Supplementary Material (ESI) for Dalton Transactions

A DFT study of the reactivity of actinidocenes (U, Np and Pu) with pyridine and pyridine *N*-oxide derivatives

Ludovic Castro[a], Ahmed Yahia[a,b] and Laurent Maron*[,a]

[a] *University of Toulouse, INSA, UPS, LPCNO, 135 avenue de Rangueil, F-31077 Toulouse (France) and CNRS, LPCNO UMR 5215, F-31077 Toulouse, France,*

[b] *Institut de Chimie Séparative de Marcoule, UMR 5257, CEA, CNRS, Université Montpellier II, ENSCM, Centre de Marcoule, BP 17171, 30207 Bagnols sur Cèze Cedex, France*

Electronic Supporting Information

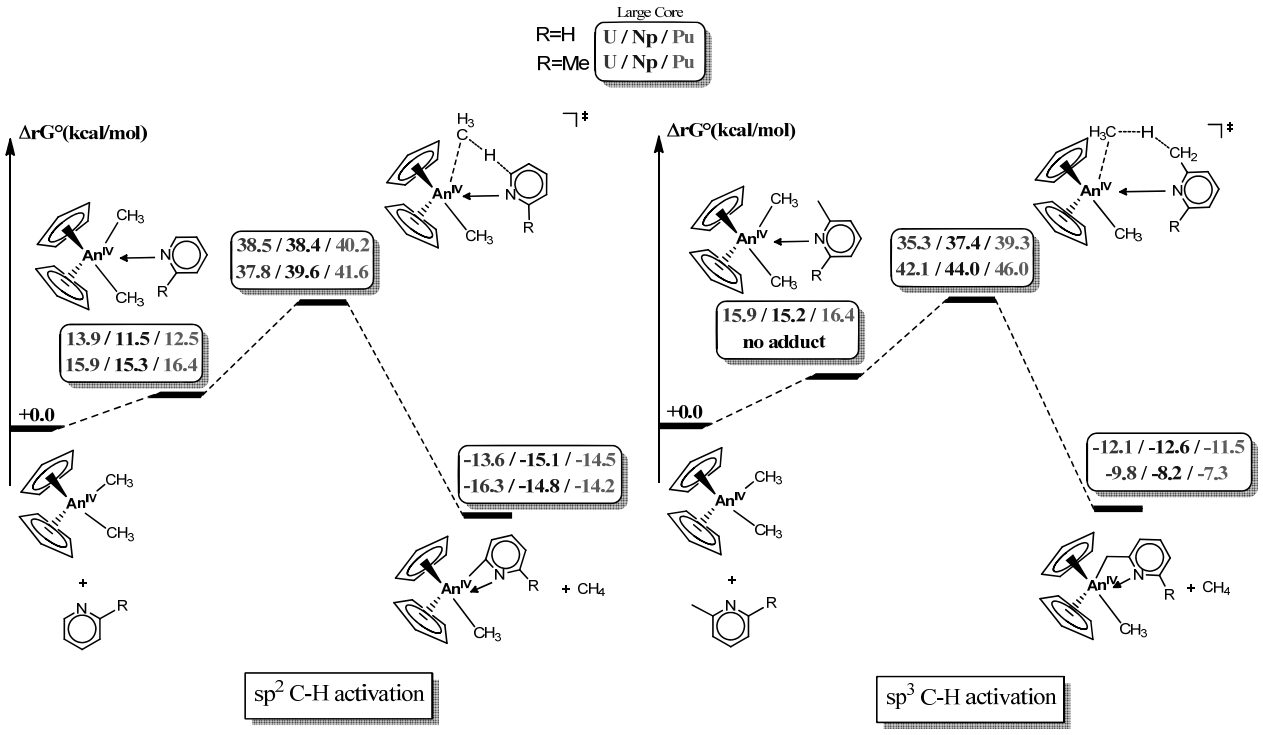

Figure 10. Free energy profiles of sp^2(left) and sp^3(right) *ortho* C-H activation of pyridine derivatives catalyzed by $Cp_2An^{IV}(CH_3)_2$ with An=U, Np and Pu using Large Core ECP. The free energies are given in $kcal.mol^{-1}$.

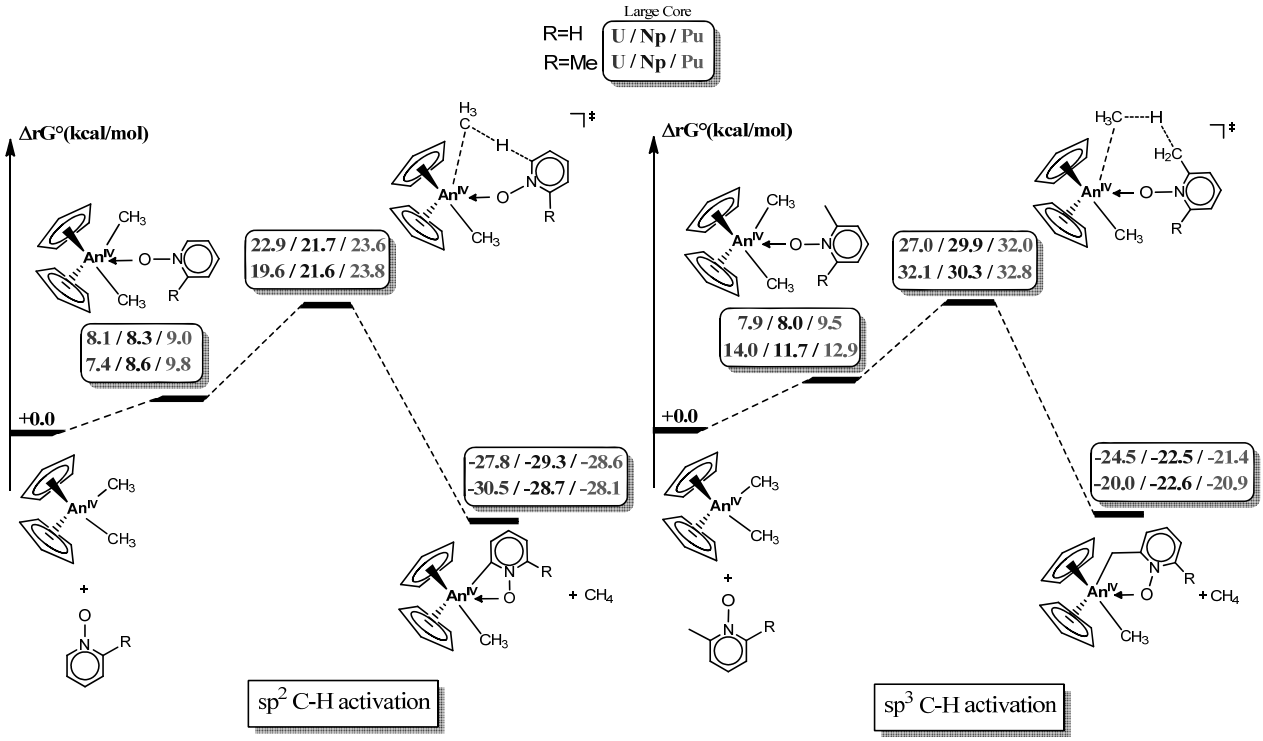

Figure 11. Free energy profiles of sp^2(left) and sp^3(right) *ortho* C-H activation of pyridine *N*-oxide derivatives catalyzed by $Cp_2An^{IV}(CH_3)_2$ with An=U, Np and Pu using Large Core ECP. The free energies are given in $kcal.mol^{-1}$.

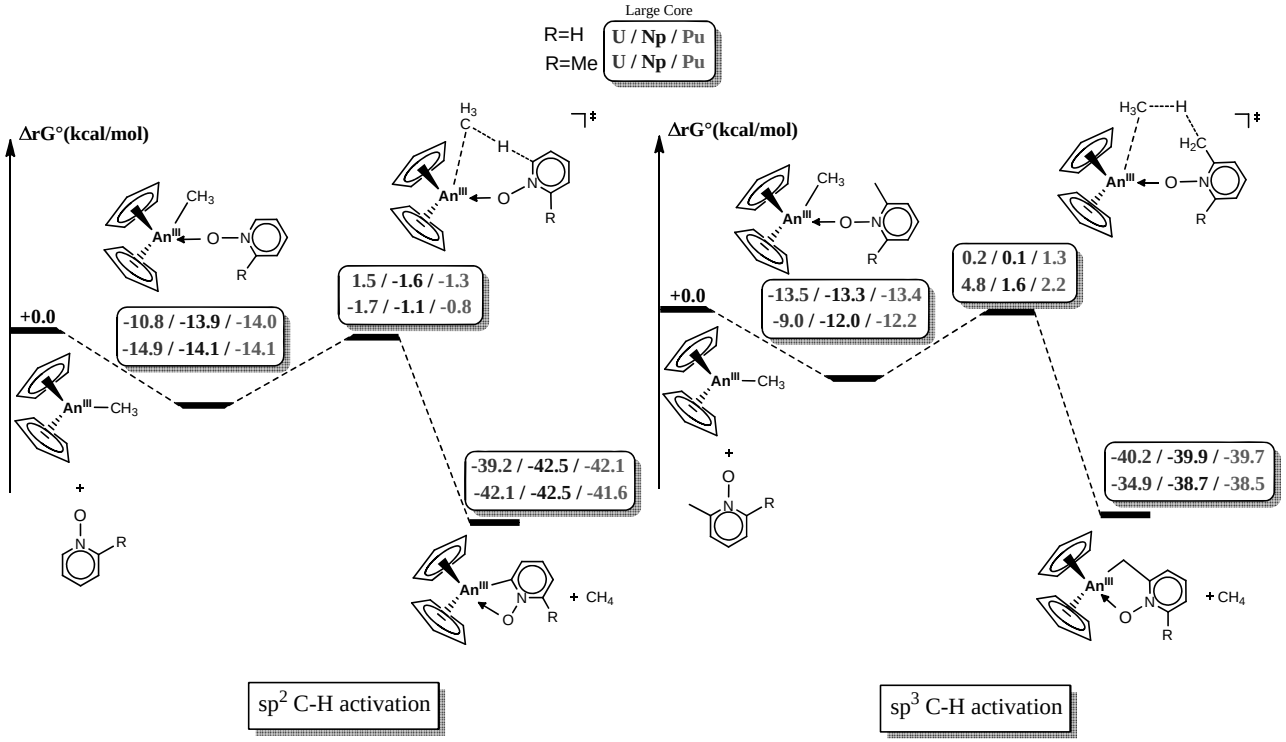

Figure 12. Free energy profiles of sp^2(left) and sp^3(right) *ortho* C-H activation of pyridine derivatives catalyzed by $Cp_2An^{III}(CH_3)$ with An=U, Np and Pu using Large Core ECP. The free energies are given in $kcal.mol^{-1}$.

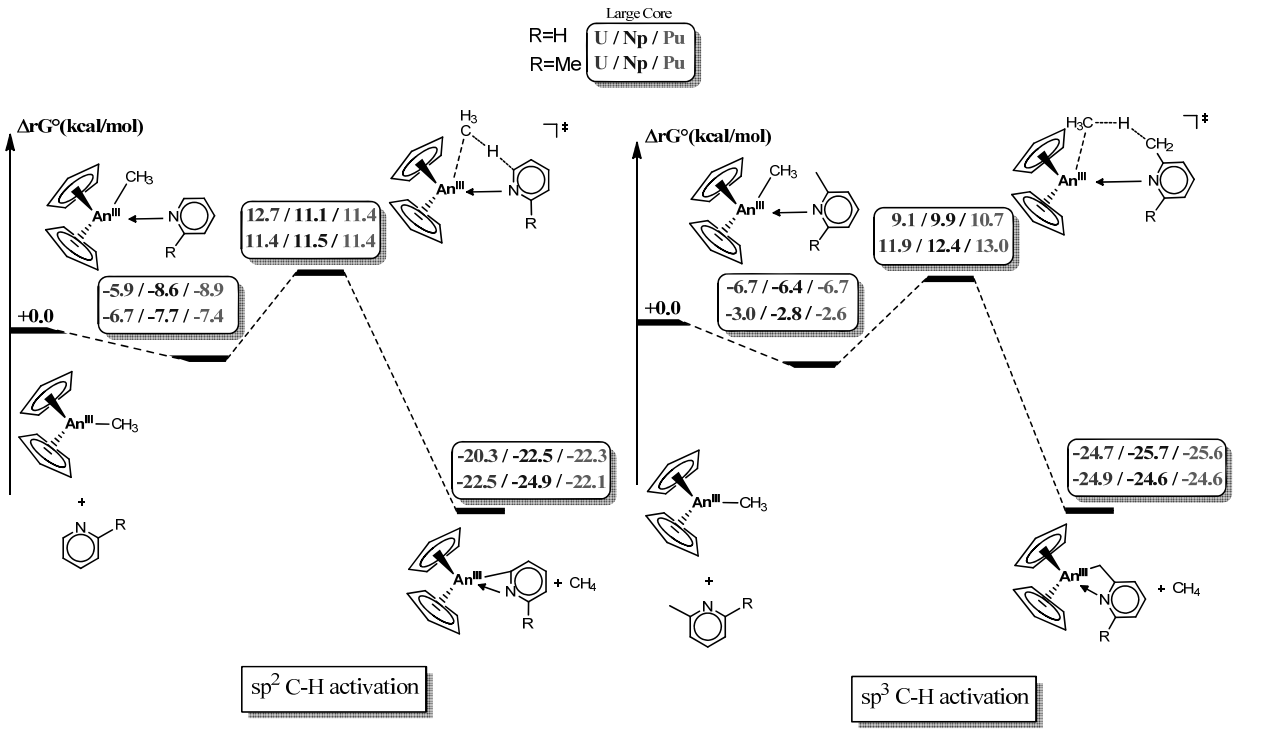

Figure 13. Free energy profiles of sp^2(left) and sp^3(right) *ortho* C-H activation of pyridine *N*-oxide derivatives catalyzed by $Cp_2An^{III}(CH_3)$ with An=U, Np and Pu using Large Core ECP. The free energies are given in $kcal.mol^{-1}$.

Optimized structures

CH4

E = -40.508109
G = -40.482693

C	-0.000004	0.000000	0.000009
H	-0.000001	0.000000	1.091768
H	1.029319	0.000000	-0.363923
H	-0.514658	-0.891417	-0.363925
H	-0.514658	0.891417	-0.363925

----Uranium(III)----

U(III) lutidine TS 11e

HF=-785.528821
G=-785.239512

U	2.414506	-2.657725	-3.249443
C	4.186684	-2.554675	-0.983074
C	5.032025	-2.894482	-2.064666
C	5.110455	-1.773108	-2.929546
C	4.321891	-0.734473	-2.370628
C	3.749532	-1.218954	-1.170520
H	3.941503	-3.191593	-0.141132
H	5.548700	-3.838260	-2.194878
H	5.720378	-1.694059	-3.822592
H	4.209484	0.265135	-2.773735
H	3.114293	-0.657859	-0.495201
C	2.308029	-1.114532	-5.627167
C	1.420097	-0.459871	-4.734142
C	0.277055	-1.281629	-4.573739
C	0.459938	-2.444524	-5.359806
C	1.712647	-2.340288	-6.013163
H	3.253537	-0.722668	-5.984464
H	1.568747	0.519048	-4.292954
H	-0.595280	-1.048618	-3.974810
H	-0.251880	-3.253765	-5.474761
H	2.126340	-3.058773	-6.711002
C	4.968391	-4.923246	-5.453874
C	4.263830	-5.647656	-4.343619
C	4.786368	-6.801615	-3.770897
C	4.087845	-7.407800	-2.720616
C	2.877596	-6.882927	-2.306836
C	2.363986	-5.742879	-2.957761
N	3.093324	-5.122613	-3.927000
C	0.528814	-2.651609	-1.272694
C	1.074420	-5.126967	-2.632402
H	4.348993	-4.912331	-6.356725
H	5.158314	-3.880523	-5.176405
H	5.924569	-5.392766	-5.695175
H	5.725705	-7.209974	-4.128362
H	4.488441	-8.298972	-2.244289
H	2.302214	-7.348643	-1.513217
H	0.500912	-5.716288	-1.913826
H	0.472209	-4.986325	-3.537952
H	0.942913	-3.909582	-1.980158
H	0.820976	-2.904987	-0.247158
H	-0.547877	-2.831591	-1.373976
H	0.660571	-1.560539	-1.371373

U(III) lutidine adduct 11e

HF=-785.553347
G=-785.263265

U	2.505247	-2.461743	-3.162036
C	4.148880	-2.033357	-0.814733
C	5.086942	-2.392652	-1.813796
C	5.129505	-1.348357	-2.770677
C	4.220184	-0.341623	-2.356946
C	3.618137	-0.765387	-1.146431
H	3.904744	-2.611348	0.069198
H	5.700357	-3.287175	-1.813444
H	5.781407	-1.295539	-3.635682
H	4.054120	0.606954	-2.854351
H	2.885512	-0.214133	-0.570162
C	2.483058	-1.626307	-5.912088
C	1.759111	-0.635075	-5.200713
C	0.525450	-1.200684	-4.793388
C	0.489400	-2.540354	-5.244158
C	1.695579	-2.803335	-5.939880
H	3.444640	-1.486098	-6.393466
H	2.074105	0.389728	-5.041321
H	-0.256835	-0.695716	-4.240603
H	-0.335639	-3.231425	-5.113116
H	1.944238	-3.728771	-6.447980
C	4.922733	-4.540849	-4.919128
C	4.155209	-5.603538	-4.191302
C	4.501427	-6.950254	-4.312873
C	3.763984	-7.906197	-3.625849
C	2.696742	-7.491993	-2.839090
C	2.396109	-6.131357	-2.757329
N	3.120328	-5.205480	-3.421128
C	0.552829	-2.254792	-1.533150
C	1.241481	-5.644919	-1.932803
H	4.263281	-3.979843	-5.590246
H	5.356983	-3.824773	-4.213269
H	5.732268	-4.970079	-5.513200
H	5.340151	-7.233603	-4.940163
H	4.016552	-8.959939	-3.703906
H	2.094227	-8.207846	-2.289842
H	0.758175	-6.469299	-1.404360
H	0.486018	-5.159339	-2.560460
H	1.557509	-4.906001	-1.188962
H	0.763838	-2.616853	-0.514428
H	-0.373050	-2.753455	-1.859690
H	0.289737	-1.191422	-1.416492

U(III) lutidine product 11e

HF=-745.062671
G=-744.814809

N	2.626374	-2.803151	-3.297195
C	3.695295	-2.815913	-2.468523
C	4.987799	-2.657092	-2.940282
C	5.182576	-2.520158	-4.326794
C	4.102294	-2.495341	-5.178523
C	2.786793	-2.585819	-4.646750
C	3.402412	-3.029967	-1.009312
C	1.587836	-2.585326	-5.431108
U	0.731462	-4.500392	-3.810752
C	2.087606	-6.919938	-3.140709
C	2.946343	-6.289779	-4.078184
C	2.308945	-6.316112	-5.341279
C	1.055055	-6.963163	-5.186398
C	0.922120	-7.342608	-3.828132
C	-1.310200	-3.616993	-1.997716
C	-1.712630	-4.915780	-2.400513
C	-2.095774	-4.850475	-3.763652
C	-1.928436	-3.512478	-4.202329
C	-1.444602	-2.751034	-3.110248
H	3.928247	-5.880541	-3.870954
H	2.309393	-7.102563	-2.094515
H	0.089845	-7.886906	-3.397487
H	0.345069	-7.175142	-5.978297
H	2.719359	-5.933270	-6.267874
H	-1.766092	-5.793473	-1.766414
H	-2.488491	-5.671045	-4.353421
H	-2.166651	-3.130665	-5.188578
H	-1.243213	-1.686083	-3.114802
H	-0.999845	-3.326573	-0.999807
H	2.685609	-2.286202	-0.646575
H	2.962475	-4.020364	-0.837296
H	4.310293	-2.963123	-0.405466
H	5.826518	-2.654937	-2.252444
H	6.189930	-2.415700	-4.722644
H	4.229749	-2.362840	-6.248262
H	1.713892	-2.484710	-6.506204
H	0.795475	-1.939897	-5.040467

U(III) lutidine N-oxide TS 11e

HF=-860.682233
G=-860.390694

C	-3.507280	-2.345679	-7.601901
N	-3.015594	-2.293963	-6.316535
C	-1.684266	-2.302877	-6.020210
C	-0.766125	-2.414796	-7.051820
C	-1.210621	-2.515057	-8.372132
C	-2.566973	-2.475596	-8.636793
O	-3.875621	-2.218304	-5.311372
U	-5.930096	-3.583532	-5.201338
C	-1.321650	-2.198386	-4.578480
C	-4.944232	-2.317806	-7.776634
C	-6.600810	-4.651470	-7.636874
C	-4.064238	-5.652274	-4.462451
C	-5.186513	-6.355369	-4.960590
C	-6.257172	-6.175882	-4.050119
C	-5.791406	-5.368036	-2.981774
C	-4.438065	-5.041625	-3.238779
C	-8.341677	-2.893067	-3.866027
C	-8.683473	-2.763753	-5.233338
C	-7.993592	-1.639803	-5.753092
C	-7.227903	-1.072155	-4.707052
C	-7.435488	-1.850288	-3.540742
H	-6.604519	-0.188323	-4.777746
H	-7.016107	-1.653931	-2.560196
H	-8.731219	-3.634900	-3.178822
H	-9.375724	-3.393291	-5.780371
H	-8.069797	-1.263059	-6.766471
H	-3.082133	-5.616591	-4.920344
H	-5.216311	-6.946763	-5.867856
H	-7.243802	-6.618109	-4.130972
H	-6.359798	-5.081233	-2.104739
H	-3.793663	-4.453482	-2.595175
H	-7.254763	-4.220856	-8.404061
H	-7.266767	-5.222194	-6.964602
H	-5.955465	-5.393586	-8.122007
H	0.289895	-2.426675	-6.807220
H	-0.496664	-2.607246	-9.184816
H	-2.941827	-2.525935	-9.653350
H	-0.236158	-2.184222	-4.465254
H	-1.747347	-1.290853	-4.139760
H	-1.733828	-3.039578	-4.013118
H	-5.665659	-3.478462	-7.585041
H	-5.414900	-1.535082	-7.170631
H	-5.208146	-2.166957	-8.825378

U(III) lutidine N-oxide adduct 11e

HF=-860.704060
G=-860.412668

C	-3.171263	-2.642577	-8.172013
N	-3.222593	-2.345982	-6.836543
C	-2.096116	-2.116854	-6.094194
C	-0.856309	-2.220504	-6.710167
C	-0.758794	-2.542962	-8.058679
C	-1.927537	-2.746273	-8.782303
O	-4.388471	-2.240022	-6.257010
U	-6.118103	-3.655555	-5.121909
C	-2.297362	-1.759614	-4.663365
C	-4.469814	-2.817087	-8.876503
C	-7.284710	-4.581018	-7.212389
C	-3.838428	-5.395188	-4.592803
C	-4.803394	-6.238472	-5.193262
C	-5.880355	-6.384799	-4.286682
C	-5.580924	-5.634019	-3.123026
C	-4.319622	-5.018345	-3.312699
C	-8.403911	-2.985148	-3.546757
C	-8.701956	-2.440491	-4.820616
C	-7.841273	-1.337892	-5.035484
C	-7.015537	-1.195173	-3.892467
C	-7.362362	-2.212815	-2.971767
H	-6.272088	-0.421034	-3.736849
H	-6.934572	-2.355287	-1.985781
H	-8.912131	-3.818911	-3.075064
H	-9.461215	-2.798095	-5.505184
H	-7.835875	-0.696237	-5.909519
H	-2.874918	-5.131910	-5.016319
H	-4.727164	-6.707728	-6.166668
H	-6.767085	-6.987018	-4.447496
H	-6.192237	-5.568303	-2.230416
H	-3.795025	-4.414603	-2.579926
H	-7.691068	-3.797887	-7.872031
H	-8.154630	-5.183386	-6.903866
H	-6.686977	-5.251357	-7.850638
H	0.029058	-2.041888	-6.109767
H	0.210600	-2.627164	-8.538562
H	-1.898078	-2.988621	-9.839018
H	-1.336668	-1.547582	-4.191262
H	-2.949339	-0.885337	-4.574507
H	-2.787468	-2.577460	-4.124746
H	-5.058660	-3.635122	-8.447041
H	-5.082061	-1.915235	-8.775415
H	-4.295404	-3.018614	-9.934700

U(III) lutidine N-oxide product 11e

HF=-820.222598
G=-819.970703

C	-3.561669	-2.160837	-6.907071
C	-2.803140	-2.024072	-5.716394
C	-1.447765	-2.288333	-6.029088
C	-1.368333	-2.592765	-7.412489
C	-2.675398	-2.517571	-7.953300
U	-2.003718	0.201061	-7.334663
C	-0.471258	0.351055	-9.521647
C	-0.996374	1.519636	-10.148006
N	-2.365368	1.732236	-10.102157
C	-2.995287	2.779873	-10.703055
C	-2.237670	3.746062	-11.340716
C	-0.841417	3.631819	-11.351120
C	-0.237130	2.538535	-10.769037
O	-3.114901	0.860633	-9.411581
C	-4.482630	2.813826	-10.596768
C	-0.574245	1.703571	-5.371883
C	-0.659262	2.586226	-6.479710
C	-2.010433	2.980872	-6.621466
C	-2.763136	2.343394	-5.601728
C	-1.873089	1.561010	-4.824744
H	-2.953989	-2.720262	-8.980914
H	-4.638267	-2.059433	-6.992238
H	-3.196825	-1.796113	-4.732583
H	-0.622954	-2.298918	-5.325305
H	-0.471767	-2.876233	-7.951849
H	-2.395741	3.674936	-7.359457
H	0.168899	2.923226	-7.091560
H	0.333435	1.256923	-4.981146
H	-2.134675	0.978051	-3.949404
H	-3.823605	2.474989	-5.415004
H	-2.743411	4.580970	-11.811598
H	-0.237386	4.391920	-11.838071
H	0.839610	2.411087	-10.797208
H	-4.878474	3.660306	-11.160990
H	-4.917811	1.884591	-10.976002
H	-4.797191	2.900186	-9.551877
H	-1.014338	-0.563885	-9.785660
H	0.604063	0.238734	-9.640370

U(III) sp3 picoline N-oxide TS 11e

HF=-821.371169
G=-821.105435

C	-3.672340	-1.908575	-6.776498
C	-3.248239	-2.670188	-5.661383
C	-1.900002	-3.051214	-5.879862
C	-1.489024	-2.516790	-7.123616
C	-2.584969	-1.804518	-7.677753
U	-1.758602	-0.210381	-5.474420
C	-0.676622	-1.219483	-3.167835
O	-3.855012	1.025141	-5.050999
N	-4.574550	0.799398	-3.963675
C	-3.943136	0.755502	-2.741122
C	-4.754760	0.473020	-1.625947
C	-6.117367	0.276304	-1.747676
C	-6.712525	0.364793	-3.012728
C	-5.910369	0.628266	-4.101305
C	-2.509569	0.936518	-2.716059
C	-0.286036	1.165387	-7.460069
C	0.710722	0.541556	-6.665496
C	0.749459	1.202737	-5.414044
C	-0.221737	2.234425	-5.433911
C	-0.859715	2.213292	-6.697771
H	-6.259077	0.709068	-5.122649
H	-0.411034	2.945674	-4.638269
H	-1.634119	2.894611	-7.031290
H	-0.531927	0.913920	-8.485231
H	1.355699	-0.271934	-6.977766
H	1.422249	0.976879	-4.595240
H	-3.858564	-2.951692	-4.810548
H	-1.299304	-3.667419	-5.221462
H	-0.521701	-2.659696	-7.591261
H	-2.602234	-1.313297	-8.643907
H	-4.660244	-1.488553	-6.923975
H	-0.019440	-0.771098	-2.413791
H	0.003333	-1.640898	-3.930899
H	-1.186031	-2.073472	-2.705202
H	-7.777584	0.228443	-3.158591
H	-6.719921	0.067900	-0.869174
H	-4.271001	0.429021	-0.655948
H	-1.713810	-0.131216	-3.049259
H	-2.190039	1.773657	-3.346263
H	-2.144361	1.082816	-1.697792

U(III) sp3 picoline N-oxide adduct 11e

HF=-821.393114
G=-821.127302

C	-3.683396	-1.703771	-6.958640
C	-3.522251	-2.394515	-5.730029
C	-2.274938	-3.061120	-5.761833
C	-1.660095	-2.776333	-7.005692
C	-2.533154	-1.940881	-7.747544
U	-1.526935	-0.281533	-5.623877
C	-0.312513	-1.185113	-3.547941
O	-3.254992	0.990017	-4.329837
N	-4.265490	0.721127	-3.551939
C	-4.094540	0.763985	-2.195819
C	-5.194288	0.494828	-1.385990
C	-6.437343	0.191910	-1.928341
C	-6.570134	0.163770	-3.315366
C	-5.471324	0.432774	-4.105539
C	-2.732972	1.098262	-1.700411
C	-0.405997	1.263822	-7.770598
C	0.688009	0.536582	-7.236103
C	0.986795	1.069936	-5.957512
C	0.074455	2.120588	-5.699865
C	-0.784962	2.242272	-6.820510
H	-5.472464	0.432054	-5.187375
H	0.056904	2.744303	-4.813120
H	-1.572606	2.977760	-6.942696
H	-0.848704	1.119789	-8.749588
H	1.229517	-0.258030	-7.737408
H	1.781558	0.740992	-5.299381
H	-4.247430	-2.446516	-4.925041
H	-1.866005	-3.686350	-4.978113
H	-0.707386	-3.164634	-7.348240
H	-2.363729	-1.575774	-8.753769
H	-4.554415	-1.135599	-7.268426
H	0.178174	-0.407333	-2.941149
H	0.493232	-1.880018	-3.833451
H	-0.956186	-1.760424	-2.861782
H	-7.515139	-0.066034	-3.794682
H	-7.284592	-0.017413	-1.284164
H	-5.049413	0.527550	-0.311437
H	-1.999121	0.364865	-2.054008
H	-2.414238	2.070670	-2.089147
H	-2.725522	1.122403	-0.609574

U(III) sp3 picoline N-oxide product 11e

HF=-780.911947
G=-780.686526

C	-3.899757	-1.581724	-7.230167
C	-3.893601	-1.955883	-5.862289
C	-2.577115	-2.350945	-5.523540
C	-1.769983	-2.228371	-6.684170
C	-2.588127	-1.755699	-7.739006
U	-2.382616	0.473059	-5.950892
C	0.203118	0.905605	-6.542044
C	0.161522	2.278624	-6.914022
N	-0.927746	2.734717	-7.637915
C	-1.046310	4.008335	-8.076266
C	-0.106140	4.962644	-7.763273
C	0.986019	4.580775	-6.965715
C	1.110200	3.270794	-6.557473
O	-1.928298	1.883011	-7.897807
C	-2.877808	0.941263	-3.178133
C	-1.932036	1.937697	-3.529304
C	-2.572728	2.869001	-4.382533
C	-3.913953	2.448579	-4.560634
C	-4.103867	1.257969	-3.814643
H	-1.943173	4.189753	-8.654951
H	-2.274105	-1.581071	-8.761562
H	-4.767139	-1.268337	-7.801363
H	-4.752100	-1.968503	-5.200888
H	-2.253169	-2.723896	-4.558235
H	-0.720931	-2.490362	-6.760087
H	-2.122780	3.761303	-4.802094
H	-0.908104	1.996160	-3.179182
H	-2.706863	0.107004	-2.506960
H	-5.032876	0.708391	-3.716260
H	-4.674130	2.970023	-5.132258
H	-0.231503	5.976650	-8.123275
H	1.741627	5.309581	-6.687893
H	1.961693	2.949879	-5.966867
H	-0.029998	0.222551	-7.366515
H	1.107692	0.619439	-6.010785

U(III) pyridine TS 11e

HF=-706.906023
G=-706.672042

U	-5.094433	-1.078488	-0.359772
C	-3.603949	-0.817718	2.078408
C	-3.856261	-2.205335	1.967784
C	-3.105995	-2.702033	0.871847
C	-2.384415	-1.619576	0.308692
C	-2.696773	-0.453245	1.051148
H	-4.012308	-0.154113	2.831724
H	-4.494553	-2.790706	2.618801
H	-3.055569	-3.736361	0.550164
H	-1.688421	-1.680411	-0.519919
H	-2.277701	0.534203	0.891611
C	-6.389585	-0.791904	-2.908093
C	-5.252666	0.049262	-2.987185
C	-4.098609	-0.773000	-3.005645
C	-4.524383	-2.125035	-2.940120
C	-5.939868	-2.134790	-2.882034
H	-6.570291	-3.015637	-2.849822
H	-7.423509	-0.466645	-2.900847
H	-5.264834	1.131070	-3.056603
H	-3.073754	-0.432730	-3.101125
H	-3.880558	-2.996770	-2.973655
C	-7.125339	-2.716642	0.499503
H	-8.048516	-2.843132	-0.079890
H	-6.449674	-3.517522	0.154086
H	-7.352661	-2.966455	1.543506
H	-7.117154	-1.245585	0.646483
C	-7.202916	0.176279	0.824687
C	-8.366803	0.636800	1.452759
C	-8.542917	1.999026	1.672511
C	-7.549158	2.890427	1.261352
C	-6.416719	2.378462	0.644545
N	-6.257177	1.062920	0.436541
H	-9.126395	-0.075437	1.764539
H	-9.441909	2.370843	2.158349
H	-7.650377	3.959933	1.415680
H	-5.612773	3.027555	0.305341

U(III) pyridine adduct 11e

HF=-706.938131
G=-706.701678

U	-5.112837	-1.351190	-0.377834
C	-3.720797	-1.067838	2.141596
C	-3.688089	-2.453655	1.857945
C	-2.837438	-2.649801	0.741487
C	-2.335415	-1.384880	0.342546
C	-2.884201	-0.406779	1.205776
H	-4.258106	-0.598441	2.958186
H	-4.210609	-3.229594	2.403490
H	-2.578998	-3.605505	0.298894
H	-1.630026	-1.203895	-0.460243
H	-2.661641	0.654821	1.186550
C	-6.465443	-0.977504	-2.906703
C	-5.480180	0.042303	-2.892055
C	-4.209798	-0.574297	-2.991165
C	-4.409859	-1.976465	-3.063187
C	-5.805686	-2.223293	-3.016788
H	-6.284619	-3.193529	-3.069078
H	-7.538876	-0.829040	-2.873336
H	-5.669446	1.109899	-2.861004
H	-3.253981	-0.065042	-3.039121
H	-3.633371	-2.723658	-3.184370
C	-6.837367	-3.122260	0.311967
H	-7.809624	-3.026329	-0.197650
H	-6.477514	-4.131653	0.055239
H	-7.050197	-3.161939	1.392579
H	-8.008855	-0.777140	1.164801
C	-7.807317	0.292020	1.166835
C	-8.714061	1.199321	1.705683
C	-8.400042	2.555247	1.678016
C	-7.190114	2.953431	1.113660
C	-6.343315	1.978837	0.598833
N	-6.640131	0.670860	0.620715
H	-9.644187	0.842493	2.135232
H	-9.085941	3.290319	2.089103
H	-6.903201	3.998845	1.070512
H	-5.390544	2.249313	0.150747

U(III) pyridine product 11e

HF=-666.436195
G=-666.241299

N	-5.287743	-1.255861	-0.548228
C	-4.769201	-1.069324	0.699169
C	-4.129024	-2.160237	1.313295
C	-4.032778	-3.384572	0.662199
C	-4.579940	-3.528964	-0.617254
C	-5.203152	-2.432105	-1.190705
U	-5.785800	1.149437	0.057125
C	-4.020322	2.345284	-1.858087
C	-3.159978	1.882827	-0.833194
C	-3.387691	2.673808	0.319413
C	-4.384847	3.632771	0.004820
C	-4.778071	3.428403	-1.340979
C	-8.544351	0.534501	0.520007
C	-7.936913	0.419376	1.793085
C	-7.554811	1.718555	2.214322
C	-7.936422	2.638307	1.204708
C	-8.542865	1.906178	0.154461
H	-7.803498	-0.497044	2.354768
H	-7.098085	1.970280	3.165311
H	-7.816656	3.714790	1.244237
H	-8.978758	2.328346	-0.744737
H	-8.973114	-0.278597	-0.055048
H	-2.860720	2.586723	1.263063
H	-2.442611	1.075560	-0.918077
H	-4.057166	1.969336	-2.874902
H	-5.495643	4.026873	-1.891415
H	-4.751032	4.412193	0.663244
H	-3.705882	-2.041831	2.307975
H	-3.537276	-4.228318	1.138147
H	-4.523189	-4.470470	-1.154633
H	-5.646187	-2.487163	-2.183461

U(III) sp2 picoline N-oxide TS 11e

HF=-821.372729
G=-821.108450

C	-4.730061	-0.506033	-0.507093
C	-3.336397	-0.247048	-0.550114
C	-2.987887	0.047684	-1.892568
C	-4.164274	-0.031153	-2.677525
C	-5.240120	-0.374657	-1.821882
U	-3.606274	-2.743017	-1.862928
C	-5.691073	-3.710279	-3.321905
O	-1.796979	-3.093873	-3.506711
N	-2.231436	-2.756478	-4.716870
C	-1.290286	-2.547650	-5.682221
C	-1.725604	-2.182583	-6.950417
C	-3.083079	-2.028048	-7.214360
C	-3.992914	-2.255391	-6.184858
C	-3.572468	-2.629044	-4.912788
C	0.136834	-2.726102	-5.292751
C	-3.946865	-4.070328	0.633545
C	-4.183895	-5.089733	-0.321983
C	-2.954665	-5.388190	-0.958921
C	-1.955783	-4.558108	-0.394349
C	-2.567313	-3.742538	0.589470
H	-4.235058	0.166272	-3.740124
H	-2.001416	0.322265	-2.248840
H	-2.665991	-0.231288	0.301429
H	-5.307669	-0.728446	0.382948
H	-6.276816	-0.485266	-2.117718
H	-5.133829	-5.575841	-0.511976
H	-4.679759	-3.648379	1.311783
H	-2.063942	-3.024951	1.227152
H	-0.904108	-4.561261	-0.657195
H	-2.799171	-6.137536	-1.726447
H	-6.405514	-3.385348	-4.088962
H	-6.213931	-3.512780	-2.367100
H	-5.604950	-4.801485	-3.406927
H	-0.979982	-2.019141	-7.721587
H	-3.419315	-1.741102	-8.206426
H	-5.061008	-2.154061	-6.358081
H	-4.534717	-3.097116	-4.042126
H	0.789346	-2.542127	-6.148610
H	0.402165	-2.042996	-4.479785
H	0.308224	-3.738146	-4.913469

U(III) sp2 picoline N-oxide product 11e

HF=-780.902440
G=-780.689636

C	-4.741592	-0.676976	-0.390966
C	-3.355346	-0.427084	-0.220390
C	-2.862156	0.123877	-1.429961
C	-3.939338	0.213730	-2.347020
C	-5.100141	-0.281483	-1.703473
U	-3.511645	-2.488860	-2.037650
C	-3.041315	-2.535429	-4.619808
N	-4.364075	-2.796050	-4.840983
C	-4.970909	-2.941074	-6.047978

C	-4.173094	-2.818701	-7.180407
C	-2.812644	-2.555795	-7.051705
C	-2.266932	-2.416466	-5.775526
O	-5.129788	-2.917255	-3.742872
C	-6.435569	-3.218457	-6.056799
C	-4.528884	-4.888630	-1.179348
C	-4.286853	-4.159368	0.010234
C	-2.883589	-4.025436	0.166101
C	-2.261305	-4.680588	-0.927285
C	-3.277215	-5.213462	-1.759569
H	-3.124671	-5.786383	-2.666668
H	-5.499841	-5.159372	-1.576377
H	-5.040230	-3.793326	0.697094
H	-2.379059	-3.549110	0.998163
H	-1.193958	-4.792232	-1.079737
H	-1.846328	0.455532	-1.611687
H	-2.788037	-0.588160	0.688357
H	-5.414554	-1.066300	0.363224
H	-6.089942	-0.341903	-2.139685
H	-3.888083	0.612022	-3.353255
H	-4.637210	-2.932521	-8.154770
H	-2.190506	-2.461108	-7.937738
H	-1.205163	-2.208105	-5.668425
H	-6.798370	-3.313251	-7.082440
H	-6.656144	-4.138035	-5.505844
H	-6.981601	-2.416356	-5.550453

U(III) sp2 picoline TS 11e

HF=-746.215818
G=-745.955106

C	-5.398265	1.986944	-0.217250
C	-6.083707	2.461529	0.930013
C	-5.907690	3.863398	0.996217
C	-5.112495	4.258833	-0.109347
C	-4.793041	3.097817	-0.856768
U	-7.578527	3.475058	-1.305993
N	-9.304574	1.722717	-0.600036
C	-9.883447	2.804143	-0.032022
C	-11.079681	2.659220	0.678786
C	-11.656261	1.399095	0.791592
C	-11.033279	0.302832	0.193443
C	-9.844059	0.491621	-0.506892
C	-9.116222	-0.630216	-1.187202
C	-6.843806	3.241505	-4.046709
C	-8.173813	2.753473	-4.017117
C	-9.037174	3.846075	-3.757392
C	-8.242291	5.011216	-3.630785
C	-6.886412	4.639132	-3.806831
C	-8.920521	5.552994	-0.116605
H	-9.035875	5.743631	0.957777
H	-9.764201	6.030386	-0.630276
H	-8.026459	6.127382	-0.413013
H	-6.294785	4.518537	1.767561
H	-6.626077	1.853796	1.644851
H	-4.770182	5.265869	-0.320515
H	-5.306965	0.950531	-0.523125
H	-4.165675	3.061219	-1.739700
H	-6.034469	5.309700	-3.803152
H	-5.954807	2.659632	-4.261592
H	-8.479926	1.729763	-4.200389
H	-10.118581	3.803557	-3.697925
H	-8.609707	6.015342	-3.454799
H	-9.365391	4.144220	-0.093622
H	-11.546097	3.527425	1.136512
H	-12.584665	1.260563	1.340853
H	-11.463440	-0.691286	0.268049
H	-8.066184	-0.648351	-0.878894
H	-9.564758	-1.599191	-0.956468
H	-9.133239	-0.495101	-2.274299

U(III) sp2 picoline adduct 11e

HF=-746.247883
G=-745.983878

C	-5.317693	1.972984	-0.424023
C	-6.063746	2.205407	0.759076
C	-5.958993	3.580630	1.080884
C	-5.149848	4.198976	0.098883
C	-4.752499	3.206128	-0.832422
U	-7.540217	3.575042	-1.335234
N	-9.623172	2.116457	-0.333708
C	-10.531588	2.893754	0.278548
C	-11.680586	2.388824	0.875166
C	-11.892754	1.014269	0.832282
C	-10.953894	0.205780	0.199363
C	-9.821986	0.783739	-0.379059
C	-8.776385	-0.037293	-1.072921
C	-7.024579	2.907848	-4.082686
C	-8.422996	2.716938	-3.970225
C	-9.027047	3.987081	-3.788764
C	-8.004465	4.963403	-3.795600
C	-6.765042	4.297536	-3.971775
C	-8.455996	5.775793	-0.396603
H	-8.552517	5.803014	0.700572
H	-9.427274	6.094287	-0.807899
H	-7.758903	6.593162	-0.642642
H	-6.401475	4.072078	1.939021
H	-6.580027	1.455039	1.347989
H	-4.864124	5.244328	0.078944
H	-5.160646	1.013819	-0.905337
H	-4.095466	3.353938	-1.681681
H	-5.793312	4.771260	-4.055298
H	-6.285545	2.135307	-4.262591
H	-8.948090	1.773283	-4.071584
H	-10.089824	4.181146	-3.698196
H	-8.146184	6.032341	-3.694585
H	-10.315265	3.960799	0.283873
H	-12.383177	3.059938	1.357108
H	-12.777203	0.575496	1.285426
H	-11.089976	-0.869816	0.149503
H	-7.801373	0.097785	-0.591805
H	-9.023940	-1.100681	-1.057744
H	-8.672655	0.277537	-2.117236

U(III) sp2 picoline product 11e

HF=-705.745823
G=-705.532353

C	-5.578001	1.863180	-0.049946
C	-6.447275	2.434441	0.911879
C	-6.223680	3.835908	0.927771
C	-5.215161	4.129929	-0.020459
C	-4.810861	2.910076	-0.620988
U	-3.831803	2.718950	2.045491
C	-2.669754	4.909359	2.494659
N	-3.556640	4.755223	3.515995
C	-3.698486	5.651738	4.513677
C	-2.915398	6.800699	4.526898
C	-1.989528	7.004700	3.499280
C	-1.866692	6.062262	2.486322
C	-4.714451	5.351515	5.578457
C	-3.243946	0.254436	3.383670
C	-2.295731	1.171883	3.906623
C	-1.384409	1.496997	2.874031
C	-1.770409	0.784119	1.709728
C	-2.915225	0.010110	2.027445
H	-0.530477	2.157299	2.963647
H	-2.251547	1.531333	4.928362
H	-1.249136	0.787873	0.758571
H	-4.045747	-0.221232	3.938571
H	-3.427566	-0.673965	1.361025
H	-5.532118	0.815914	-0.325077
H	-7.192066	1.899660	1.491811
H	-6.758675	4.560846	1.530703
H	-4.833013	5.115014	-0.258544
H	-4.081115	2.803220	-1.416254
H	-1.148880	6.214048	1.684121
H	-1.372300	7.900981	3.501781
H	-3.027336	7.524540	5.328810
H	-4.477138	4.409249	6.084635
H	-4.753355	6.142936	6.330808
H	-5.713252	5.244000	5.141419

U(III) sp3 picoline TS 11e

HF=-746.219642
G=-745.956822

U	-0.286597	1.501660	-1.691410
C	0.480831	-0.267051	-3.830463
H	0.814067	-1.264821	-3.569441
C	-0.847921	0.115156	-4.132247
H	-1.714079	-0.535807	-4.133270
C	-0.842993	1.493251	-4.464433
H	-1.700775	2.076741	-4.779510
C	0.494108	1.959864	-4.375918
H	0.835130	2.962454	-4.606291
C	1.310653	0.872266	-3.981369
H	2.386536	0.896114	-3.850748
C	-0.711052	4.314514	-1.824027
C	0.418433	4.170940	-0.978993
H	1.428728	4.491013	-1.209296
C	-0.021921	3.611452	0.248045
H	0.598315	3.405313	1.112556
C	-1.416021	3.396435	0.155454
H	-2.053028	2.996223	0.935344
C	-1.843221	3.828542	-1.126064
H	-2.864199	3.826460	-1.490486
C	-2.595253	0.223109	-0.979991
H	-2.924444	-0.769872	-1.307683
H	-3.019430	0.935918	-1.708132
H	-3.082087	0.441535	-0.022580
C	-0.099117	-0.866619	-0.050147
H	-1.250701	-0.222529	-0.477008

H	0.233151	-1.407983	-0.943961
C	1.019347	-0.161566	0.579525
N	1.747690	0.652560	-0.236021
C	2.814447	1.302248	0.255859
H	3.357942	1.924405	-0.451881
C	3.212378	1.217022	1.579578
H	4.088071	1.753545	1.927778
C	2.432952	0.438727	2.445660
H	2.695217	0.361535	3.497611
C	1.336853	-0.245857	1.952124
H	0.730016	-0.871943	2.598783
H	-0.587364	-1.568313	0.629260
H	-0.712953	4.749551	-2.816457

U(III) sp3 picoline adduct 11e

HF=-746.246297
G=-745.983856

U	-0.568725	1.725560	-1.675092
C	0.161336	-0.358001	-3.556868
H	0.076313	-1.388723	-3.231608
C	-0.854289	0.391483	-4.194822
H	-1.854822	0.043030	-4.419961
C	-0.325420	1.670327	-4.501444
H	-0.843222	2.464522	-5.027297
C	1.021951	1.706011	-4.058519
H	1.709579	2.535176	-4.181367
C	1.322041	0.452323	-3.474775
H	2.283189	0.150657	-3.073512
C	-0.787266	4.549027	-2.050808
C	0.162947	4.436037	-1.006200
H	1.209805	4.713189	-1.072324
C	-0.514374	3.979484	0.153162
H	-0.074619	3.831851	1.133445
C	-1.880818	3.810358	-0.175231
H	-2.664887	3.485865	0.497909
C	-2.049642	4.160258	-1.536244
H	-2.986606	4.156097	-2.081376
C	-2.762270	0.504133	-1.183228
H	-2.765651	-0.567836	-1.433820
H	-3.572757	0.949004	-1.783063
H	-3.105410	0.583120	-0.138489
C	-0.024446	-1.318850	0.468784
H	-0.963913	-0.757031	0.459650
H	0.100893	-1.750420	-0.531311
C	1.142232	-0.439258	0.806080
N	1.222581	0.755146	0.184848
C	2.270277	1.553148	0.446159
H	2.282240	2.509242	-0.071937
C	3.287958	1.214567	1.327731
H	4.110938	1.899574	1.500358
C	3.208788	-0.014774	1.976623
H	3.978112	-0.321603	2.679491
C	2.125722	-0.844981	1.713392
H	2.032590	-1.808856	2.203455
H	-0.119030	-2.142959	1.179261
H	-0.590275	4.910200	-3.053501

U(III) sp3 picoline product 11e

HF=-705.753601
G=-705.532353

C	0.584612	1.801521	-1.754732
C	0.777087	0.900269	-2.839710
N	1.379531	-0.314561	-2.595016
C	1.673564	-0.671300	-1.329328
C	1.444868	0.137633	-0.234657
C	0.905370	1.416601	-0.472441
C	0.499521	1.199940	-4.211208
U	2.798950	-0.020529	-4.746620
C	4.713414	2.021433	-5.243624
C	5.493630	0.867183	-4.986503
C	5.351322	0.540681	-3.614369
C	4.492179	1.501338	-3.021165
C	4.097627	2.415372	-4.027051
C	2.995002	-0.991149	-7.414750
C	1.599323	-0.979606	-7.163200
C	1.316269	-1.996705	-6.219284
C	2.535051	-2.637665	-5.886893
C	3.573679	-2.017560	-6.626235
H	0.335857	-2.259596	-5.839350
H	0.871551	-0.331867	-7.638560
H	3.521363	-0.359666	-8.121651
H	4.618743	-2.305668	-6.624673
H	2.646271	-3.484575	-5.218317
H	5.857103	-0.268040	-3.097599
H	4.204532	1.542507	-1.977085
H	3.460065	3.279795	-3.886103
H	4.640985	2.541846	-6.192356
H	-0.017742	0.401563	-4.750957
H	2.120964	-1.656697	-1.209501
H	1.688619	-0.201715	0.765879
H	0.726857	2.094586	0.358601
H	0.144562	2.773710	-1.954647
H	0.086119	2.183377	-4.419730
H	6.113528	0.344464	-5.705527

U(III) pyridine N-oxide TS 11e

HF=-782.061330
G=-781.822710

C	0.891141	1.257172	-2.187766
N	0.150023	0.260727	-2.729360
C	0.039505	-0.976919	-2.175615
C	0.741696	-1.196831	-0.991737
C	1.516255	-0.204954	-0.395850
C	1.583548	1.045083	-1.010971
O	-0.484327	0.516076	-3.865662
U	-1.163980	-1.610088	-4.929665
C	-2.031599	-2.881350	-2.687507
C	-3.801489	-0.515098	-5.215892
C	-3.920889	-1.853448	-5.666164
C	-3.202267	-1.973203	-6.881399
C	-2.639963	-0.705866	-7.182917
C	-3.013679	0.194130	-6.154415
C	0.449362	-2.868185	-6.898302
C	1.324966	-1.950283	-6.265136
C	1.589564	-2.428841	-4.957171
C	0.873628	-3.637787	-4.779863
C	0.168448	-3.909192	-5.978760
H	2.250739	-1.968745	-4.232520
H	1.751816	-1.061564	-6.716876
H	0.086522	-2.803117	-7.917257
H	-0.446019	-4.781234	-6.173520
H	0.885449	-4.261180	-3.893743
H	-4.256251	-0.099625	-4.323930
H	-4.489248	-2.639390	-5.182009
H	-3.129365	-2.864235	-7.494510
H	-2.063801	-0.459805	-8.067835
H	-2.754320	1.245119	-6.100635
H	-1.664129	-3.479599	-1.844147
H	-2.317686	-3.634226	-3.446482
H	-2.965015	-2.405841	-2.358022
H	0.886250	2.184422	-2.746580
H	2.168358	1.857028	-0.592565
H	2.053843	-0.394103	0.528368
H	0.661311	-2.178970	-0.532971
H	-0.923128	-1.891254	-2.550320

U(III) pyridine N-oxide adduct 11e

HF=-782.082425
G=-781.842295

C	1.090316	1.170371	-2.157044
N	0.459954	0.010475	-2.474772
C	-0.157712	-0.725027	-1.513647
C	-0.154280	-0.294469	-0.198577
C	0.484093	0.892614	0.152295
C	1.112921	1.625815	-0.852262
O	0.468909	-0.385629	-3.712697
U	-0.889902	-1.967669	-5.130066
C	-1.517517	-3.471754	-3.119104
C	-3.186873	-0.266312	-4.668264
C	-3.728575	-1.511261	-5.068484
C	-3.412531	-1.705728	-6.435542
C	-2.679904	-0.575746	-6.881934
C	-2.542105	0.313594	-5.789559
C	0.293901	-2.929197	-7.559136
C	1.393336	-2.414215	-6.830776
C	1.619111	-3.264611	-5.718885
C	0.660343	-4.304687	-5.759732
C	-0.162446	-4.095797	-6.894627
H	2.407243	-3.153846	-4.982561
H	1.981987	-1.543050	-7.097443
H	-0.107535	-2.523238	-8.480573
H	-0.970470	-4.740223	-7.222932
H	0.577843	-5.124009	-5.056166
H	-3.285276	0.182557	-3.685931
H	-4.296725	-2.188685	-4.442903
H	-3.714757	-2.549180	-7.046201
H	-2.320777	-0.407582	-7.890827

H -2.056062 1.282813 -5.815680

H -0.671591 -3.895763 -2.552956

H -2.021646 -4.348794 -3.559114

H -2.236475 -3.088267 -2.376654

H 1.549438 1.671967 -2.998593

H 1.625925 2.556959 -0.637671

H 0.492673 1.237495 1.180476

H -0.659013 -0.906262 0.541214

H -0.629518 -1.636975 -1.872930

U(III) pyridine N-oxide product 11e

HF=-741.602937
G=-741.404162

C 1.387432 1.742781 -2.505722

C 0.785028 0.893041 -3.467281

C 0.113882 -0.146662 -2.772567

C 0.306690 0.057086 -1.385803

C 1.096745 1.223136 -1.220430

U 2.894593 -0.684195 -2.366235

O 2.543762 -3.015050 -1.658156

N 2.920064 -2.900341 -0.375527

C 2.873545 -4.012030 0.392007

C 3.251656 -3.938325 1.719421

C 3.673722 -2.712657 2.234486

C 3.700199 -1.601774 1.392479

C 3.320008 -1.663859 0.047792

C 5.342904 0.719349 -2.789729

C 5.754960 -0.587521 -2.419542

C 5.417539 -1.468158 -3.474312

C 4.796203 -0.708024 -4.497884

C 4.758113 0.645592 -4.077586

H -0.095280 -0.557751 -0.589273

H -0.474582 -0.938816 -3.222742

H 0.789985 1.044083 -4.541140

H 1.943423 2.648908 -2.717403

H 1.391064 1.661117 -0.273449

H 6.263470 -0.858874 -1.502391

H 5.495691 1.623633 -2.211032

H 4.376227 1.480766 -4.653161

H 4.461484 -1.085304 -5.458422

H 5.621036 -2.532309 -3.504454

H 2.530794 -4.908454 -0.109697

H 3.212064 -4.833450 2.330725

H 3.975493 -2.630335 3.274841

H 4.027648 -0.642769 1.785840

U(III) lutidine TS SDDAll

HF=-1230.733686
G=-1230.443060

U 2.401085 -2.721049 -3.265753

C 4.272081 -2.931140 -1.246696

C 5.030244 -2.822995 -2.439594

C 4.849152 -1.517110 -2.959000

C 3.981161 -0.815475 -2.082665

C 3.630259 -1.688303 -1.024175

H 4.223091 -3.799800 -0.600777

H 5.668392 -3.594011 -2.854054

H 5.327443 -1.107487 -3.840524

H 3.675098 0.218465 -2.184964

H 2.996626 -1.442526 -0.181196

C 2.505166 -1.239993 -5.571460

C 1.651084 -0.505056 -4.709083

C 0.451481 -1.241242 -4.550278

C 0.563823 -2.433004 -5.307019

C 1.831036 -2.430347 -5.941661

H 3.480285 -0.922760 -5.920791

H 1.862925 0.468172 -4.283533

H -0.409668 -0.936227 -3.968680

H -0.200473 -3.193947 -5.414186

H 2.204335 -3.193527 -6.613573

C 4.835685 -5.012300 -5.559490

C 4.213621 -5.638528 -4.345308

C 4.803227 -6.707974 -3.684428

C 4.181286 -7.224477 -2.539786

C 2.973507 -6.701174 -2.119520

C 2.384850 -5.659048 -2.864662

N 3.040703 -5.114118 -3.926356

C 0.482069 -2.481334 -1.460342

C 1.078682 -5.063577 -2.561704

H 4.177904 -5.127812 -6.427177

H 4.987859 -3.938085 -5.409550

H 5.800853 -5.467501 -5.792893

H 5.738656 -7.121788 -4.046081

H 4.640679 -8.045682 -1.995735

H 2.455532 -7.098312 -1.252376

H 0.550167 -5.594032 -1.766959

H 0.449499 -5.031186 -3.458394

H 0.915541 -3.816090 -2.030333

H 0.615070 -2.736484 -0.402825

H -0.582893 -2.574655 -1.703299

H 0.734074 -1.411987 -1.558857

U(III) lutidine adduct SDDAll

HF=-1230.753405
G=-1230.461698

U 2.498566 -2.511923 -3.170311

C 4.101553 -2.199857 -0.936782

C 5.018730 -2.467326 -1.983104

C 4.998461 -1.366102 -2.876160

C 4.074126 -0.414782 -2.372687

C 3.523631 -0.929443 -1.173302

H 3.901371 -2.839712 -0.084770

H 5.654276 -3.342187 -2.060008

H 5.620214 -1.240525 -3.754894

H 3.861213 0.554298 -2.806512

H 2.792221 -0.438456 -0.544562

C 2.586653 -1.646975 -5.784100

C 1.880858 -0.642758 -5.071732

C 0.628307 -1.178096 -4.682264

C 0.560037 -2.512351 -5.148585

C 1.765408 -2.801117 -5.835223

H 3.558714 -1.530051 -6.248375

H 2.222850 0.369825 -4.896981

H -0.143956 -0.659534 -4.128964

H -0.282920 -3.183439 -5.028825

H 1.992627 -3.730116 -6.345221

C 4.860154 -4.524039 -5.012612

C 4.141818 -5.558163 -4.200247

C 4.526144 -6.898894 -4.253631

C 3.813895 -7.843518 -3.525657

C 2.731026 -7.421537 -2.762502

C 2.396775 -6.068372 -2.741777

N 3.098429 -5.150701 -3.444577

C 0.593428 -2.219589 -1.606454

C 1.229771 -5.571210 -1.940646

H 4.305505 -4.308530 -5.932036

H 4.957486 -3.582168 -4.461968

H 5.859734 -4.865492 -5.292539

H 5.375246 -7.186753 -4.865155

H 4.096881 -8.891982 -3.552761

H 2.145638 -8.126853 -2.181721

H 0.762745 -6.381513 -1.376772

H 0.464543 -5.131044 -2.589769

H 1.528077 -4.795654 -1.226516

H 0.794660 -2.588018 -0.587046

H -0.326648 -2.721266 -1.947898

H 0.326427 -1.158304 -1.487799

U(III) lutidine product SDDAll

HF=-1190.263102
G=-1190.015215

N 2.504223 -2.856473 -3.266726

C 3.451353 -2.976627 -2.304219

C 4.797771 -2.846884 -2.590794

C 5.184193 -2.621351 -3.927253

C 4.233335 -2.491876 -4.911578

C 2.854512 -2.563225 -4.566410

C 2.949531 -3.253416 -0.915242

C 1.767182 -2.484760 -5.490191

U 0.762027 -4.427814 -4.103656

C 2.605149 -6.378477 -3.578345

C 2.773816 -6.083952 -4.954360

C 1.615571 -6.525186 -5.640455

C 0.731679 -7.100038 -4.690786

C 1.343674 -7.007551 -3.414877

C -0.993520 -3.492467 -2.194275

C -1.361645 -4.845124 -2.403597

C -1.899964 -4.955727 -3.710739

C -1.864903 -3.668034 -4.306933

C -1.307736 -2.764256 -3.367984

H 3.640348 -5.612318 -5.401284

H 3.332866 -6.189423 -2.797877

H 0.935932 -7.389350 -2.486527

H -0.222709 -7.564643 -4.905964

H 1.448984 -6.460735 -6.710243

H -1.280013 -5.648693 -1.681319

H -2.312590 -5.853353 -4.154690

H -2.235247 -3.412378 -5.293902

H -1.169207 -1.699105 -3.510634

H -0.572048 -3.077551 -1.286264

H 2.366346 -2.404438 -0.541959

H 2.287966 -4.126995 -0.905539

H 3.772757 -3.440178 -0.221879

H 5.536607 -2.931911 -1.801160

H 6.239330 -2.535840 -4.175593

H 4.508714 -2.294055 -5.942746

H 2.018370 -2.339414 -6.537670

H 0.930177 -1.861941 -5.156235

U(III) lutidine N-oxide TS SDDAll

HF=-1305.884129
G=-1305.590216

C -3.416547 -2.292479 -7.462631

N -2.978807 -2.307737 -6.159173

C -1.661564 -2.303829 -5.808159

C -0.701942 -2.332726 -6.807711

C -1.090923 -2.361287 -8.148641

C -2.437316 -2.335067 -8.465481

O -3.882468 -2.311227 -5.189671

U -5.933273 -3.583225 -5.281641

C -1.358815 -2.280183 -4.349263

C -4.849731 -2.268240 -7.683746

C -6.646612 -4.489577 -7.670252

C -4.283731 -5.762832 -4.874649

C -5.526093 -6.328280 -5.251722

C -6.458694 -6.073946 -4.217449

C -5.789696 -5.357904 -3.191974

C -4.446976 -5.166527 -3.599102

C -7.733913 -2.565641 -3.494965

C -8.533452 -3.160287 -4.505574

C -8.395687 -2.386531 -5.683322

C -7.513730 -1.312939 -5.401610

C -7.104422 -1.423303 -4.050246

H -7.240738 -0.517520 -6.085298

H -6.442645 -0.742032 -3.527891

H -7.656228 -2.897745 -2.467201

H -9.163590 -4.033141 -4.385595

H -8.897110 -2.567555 -6.626132

H -3.363170 -5.809706 -5.445407

H -5.724325 -6.874312 -6.165412

H -7.490317 -6.403403 -4.193564

H -6.217991 -5.051712 -2.245829

H -3.676412 -4.666956 -3.023970

H -7.233500 -3.970688 -8.437680

H -7.379773 -4.992772 -7.012925

H -6.073964 -5.284254 -8.162524

H 0.343755 -2.338631 -6.521768

H -0.343387 -2.387732 -8.935467

H -2.771178 -2.330111 -9.497462

H -0.279754 -2.237445 -4.191181

H -1.833919 -1.418029 -3.871704

H -1.761307 -3.170157 -3.856564

H -5.603043 -3.397293 -7.567750

H -5.334917 -1.502947 -7.064403

H -5.079591 -2.073133 -8.733278

U(III) lutidine N-oxide adduct SDDAll

HF=-1305.904998
G=-1305.611259

C -3.341867 -2.164473 -8.097817

N -3.162696 -2.276799 -6.740218

C -1.915922 -2.309863 -6.164897

C -0.802868 -2.287822 -6.988900

C -0.937705 -2.212326 -8.373825

C -2.220913 -2.141500 -8.912237

O -4.220427 -2.313103 -5.958608

U -5.917736 -3.691119 -5.040964

C -1.864743 -2.355409 -4.679069

C -4.741780 -2.071448 -8.590133

C -6.689501 -4.823849 -7.106087

C -4.190039 -5.773989 -4.409992

C -5.446454 -6.389789 -4.624451

C -6.312057 -5.993404 -3.577323

C -5.590445 -5.138547 -2.707306

C -4.278207 -5.003551 -3.221193

C -8.429644 -3.220177 -4.028513

C -8.505473 -2.775983 -5.370438

C -7.691325 -1.624558 -5.496224

C -7.116871 -1.351087 -4.229893

C -7.571182 -2.339093 -3.321665

H -6.461012 -0.520541 -3.994071

H -7.335981 -2.390088 -2.265450

H -8.959377 -4.065587 -3.606964

H -9.085650 -3.234362 -6.160828

H -7.551265 -1.040200 -6.398222

H -3.306269 -5.905823 -5.024791

H -5.699146 -7.050008 -5.443570

H -7.339567 -6.311165 -3.448239

H -5.964095 -4.697467 -1.791668

H -3.471630 -4.454282 -2.748495

H -7.148278 -4.175867 -7.869260

H -7.469782 -5.551882 -6.832482

H -5.903746 -5.409268 -7.612394

H 0.175853 -2.323907 -6.522386

H -0.064421 -2.197793 -9.016750

H -2.374744 -2.062951 -9.983194

H -0.828253 -2.400203 -4.340679

H -2.345838 -1.470633 -4.248733

H -2.410496 -3.223646 -4.296714

H -5.329045 -2.944691 -8.283935

H -5.241858 -1.193533 -8.167879

H -4.749383 -1.997782 -9.678955

U(III) lutidine N-oxide product SDDAll

HF=-1265.423566
G=-1265.170835

C -3.417904 -2.161228 -6.892479

C -2.673578 -1.944773 -5.703110

C -1.299649 -2.077227 -6.018373

C -1.192595 -2.375797 -7.399588

C -2.502953 -2.434693 -7.939414

U -2.125406 0.217920 -7.326556

C -0.605524 0.423048 -9.418099

C -1.092813 1.570450 -10.110579

N -2.453725 1.816454 -10.064387

C -3.078142 2.822929 -10.732781

C -2.310644 3.723928 -11.450143

C -0.916225 3.585399 -11.462639

C -0.321627 2.527562 -10.807566

O -3.195940 1.023232 -9.277756

C -4.562335 2.893144 -10.602018

C -0.758825 1.342981 -5.235822

C -0.506343 2.201180 -6.335664

C -1.717075 2.857477 -6.667800

C -2.718993 2.403857 -5.774348

C -2.126891 1.469649 -4.886115

H -2.761345 -2.672438 -8.964962

H -4.499449 -2.163157 -6.976975

H -3.085529 -1.751767 -4.720088

H -0.476651 -1.993950 -5.318997

H -0.272752 -2.559726 -7.942259

H -1.846978 3.593735 -7.452262

H 0.448669 2.344747 -6.826069

H -0.027447 0.726257 -4.727875

H -2.621978 0.971386 -4.061563

H -3.749853 2.740620 -5.749891

H -2.806365 4.531676 -11.975884

H -0.305235 4.298985 -12.007884

H 0.752579 2.380850 -10.836267

H -4.954394 3.702835 -11.220092

H -5.022189 1.947384 -10.903735

H -4.851962 3.062825 -9.560219

H -1.171368 -0.487929 -9.665797

H 0.466786 0.269480 -9.521804

U(III) pyridine TS SDDAll

HF=-1152.107120
G=-1151.871699

U -5.147640 -1.098943 -0.374885

C -3.825824 -0.720096 2.027089

C -4.030978 -2.115184 1.919930

C -3.245792 -2.593291 0.838371

C -2.549665 -1.487190 0.281553

C -2.916824 -0.328833 1.014149

H -4.279869 -0.065979 2.761377

H -4.663458 -2.716054 2.561938

H -3.154695 -3.627071 0.524626

H -1.835016 -1.528183 -0.531333

H -2.540925 0.674673 0.850175

C -6.343118 -0.748550 -2.850431

C -5.160742 0.032159 -2.899566

C -4.051101 -0.850930 -2.913444

C -4.551854 -2.176389 -2.874744

C -5.966133 -2.114284 -2.841749

H -6.641665 -2.960883 -2.826477

H -7.358127 -0.368351 -2.849202

H -5.114983 1.114174 -2.945445

H -3.007761 -0.566326 -2.977622

H -3.953122 -3.080192 -2.889104

C -7.070813 -2.749129 0.360673

H -7.856611 -2.878023 -0.392941

H -6.311683 -3.526611 0.164969

H -7.501770 -3.011254 1.335086

H -7.030723 -1.290781 0.687623

C -7.057461 0.098722 0.915766

C -8.159254 0.555531 1.639433

C -8.352680 1.927372 1.800111

C -7.446369 2.814985 1.216066

C -6.374889 2.300756 0.497896

N -6.192412 0.977558 0.363200

H -8.852716 -0.157342 2.077417

H -9.196308 2.304650 2.372304

H -7.566169 3.889085 1.316547

H -5.639771 2.947714 0.025997

U(III) pyridine adduct SDDAll

HF=-1152.138830
G=-1151.902903

U -5.281097 -1.408966 -0.323042

C -4.089444 -1.893121 2.115727

C -3.522455 -2.830444 1.219183

C -2.705808 -2.120974 0.301168

C -2.770334 -0.743856 0.632083

C -3.625297 -0.604126 1.753636

H -4.750338 -2.126852 2.941906

H -3.676422 -3.902881 1.241955

H -2.103867 -2.557451 -0.486307

H -2.229563 0.053410 0.135949

H -3.855953 0.321498 2.268023

C -6.519124 -1.481935 -2.786382

C -5.864936 -0.224882 -2.763599

C -4.466871 -0.456624 -2.792309

C -4.257497 -1.858003 -2.832577

C -5.527310 -2.490732 -2.829545

H -5.710155 -3.558198 -2.866555

H -7.590241 -1.645772 -2.785561

H -6.351711 0.743583 -2.763837

H -3.692463 0.300818 -2.820926

H -3.297730 -2.355429 -2.898510

C -6.960386 -3.099911 0.375356

H -7.949235 -2.958503 -0.089956

H -6.643412 -4.114146 0.084080

H -7.123788 -3.146437 1.463899

H -7.929837 -0.534477 1.309575

C -7.619332 0.501204 1.186870

C -8.364276 1.543681 1.724190

C -7.925166 2.852204 1.536518

C -6.749353 3.063140 0.812138

C -6.065048 1.967814 0.308969

N -6.482151 0.698893 0.489009

H -9.271731 1.326022 2.277957

H -8.484196 3.689685 1.942665

H -6.366875 4.063463 0.637224

H -5.148422 2.092288 -0.261116

U(III) pyridine product SDDAll

HF=-1111.638116
G=-1111.441707

N -5.257166 -1.050934 -0.311578

C -4.637508 -1.090565 0.898900

C -4.036750 -2.303692 1.284099

C -4.083643 -3.411196 0.447157

C -4.734991 -3.316645 -0.790119

C -5.314776 -2.108132 -1.136570

U -5.549920 1.172766 0.580080

C -4.126367 1.902607 -1.638057

C -3.180450 1.916770 -0.583071

C -3.513759 2.987469 0.284922

C -4.658673 3.641421 -0.238390

C -5.039092 2.968120 -1.426453

C -8.213054 0.578920 0.401995

C -7.898250 0.416757 1.774213

C -7.615355 1.699273 2.309444

C -7.765489 2.654688 1.272055

C -8.130820 1.960934 0.091119

H -7.895111 -0.518722 2.320714

H -7.369686 1.915686 3.344050

H -7.651468 3.727437 1.369885

H -8.346297 2.412388 -0.869912

H -8.495419 -0.213418 -0.280902

H -2.963062 3.280780 1.172760

H -2.342199 1.239940 -0.469863

H -4.131071 1.214689 -2.475041

H -5.859458 3.243660 -2.078149

H -5.138388 4.519534 0.176527

H -3.532235 -2.373887 2.245073

H -3.620002 -4.349871 0.743295

H -4.788965 -4.164079 -1.466320

H -5.834305 -1.973637 -2.083233

U(III) pyridine N-oxide TS SDDAll

HF=-1227.262247
G=-1227.022522

C 0.839150 1.315391 -2.297228

N 0.076898 0.330982 -2.827478

C -0.051334 -0.901888 -2.262953

C 0.651995 -1.130694 -1.082195

C 1.438142 -0.144034 -0.492876

C 1.526725 1.100239 -1.117148

O -0.560592 0.578900 -3.963800

U -1.124399 -1.594404 -4.881958

C -1.921231 -3.002563 -2.801776

C -3.596366 -0.411093 -5.140017

C -3.830930 -1.795822 -5.320541

C -3.216922 -2.191411 -6.535782

C -2.607618 -1.045202 -7.109309

C -2.840340 0.053216 -6.244122

C 0.542082 -2.452167 -6.868679

C 1.394613 -1.827646 -5.921879

C 1.428360 -2.639696 -4.760368

C 0.593387 -3.762526 -4.987242

C 0.047624 -3.647973 -6.288762

H 2.017417 -2.454654 -3.870319

H 1.951060 -0.909569 -6.074112

H 0.340768 -2.101094 -7.873104

H -0.608428 -4.363050 -6.770305

H 0.423674 -4.578042 -4.294862

H -3.940886 0.192266 -4.308303

H -4.396488 -2.437122 -4.655321

H -3.246183 -3.182084 -6.972839

H -2.092707 -1.008631 -8.061412

H -2.510783 1.073466 -6.402359

H -1.435734 -3.634503 -2.047234

H -2.186289 -3.696172 -3.622135

H -2.869049 -2.650396 -2.374868

H 0.852472 2.236366 -2.866239

H 2.124700 1.905097 -0.703911

H 1.969731 -0.334417 0.434385

H 0.560068 -2.110589 -0.621799

H -0.937319 -1.853655 -2.610854

U(III) pyridine N-oxide adduct SDDAll

HF=-1227.284755
G=-1227.043834

C 0.983735 1.096291 -2.293071

N 0.149751 0.012893 -2.358749

C 0.055904 -0.866651 -1.312105

C 0.812810 -0.667663 -0.179694

C 1.682917 0.427452 -0.081985

C 1.749550 1.310602 -1.170197

O -0.579084 -0.174163 -3.441119

U -1.214810 -1.682488 -5.022573

C -2.022772 -3.280593 -3.348620

C -3.644352 -0.418280 -5.229723

C -3.930327 -1.782962 -5.474840

C -3.338105 -2.138696 -6.711338

C -2.692820 -0.990948 -7.237030

C -2.877485 0.071083 -6.317815

C 0.522158 -2.391683 -7.040660

C 1.343351 -1.909125 -5.992043

C 1.278202 -2.837757 -4.921418

C 0.419952 -3.895113 -5.309353

C -0.049953 -3.616637 -6.614630

H 1.811141 -2.763500 -3.980068

H 1.937631 -1.002118 -6.014564

H 0.380666 -1.923176 -8.006824

H -0.715937 -4.242228 -7.196611

H 0.170110 -4.763374 -4.714290

H -3.967038 0.156497 -4.369602

H -4.506773 -2.437343 -4.834158

H -3.394926 -3.110564 -7.186889

H -2.175228 -0.929550 -8.186390

H -2.519366 1.087766 -6.437355

H -1.224897 -3.638618 -2.676931

H -2.458156 -4.184433 -3.800268

H -2.811445 -2.845050 -2.714362

H 0.972076 1.730070 -3.169462

H 2.401198 2.177840 -1.150751

H 2.284990 0.586241 0.804739

H 0.717810 -1.383472 0.630238

H -0.628618 -1.690953 -1.467820

U(III) pyridine N-oxide product SDDAll

HF=-1186.802984
G=-1186.602909

C 1.689434 1.670346 -2.041016

C 1.150928 1.207610 -3.267323

C 0.303490 0.104694 -2.982963

C 0.315545 -0.109460 -1.582232

C 1.173895 0.857119 -1.000856

U 2.828900 -0.798861 -2.442752

O 2.460315 -3.035059 -1.678449

N 2.886658 -2.893230 -0.409099

C 2.834374 -3.969945 0.403374

C 3.265904 -3.846074 1.710943

C 3.742338 -2.609940 2.150485

C 3.769019 -1.537856 1.260009

C 3.334500 -1.652000 -0.064836

C 4.985147 0.797930 -3.047707

C 5.534522 -0.335744 -2.396773

C 5.367596 -1.455935 -3.249736

C 4.711549 -1.014296 -4.425979

C 4.479082 0.380262 -4.303160

H -0.245879 -0.867145 -1.048400

H -0.282928 -0.452158 -3.706322

H 1.326155 1.642497 -4.243920

H 2.353538 2.517330 -1.918951

H 1.378239 0.967939 0.056890

H 6.020058 -0.342952 -1.428633

H 4.982859 1.812161 -2.667253

H 4.025691 1.019867 -5.050748

H 4.469148 -1.627777 -5.287349

H 5.699553 -2.467372 -3.046184

H 2.446591 -4.876430 -0.044933

H 3.225212 -4.709443 2.366143

H 4.085882 -2.490662 3.174270

H 4.138245 -0.572583 1.597115

U(III) sp2 picoline TS SDDAll

HF=-1191.423814
G=-1191.161899

C -5.821826 2.007458 0.189070

C -6.245466 3.019104 1.086554

C -5.754801 4.259417 0.608841

C -5.028987 4.016461 -0.583705

C -5.070771 2.622969 -0.845396

U -7.641055 3.487569 -1.239957

N -9.202848 1.680378 -0.687214

C -9.823508 2.718282 -0.092451

C -11.030476 2.522753 0.587178

C -11.571557 1.244601 0.636208

C -10.904442 0.187403 0.009084

C -9.706884 0.430341 -0.656605

C -8.932749 -0.641732 -1.362931

C -6.908375 3.296113 -3.873572

C -8.264318 2.879248 -3.842589

C -9.064506 4.007793 -3.536003

C -8.204619 5.122471 -3.378568

C -6.873131 4.685041 -3.587158

C -8.916213 5.475322 -0.044682

H -8.945072 5.620514 1.042067

H -9.809446 5.947047 -0.471543

H -8.060423 6.072426 -0.402317

H -5.894106 5.222363 1.085450

H -6.819335 2.868112 1.993428

H -4.504974 4.758258 -1.174022

H -6.004537 0.944900 0.298873

H -4.576441 2.114961 -1.664706

H -5.986569 5.307296 -3.568018

H -6.054461 2.675772 -4.118117

H -8.628702 1.880729 -4.053224

H -10.145475 4.021775 -3.460464

H -8.515021 6.136293 -3.155945

H -9.372322 4.046658 -0.075909

H -11.529192 3.360543 1.066147

H -12.507579 1.059464 1.157487

H -11.310942 -0.818919 0.036088

H -7.898365 -0.665587 -1.005895

H -9.379586 -1.626495 -1.209161

H -8.897670 -0.442094 -2.439386

U(III) sp2 picoline adduct SDDAll

HF=-1191.447016
G=-1191.183603

C -5.988304 2.091043 0.394551

C -6.218083 3.282204 1.128412

C -5.585441 4.347655 0.445206

C -4.971669 3.819137 -0.717934

C -5.219940 2.422530 -0.749893

U -7.653111 3.619137 -1.209171

N -9.398355 1.823250 -0.541910

C -10.263474 2.599854 0.126700

C -11.431245 2.144222 0.723013

C -11.709936 0.783854 0.611980

C -10.817058 -0.035585 -0.082383

C -9.665471 0.503413 -0.654742

C -8.678608 -0.325598 -1.417276

C -7.104485 3.117433 -3.857522

C -8.513805 2.994981 -3.767997

C -9.049897 4.279807 -3.499977

C -7.975249 5.197689 -3.430153

C -6.772176 4.480885 -3.648767

C -8.568690 5.699088 -0.187154

H -8.638967 5.679631 0.912205

H -9.553102 6.020914 -0.562928

H -7.881359 6.527293 -0.422014

H -5.572667 5.383247 0.760596

H -6.758933 3.361381 2.064562

H -4.379412 4.374837 -1.434205

H -6.306457 1.096520 0.686358

H -4.850096 1.728834 -1.495697

H -5.776781 4.905092 -3.691931

H -6.405710 2.321667 -4.085963

H -9.088240 2.088963 -3.924172

H -10.100653 4.523557 -3.392861

H -8.061187 6.261232 -3.247627

H -10.007257 3.663368 0.191024

H -12.085722 2.830983 1.248077

H -12.606413 0.360254 1.055802

H -11.011452 -1.098808 -0.183985

H -7.678442 -0.223146 -0.983655

H -8.955580 -1.381836 -1.416922

H -8.613983 0.018388 -2.455178

U(III) sp2 picoline product SDDAll

HF=-1150.947667
G=-1150.726439

C -5.463115 1.887174 0.036436

C -6.130889 2.219790 1.241250

C -6.094771 3.630596 1.387176

C -5.407875 4.171843 0.272137

C -5.010982 3.093347 -0.558135

U -3.494879 2.832775 1.714019

C -2.425319 4.976540 2.251382

N -3.351117 4.720264 3.212541

C -3.592141 5.535275 4.259228

C -2.867826 6.714600 4.384151

C -1.902439 7.029563 3.420188

C -1.680859 6.164367 2.357169

C -4.643531 5.114007 5.243592

C -3.623742 0.517274 3.177851

C -2.750887 1.369755 3.903306

C -1.559563 1.523087 3.151742

C -1.699371 0.771033 1.958088

C -2.971313 0.143549 1.976369

H -0.689306 2.097236 3.446312

H -2.944024 1.798633 4.879181

H -0.945983 0.661456 1.184916

H -4.599920 0.177716 3.502725

H -3.363568 -0.528010 1.222362

H -5.348320 0.890730 -0.372749

H -6.616463 1.521222 1.911723

H -6.546981 4.200479 2.189943

H -5.232316 5.223636 0.080962

H -4.489413 3.179961 -1.505765

H -0.931337 6.404516 1.606939

H -1.332476 7.951877 3.513257

H -3.054814 7.378125 5.223340

H -4.376905 4.157647 5.706185

H -4.772470 5.855729 6.035502

H -5.606256 4.971449 4.741599

U(III) sp2 picoline N-oxide TS SDDAll

HF=-1266.574272
G=-1266.308265

C	-4.706342	-0.635209	-0.541400
C	-3.310493	-0.386517	-0.567658
C	-2.946827	-0.080275	-1.904262
C	-4.117276	-0.139975	-2.701825
C	-5.203305	-0.485052	-1.858721
U	-3.595774	-2.739071	-1.924764
C	-5.727523	-3.623998	-3.199300
O	-1.749321	-3.134173	-3.435487
N	-2.201092	-2.802279	-4.642203
C	-1.280891	-2.546289	-5.613759
C	-1.745850	-2.193060	-6.875598
C	-3.111616	-2.088893	-7.121879
C	-4.001819	-2.349234	-6.083058
C	-3.549273	-2.720995	-4.822121
C	0.155329	-2.665894	-5.235523
C	-3.986180	-3.969042	0.486429
C	-4.201466	-4.992450	-0.471121
C	-2.960936	-5.283961	-1.088684
C	-1.975990	-4.445863	-0.511378
C	-2.607395	-3.633511	0.463232
H	-4.178712	0.075992	-3.761436
H	-1.954198	0.187218	-2.248540
H	-2.648330	-0.385227	0.289344
H	-5.292980	-0.869130	0.338668
H	-6.236728	-0.590174	-2.166208
H	-5.146166	-5.479847	-0.680364
H	-4.731720	-3.549862	1.151291
H	-2.117974	-2.913014	1.107149
H	-0.923175	-4.435562	-0.767804
H	-2.790247	-6.025893	-1.860047
H	-6.442195	-3.206082	-3.919610
H	-6.175858	-3.421674	-2.208476
H	-5.734405	-4.714356	-3.325514
H	-1.017043	-1.998311	-7.655427
H	-3.470805	-1.813027	-8.108871
H	-5.074581	-2.279240	-6.239128
H	-4.509891	-3.139814	-3.977186
H	0.793149	-2.446703	-6.093994
H	0.395351	-1.978291	-4.418490
H	0.372569	-3.672567	-4.865568

U(III) sp2 picoline N-oxide adduct SDDAll

HF=-1266.5961482
G=-1266.329844

C	-4.444493	-0.621598	-0.269977
C	-3.043595	-0.434725	-0.377377
C	-2.750689	-0.116831	-1.726878
C	-3.971017	-0.109020	-2.450464
C	-5.017582	-0.416877	-1.547681
U	-3.554612	-2.751905	-1.786828
C	-5.761353	-3.332714	-2.712594
O	-2.491638	-3.216871	-3.800088
N	-2.569686	-2.926892	-5.082690
C	-1.487875	-2.350676	-5.704270
C	-1.586037	-2.068144	-7.056960
C	-2.741127	-2.364334	-7.785280
C	-3.811479	-2.962783	-7.112154
C	-3.711155	-3.236666	-5.767111
C	-0.292122	-2.083119	-4.858997
C	-3.905630	-4.017900	0.625569
C	-4.274049	-4.984096	-0.343061
C	-3.106096	-5.365248	-1.046399
C	-2.013650	-4.638515	-0.509811
C	-2.506913	-3.805927	0.524946
H	-4.088700	0.121529	-3.503488
H	-1.769975	0.120774	-2.124478
H	-2.328590	-0.492748	0.434055
H	-4.985769	-0.855522	0.638745
H	-6.069802	-0.480234	-1.792096
H	-5.271874	-5.367624	-0.512450
H	-4.570205	-3.548255	1.340570
H	-1.915840	-3.148614	1.151042
H	-0.978251	-4.724384	-0.820521
H	-3.053706	-6.094715	-1.846131
H	-6.065072	-2.668054	-3.538705
H	-6.576233	-3.284794	-1.975086
H	-5.770911	-4.363973	-3.104493
H	-0.728829	-1.609489	-7.539218
H	-2.802913	-2.136633	-8.843343
H	-4.733138	-3.217791	-7.623967
H	-4.490384	-3.682010	-5.161926
H	0.497315	-1.627475	-5.459150
H	-0.542505	-1.414329	-4.028272
H	0.083645	-3.009610	-4.412652

U(III) sp2 picoline N-oxide product SDDAll

HF=-1226.114492
G=-1225.888530

C	-4.342905	-0.566281	-0.042364
C	-3.093686	-0.452178	-0.700972
C	-3.333668	0.002660	-2.022000
C	-4.732079	0.169092	-2.182095
C	-5.356270	-0.185041	-0.959849
U	-4.365978	-2.541845	-1.952779
C	-3.264335	-2.572492	-4.270792
N	-4.473343	-2.797362	-4.860806
C	-4.715773	-2.939645	-6.189943
C	-3.623650	-2.848126	-7.044781
C	-2.349519	-2.620076	-6.529851
C	-2.185401	-2.485093	-5.152219
O	-5.523905	-2.883475	-4.016395
C	-6.123934	-3.180012	-6.615710
C	-4.680184	-4.895128	-0.581201
C	-3.848092	-4.102054	0.251169
C	-2.595757	-3.957694	-0.395338
C	-2.651820	-4.663613	-1.623502
C	-3.939474	-5.245126	-1.737624
H	-4.289292	-5.863310	-2.556098
H	-5.692052	-5.213550	-0.353333
H	-4.111128	-3.706832	1.224913
H	-1.735852	-3.428501	-0.003104
H	-1.845543	-4.764136	-2.339413
H	-2.580770	0.208739	-2.772520
H	-2.123208	-0.645198	-0.260117
H	-4.493750	-0.857737	0.990057
H	-6.419563	-0.133730	-0.750097
H	-5.233768	0.523559	-3.074860
H	-3.790152	-2.957930	-8.111478
H	-1.497967	-2.549103	-7.201404
H	-1.194867	-2.306771	-4.741913
H	-6.182020	-3.273938	-7.702078
H	-6.516220	-4.089795	-6.150692
H	-6.770163	-2.360393	-6.286456

U(III) sp3 picoline TS SDDAll

HF=-1191.418738
G=-1191.418738

U	-0.272382	1.442197	-1.648628
C	0.730397	-0.149661	-3.686266
H	1.126213	-1.120773	-3.412817
C	-0.613207	0.138806	-4.024938
H	-1.427061	-0.574702	-4.070495
C	-0.698424	1.524545	-4.330765
H	-1.582483	2.050916	-4.670585
C	0.600012	2.081037	-4.190054
H	0.874011	3.110302	-4.383975
C	1.477661	1.049287	-3.788108
H	2.540372	1.152164	-3.602550
C	-1.226224	4.035800	-1.735996
C	0.168211	4.171139	-1.506952
H	0.885787	4.602731	-2.193861
C	0.445330	3.697749	-0.202450
H	1.413305	3.696898	0.283441
C	-0.774500	3.260665	0.376317
H	-0.901013	2.872539	1.380005
C	-1.805472	3.479559	-0.570620
H	-2.857226	3.266558	-0.423990
C	-2.645529	0.370971	-1.257672
H	-2.991684	-0.620533	-1.571813
H	-2.930173	1.065588	-2.067520
H	-3.219088	0.664920	-0.371664
C	-0.299375	-0.814643	-0.074655
H	-1.375319	-0.158852	-0.611408
H	0.051958	-1.430181	-0.911987
C	0.828131	-0.140447	0.579228
N	1.654183	0.548593	-0.259009
C	2.760638	1.130780	0.236496
H	3.383336	1.651269	-0.487358
C	3.095725	1.097553	1.577710
H	4.007155	1.568890	1.929002
C	2.206966	0.466341	2.463164
H	2.419717	0.445747	3.528691
C	1.069138	-0.143944	1.970326
H	0.376519	-0.657657	2.629958
H	-0.878433	-1.434029	0.613116
H	-1.755462	4.338071	-2.631567

U(III) sp3 picoline adduct SDDAll

HF=-1191.446805
G=-1191.182326

U	-0.528049	1.695713	-1.673624
C	0.248205	-0.236141	-3.494997
H	0.102765	-1.275563	-3.223265
C	-0.689916	0.580415	-4.170966
H	-1.679088	0.278555	-4.491737
C	-0.100888	1.856476	-4.361372
H	-0.549073	2.693397	-4.882687
C	1.205913	1.823540	-3.806456
H	1.924294	2.634269	-3.827448
C	1.420736	0.528719	-3.275199
H	2.331950	0.175044	-2.806897
C	-1.191865	4.320390	-2.141986
C	-0.000677	4.387514	-1.374479
H	0.955023	4.763515	-1.720556
C	-0.302782	3.941068	-0.063395
H	0.383399	3.908952	0.775219
C	-1.676188	3.593211	-0.024033
H	-2.218643	3.228579	0.840548
C	-2.226309	3.831186	-1.306087
H	-3.258262	3.671391	-1.592946
C	-2.689689	0.500346	-1.457099
H	-2.607930	-0.585042	-1.626949
H	-3.444795	0.858779	-2.173439
H	-3.144370	0.634586	-0.461120
C	-0.238173	-1.181629	0.638084
H	-1.136140	-0.555797	0.616482
H	-0.186137	-1.696310	-0.328606
C	0.998990	-0.365436	0.867080
N	1.148329	0.753290	0.124765
C	2.262721	1.490795	0.283631
H	2.335149	2.381611	-0.336742
C	3.272671	1.165100	1.174840
H	4.148895	1.798884	1.259824
C	3.120936	0.016257	1.951590
H	3.882740	-0.274085	2.669098
C	1.972916	-0.751317	1.791485
H	1.820864	-1.651879	2.378054
H	-0.364566	-1.939101	1.414691
H	-1.299696	4.629646	-3.174383

U(III) sp3 picoline product SDDAll

HF=-1150.949653
G=-1150.725292

C	0.691680	1.816710	-1.774662
C	0.805978	0.927417	-2.881541
N	1.348976	-0.324840	-2.678365
C	1.669013	-0.720291	-1.427581
C	1.513993	0.078385	-0.315219
C	1.028669	1.388670	-0.511722
C	0.532147	1.258205	-4.243034
U	2.726361	-0.000689	-4.734519
C	4.525768	2.017547	-5.262527
C	5.310491	0.853396	-5.064766
C	5.217664	0.494580	-3.694825
C	4.389065	1.445914	-3.047370
C	3.961850	2.384702	-4.015558
C	3.131545	-1.003471	-7.304399
C	1.727150	-0.944731	-7.124753
C	1.368254	-1.920359	-6.158739
C	2.554359	-2.577989	-5.742796
C	3.640779	-2.012524	-6.452956
H	0.363223	-2.149263	-5.824284
H	1.042965	-0.292684	-7.656127
H	3.712149	-0.397875	-7.990511
H	4.679865	-2.309695	-6.373590
H	2.612263	-3.393977	-5.030933
H	5.729837	-0.333736	-3.217377
H	4.128935	1.457967	-1.995367
H	3.318871	3.237047	-3.833140
H	4.404579	2.551574	-6.198473
H	-0.000644	0.479192	-4.799408
H	2.068332	-1.729256	-1.340902
H	1.771694	-0.290227	0.671441
H	0.908698	2.056230	0.337967
H	0.297229	2.814201	-1.943024
H	0.168481	2.260899	-4.451436
H	5.900159	0.345887	-5.817867

U(III) sp3 picoline N-oxide TS SDDAll

HF=-1266.573027
G=-1266.305839

C	-3.520891	-1.751596	-6.902143
C	-3.307765	-2.484019	-5.708002
C	-1.970068	-2.950694	-5.716218
C	-1.353085	-2.498884	-6.907113
C	-2.314173	-1.757924	-7.643254
U	-1.780076	-0.198735	-5.456146
C	-0.587569	-1.225593	-3.320761
O	-3.887124	0.913904	-5.066636
N	-4.593331	0.737018	-3.962916
C	-3.940589	0.687594	-2.754228
C	-4.734972	0.461380	-1.617413
C	-6.108122	0.317952	-1.707612
C	-6.724786	0.408232	-2.961476
C	-5.936918	0.619665	-4.072399
C	-2.498693	0.831582	-2.770753
C	-0.438394	1.111308	-7.441965
C	0.579183	0.481193	-6.679133
C	0.647154	1.129170	-5.422032
C	-0.326321	2.159790	-5.406751
C	-0.996764	2.149301	-6.654451
H	-6.303314	0.693833	-5.087988
H	-0.494290	2.864488	-4.600525
H	-1.784379	2.828731	-6.959176
H	-0.708633	0.871671	-8.462883
H	1.213876	-0.330021	-7.014210
H	1.338120	0.894877	-4.621491
H	-4.047700	-2.683918	-4.941069
H	-1.506055	-3.562047	-4.952446
H	-0.339668	-2.715123	-7.222653
H	-2.164171	-1.312856	-8.619121
H	-4.446511	-1.272853	-7.198723
H	0.085713	-0.733873	-2.608463
H	0.057184	-1.599404	-4.137940
H	-1.012686	-2.109029	-2.830144
H	-7.797204	0.310663	-3.083017
H	-6.700026	0.150136	-0.813394
H	-4.232654	0.415799	-0.656921
H	-1.704273	-0.208877	-3.127100
H	-2.190194	1.683118	-3.390662
H	-2.103336	0.961945	-1.761361

U(III) sp3 picoline N-oxide adduct SDDAll

HF=-1266.5961485
G=-1266.329454

C	-3.621153	-1.762764	-6.709694
C	-3.199424	-2.519900	-5.586718
C	-1.893679	-3.000800	-5.847661
C	-1.505423	-2.534904	-7.126436
C	-2.572256	-1.770513	-7.662188
U	-1.607399	-0.263577	-5.573391
C	-0.282505	-1.196268	-3.726478
O	-3.146341	0.872002	-4.282698
N	-4.231242	0.717997	-3.550045
C	-4.132019	0.770680	-2.178724
C	-5.290274	0.609470	-1.436832
C	-6.533709	0.409090	-2.044857
C	-6.587366	0.381447	-3.442576
C	-5.433928	0.538813	-4.175566
C	-2.776045	0.995769	-1.607718
C	-0.575975	1.120038	-7.710655
C	0.515190	0.373139	-7.197224
C	0.860439	0.911814	-5.933508
C	-0.020717	1.986380	-5.661846
C	-0.906261	2.117843	-6.761031
H	-5.378415	0.532369	-5.255437
H	-0.008377	2.611964	-4.776725
H	-1.685621	2.864378	-6.864059
H	-1.048774	0.975805	-8.674536
H	1.018622	-0.444301	-7.699134
H	1.658611	0.565292	-5.289763
H	-3.783941	-2.719861	-4.695567
H	-1.298645	-3.615962	-5.185583
H	-0.565395	-2.747297	-7.620966
H	-2.595616	-1.307081	-8.640681
H	-4.593937	-1.302471	-6.842104
H	0.145602	-0.399653	-3.096298
H	0.567185	-1.811392	-4.058165
H	-0.883245	-1.841968	-3.064788
H	-7.522916	0.237747	-3.972428
H	-7.429499	0.282043	-1.447933
H	-5.202494	0.645607	-0.355825
H	-2.079166	0.211164	-1.922451
H	-2.358388	1.944797	-1.959885
H	-2.829131	1.011934	-0.517764

U(III) sp3 picoline N-oxide product SDDAll

HF=-1226.112763
G=-1225.886023

C	-3.781032	-1.525157	-7.284418
C	-3.959299	-1.800927	-5.903115
C	-2.696802	-2.141388	-5.359937
C	-1.738539	-2.077829	-6.402121
C	-2.409604	-1.703545	-7.594453
U	-2.504809	0.539265	-6.012609
C	0.012332	0.950920	-6.537018
C	0.079567	2.317695	-6.930035
N	-0.999438	2.840420	-7.618567
C	-1.039830	4.099534	-8.104521
C	-0.010085	4.982039	-7.868963
C	1.080503	4.539301	-7.101459
C	1.119085	3.237838	-6.647842
O	-2.079083	2.064166	-7.772160
C	-2.775909	0.725767	-3.291306
C	-1.887794	1.775178	-3.636893
C	-2.616479	2.744409	-4.369085
C	-3.955087	2.293321	-4.479211
C	-4.055913	1.046608	-3.809750
H	-1.947526	4.335077	-8.645677
H	-1.960243	-1.597765	-8.575257
H	-4.563913	-1.267750	-7.989908
H	-4.900737	-1.791261	-5.367418
H	-2.502541	-2.426047	-4.333111
H	-0.683555	-2.308998	-6.312801
H	-2.224118	3.676549	-4.758385
H	-0.839428	1.836101	-3.371542
H	-2.529833	-0.149528	-2.702472
H	-4.958823	0.462217	-3.681814
H	-4.768556	2.826623	-4.959274
H	-0.068384	5.990276	-8.260850
H	1.902555	5.214163	-6.882013
H	1.968220	2.869548	-6.082098
H	-0.272875	0.288470	-7.368197
H	0.902891	0.592723	-6.024722

--------Uranium (IV)

U(IV) lutidine TS SDDAll

HF=-1270.5979796
G=-1270.271667

N	2.554830	-2.596658	-3.748636
C	3.373877	-2.055177	-2.814469
C	4.727639	-2.392221	-2.729723
C	5.228859	-3.359928	-3.589564
C	4.365453	-3.973362	-4.491204
C	3.027848	-3.571741	-4.547310
C	2.693921	-1.064254	-1.965078
C	2.339677	0.921754	-3.949507
U	0.385562	-0.827474	-3.390482
C	-0.153354	-0.060979	-0.766788
C	0.296233	1.106012	-1.428332
C	-0.687058	1.472270	-2.377203
C	-1.746624	0.534755	-2.291237
C	-1.414863	-0.413249	-1.299648
C	-0.846877	-2.048119	-5.555107
C	0.292387	-1.408383	-6.100261
C	0.081922	-0.009614	-6.030948
C	-1.178312	0.214700	-5.435549
C	-1.750763	-1.046401	-5.136394
C	-0.401878	-3.004891	-2.611459
H	-1.013423	-3.113918	-5.474592
H	1.160723	-1.891555	-6.525915
H	0.762990	0.751753	-6.388215
H	-1.636040	1.179849	-5.261380
H	-2.719259	-1.219702	-4.684738
H	-2.663740	0.556930	-2.864520
H	-0.650957	2.336695	-3.028804
H	-2.020641	-1.255334	-0.993582
H	0.362326	-0.580648	0.031462
H	1.221456	1.633790	-1.235996
H	-0.037221	-3.165857	-1.583319
H	-1.495771	-3.099480	-2.573605
H	-0.025023	-3.842671	-3.212162
H	3.067376	1.532263	-3.400934
H	2.844545	0.529534	-4.840094
H	1.546895	1.607443	-4.275097
H	2.390275	-0.053269	-2.844704
H	1.932820	-1.556343	-1.344748
H	3.357418	-0.515789	-1.292621
H	5.355757	-1.914466	-1.984618
H	6.274452	-3.653013	-3.542942
H	4.714853	-4.760807	-5.152084
C	2.089571	-4.248936	-5.505406
H	1.053615	-4.028880	-5.254232
H	2.274169	-3.930031	-6.537671
H	2.235673	-5.333155	-5.474778

U(IV) lutidine adduct SDDAll

HF=-1270.622777
G=-1270.297102

N	2.851696	-2.388912	-3.389776
C	3.678819	-2.192380	-2.343520
C	4.888968	-2.877613	-2.205753
C	5.258838	-3.807137	-3.167527
C	4.406127	-4.016303	-4.241848
C	3.216501	-3.287540	-4.325931
C	3.251956	-1.225073	-1.282218
C	2.073172	0.532828	-4.498495
U	0.171019	-0.779321	-3.679502
C	0.034616	0.006061	-1.014087
C	0.350195	1.171487	-1.754239
C	-0.777406	1.499034	-2.544110
C	-1.793334	0.546269	-2.275510
C	-1.289954	-0.375986	-1.333339
C	-1.169005	-2.028936	-5.735152
C	-0.178900	-1.267060	-6.401746
C	-0.496204	0.103346	-6.245627
C	-1.677092	0.191786	-5.478382
C	-2.089230	-1.125582	-5.152788
C	-0.272431	-2.997890	-2.734644
H	-1.225357	-3.108896	-5.683162
H	0.651738	-1.655791	-6.974532
H	0.068233	0.934162	-6.648123
H	-2.190162	1.104758	-5.205306
H	-2.967676	-1.397014	-4.580176
H	-2.787877	0.539066	-2.702282
H	-0.855593	2.343305	-3.218158
H	-1.820735	-1.224923	-0.922975
H	0.670087	-0.485423	-0.290226
H	1.279135	1.726403	-1.718726
H	0.203930	-3.133129	-1.752488
H	-1.350000	-3.165517	-2.590314
H	0.090409	-3.817049	-3.372485
H	2.868774	0.653738	-3.748818
H	2.539920	0.063764	-5.377046
H	1.768970	1.544985	-4.803261
H	2.823680	-0.322657	-1.723675
H	2.488452	-1.682895	-0.644796
H	4.092089	-0.936681	-0.645691
H	5.520946	-2.679364	-1.345927
H	6.192027	-4.356938	-3.081421
H	4.651326	-4.731357	-5.020752
C	2.320700	-3.471192	-5.512556
H	1.269554	-3.467433	-5.216329
H	2.473193	-2.653502	-6.224957
H	2.533348	-4.410111	-6.029848

U(IV) lutidine product SDDAll

HF=-1230.148764
G=-1229.865441

C	2.159049	-3.321256	-3.137415
C	3.073340	-2.251184	-3.272404
C	4.017794	-2.605655	-4.265269
C	3.700064	-3.905370	-4.730657
C	2.547227	-4.346376	-4.040449
U	1.642264	-2.330964	-5.618726
C	1.372478	-0.086885	-4.712603
N	3.086005	-1.164851	-7.395042
C	3.541424	-2.413392	-7.743595
C	4.931672	-2.643406	-7.913774
C	5.793794	-1.572100	-7.867033
C	5.291402	-0.276081	-7.651877
C	3.936777	-0.105139	-7.412885
C	2.513417	-3.402848	-7.773646
C	3.346432	1.259221	-7.209829
C	-0.878884	-2.728765	-4.619440
C	-0.557391	-3.945326	-5.273966
C	-0.509530	-3.694963	-6.663004
C	-0.798623	-2.320399	-6.871283
C	-1.042503	-1.730379	-5.608519
H	3.052219	-1.323764	-2.715976
H	4.845758	-1.995100	-4.605968
H	4.248084	-4.462982	-5.478608
H	2.067755	-5.310262	-4.156926
H	1.329434	-3.363855	-2.443048

H -1.008377 -2.592661 -3.552956

H -0.400810 -4.903363 -4.794948

H -1.304997 -0.696669 -5.428929

H -0.852878 -1.817006 -7.829577

H -0.299865 -4.426606 -7.432610

H 0.853807 0.594293 -5.402062

H 0.781108 -0.115076 -3.785806

H 2.337571 0.370500 -4.451406

H 1.634129 -3.104446 -8.347803

H 2.806709 -4.437553 -7.935119

H 5.281517 -3.646793 -8.135129

H 6.858496 -1.718876 -8.031607

H 5.949616 0.586036 -7.673972

H 2.935539 1.373514 -6.204075

H 4.097853 2.036001 -7.369963

H 2.522285 1.419245 -7.912305

U(IV) lutidine N-oxide TS SDDAll

HF=-1345.757680
G=-1345.428161

C -3.446568 -1.745029 -7.131712

C -2.781550 -2.591838 -6.217842

C -1.410200 -2.628302 -6.569782

C -1.228881 -1.806907 -7.705069

C -2.484181 -1.255026 -8.049428

U -1.854796 -0.007447 -5.690403

C -3.501589 2.020957 -4.864831

C -4.293722 1.279246 -5.776354

C -3.770566 1.488280 -7.073853

C -2.652851 2.344652 -6.966645

C -2.487817 2.675694 -5.601056

O -0.666512 1.171535 -3.936196

N 0.052609 0.734234 -2.920017

C 0.394484 1.630156 -1.949954

C 1.112122 1.179953 -0.851836

C 1.472295 -0.163610 -0.749038

C 1.124032 -1.037539 -1.766318

C 0.416646 -0.585906 -2.883663

C -0.049505 3.037778 -2.151011

C -0.053444 -1.383356 -4.005615

C -2.862733 -1.179818 -3.503890

C 0.102069 0.782767 -6.943287

H -0.644242 -3.217757 -6.082504

H -0.298124 -1.638935 -8.229198

H -2.673870 -0.599184 -8.889050

H -4.507769 -1.531592 -7.143283

H -3.243007 -3.137980 -5.406160

H -3.644618 2.069436 -3.792245

H -5.165740 0.685889 -5.528428

H -4.173656 1.081611 -7.991622

H -2.034788 2.692809 -7.783842

H -1.707485 3.301988 -5.190465

H -2.892176 -2.183898 -3.065502

H -3.826573 -1.043263 -4.015658

H -2.814134 -0.452097 -2.683303

H 0.415189 1.742099 -6.506283

H 0.966912 0.103867 -6.871340

H -0.071075 0.948764 -8.014660

H 1.377661 1.895295 -0.081479

H 2.029604 -0.517437 0.112667

H 1.403762 -2.084792 -1.730814

H 0.286779 3.660136 -1.319849

H 0.349661 3.435669 -3.089098

H -1.139602 3.091837 -2.228444

H -1.426272 -1.325576 -3.894737

H 0.399744 -1.023457 -4.942671

H 0.191987 -2.439295 -3.890229

U(IV) lutidine N-oxide adduct SDDAll

HF=-1345.782389
G=-1345.451234

C -3.569187 -1.722634 -6.830330

C -2.683944 -2.449869 -6.001537

C -1.396810 -2.401276 -6.591282

C -1.488900 -1.654699 -7.790000

C -2.828969 -1.234962 -7.938636

U -1.943883 0.214115 -5.780508

C -3.600809 2.227209 -4.847740

C -4.377838 1.482843 -5.767932

C -3.871452 1.731478 -7.067702

C -2.772728 2.610087 -6.950539

C -2.602428 2.915219 -5.578405

O 0.026313 0.384362 -4.329475

N 0.324765 0.205751 -3.067581

C 0.235077 1.267231 -2.210211

C 0.580945 1.085675 -0.877836

C 1.020669 -0.149756 -0.419104

C 1.119109 -1.197584 -1.325820

C 0.774041 -1.019297 -2.658881

C -0.222020 2.559388 -2.784660

C 0.869667 -2.080934 -3.693928

C -2.707787 -0.527188 -3.532857

C -0.089899 1.028987 -7.174001

H -0.503686 -2.892850 -6.225804

H -0.677920 -1.448773 -8.475429

H -3.223047 -0.668339 -8.772142

H -4.630365 -1.588455 -6.662076

H -2.949402 -2.957616 -5.083549

H -3.757952 2.264940 -3.777122

H -5.229358 0.860928 -5.521508

H -4.276174 1.341067 -7.991817

H -2.168337 2.989400 -7.763703

H -1.856803 3.589369 -5.174138

H -2.198660 -1.423140 -3.144973

H -3.780855 -0.767217 -3.549814

H -2.581910 0.260115 -2.772442

H 0.270519 1.986505 -6.767843

H 0.750668 0.320560 -7.121931

H -0.320405 1.189321 -8.235305

H 0.499207 1.936296 -0.209937

H 1.288725 -0.291042 0.622693

H 1.467961 -2.176947 -1.016881

H -0.189854 3.341492 -2.024353

H 0.405621 2.844147 -3.634653

H -1.243845 2.468087 -3.165540

H -0.119817 -2.294358 -4.109129

H 1.496856 -1.749864 -4.527386

H 1.284705 -2.992554 -3.260846

U(IV) lutidine N-oxide product SDDAll

HF=-1305.309208
G=-1305.021919

C -2.770521 -1.664864 -7.370550

N -1.759986 -2.322565 -6.702589

C -0.448848 -2.293694 -7.057279

C -0.095658 -1.626079 -8.218557

C -1.087229 -1.010525 -8.992400

C -2.402687 -1.024683 -8.571574

O -2.116794 -3.060766 -5.644893

U -4.224240 -4.084953 -5.613053

C -3.048373 -5.145983 -3.779398

C 0.504885 -3.022043 -6.171795

C -4.069121 -1.762492 -6.785914

C -5.132893 -5.424056 -7.796400

C -3.903585 -4.872627 -8.232420

C -2.861426 -5.531931 -7.540199

C -3.440492 -6.496660 -6.681917

C -4.845152 -6.431297 -6.839169

C -5.830684 -2.786129 -3.815887

C -6.528925 -2.682745 -5.048073

C -6.986945 -3.971835 -5.400578

C -6.576962 -4.873858 -4.388227

C -5.872792 -4.140124 -3.405181

H -5.380110 -1.967749 -3.265768

H -5.446343 -4.541962 -2.496514

H -6.788970 -5.935041 -4.354818

H -7.567817 -4.220766 -6.279424

H -6.699338 -1.772624 -5.608486

H -3.782595 -4.091967 -8.972604

H -6.115241 -5.150771 -8.160160

H -5.569827 -7.061799 -6.339937

H -2.904695 -7.167087 -6.022646

H -1.802219 -5.334851 -7.649905

H -2.042150 -5.397300 -4.145555

H -2.918940 -4.439008 -2.945958

H -3.492923 -6.061492 -3.367722

H 0.946810 -1.608742 -8.514569

H -0.816773 -0.499697 -9.911991

H -3.179359 -0.517110 -9.133131

H 1.525038 -2.900759 -6.540327

H 0.440079 -2.648702 -5.145353

H 0.259436 -4.087436 -6.128465

H -4.062717 -1.431758 -5.735345

H -4.845217 -1.250806 -7.352179

U(IV) pyridine TS SDDAll

HF=-1191.9867029
G=-1191.713294

U -5.022296 -0.672008 -0.436003

C -3.921538 -1.042110 2.034546
C -4.143634 -2.344168 1.525006
C -5.541823 -2.571449 1.497554
C -6.180966 -1.407898 1.982686
C -5.181523 -0.459767 2.311414
C -2.692358 0.074556 -0.514644
C -7.725792 -0.319447 -0.463182
C -4.687602 -1.176007 -3.112117
C -5.933449 -1.758091 -2.779136
C -5.686996 -2.868612 -1.936233
C -4.284979 -2.983085 -1.763455
C -3.668632 -1.939621 -2.488545
C -5.907080 1.783964 -0.131281
C -6.262244 3.014648 0.429242
C -5.717644 4.176893 -0.109764
C -4.833574 4.087319 -1.188336
C -4.523295 2.830253 -1.692855
N -5.066537 1.722463 -1.177741
H -2.413268 0.492266 -1.492161
H -2.587810 0.888443 0.221928
H -1.942467 -0.686266 -0.258561
H -8.086959 0.035527 -1.435522
H -8.434408 0.016152 0.303346
H -7.757024 -1.416843 -0.465897
H -6.905999 -1.415315 -3.109300
H -4.537864 -0.312924 -3.748839
H -6.436615 -3.531777 -1.522070
H -2.604921 -1.762610 -2.565632
H -3.774433 -3.750424 -1.196058
H -6.034135 -3.483198 1.182919
H -3.375084 -3.049488 1.235722
H -2.956593 -0.580796 2.194573
H -5.350303 0.523864 2.731909
H -7.247664 -1.272613 2.101045
H -6.716366 0.733629 -0.071560
H -6.950397 3.057051 1.268531
H -5.971972 5.148843 0.305694
H -4.386529 4.974932 -1.624111
H -3.823961 2.697943 -2.514078

U(IV) pyridine adduct SDDAll

HF=-1192.018962
G=-1191.744998

U -5.033355 -0.898811 -0.388405
C -4.028331 -1.424079 2.104705
C -4.255571 -2.686474 1.507861
C -5.658546 -2.879546 1.409483
C -6.295986 -1.736491 1.941319
C -5.289308 -0.830888 2.358837
C -2.815194 0.168855 -0.321724
C -7.430385 -0.364606 -0.572303
C -4.764617 -1.094016 -3.126271
C -5.863555 -1.922465 -2.791014
C -5.367574 -3.025341 -2.056805
C -3.958554 -2.886735 -1.954801
C -3.586351 -1.698117 -2.621447
C -6.047929 2.435665 0.471188
C -6.231788 3.813914 0.457825
C -5.683009 4.552740 -0.586705
C -4.963061 3.880008 -1.570190
C -4.812085 2.501841 -1.463469
N -5.345984 1.780716 -0.465927
H -2.512588 0.736753 -1.212695
H -2.758384 0.860716 0.532498
H -2.040945 -0.597346 -0.163820
H -7.612586 0.198357 -1.500933
H -7.873211 0.221037 0.245304
H -8.016308 -1.293662 -0.643690
H -6.898871 -1.743535 -3.048600
H -4.814099 -0.181342 -3.709557
H -5.956522 -3.847270 -1.669099
H -2.579149 -1.318529 -2.727257
H -3.283088 -3.582419 -1.472660
H -6.154686 -3.758932 1.017977
H -3.492885 -3.394394 1.207876
H -3.062738 -0.989026 2.325306
H -5.452125 0.128887 2.836023
H -7.363979 -1.582549 2.015977
H -6.482701 1.825008 1.256059
H -6.801145 4.289767 1.249553
H -5.813697 5.630035 -0.633393
H -4.515882 4.408484 -2.405744
H -4.236238 1.947671 -2.198016

U(IV) pyridine product SDDAll

HF=-1151.5347885
G=-1151.305480

N -4.190705 -0.548103 -0.173654
C -3.781600 -1.064223 1.002382
C -4.219142 -2.351476 1.360305
C -5.055825 -3.054276 0.503892
C -5.451909 -2.477680 -0.712604
C -4.994203 -1.209662 -1.023892
U -2.787130 1.124440 0.839833
C -4.299842 2.037149 2.461839
C -0.086859 1.008698 1.213076
C -0.526229 1.995760 2.134585
C -1.274229 1.351166 3.146038
C -1.308428 -0.030438 2.847270
C -0.571222 -0.244456 1.656737
C -4.041148 2.531338 -1.137285
C -2.858529 2.029208 -1.739802
C -1.757737 2.714726 -1.176767
C -2.260136 3.637202 -0.224419
C -3.669701 3.529321 -0.206544
H -5.300055 2.121150 2.006396
H -4.385593 1.316674 3.290395
H -4.063565 3.013832 2.903234
H -2.808633 1.265686 -2.507281
H -5.052973 2.215458 -1.359848
H -0.717516 2.575341 -1.442674
H -4.344588 4.107095 0.410433
H -1.669140 4.321230 0.371140
H 0.540638 1.179012 0.347084
H -0.300222 3.053348 2.088666
H -1.742381 1.830786 3.995393
H -1.811570 -0.794034 3.426209
H -0.402144 -1.201509 1.177396
H -3.906488 -2.791294 2.303750
H -5.407640 -4.049232 0.767516
H -6.104700 -3.007667 -1.399017
H -5.265370 -0.707999 -1.950025

U(IV) pyridine N-oxide TS SDDAll

HF=-1267.142037
G=-1266.865476

C 0.404090 1.630934 -1.718965
C -0.192280 0.603633 -2.491539
C 0.462358 -0.610226 -2.182656
C 1.454011 -0.336359 -1.211266
C 1.421738 1.051906 -0.929257
U -0.912410 0.006718 0.119732
C -0.005414 -1.475951 2.275718
C 1.012932 -0.528374 2.015869
C 0.508472 0.756761 2.331868
C -0.822658 0.599404 2.792056
C -1.137470 -0.778542 2.756624
O -3.199590 -0.332914 0.839007
N -3.890118 -0.308448 -0.284200
C -3.317805 0.352050 -1.325728
C -4.018420 0.380099 -2.529486
C -5.247842 -0.260310 -2.657284
C -5.779307 -0.930630 -1.552806
C -5.076687 -0.949475 -0.362156
C -2.000378 2.437486 0.008178
C -1.347682 -2.323137 -0.485593
H -0.981365 0.731752 -3.221422
H 0.251100 -1.576889 -2.618412
H 2.136752 -1.060305 -0.785308
H 2.075474 1.579394 -0.246259
H 0.141196 2.679944 -1.746540
H -1.485695 1.394823 3.110665
H 1.054103 1.690256 2.263892
H 2.013081 -0.749922 1.667262
H 0.070136 -2.546471 2.136491
H -2.089255 -1.217497 3.023896
H -2.124233 3.181054 -0.786719
H -1.064360 2.699876 0.528255
H -2.819652 2.555616 0.726794
H -2.002338 -2.781957 0.268087
H -1.864086 -2.395283 -1.455405
H -0.448764 -2.949476 -0.563460
H -5.391131 -1.451667 0.543836
H -6.732897 -1.444284 -1.606824
H -5.788422 -0.241501 -3.598540
H -3.586351 0.917079 -3.368723
H -2.549069 1.278026 -0.864595

U(IV) pyridine N-oxide adduct SDDAll

HF=-1267.160908
G=-1266.884667

C	-4.847453	-0.509722	-0.337116
N	-3.844328	-0.451708	-1.248120
C	-4.048423	0.124170	-2.458413
C	-5.282885	0.654462	-2.785745
C	-6.329323	0.604266	-1.867704
C	-6.094285	0.011091	-0.629008
O	-2.692569	-0.986374	-0.971238
U	-0.592258	-0.229324	0.009522
C	-0.422505	-2.644493	-0.425132
C	-2.023037	1.794990	-0.180689
C	-1.087684	0.695032	2.570458
C	0.318939	0.674111	2.433210
C	0.732654	-0.681912	2.364736
C	-0.419351	-1.495785	2.459906
C	-1.545654	-0.645216	2.574783
C	2.043813	0.049576	-0.702600
C	1.462817	-0.631821	-1.795862
C	0.577973	0.261922	-2.447324
C	0.626990	1.502744	-1.766994
C	1.524812	1.370340	-0.682635
H	-0.008078	0.040384	-3.332287
H	1.657563	-1.656170	-2.083080
H	2.778363	-0.357411	-0.019513
H	1.792270	2.151468	0.017748
H	0.075720	2.396604	-2.027178
H	-1.704010	1.580139	2.655062
H	0.967686	1.540706	2.416841
H	1.752849	-1.035279	2.283441
H	-0.435766	-2.577229	2.443014
H	-2.575288	-0.966978	2.684449
H	-2.303105	2.024877	-1.221259
H	-1.497471	2.683674	0.196927
H	-2.959604	1.723076	0.395165
H	-1.225618	-3.181349	0.100911
H	-0.551161	-2.848976	-1.498427
H	0.531472	-3.094342	-0.116826
H	-4.577206	-0.986617	0.595411
H	-6.871536	-0.052965	0.124634
H	-7.302074	1.017865	-2.110146
H	-5.408755	1.107944	-3.762798
H	-3.182584	0.123322	-3.106595

U(IV) pyridine N-oxide product SDDAll

HF=-1226.692580
G=-1226.460344

U	-0.137503	-0.010572	0.030336
O	2.029302	0.722730	0.532070
N	2.060930	1.900672	-0.121213
C	3.183201	2.645979	-0.073169
H	4.000844	2.233318	0.505018
C	3.205419	3.851747	-0.749294
H	4.101676	4.461393	-0.719251
C	2.066769	4.250201	-1.454320
H	2.064401	5.194374	-1.992181
C	0.941220	3.428559	-1.458424
H	0.054073	3.737474	-2.005453
C	0.910419	2.205529	-0.776883
C	0.520599	-1.755821	1.560843
H	0.722589	-1.319778	2.550966
H	-0.190347	-2.581397	1.702549
H	1.465866	-2.190890	1.201477
C	-1.356947	1.365955	2.060916
H	-0.705295	1.771093	2.826467
C	-1.964640	0.087234	2.080410
H	-1.852018	-0.659386	2.855070
C	-2.743777	-0.041500	0.906046
H	-3.339459	-0.903838	0.631360
C	-2.628356	1.161005	0.165444
H	-3.126117	1.381555	-0.770707
C	-1.777456	2.035535	0.882859
H	-1.511600	3.044004	0.596156
C	1.006954	-1.359731	-2.066521
H	2.079454	-1.503961	-2.013409
C	0.343958	-0.259094	-2.664261
H	0.817558	0.570842	-3.171291
C	-1.050840	-0.456465	-2.510509
H	-1.831358	0.198886	-2.877199
C	-1.245972	-1.682995	-1.828538
H	-2.201873	-2.124645	-1.573781
C	0.025560	-2.243198	-1.557098
H	0.214284	-3.179217	-1.048016

U(IV) sp2 picoline TS SDDAll

HF=-1231.296111
G=-1230.996202

N	-5.038234	1.780424	-1.157252
C	-5.888529	1.776410	-0.117312
C	-6.282656	2.962213	0.505396
C	-5.759887	4.159528	0.027340
C	-4.873910	4.141748	-1.049998
C	-4.514560	2.924695	-1.632614
U	-4.989351	-0.655632	-0.447737
C	-2.636581	0.019905	-0.500524
C	-4.156997	-2.300681	1.551908
C	-3.933259	-0.994106	2.049097
C	-5.192544	-0.399155	2.298323
C	-6.194256	-1.342592	1.963437
C	-5.556398	-2.517239	1.503969
C	-7.694356	-0.320037	-0.531919
C	-4.620687	-1.243946	-3.109576
C	-5.882859	-1.791841	-2.781266
C	-5.672270	-2.882604	-1.904015
C	-4.275674	-3.020038	-1.705868
C	-3.627204	-2.009707	-2.448546
H	-2.316962	0.374682	-1.489580
H	-2.524284	0.864092	0.200032
H	-1.919039	-0.751158	-0.189083
H	-8.019665	0.026171	-1.519885
H	-8.419691	0.040510	0.207229
H	-7.740313	-1.416001	-0.516180
H	-6.842884	-1.440112	-3.137477
H	-4.442919	-0.407884	-3.774200
H	-6.441598	-3.519189	-1.484579
H	-2.558925	-1.857170	-2.513815
H	-3.789924	-3.780710	-1.108586
H	-6.050730	-3.429277	1.193632
H	-3.389337	-3.015748	1.285384
H	-2.967659	-0.537790	2.219343
H	-5.359797	0.591013	2.703497
H	-7.261660	-1.197600	2.061959
H	-6.685465	0.728969	-0.103866
H	-6.981963	2.943077	1.335858
H	-6.037166	5.106151	0.484789
H	-4.455964	5.065359	-1.438543
C	-3.547749	2.838073	-2.774135
H	-3.937973	2.184706	-3.559130
H	-3.348118	3.823717	-3.201008
H	-2.599474	2.408448	-2.434977

U(IV) sp2 picoline product SDDAll

HF=-1190.8451011
G=-1190.590854

C	-4.659182	1.959412	-0.430690
C	-5.185283	2.238996	0.853170
C	-5.857058	3.485800	0.794427
C	-5.754969	3.970476	-0.532354
C	-5.014655	3.027165	-1.288808
U	-7.397529	1.800796	-0.702862
C	-6.662109	-0.459174	-1.201522
N	-8.182703	0.813784	1.351954
C	-8.833077	1.984534	1.215029
C	-9.761269	2.363946	2.197656
C	-9.976963	1.521481	3.279873
C	-9.276538	0.311886	3.377272
C	-8.365482	-0.033780	2.385963
C	-7.568992	-1.303249	2.405893
C	-7.910035	2.574723	-3.285306
C	-8.488909	1.288482	-3.153872
C	-9.592521	1.396226	-2.273813
C	-9.706292	2.751901	-1.873291
C	-8.664542	3.478121	-2.495912
H	-6.034420	-0.900633	-0.415692
H	-7.524399	-1.129703	-1.340681
H	-6.078988	-0.498599	-2.134797
H	-6.349025	3.984547	1.619796
H	-5.078466	1.615568	1.732131
H	-6.150923	4.909585	-0.899735
H	-4.090159	1.081548	-0.708008
H	-4.749836	3.118004	-2.335366
H	-8.483459	4.541714	-2.398156
H	-7.056156	2.829287	-3.901364
H	-8.149142	0.383000	-3.639335

H -10.248448 0.587431 -1.973315

H -10.461826 3.157828 -1.213379

H -10.302037 3.302746 2.112750

H -10.689368 1.790867 4.056898

H -9.439156 -0.356532 4.217529

H -6.496900 -1.083230 2.442487

H -7.826258 -1.921402 3.269369

H -7.743325 -1.879647 1.492396

U(IV) sp2 picoline N-oxide TS SDDAll

HF=-1306.454362
G=-1306.151781

C -5.084239 -0.986417 -0.416994

N -3.893270 -0.335976 -0.331630

C -3.307178 0.345037 -1.352032

C -3.982365 0.397613 -2.566534

C -5.208191 -0.244723 -2.718129

C -5.752922 -0.932262 -1.634442

O -3.208664 -0.374404 0.799732

U -0.921502 -0.008235 0.103277

C -1.314345 -2.346124 -0.507413

C -2.017584 2.422569 0.021677

C -0.852253 0.574724 2.779370

C 0.480112 0.746908 2.328331

C 0.999189 -0.531893 2.010669

C -0.011283 -1.490383 2.259886

C -1.153202 -0.805999 2.736393

C 1.456373 -0.320510 -1.216468

C 0.472415 -0.592544 -2.196297

C -0.188429 0.619555 -2.498640

C 0.395436 1.643824 -1.712639

C 1.412509 1.064792 -0.922132

H -0.973633 0.748559 -3.232375

H 0.270518 -1.556714 -2.641983

H 2.141151 -1.043667 -0.792366

H 2.058154 1.590640 -0.230253

H 0.125171 2.691166 -1.732297

H -1.524988 1.362548 3.096354

H 1.016767 1.686035 2.267337

H 2.003330 -0.742187 1.666525

H 0.076091 -2.559475 2.116857

H -2.102204 -1.255124 2.996479

H -2.148608 3.172954 -0.765658

H -1.082864 2.685783 0.542968

H -2.837484 2.526380 0.741757

H -1.958084 -2.824008 0.243806

H -1.834169 -2.416249 -1.475830

H -0.406376 -2.957770 -0.595650

C -5.557005 -1.704541 0.799161

H -6.706374 -1.443166 -1.718656

H -5.738876 -0.213030 -3.664978

H -3.539615 0.952185 -3.388240

H -2.552863 1.270703 -0.864414

H -6.521074 -2.179785 0.609016

H -4.828697 -2.464864 1.097622

H -5.651835 -1.013236 1.642298

U(IV) sp2 picoline N-oxide adduct SDDAll

HF=-1306.473281
G=-1306.170598

C -5.073471 -0.687751 -0.663199

N -3.891001 -0.466911 -1.309590

C -3.829282 0.283033 -2.437594

C -4.967179 0.847003 -2.977358

C -6.194368 0.646138 -2.348745

C -6.229965 -0.123802 -1.192050

O -2.805806 -1.023718 -0.847975

U -0.717858 -0.279121 0.144995

C -0.553319 -2.704408 -0.230394

C -2.218400 1.707170 0.190795

C -0.954850 0.608805 2.756366

C 0.419603 0.709258 2.441978

C 0.937217 -0.605827 2.317105

C -0.118329 -1.515584 2.551271

C -1.291683 -0.765996 2.811151

C 1.805225 0.098892 -0.854646

C 1.156454 -0.645667 -1.864885

C 0.169029 0.183353 -2.450663

C 0.215465 1.445411 -1.810012

C 1.220752 1.391642 -0.816718

H -0.477840 -0.098402 -3.274031

H 1.374267 -1.668380 -2.142079

H 2.626540 -0.247538 -0.240673

H 1.513373 2.206662 -0.166895

H -0.403775 2.303735 -2.036051

H -1.629371 1.437313 2.925738

H 0.983093 1.628710 2.345629

H 1.966278 -0.870199 2.109690

H -0.042483 -2.594281 2.536087

H -2.265827 -1.175962 3.053308

H -2.602215 2.017546 -0.792957

H -1.690894 2.580870 0.600096

H -3.095340 1.543446 0.838212

H -1.300646 -3.232968 0.381036

H -0.779853 -2.933006 -1.282132

H 0.426620 -3.144039 0.000493

C -5.019048 -1.527654 0.563226

H -7.164586 -0.303574 -0.671401

H -7.103319 1.080767 -2.750775

H -4.878252 1.441308 -3.879850

H -2.832005 0.388839 -2.842843

H -6.022159 -1.670930 0.968058

H -4.566820 -2.499297 0.342685

H -4.386945 -1.053550 1.321166

U(IV) sp2 picoline N-oxide product SDDAll

HF=-1265.999828
G=-1265.739107

C -5.060940 -0.908113 -0.407291

C -3.658518 -0.722447 -0.342372

C -3.280570 0.138427 -1.401933

C -4.440886 0.466127 -2.134198

C -5.541681 -0.188251 -1.522839

U -4.045915 -2.227119 -2.607251

C -1.696638 -1.920930 -2.978918

C -5.349955 -1.255924 -4.600356

N -4.826718 -2.198813 -5.428524

C -4.971452 -2.285466 -6.773985

C -5.768458 -1.317142 -7.376665

C -6.360382 -0.318308 -6.607320

C -6.136859 -0.291604 -5.230048

C -4.279427 -3.401856 -7.478633

O -4.095347 -3.132976 -4.792025

C -4.876095 -4.799212 -2.312382

C -5.098758 -4.196727 -1.049387

C -3.832728 -3.967174 -0.451552

C -2.835768 -4.411013 -1.345630

C -3.479424 -4.919786 -2.498779

H -4.484559 1.107566 -3.005008

H -2.277408 0.486096 -1.608477

H -2.993045 -1.129795 0.407683

H -5.660237 -1.492615 0.278859

H -6.573765 -0.136702 -1.849661

H -5.638307 -5.103093 -3.020000

H -6.063653 -3.997469 -0.598395

H -3.663540 -3.542447 0.529096

H -1.766930 -4.363986 -1.182596

H -2.991373 -5.316839 -3.379860

H -1.339992 -2.781574 -3.563752

H -1.591531 -1.028262 -3.618870

H -1.020734 -1.791496 -2.126245

H -5.914456 -1.362027 -8.451028

H -6.985519 0.432249 -7.083578

H -6.582808 0.493491 -4.625002

H -4.470929 -3.351054 -8.552314

H -3.200614 -3.358242 -7.299602

H -4.619538 -4.368745 -7.094781

U(IV) sp3 picoline TS SDDAll

HF=-1231.2961109
G=-1230.998294

C 0.224910 1.509348 -1.723786

C -0.493310 -2.160700 -5.553744

H -0.375416 -3.235244 -5.498373

U 0.365993 -0.750934 -3.325175

C 0.446620 -1.234244 -6.061709

H 1.421702 -1.467058 -6.471233

C -0.112157 0.061980 -5.948256

H 0.354686 0.985391 -6.268043

C -1.398862 -0.067428 -5.376074

H -2.091011 0.741311 -5.181907

C -1.632376 -1.438933 -5.124695

H -2.527367 -1.867226 -4.691643

C -1.772988 0.492828 -2.198137

H -2.733814 0.266158 -2.642643

C -0.898498 1.542996 -2.582104

H	-1.075457	2.265684	-3.369083
C	-1.187434	-0.185878	-1.104831
H	-1.612693	-1.029226	-0.577683
C	0.046656	0.440454	-0.815170
H	0.725302	0.169028	-0.016523
H	1.064724	2.191439	-1.745918
C	-0.424375	-2.875386	-2.404039
H	-0.058212	-3.050608	-1.380532
H	-1.522163	-2.909705	-2.347818
H	-0.105722	-3.736313	-3.005792
C	2.464200	0.791813	-3.845282
H	3.190229	1.416608	-3.312369
H	2.983625	0.318886	-4.686399
H	1.711237	1.481773	-4.253451
H	2.412699	-0.126775	-2.708302
C	2.622824	-1.181198	-1.804546
H	1.812835	-1.612014	-1.200930
H	3.342221	-0.721660	-1.123473
C	3.184190	-2.194642	-2.709233
C	4.459140	-2.772433	-2.641862
H	5.129901	-2.496419	-1.834168
C	4.830442	-3.705693	-3.599254
H	5.809745	-4.175060	-3.557734
C	3.926819	-4.044894	-4.609782
H	4.174819	-4.778227	-5.369818
C	2.695486	-3.405683	-4.631360
H	1.968667	-3.622175	-5.409100
N	2.337891	-2.488530	-3.723242

U(IV) sp3 picoline product SDDAll

HF=-1190.8425702
G=-1190.584545

N	0.882030	0.341355	-1.896354
C	0.277106	-0.523948	-2.776280
C	0.484138	-1.924805	-2.632286
C	1.365527	-2.386561	-1.681825
C	2.029746	-1.477475	-0.831851
C	1.735484	-0.137150	-0.967791
C	-0.635595	0.112974	-3.659835
U	-1.275321	1.609764	-1.670196
C	-2.747575	2.461619	-3.388734
C	-3.324414	1.220993	0.060025
C	-2.219986	0.535233	0.633026
C	-1.939540	-0.590359	-0.177059
C	-2.862807	-0.597688	-1.250604
C	-3.722926	0.515925	-1.099871
C	0.150326	3.916768	-1.946127
C	0.702391	3.312609	-0.788565
C	-0.270095	3.352745	0.235284
C	-1.424746	3.991480	-0.285205
C	-1.160087	4.350173	-1.627278
H	0.655197	4.053520	-2.895172
H	1.699881	2.900059	-0.709392
H	-0.149353	2.980370	1.245118
H	-2.335028	4.203322	0.260736
H	-1.837517	4.867197	-2.292846
H	-3.803829	2.104493	0.461745
H	-1.707999	0.805547	1.548325
H	-4.539964	0.782283	-1.757062
H	-2.906183	-1.332186	-2.044416
H	-1.153440	-1.316931	-0.009615
H	-3.231748	1.625809	-3.913092
H	-3.545544	3.120688	-3.018528
H	-2.184993	3.031936	-4.144081
H	-0.258998	1.019653	-4.144586
H	-1.248942	-0.501934	-4.311281
H	-0.026854	-2.605372	-3.306192
H	1.559740	-3.452543	-1.592983
H	2.741574	-1.814162	-0.086355
H	2.187324	0.605845	-0.313964

U(IV) sp3 picoline N-oxide TS SDDAll

HF=-1306.446085
G=-1306.144073

C	-3.522623	-1.814400	-7.191985
N	-2.886868	-2.595041	-6.263260
C	-1.555219	-2.836695	-6.308967
C	-0.779081	-2.327637	-7.328373
C	-1.388159	-1.553660	-8.321568
C	-2.748723	-1.305452	-8.243172
O	-3.581250	-3.144565	-5.288445
U	-5.971652	-3.402194	-4.986408
C	-5.528904	-1.560724	-3.426303
H	-1.190751	-3.456974	-5.500568
C	-4.957056	-1.682930	-7.007714
C	-5.643376	-4.426376	-7.436390
C	-8.577419	-3.023432	-4.248568
C	-8.651045	-3.940789	-5.326644
C	-8.305919	-3.248242	-6.508344
C	-8.019136	-1.904861	-6.163808
C	-8.193989	-1.765652	-4.768442
C	-4.732978	-5.719480	-4.206664
C	-6.108121	-6.061225	-4.227216
C	-6.738436	-5.385107	-3.156721
C	-5.763112	-4.615571	-2.484855
C	-4.522268	-4.824438	-3.133028
H	-7.755559	-1.113510	-6.853859
H	-8.069434	-0.855673	-4.198037
H	-8.800627	-3.234273	-3.210799
H	-8.944534	-4.980890	-5.262741
H	-8.287294	-3.665170	-7.506262
H	-3.977932	-6.072544	-4.897927
H	-6.586249	-6.745455	-4.918328
H	-7.783819	-5.460885	-2.888469
H	-5.931052	-3.984270	-1.621885
H	-3.580622	-4.362790	-2.867587
H	-6.002634	-4.222610	-8.451448
H	-6.274965	-5.239112	-7.047558
H	-4.617374	-4.811015	-7.509705
H	-4.510182	-1.707637	-3.039056
H	-5.552073	-0.561945	-3.890312
H	-6.206980	-1.516368	-2.564029
H	0.283120	-2.542899	-7.340831
H	-0.802338	-1.144480	-9.138435
H	-3.249875	-0.696662	-8.988148
H	-5.416037	-2.973978	-7.150244
H	-5.177165	-1.179630	-6.053319
H	-5.428900	-1.121256	-7.813942

U(IV) sp3 picoline N-oxide adduct SDDAll

HF=-1306.473223
G=-1306.171059

C	-3.374121	-1.296982	-7.564056
N	-3.350360	-2.362482	-6.709545
C	-2.273354	-2.617136	-5.925375
C	-1.158914	-1.804339	-5.965550
C	-1.143647	-0.705237	-6.821778
C	-2.259856	-0.465981	-7.614862
O	-4.371909	-3.171360	-6.683885
U	-6.124283	-3.825320	-5.137244
C	-5.072368	-1.807304	-4.139097
H	-2.380845	-3.487500	-5.292431
C	-4.603596	-1.124707	-8.383163
C	-6.275921	-5.285297	-7.112929
C	-8.501977	-3.020196	-4.017228
C	-8.858494	-4.038924	-4.938014
C	-8.645914	-3.542374	-6.244083
C	-8.149523	-2.220704	-6.133151
C	-8.072366	-1.894871	-4.756678
C	-5.448771	-6.386321	-4.313437
C	-6.499668	-5.968145	-3.466825
C	-6.008131	-4.926863	-2.637209
C	-4.650125	-4.709616	-2.967842
C	-4.307817	-5.604046	-4.010985
H	-7.913781	-1.559677	-6.959587
H	-7.743784	-0.950981	-4.343038
H	-8.574370	-3.081053	-2.938596
H	-9.251769	-5.016290	-4.688928
H	-8.832101	-4.078285	-7.164862
H	-5.505230	-7.165770	-5.061355
H	-7.496100	-6.389737	-3.436670
H	-6.561770	-4.410991	-1.862816
H	-3.994498	-3.986770	-2.500036
H	-3.334593	-5.706457	-4.478038
H	-6.501977	-4.693198	-8.012770
H	-7.039258	-6.071994	-7.039373
H	-5.307578	-5.777054	-7.286408
H	-3.991390	-1.902918	-3.955989
H	-5.211298	-0.916824	-4.773496
H	-5.526437	-1.570039	-3.166353
H	-0.317783	-2.039330	-5.322991
H	-0.280815	-0.049628	-6.870668
H	-2.288790	0.377793	-8.296125

H -4.798071 -2.024522 -8.975023

H -5.475897 -0.982410 -7.737177

H -4.499320 -0.263919 -9.045536

U(IV) sp3 picoline N-oxide product SDDAll

HF=-1265.998082
G=-1265.737333

C -3.529953 -2.190559 -6.723148

C -3.063646 -1.726403 -5.471377

C -1.647643 -1.702837 -5.515722

C -1.243063 -2.162744 -6.795266

C -2.407279 -2.462401 -7.540947

U -2.381982 0.270566 -7.225379

C -3.579561 1.701417 -5.379401

C -4.928280 1.251186 -5.306568

N -5.470656 0.775443 -6.480565

C -6.748100 0.360928 -6.608252

C -7.583166 0.321714 -5.513532

C -7.067618 0.716198 -4.267990

C -5.768924 1.174284 -4.172089

O -4.660117 0.689671 -7.539590

C -2.684509 -0.009064 -9.609123

C -0.954633 2.574314 -7.632610

C -0.595306 2.164283 -6.320868

C 0.177201 0.986804 -6.427835

C 0.297472 0.665192 -7.802059

C -0.391554 1.651710 -8.545899

H -7.017082 0.047387 -7.609072

H -1.523815 3.459760 -7.892326

H -0.469184 1.695657 -9.623436

H 0.842616 -0.173630 -8.216273

H 0.615268 0.436801 -5.604685

H -0.848446 2.677135 -5.402018

H -3.678376 -1.449652 -4.624225

H -0.992361 -1.417023 -4.702409

H -0.222624 -2.290852 -7.132669

H -2.434973 -2.834486 -8.556760

H -4.566932 -2.310198 -7.011615

H -3.586993 -0.623122 -9.744295

H -2.886240 0.966063 -10.078231

H -1.869037 -0.482106 -10.171175

H -8.602831 -0.024741 -5.630694

H -7.696671 0.682416 -3.383396

H -5.366082 1.517884 -3.225337

H -3.443700 2.455807 -6.169832

H -3.173687 2.046368 -4.430619

U(IV) lutidine TS 12e

HF=-831.079674
G=-830.751747

N 2.534247 -2.639680 -3.787326

C 3.278857 -2.233616 -2.729741

C 4.603396 -2.658470 -2.549937

C 5.143307 -3.569263 -3.441315

C 4.344717 -4.050856 -4.477395

C 3.042577 -3.572802 -4.620634

C 2.586655 -1.274611 -1.860161

C 2.547809 0.716750 -3.903955

U 0.322847 -0.764488 -3.403307

C 0.066455 0.383916 -0.823145

C 0.243519 1.475743 -1.705778

C -0.894664 1.550624 -2.544482

C -1.776085 0.500782 -2.176838

C -1.179500 -0.219543 -1.112092

C -0.587379 -2.028731 -5.722933

C 0.349849 -1.067981 -6.171667

C -0.216388 0.218606 -5.976717

C -1.505257 0.046734 -5.421180

C -1.729821 -1.337976 -5.248251

C -0.393269 -2.969508 -2.460606

H -0.469298 -3.102370 -5.742066

H 1.322658 -1.263273 -6.604219

H 0.243816 1.161860 -6.244368

H -2.200244 0.839285 -5.175542

H -2.625755 -1.797402 -4.849285

H -2.749754 0.303115 -2.607250

H -1.074812 2.299857 -3.305364

H -1.607959 -1.072809 -0.603853

H 0.758139 0.074922 -0.050680

H 1.093819 2.145046 -1.727631

H -0.045202 -3.170376 -1.437859

H -1.491713 -3.026020 -2.426071

H -0.051541 -3.810940 -3.076506

H 3.335134 1.239406 -3.348028

H 3.022213 0.239978 -4.768346

H 1.867998 1.497129 -4.270505

H 2.421196 -0.206842 -2.803421

H 1.783202 -1.783897 -1.313209

H 3.230676 -0.781489 -1.128553

H 5.173126 -2.284594 -1.705128

H 6.164436 -3.922721 -3.323797

H 4.723094 -4.791436 -5.174625

C 2.165159 -4.118452 -5.710117

H 1.237755 -4.514024 -5.286127

H 1.894505 -3.350899 -6.439467

H 2.668793 -4.927235 -6.244716

U(IV) lutidine adduct 12e

no adduct

U(IV) lutidine product 12e

HF=-790.636452
G=-790.351081

C 2.005527 -2.764829 -2.788123

C 2.839898 -1.637950 -2.982650

C 3.859075 -2.000805 -3.897857

C 3.666771 -3.358680 -4.254379

C 2.515709 -3.830801 -3.578508

U 1.501259 -2.017095 -5.388846

C 1.239029 0.390084 -4.767830

N 2.700617 -0.786707 -7.411433

C 3.477816 -1.909829 -7.538016

C 4.879315 -1.791668 -7.698759

C 5.422075 -0.537690 -7.888564

C 4.587348 0.588566 -7.920083

C 3.230576 0.433152 -7.664324

C 2.733569 -3.128058 -7.378254

C 2.305164 1.616192 -7.675752

C -1.093864 -2.445915 -4.579320

C -0.697522 -3.676577 -5.170055

C -0.580617 -3.472709 -6.564985

C -0.897770 -2.117537 -6.838214

C -1.228249 -1.487871 -5.613951

H 2.721865 -0.670274 -2.514274

H 4.657335 -1.358147 -4.248930

H 4.292688 -3.935900 -4.921552

H 2.117961 -4.837321 -3.626321

H 1.150006 -2.816317 -2.125593

H -1.300134 -2.280199 -3.528876

H -0.545156 -4.613890 -4.649019

H -1.528034 -0.456257 -5.487364

H -0.906014 -1.651027 -7.815957

H -0.308987 -4.224585 -7.294948

H 0.633024 0.968236 -5.474921

H 0.715979 0.433754 -3.800200

H 2.189201 0.924423 -4.634923

H 1.877886 -3.186682 -8.054202

H 3.305171 -4.053810 -7.355402

H 5.491059 -2.687652 -7.731887

H 6.490777 -0.424302 -8.054393

H 4.988387 1.574546 -8.131253

H 2.257736 2.092956 -6.692221

H 2.651821 2.363693 -8.395059

H 1.292524 1.309151 -7.944265

U(IV) lutidine N-oxide TS 12e

HF=-906.237808
G=-905.907480

C -3.501906 -1.793034 -7.151792

C -2.812482 -2.621855 -6.235743

C -1.448688 -2.660963 -6.619679

C -1.296159 -1.860815 -7.776300

C -2.562261 -1.319856 -8.103020

U -1.889507 -0.011005 -5.745696

C -3.456646 2.149400 -4.896776

C -4.309731 1.393059 -5.740943

C -3.835227 1.526104 -7.068526

C -2.684351 2.349929 -7.044270

C -2.455334 2.738265 -5.701263

O -0.666898 1.205936 -3.930433

N 0.040080 0.750897 -2.915152

C 0.327214 1.619967 -1.903727

C 1.042680 1.162331 -0.806407

C 1.457385 -0.166548 -0.744553

C 1.164089 -1.014814 -1.800535

C 0.458990 -0.556577 -2.917222

C	-0.168878	3.015780	-2.061094
C	0.033849	-1.348819	-4.060470
C	-2.759109	-1.176603	-3.432562
C	0.223847	0.701343	-6.889658
H	-0.667261	-3.229930	-6.133190
H	-0.376605	-1.695268	-8.320747
H	-2.776091	-0.683346	-8.952443
H	-4.564088	-1.581883	-7.142402
H	-3.253621	-3.150808	-5.401514
H	-3.553915	2.250421	-3.823222
H	-5.189543	0.841704	-5.430594
H	-4.290651	1.094679	-7.950093
H	-2.092631	2.646744	-7.900773
H	-1.637675	3.352953	-5.350036
H	-2.774956	-2.202939	-3.047275
H	-3.751827	-1.011490	-3.878508
H	-2.672647	-0.498000	-2.575225
H	0.595696	1.627321	-6.430072
H	1.055350	-0.018485	-6.862871
H	0.050862	0.916289	-7.954395
H	1.263236	1.861033	-0.007155
H	2.013491	-0.529459	0.114186
H	1.486523	-2.050318	-1.796984
H	0.126516	3.619075	-1.200731
H	0.230622	3.464154	-2.975925
H	-1.258620	3.030250	-2.158302
H	-1.363871	-1.300594	-3.903759
H	0.484198	-0.959955	-4.985105
H	0.304057	-2.399661	-3.953038

U(IV) lutidine N-oxide adduct 12e

HF=-906.268427
G=-905.936392

C	-3.582978	-1.826535	-6.876692
C	-2.657396	-2.523765	-6.063714
C	-1.382678	-2.424189	-6.674689
C	-1.519387	-1.679525	-7.871039
C	-2.877917	-1.308043	-7.997332
U	-2.031660	0.203640	-5.844335
C	-3.563052	2.330310	-4.835984
C	-4.426498	1.584006	-5.675122
C	-3.999482	1.768550	-7.015347
C	-2.863737	2.612938	-7.002292
C	-2.594707	2.959792	-5.655915
O	0.059841	0.411045	-4.343283
N	0.321601	0.218156	-3.079668
C	0.215943	1.269879	-2.210710
C	0.526325	1.075080	-0.871597
C	0.950445	-0.165770	-0.412657
C	1.073537	-1.202865	-1.328756
C	0.762978	-1.009749	-2.668152
C	-0.213073	2.571551	-2.786779
C	0.893570	-2.057929	-3.714058
C	-2.620669	-0.534742	-3.486478
C	0.018881	1.019003	-7.043488
H	-0.463998	-2.873090	-6.318557
H	-0.724585	-1.435779	-8.563058
H	-3.309206	-0.756087	-8.823291
H	-4.646770	-1.733787	-6.693527
H	-2.888169	-3.039526	-5.140809
H	-3.646598	2.407010	-3.759393
H	-5.280061	1.001941	-5.349767
H	-4.476729	1.357098	-7.895903
H	-2.298249	2.938595	-7.865612
H	-1.793850	3.609033	-5.324699
H	-2.090300	-1.416630	-3.098139
H	-3.688059	-0.808195	-3.487225
H	-2.515624	0.243427	-2.715656
H	0.397398	1.960192	-6.620974
H	0.850280	0.302224	-6.995225
H	-0.179111	1.206111	-8.110369
H	0.430314	1.919931	-0.198044
H	1.190381	-0.318209	0.634365
H	1.415387	-2.185417	-1.021637
H	-0.173404	3.352361	-2.025175
H	0.427251	2.843150	-3.631462
H	-1.233218	2.500663	-3.175705
H	-0.086252	-2.288513	-4.143026
H	1.523308	-1.701883	-4.535025
H	1.322164	-2.965961	-3.286177

U(IV) lutidine N-oxide product 12e

HF=-865.795087
G=-865.507282

C	-2.885856	-1.666955	-7.193339
N	-1.884942	-2.329586	-6.519587
C	-0.576317	-2.313864	-6.886610
C	-0.220910	-1.649362	-8.051337
C	-1.203709	-1.018720	-8.817988
C	-2.518794	-1.021714	-8.386586
O	-2.232792	-3.052985	-5.457036
U	-4.453897	-4.092574	-5.434060
C	-3.095400	-5.054082	-3.581234
C	0.374812	-3.052839	-6.007941
C	-4.193596	-1.763183	-6.604137
C	-5.020358	-6.515015	-6.599913
C	-5.378436	-5.553549	-7.581683
C	-4.185347	-4.972900	-8.079196
C	-3.094498	-5.571908	-7.403289
C	-3.606428	-6.526703	-6.492893
C	-5.971559	-2.670966	-3.575304
C	-6.719851	-2.582620	-4.777942
C	-7.222566	-3.871067	-5.076105
C	-6.789786	-4.756260	-4.055790
C	-6.023916	-4.013060	-3.125158
H	-5.476905	-1.849871	-3.069063
H	-5.562832	-4.401330	-2.227243
H	-7.030051	-5.809911	-3.980840
H	-7.852217	-4.127965	-5.919155
H	-6.893322	-1.683839	-5.355811
H	-4.119524	-4.211591	-8.846154
H	-6.383478	-5.327149	-7.916001
H	-5.704684	-7.153102	-6.054225
H	-3.023649	-7.155750	-5.833153
H	-2.048193	-5.341425	-7.559168
H	-2.097564	-5.336004	-3.940045
H	-2.943786	-4.321414	-2.775708
H	-3.545093	-5.945734	-3.120918
H	0.820840	-1.646192	-8.351155
H	-0.932248	-0.507014	-9.736655
H	-3.293506	-0.503034	-8.940857
H	1.393632	-2.949712	-6.386004
H	0.323757	-2.675555	-4.982189
H	0.111027	-4.113522	-5.956121
H	-4.185158	-1.338347	-5.588286
H	-4.962791	-1.275540	-7.203283

U(IV) pyridine TS 12e

HF=-752.464553
G=-752.191208

U	-5.046618	-0.752332	-0.375621
C	-3.957473	-1.213273	2.143093
C	-4.139510	-2.494892	1.567084
C	-5.533116	-2.748792	1.489694
C	-6.209280	-1.620159	2.012585
C	-5.236229	-0.669889	2.412460
C	-2.808817	0.350585	-0.291583
C	-7.738989	-0.156167	-0.375183
C	-4.521099	-1.139855	-3.098101
C	-5.807764	-1.689841	-2.892797
C	-5.664615	-2.850984	-2.090894
C	-4.284888	-3.018531	-1.808831
C	-3.578830	-1.957911	-2.427310
C	-5.820312	1.820186	-0.055574
C	-5.914639	3.091176	0.516318
C	-5.504660	4.201209	-0.221188
C	-4.982082	4.017045	-1.500903
C	-4.892137	2.720844	-2.001492
N	-5.324670	1.669119	-1.304327
H	-2.563066	0.818813	-1.254474
H	-2.759595	1.143705	0.467503
H	-1.996936	-0.355410	-0.064568
H	-8.064930	0.256794	-1.336026
H	-8.438915	0.192770	0.393652
H	-7.857443	-1.248795	-0.417615
H	-6.739420	-1.298866	-3.283546
H	-4.294417	-0.246976	-3.666754
H	-6.464415	-3.513482	-1.782064
H	-2.508017	-1.804222	-2.402940
H	-3.845739	-3.832473	-1.246079
H	-5.997331	-3.655845	1.122444
H	-3.348533	-3.172739	1.270844
H	-3.007729	-0.736891	2.343844
H	-5.434832	0.294165	2.863243
H	-7.281358	-1.510101	2.108524
H	-6.697460	0.773628	0.081965

H -6.312255 3.210745 1.520503

H -5.587324 5.202672 0.194630

H -4.645357 4.857486 -2.099306

H -4.465938 2.521710 -2.982177

U(IV) pyridine adduct 12e

HF=-752.508037
G=-752.230457

U -5.070599 -0.963214 -0.296628

C -4.074846 -1.617232 2.235772

C -4.253668 -2.844250 1.554364

C -5.651417 -3.064112 1.406066

C -6.330404 -1.970007 1.991010

C -5.356329 -1.069600 2.490963

C -2.866460 0.233309 -0.006383

C -7.490071 -0.252449 -0.416054

C -5.061235 -0.930994 -3.116908

C -5.993574 -1.933925 -2.755777

C -5.279074 -2.992623 -2.146842

C -3.900017 -2.644387 -2.137794

C -3.766592 -1.373957 -2.747373

C -5.972727 2.482284 0.287795

C -6.065972 3.869144 0.235704

C -5.449046 4.543052 -0.814033

C -4.751422 3.797892 -1.760595

C -4.689803 2.416812 -1.612130

N -5.293482 1.756116 -0.612681

H -2.539772 0.839994 -0.861600

H -2.844986 0.900050 0.867716

H -2.080146 -0.520785 0.155490

H -7.721362 0.358213 -1.299401

H -7.876397 0.298093 0.454015

H -8.106973 -1.161815 -0.490372

H -7.063219 -1.893343 -2.913201

H -5.301822 -0.003094 -3.621895

H -5.703200 -3.921313 -1.784901

H -2.836321 -0.843163 -2.902177

H -3.089212 -3.258583 -1.764720

H -6.116481 -3.934415 0.958931

H -3.464977 -3.516334 1.237654

H -3.126765 -1.172717 2.506722

H -5.556803 -0.142587 3.016034

H -7.403319 -1.842546 2.043643

H -6.469446 1.922876 1.074164

H -6.621446 4.400970 1.001247

H -5.510231 5.624619 -0.892984

H -4.252338 4.272827 -2.598972

H -4.130332 1.808839 -2.315851

U(IV) pyridine product 12e

HF=-712.022279
G=-711.790858

N -4.375535 -0.587393 -0.300597

C -3.822448 -0.944355 0.879988

C -4.100174 -2.223600 1.389159

C -4.928198 -3.083866 0.676843

C -5.479183 -2.670037 -0.542891

C -5.176604 -1.399643 -1.006281

U -3.024846 1.351233 0.451761

C -3.828921 2.284732 -1.711194

C -0.441558 2.308953 0.203022

C -0.354537 1.281860 1.181615

C -0.560584 0.040741 0.531193

C -0.784117 0.300310 -0.844608

C -0.700551 1.698979 -1.049431

C -3.407905 3.638115 1.956516

C -4.601256 3.526149 1.200725

C -5.312473 2.396161 1.673098

C -4.568873 1.816021 2.731116

C -3.387360 2.578197 2.903449

H -3.508709 1.667533 -2.562212

H -4.926801 2.320015 -1.744165

H -3.472635 3.306123 -1.908253

H -0.543774 -0.934482 1.000460

H -0.967387 -0.444012 -1.610213

H -0.135114 1.420450 2.233609

H -0.815696 2.211506 -1.995261

H -0.296671 3.368660 0.376900

H -2.621787 2.405405 3.650623

H -2.660872 4.416537 1.856132

H -4.913641 4.186077 0.402177

H -6.267744 2.046253 1.300818

H -4.855699 0.947336 3.309601

H -3.669747 -2.539623 2.336140

H -5.151921 -4.077256 1.059866

H -6.128505 -3.323333 -1.117224

H -5.569739 -1.015818 -1.944702

U(IV) pyridine N-oxide TS 12e

HF=-827.626475
G=-827.348812

C 0.705504 1.710428 -1.485834

C -0.104438 0.978703 -2.396183

C 0.320941 -0.367854 -2.375691

C 1.386196 -0.475019 -1.445563

C 1.635155 0.814146 -0.914697

U -0.861156 0.030485 0.125602

C -0.050619 -1.410362 2.379032

C 1.006987 -0.509619 2.091949

C 0.556048 0.803328 2.382418

C -0.780106 0.711091 2.847818

C -1.150540 -0.654068 2.846845

O -3.215329 -0.345692 0.845107

N -3.901936 -0.369323 -0.276390

C -3.308805 0.204296 -1.359810

C -4.009817 0.172151 -2.564475

C -5.254513 -0.443831 -2.655339

C -5.811476 -1.012039 -1.506827

C -5.114504 -0.964872 -0.314015

C -2.147284 2.420903 -0.106069

C -1.356170 -2.333354 -0.525440

H -0.889712 1.392669 -3.016181

H -0.093817 -1.179709 -2.958233

H 1.933450 -1.380038 -1.211644

H 2.404220 1.070063 -0.196907

H 0.639759 2.773394 -1.290623

H -1.406520 1.539226 3.156565

H 1.139654 1.712039 2.293036

H 1.996594 -0.782068 1.746943

H -0.018701 -2.486430 2.267554

H -2.119124 -1.047067 3.124777

H -2.119392 3.094810 -0.969313

H -1.341657 2.751762 0.567676

H -3.088862 2.579479 0.430885

H -1.999863 -2.814057 0.222165

H -1.853535 -2.442481 -1.498207

H -0.430624 -2.924059 -0.583410

H -5.451454 -1.385109 0.625065

H -6.781135 -1.497313 -1.527886

H -5.788817 -0.481637 -3.599567

H -3.561847 0.639060 -3.436773

H -2.582989 1.185160 -0.923274

U(IV) pyridine N-oxide adduct 12e

HF=-827.647687
G=-827.369714

C -4.849957 -0.459954 -0.295264

N -3.847384 -0.465084 -1.210739

C -4.054869 0.053047 -2.448042

C -5.283903 0.581572 -2.796955

C -6.327205 0.592730 -1.873989

C -6.091898 0.060288 -0.608254

O -2.707289 -1.005779 -0.917303

U -0.500920 -0.186900 0.050544

C -0.535694 -2.639511 -0.508275

C -2.076059 1.783563 -0.226133

C -1.107578 0.663671 2.650238

C 0.304129 0.663025 2.551511

C 0.737298 -0.688704 2.465534

C -0.407795 -1.519423 2.510839

C -1.546142 -0.683033 2.613575

C 2.126355 0.091548 -0.756579

C 1.525661 -0.601639 -1.833770

C 0.629483 0.287393 -2.477048

C 0.689504 1.536580 -1.811777

C 1.606174 1.415020 -0.740419

H 0.024443 0.055761 -3.345966

H 1.710122 -1.630635 -2.111205

H 2.875864 -0.306906 -0.083515

H 1.888830 2.203474 -0.053317

H 0.130056 2.425968 -2.069377

H -1.737889 1.539333 2.731036

H 0.943119 1.537545 2.571946

H 1.765086 -1.026766 2.410511

H -0.411922 -2.600095 2.464887

H -2.573967 -1.019867 2.679795

H -2.359776 2.019944 -1.262865

H -1.557060 2.678792 0.151127

H -3.015834 1.721630 0.343228

H -1.340332 -3.180423 0.007458

H -0.675930 -2.825033 -1.582127

H 0.412704 -3.120029 -0.220649

H -4.583011 -0.892239 0.659449

H -6.865932 0.044307 0.151375

H -7.296077 1.005015 -2.133326

H -5.408640 0.985133 -3.795921

H -3.193853 0.005773 -3.100707

U(IV) pyridine N-oxide product 12e

HF=-787.180761
G=-786.946306

U -0.230975 0.026094 -0.061226

O 1.999618 0.763303 0.621783

N 2.077581 1.917633 -0.046918

C 3.193674 2.668532 0.056718

H 3.971335 2.268717 0.695652

C 3.263571 3.862054 -0.640328

H 4.158531 4.469444 -0.560002

C 2.180150 4.251901 -1.427764

H 2.216497 5.185308 -1.982288

C 1.055281 3.428144 -1.490994

H 0.207233 3.725741 -2.102600

C 0.977506 2.222227 -0.790072

C 0.650247 -1.668671 1.521051

H 0.867112 -1.204784 2.492945

H -0.025716 -2.515612 1.708443

H 1.598322 -2.084056 1.153728

C -1.401970 1.386087 2.078192

H -0.727807 1.791660 2.823014

C -1.980443 0.093457 2.098019

H -1.824688 -0.661351 2.857089

C -2.801914 -0.034692 0.949456

H -3.403270 -0.898228 0.690919

C -2.736488 1.184426 0.224090

H -3.276540 1.414148 -0.686558

C -1.876877 2.063857 0.926910

H -1.631610 3.078289 0.640373

C 0.963561 -1.381708 -2.154379

H 2.041292 -1.482598 -2.113152

C 0.248319 -0.337283 -2.792269

H 0.683142 0.494308 -3.331437

C -1.135902 -0.579193 -2.609841

H -1.945263 0.026842 -2.999032

C -1.274677 -1.781379 -1.867121

H -2.209078 -2.255376 -1.591321

C 0.024310 -2.278317 -1.589735

H 0.257453 -3.183332 -1.044874

U(IV) sp2 picoline TS 12e

HF=-791.773445
G=-791.473295

N -5.184356 1.758542 -1.231471

C -5.741642 1.820349 -0.002612

C -5.865172 3.037565 0.668460

C -5.411770 4.195615 0.040801

C -4.830115 4.105312 -1.221387

C -4.710156 2.856103 -1.838946

U -4.991033 -0.730779 -0.361253

C -2.732267 0.318485 -0.173962

C -4.184906 -2.460474 1.628521

C -4.046432 -1.178695 2.217088

C -5.342315 -0.646682 2.413923

C -6.283773 -1.602904 1.955295

C -5.569661 -2.725594 1.472057

C -7.674471 -0.105661 -0.522344

C -4.357142 -1.176118 -3.053531

C -5.661744 -1.698082 -2.894363

C -5.574603 -2.849617 -2.070806

C -4.211272 -3.041128 -1.731899

C -3.459595 -2.003085 -2.333015

H -2.418472 0.771413 -1.124759

H -2.701361 1.116701 0.580479

H -1.953134 -0.407620 0.100322

H -7.932711 0.340105 -1.489100

H -8.411510 0.239820 0.212545

H -7.812205 -1.193528 -0.603737

H -6.568652 -1.296200 -3.329876

H -4.089435 -0.299149 -3.627417

H -6.399933 -3.490987 -1.785555

H -2.387649 -1.870650 -2.266767

H -3.812551 -3.853958 -1.138217

H -6.004990 -3.635970 1.078983

H -3.372493 -3.130179 1.374898

H -3.113681 -0.694595 2.471817

H -5.574186 0.314803 2.853817

H -7.360517 -1.501078 1.988825

H -6.640379 0.790043 0.024371

H -6.317505 3.078294 1.655361

H -5.508610 5.164583 0.525183

H -4.465756 4.992677 -1.730072

C -4.063678 2.693673 -3.183295

H -4.750419 2.209473 -3.884770

H -3.763691 3.657399 -3.601410

H -3.173526 2.061453 -3.102654

U(IV) sp2 picoline adduct 12e

HF=-791.814071
G=-791.510627

N -5.361929 1.813674 -0.629751

C -5.671323 2.671646 0.363644

C -5.773938 4.047465 0.137620

C -5.554884 4.559937 -1.134714

C -5.236795 3.673353 -2.158096

C -5.153858 2.320386 -1.854104

U -5.152324 -0.961433 -0.235288

C -7.543517 -0.245531 -0.610655

C -3.022584 0.231194 0.405122

C -4.519912 -2.979585 -2.019536

C -5.646791 -2.345360 -2.600314

C -5.242042 -1.066469 -3.051776

C -3.867382 -0.907442 -2.744648

C -3.421503 -2.088003 -2.104507

C -4.581197 -3.084664 1.424878

C -4.421888 -1.968201 2.278749

C -5.702367 -1.404731 2.500889

C -6.656962 -2.179618 1.797773

C -5.965710 -3.214775 1.125397

H -2.659747 0.897531 -0.389140

H -3.034390 0.832593 1.325240

H -2.241779 -0.531169 0.555357

H -7.662359 0.361198 -1.518586

H -8.036623 0.314869 0.196449

H -8.148034 -1.154225 -0.760003

H -6.640167 -2.765877 -2.694945

H -5.879735 -0.350449 -3.555278

H -4.495294 -3.981779 -1.610266

H -3.249425 -0.046790 -2.968924

H -2.415048 -2.276442 -1.752295

H -6.418060 -3.990411 0.519112

H -3.790216 -3.743996 1.088012

H -3.487482 -1.610010 2.689611

H -5.919298 -0.557462 3.138922

H -7.725363 -2.010950 1.776558

C -5.902825 2.095447 1.725761

H -6.025440 4.703161 0.965371

H -5.631612 5.627103 -1.322413

H -5.055804 4.013071 -3.172443

H -4.908826 1.603327 -2.629747

H -6.720756 1.368141 1.694030

H -5.004493 1.574318 2.072611

H -6.156791 2.870243 2.452520

U(IV) sp2 picoline product 12e

HF=-751.331893
G=-751.076182

C -4.520136 2.214879 -0.441890

C -5.019476 2.534621 0.844106

C -5.751748 3.744943 0.746121

C -5.719032 4.165896 -0.605752

C -4.957110 3.218270 -1.341748

U -7.282825 1.883596 -0.662705

C -6.351076 -0.388298 -1.096786

N -8.286339 0.764342 1.320337

C -8.648016 2.064317 1.376171

C -9.440122 2.502426 2.447757

C -9.828053 1.589249 3.420483

C -9.428798 0.251829 3.321643

C -8.644504 -0.150017 2.244805

C -8.175896 -1.561688 2.055613

C -8.010404 2.450743 -3.268804

C -8.454875 1.119585 -3.074990

C -9.530459 1.148379 -2.153696

C -9.763765 2.497679 -1.788101

C	-8.819878	3.303969	-2.470315
H	-5.717496	-0.744797	-0.272805
H	-7.143182	-1.137885	-1.230965
H	-5.731345	-0.419073	-2.005153
H	-6.243083	4.259154	1.561934
H	-4.853603	1.964417	1.750297
H	-6.165811	5.070185	-1.001661
H	-3.913265	1.355232	-0.693496
H	-4.718303	3.274406	-2.397151
H	-8.751300	4.384197	-2.419694
H	-7.217716	2.766906	-3.936486
H	-8.044417	0.236122	-3.545995
H	-10.088312	0.288952	-1.801994
H	-10.529840	2.850902	-1.110048
H	-9.744940	3.543386	2.516577
H	-10.441047	1.904767	4.262333
H	-9.724091	-0.472820	4.074671
H	-7.086065	-1.595927	1.965629
H	-8.481958	-2.198722	2.888990
H	-8.582110	-1.980217	1.129104

U(IV) sp2 picoline N-oxide TS 12e

HF=-866.938564
G=-866.634866

C	-5.106060	-1.035619	-0.382433
N	-3.895839	-0.417098	-0.333087
C	-3.289573	0.182454	-1.394610
C	-3.959246	0.166088	-2.614373
C	-5.194003	-0.465116	-2.733528
C	-5.763137	-1.057686	-1.606868
O	-3.220537	-0.399721	0.800378
U	-0.867311	0.018654	0.106815
C	-1.316693	-2.344830	-0.582902
C	-2.179876	2.398934	-0.093302
C	-0.805963	0.666506	2.838559
C	0.532679	0.772441	2.383478
C	0.993755	-0.534013	2.080674
C	-0.059889	-1.444676	2.349713
C	-1.167661	-0.700818	2.819055
C	1.395577	-0.436184	-1.459497
C	0.334934	-0.317364	-2.393586
C	-0.100476	1.026091	-2.388125
C	0.698317	1.744329	-1.457429
C	1.631667	0.843138	-0.900089
H	-0.885943	1.447072	-3.003090
H	-0.070262	-1.119489	-2.995858
H	1.948095	-1.341858	-1.241053
H	2.394515	1.089428	-0.172386
H	0.623249	2.802436	-1.240272
H	-1.439559	1.487192	3.152510
H	1.110965	1.685824	2.308620
H	1.987055	-0.796120	1.738240
H	-0.020087	-2.519102	2.225715
H	-2.135554	-1.102895	3.086009
H	-2.160161	3.085001	-0.947156
H	-1.380239	2.731858	0.586374
H	-3.125247	2.535519	0.442943
H	-1.955779	-2.850126	0.152575
H	-1.807138	-2.444529	-1.560154
H	-0.381215	-2.919101	-0.646119
C	-5.608430	-1.647705	0.878997
H	-6.726668	-1.553475	-1.662291
H	-5.713917	-0.496076	-3.686340
H	-3.500543	0.653916	-3.469191
H	-2.588667	1.170754	-0.928030
H	-6.584913	-2.107618	0.716200
H	-4.904836	-2.404272	1.240325
H	-5.688342	-0.893452	1.668055

U(IV) sp2 picoline N-oxide adduct 12e

HF=-866.958188
G=-866.654350

C	-5.213486	-1.084787	-0.389975
N	-4.061685	-0.377091	-0.620121
C	-3.870110	0.273065	-1.799628
C	-4.820465	0.231094	-2.800677
C	-5.998306	-0.484677	-2.604989
C	-6.178716	-1.133733	-1.387601
O	-3.167971	-0.337323	0.314311
U	-0.618022	0.086746	0.111410
C	-1.271514	-2.147996	-0.855302
C	-1.790696	2.327017	-0.044565
C	-0.883545	0.673891	2.845865
C	0.505570	0.663701	2.569085
C	0.888913	-0.676202	2.295753
C	-0.265034	-1.492291	2.405915
C	-1.355986	-0.656766	2.741495
C	1.806831	-0.331837	-1.146608
C	0.878559	-0.347963	-2.216078
C	0.364788	0.961182	-2.367015
C	0.996485	1.796754	-1.409261
C	1.889778	1.000672	-0.659560
H	-0.354733	1.283553	-3.110706
H	0.606877	-1.212977	-2.805682
H	2.384107	-1.178263	-0.794540
H	2.537916	1.348581	0.135475
H	0.822461	2.856559	-1.279097
H	-1.477443	1.545056	3.091064
H	1.164141	1.523818	2.588092
H	1.893208	-1.018794	2.078073
H	-0.303268	-2.564092	2.257978
H	-2.380952	-0.976134	2.875801
H	-1.980448	2.741055	-1.046579
H	-1.130980	3.060826	0.445806
H	-2.744703	2.353929	0.498301
H	-1.944559	-2.684022	-0.172843
H	-1.795529	-2.085552	-1.822152
H	-0.402784	-2.799878	-1.027177
C	-5.323065	-1.752562	0.934990
H	-7.081518	-1.701797	-1.188544
H	-6.757502	-0.534535	-3.377922
H	-4.625171	0.766474	-3.723394
H	-2.951307	0.844235	-1.853343
H	-6.270833	-2.288234	1.011768
H	-4.493397	-2.451843	1.078283
H	-5.253751	-1.016256	1.742169

U(IV) sp2 picoline N-oxide product 12e

HF=-826.491103
G=-826.231375

C	-5.000209	-0.448426	-0.780618
C	-3.600743	-0.566274	-0.608392
C	-3.191786	-1.797037	-1.183890
C	-4.337632	-2.428808	-1.727773
C	-5.458113	-1.604317	-1.471448
U	-4.710896	-2.522699	1.043685
C	-3.090159	-1.269467	2.446439
C	-3.016603	-4.392786	1.641795
N	-3.677724	-5.326141	0.903968
C	-3.332536	-6.629451	0.745211
C	-2.185187	-7.058229	1.404808
C	-1.446677	-6.169584	2.182748
C	-1.870315	-4.844501	2.293148
C	-4.205051	-7.478470	-0.114955
O	-4.775240	-4.863668	0.289668
C	-6.893275	-1.368898	2.296229
C	-7.417041	-2.517835	1.640070
C	-6.926768	-3.661626	2.311709
C	-6.089288	-3.227110	3.369284
C	-6.079547	-1.808649	3.367082
H	-4.357627	-3.387619	-2.229418
H	-2.176529	-2.172634	-1.226467
H	-2.955437	0.155543	-0.126130
H	-5.611082	0.390861	-0.469832
H	-6.478098	-1.801816	-1.779293
H	-7.134127	-4.690189	2.046161
H	-8.098420	-2.516526	0.797554
H	-7.108211	-0.337560	2.041952
H	-5.545178	-1.175117	4.062078
H	-5.571314	-3.864995	4.074852
H	-2.994872	-1.717358	3.444894
H	-2.086367	-1.270443	1.999820
H	-3.372824	-0.216411	2.594629
H	-1.884760	-8.095454	1.296384
H	-0.551428	-6.512364	2.694377
H	-1.306834	-4.136889	2.894707
H	-3.820380	-8.499451	-0.158250
H	-5.229368	-7.493152	0.270421
H	-4.261497	-7.069534	-1.128704

U(IV) sp3 picoline TS 12e

HF=-791.779103
G=-791.477349

C	0.163072	1.657484	-1.873005
C	-0.409662	-2.168402	-5.633206
H	-0.191103	-3.228206	-5.611445

U	0.332503	-0.725617	-3.341333
C	0.433346	-1.138985	-6.112098
H	1.423746	-1.260755	-6.533081
C	-0.250665	0.094200	-5.955123
H	0.116860	1.068615	-6.254096
C	-1.521320	-0.181690	-5.394568
H	-2.291856	0.547029	-5.178918
C	-1.615733	-1.575968	-5.182773
H	-2.465562	-2.105068	-4.770271
C	-1.811511	0.524856	-2.131018
H	-2.789627	0.225557	-2.487107
C	-1.026073	1.591156	-2.637574
H	-1.296578	2.256521	-3.448123
C	-1.109642	-0.060541	-1.047668
H	-1.453276	-0.889323	-0.443500
C	0.110147	0.638373	-0.889804
H	0.863114	0.443213	-0.137640
H	0.960510	2.377834	-1.999960
C	-0.413570	-2.874950	-2.293610
H	-0.061755	-3.053506	-1.268291
H	-1.512448	-2.899781	-2.246946
H	-0.101509	-3.741922	-2.889491
C	2.629866	0.731872	-3.710730
H	3.129763	1.464769	-3.068061
H	3.390544	0.251860	-4.335119
H	1.977908	1.313682	-4.378838
H	2.451112	-0.198206	-2.650000
C	2.590722	-1.321613	-1.731987
H	1.739094	-1.757827	-1.196051
H	3.301798	-0.935546	-0.999330
C	3.145142	-2.276647	-2.690528
C	4.402986	-2.898490	-2.620937
H	5.037591	-2.714381	-1.759644
C	4.798026	-3.756012	-3.634420
H	5.760812	-4.257922	-3.586039
C	3.936870	-3.979589	-4.713795
H	4.203181	-4.650074	-5.523876
C	2.726712	-3.305459	-4.736371
H	2.039586	-3.433025	-5.567539
N	2.342589	-2.456106	-3.771299

U(IV) sp3 picoline product 12e

HF=-751.328590
G=-751.069520

N	0.848198	0.283893	-1.719387
C	0.356511	-0.463840	-2.763599
C	0.544151	-1.875510	-2.751386
C	1.322911	-2.447574	-1.771669
C	1.903238	-1.645843	-0.765427
C	1.614665	-0.297507	-0.775159
C	-0.422394	0.291630	-3.683102
U	-1.300869	1.636772	-1.591061
C	-2.845117	2.356203	-3.403961
C	-3.337524	1.144064	0.193253
C	-2.216699	0.441916	0.716067
C	-1.950762	-0.652029	-0.142816
C	-2.892858	-0.619075	-1.200620
C	-3.756751	0.484116	-0.987001
C	0.144606	3.973694	-2.070508
C	0.740617	3.434501	-0.902961
C	-0.197095	3.524719	0.152105
C	-1.374206	4.133787	-0.361576
C	-1.158875	4.417294	-1.731234
H	0.616497	4.066725	-3.041445
H	1.739614	3.022800	-0.836440
H	-0.034630	3.216699	1.178121
H	-2.265339	4.375530	0.205259
H	-1.861907	4.893930	-2.400913
H	-3.810139	2.010372	0.640238
H	-1.687703	0.678035	1.631811
H	-4.589078	0.771130	-1.615302
H	-2.951712	-1.323232	-2.020740
H	-1.159809	-1.381499	-0.016817
H	-3.338442	1.506447	-3.891276
H	-3.637057	3.025841	-3.036378
H	-2.307382	2.904301	-4.190210
H	0.054790	1.206994	-4.044442
H	-0.972613	-0.235479	-4.456609
H	0.107177	-2.473172	-3.545280
H	1.505671	-3.519337	-1.781351
H	2.538979	-2.071054	0.003090
H	1.988315	0.365006	0.003562

U(IV) sp3 picoline N-oxide TS 12e

HF=-866.926729
G=-866.623132

C	-3.518296	-1.827037	-7.190480
N	-2.879907	-2.642071	-6.288794
C	-1.561866	-2.935556	-6.391847
C	-0.802374	-2.451916	-7.436941
C	-1.415314	-1.646612	-8.400336
C	-2.761120	-1.344458	-8.266207
O	-3.548623	-3.161762	-5.282667
U	-6.019919	-3.414295	-4.941484
C	-5.449530	-1.433169	-3.516153
H	-1.190848	-3.573957	-5.600767
C	-4.941875	-1.641874	-6.969851
C	-5.591792	-4.392966	-7.451752
C	-8.703261	-3.134041	-4.277051
C	-8.699635	-3.930431	-5.451373
C	-8.312872	-3.103883	-6.534442
C	-8.065421	-1.805127	-6.028711
C	-8.309961	-1.823844	-4.633835
C	-4.603070	-5.658533	-4.034489
C	-5.933605	-6.119751	-4.198282
C	-6.732067	-5.504977	-3.203111
C	-5.900888	-4.652834	-2.436787
C	-4.583236	-4.752626	-2.950014
H	-7.771160	-0.940297	-6.609313
H	-8.221279	-0.981878	-3.961122
H	-8.982325	-3.460949	-3.283415
H	-8.980085	-4.974697	-5.516931
H	-8.234342	-3.410156	-7.569048
H	-3.753346	-5.935919	-4.644373
H	-6.273612	-6.841596	-4.931504
H	-7.788571	-5.676660	-3.043880
H	-6.209450	-4.046829	-1.594086
H	-3.718617	-4.210795	-2.589975
H	-5.911068	-4.144652	-8.471063
H	-6.260169	-5.202637	-7.122553
H	-4.577837	-4.807449	-7.513118
H	-4.390571	-1.484416	-3.229739
H	-5.608402	-0.444461	-3.971407
H	-6.035893	-1.432992	-2.585546
H	0.248975	-2.710283	-7.488840
H	-0.845621	-1.254172	-9.236621
H	-3.264800	-0.709414	-8.987173
H	-5.399543	-2.961353	-7.126563
H	-5.121632	-1.136323	-6.010424
H	-5.413781	-1.068847	-7.768298

U(IV) sp3 picoline N-oxide adduct 12e

HF=-866.959737
G=-866.653586

C	-3.312483	-1.232305	-7.425034
N	-3.306949	-2.167571	-6.427689
C	-2.327570	-3.103926	-6.350658
C	-1.299847	-3.138782	-7.271194
C	-1.270030	-2.201046	-8.301108
C	-2.285576	-1.253557	-8.362642
O	-4.232158	-2.121445	-5.516521
U	-6.193745	-3.583166	-4.820199
C	-5.873537	-1.542040	-3.384684
H	-2.439115	-3.791278	-5.523444
C	-4.431130	-0.252184	-7.407712
C	-5.391963	-4.331908	-7.107859
C	-8.902958	-3.459985	-4.272382
C	-8.789672	-4.404399	-5.329377
C	-8.428730	-3.703630	-6.503403
C	-8.308637	-2.330674	-6.172555
C	-8.615394	-2.178369	-4.798062
C	-4.590126	-5.818949	-4.229136
C	-5.927009	-6.187812	-3.941815
C	-6.347155	-5.455807	-2.798975
C	-5.272466	-4.630573	-2.387401
C	-4.191175	-4.852658	-3.273162
H	-8.061579	-1.530666	-6.860784
H	-8.621190	-1.249536	-4.244162
H	-9.193133	-3.675640	-3.251162
H	-8.976660	-5.469027	-5.255947
H	-8.269304	-4.138766	-7.480779
H	-3.987785	-6.215030	-5.036561
H	-6.511833	-6.923222	-4.480954
H	-7.309319	-5.539004	-2.308536

H	-5.275667	-3.948253	-1.547758
H	-3.222432	-4.371675	-3.208051
H	-5.564875	-3.596539	-7.909360
H	-5.968308	-5.226281	-7.390889
H	-4.336117	-4.625905	-7.185985
H	-4.854685	-1.476028	-2.980897
H	-6.051309	-0.604682	-3.931387
H	-6.563977	-1.542710	-2.526824
H	-0.536665	-3.902914	-7.173557
H	-0.474286	-2.207364	-9.038211
H	-2.301868	-0.504715	-9.147602
H	-5.390393	-0.768279	-7.519097
H	-4.468610	0.267357	-6.445371
H	-4.314201	0.471765	-8.215963

U(IV) sp3 picoline N-oxide product 12e

HF=-826.483995
G=-826.221884

C	-3.236498	-1.862098	-6.658304
C	-2.752625	-1.473003	-5.386141
C	-1.337782	-1.414959	-5.455936
C	-0.950761	-1.772839	-6.774006
C	-2.127355	-2.050756	-7.516081
U	-2.127083	0.693782	-7.046780
C	-3.492648	2.018785	-5.231697
C	-4.831769	1.505933	-5.177654
N	-5.331783	1.028659	-6.367685
C	-6.585928	0.549257	-6.506684
C	-7.427963	0.451436	-5.418478
C	-6.951725	0.858751	-4.165851
C	-5.676165	1.383560	-4.056526
O	-4.523113	1.011109	-7.421969
C	-2.567307	0.565568	-9.491711
C	0.532383	1.333202	-7.619321
C	0.403582	1.585666	-6.229836
C	-0.444349	2.706027	-6.066845
C	-0.840101	3.148196	-7.356654
C	-0.227652	2.304628	-8.315003
H	-6.832347	0.237885	-7.513857
H	-1.468477	4.004574	-7.573229
H	-0.320923	2.388481	-9.389190
H	1.134182	0.555403	-8.073594
H	0.887595	1.033803	-5.433323
H	-0.723909	3.159996	-5.124698
H	-3.354581	-1.266388	-4.510067
H	-0.670223	-1.172564	-4.638145
H	0.065870	-1.854306	-7.138546
H	-2.169102	-2.355604	-8.553430
H	-4.276408	-1.986011	-6.932271
H	-3.433648	-0.077526	-9.691782
H	-2.809192	1.555132	-9.905646
H	-1.722545	0.174252	-10.076542
H	-8.426353	0.052158	-5.552117
H	-7.586791	0.784658	-3.288207
H	-5.299648	1.740384	-3.103725
H	-3.431881	2.860037	-5.939747
H	-3.115508	2.325387	-4.256372

Cp2Np(IV)Me2 – Large core

E = -505.081640
G = -504.890287

C	0.054125	0.066029	0.024822
C	0.303875	0.123286	1.417715
C	1.287351	-0.145341	-0.638985
C	2.302451	-0.233671	0.345894
C	1.693770	-0.066835	1.619224
Np	0.823673	-2.511529	0.730180
C	2.539391	-3.610314	2.566327
C	1.449573	-4.515913	2.539443
C	1.453348	-5.163716	1.279818
C	2.550727	-4.672430	0.531353
C	3.221447	-3.707532	1.323410
C	0.327199	-3.227529	-1.560315
C	-1.329140	-2.778736	1.872160
H	-0.465908	-2.606644	-2.001482
H	1.178851	-3.184768	-2.252786
H	-0.034093	-4.266047	-1.572883
H	-1.319645	-2.516991	2.939167
H	-2.102233	-2.152461	1.403873
H	-1.678701	-3.819486	1.809107
H	3.361641	-0.365092	0.158851
H	2.207941	-0.050463	2.572878
H	-0.436320	0.286897	2.190478
H	-0.912472	0.177013	-0.451845
H	1.428486	-0.222402	-1.709428
H	2.826589	-2.982714	3.401777
H	4.119086	-3.167428	1.046495
H	2.827846	-4.982378	-0.468238
H	0.745603	-5.914606	0.949506
H	0.741544	-4.685328	3.340435

Cp2Np(IV)Me2 – Small core

E = -981.321782
G = -981.133095

C	0.085126	0.009362	0.049906
C	0.301730	0.036464	1.448990
C	1.329230	-0.213888	-0.588720
C	2.315438	-0.341983	0.418371
C	1.680596	-0.186515	1.677599
Np	0.752852	-2.539217	0.697518
C	2.559584	-3.479363	2.489374
C	1.476471	-4.387934	2.556968
C	1.423835	-5.090825	1.328805
C	2.481826	-4.630972	0.507521
C	3.181017	-3.629804	1.222868
C	0.373974	-3.202132	-1.563957
C	-1.323006	-2.792648	1.849572
H	-0.432793	-2.574520	-1.977991
H	1.206521	-3.166010	-2.278089
H	-0.002769	-4.238634	-1.560497
H	-1.373898	-2.539191	2.916295
H	-2.084298	-2.181150	1.337160
H	-1.645270	-3.842987	1.752950
H	3.374187	-0.501959	0.255634
H	2.170225	-0.209162	2.643534
H	-0.454412	0.195284	2.207010
H	-0.868626	0.142607	-0.447512
H	1.493434	-0.279349	-1.656551
H	2.876066	-2.806528	3.276925
H	4.054140	-3.091613	0.874995
H	2.710086	-4.980791	-0.491016
H	0.700944	-5.854062	1.064544
H	0.803795	-4.519610	3.394745

Cp2Pu(IV)Me2 – Large core

E = -505.837497
G = -505.645717

C	0.056266	0.048320	0.028524
C	0.306624	0.105780	1.421292
C	1.289331	-0.162814	-0.635562
C	2.304904	-0.250621	0.348885
C	1.696633	-0.083758	1.622434
Pu	0.829114	-2.509644	0.732464
C	2.533045	-3.594791	2.561584
C	1.442936	-4.500057	2.534173
C	1.446736	-5.147703	1.274548
C	2.544557	-4.656640	0.526541
C	3.215541	-3.692240	1.318884
C	0.322947	-3.223312	-1.539246
C	-1.315051	-2.779100	1.855148
H	-0.472122	-2.602617	-1.976475
H	1.172498	-3.179005	-2.234119
H	-0.036665	-4.262115	-1.549848
H	-1.308638	-2.516717	2.921971
H	-2.086348	-2.153539	1.383559
H	-1.661973	-3.820377	1.791064
H	3.363849	-0.382723	0.161457
H	2.210899	-0.068042	2.575945
H	-0.433491	0.268111	2.194325
H	-0.910734	0.157010	-0.447635
H	1.429946	-0.240980	-1.705931
H	2.819586	-2.966808	3.396846
H	4.112673	-3.151604	1.041771
H	2.821121	-4.965662	-0.473437
H	0.737843	-5.896958	0.943324
H	0.733977	-4.668525	3.334463

Cp2Pu(IV)Me2 – Small core

E = -1020.792944
G = -1020.605941

C	4.199678	-3.285025	1.223609
C	3.813103	-3.063259	2.570413
C	2.897370	-4.078120	2.939152
C	2.722171	-4.925684	1.817411
C	3.519906	-4.436597	0.755705
Pu	5.281631	-5.351375	2.620951
C	4.485043	-6.369086	4.619404
C	5.382934	-7.137045	1.051950
C	7.808620	-5.930667	3.432986
C	7.389886	-4.875776	4.278887
C	7.270680	-3.709184	3.484201
C	7.622015	-4.046575	2.151682
C	7.957178	-5.421890	2.119309
H	4.371694	-7.565470	0.965223
H	5.740545	-6.929774	0.035453
H	6.036168	-7.914990	1.478997
H	4.880123	-2.667752	0.649065
H	4.151429	-2.249814	3.201550
H	2.409994	-4.183412	3.899622
H	2.087918	-5.804021	1.779828
H	3.593059	-4.866209	-0.235210
H	6.980344	-2.725343	3.833630
H	7.643605	-3.365030	1.309419
H	8.278833	-5.983195	1.251678
H	7.981743	-6.956246	3.738581
H	7.201269	-4.949370	5.342170
H	3.517505	-6.844388	4.391883
H	5.189986	-7.168761	4.897014
H	4.340069	-5.736466	5.504401

Cp2Np(III)Me – Large core

E = -459.399147
G = -459.243201

C	-1.847507	-3.065666	1.603387
C	-1.649313	-3.534077	0.278029
C	-0.857797	-4.710256	0.341303
C	-0.551775	-4.955483	1.700224
C	-1.165380	-3.940223	2.481291
Np	0.875107	-2.590063	1.015000
C	2.335603	-3.735147	-0.687876
C	0.495321	-0.077003	-0.147002
C	0.210248	0.149894	1.225083
C	1.424126	0.050906	1.944612
C	2.462723	-0.228110	1.016901
C	1.891274	-0.298965	-0.274681
H	-2.081201	-3.104675	-0.619134
H	-2.441625	-2.206776	1.892728
H	-1.156428	-3.874265	3.564122
H	0.013313	-5.799599	2.080446
H	-0.549236	-5.317260	-0.500400
H	-0.761148	0.386868	1.642859
H	-0.218664	-0.024558	-0.961458
H	2.426239	-0.481960	-1.198046
H	3.517561	-0.325460	1.249334
H	1.546085	0.212501	3.010502
H	2.423051	-4.819917	-0.523655
H	1.952147	-3.620143	-1.713425
H	3.360792	-3.334900	-0.708303

Cp2Np(III)Me – Small core

E = -941.436222
G = -941.279414

C	-1.743911	-2.994179	1.698189
C	-1.563656	-3.296823	0.324485
C	-0.807801	-4.493731	0.231662
C	-0.508552	-4.917917	1.548021
C	-1.088460	-3.995666	2.454825
Np	0.905455	-2.582202	1.162364
C	2.271239	-3.699796	-0.514864
C	0.431065	-0.288776	-0.192351
C	0.151722	0.046348	1.157204
C	1.376717	0.048356	1.867113
C	2.410977	-0.280410	0.955011
C	1.830364	-0.480534	-0.320264
H	-1.970262	-2.734049	-0.507488
H	-2.303166	-2.156317	2.097026
H	-1.064989	-4.064071	3.537217
H	0.048432	-5.809474	1.814617
H	-0.514976	-4.996833	-0.680440
H	-0.823640	0.281356	1.565884
H	-0.295083	-0.348208	-0.994783
H	2.360982	-0.728776	-1.229855
H	3.469105	-0.339601	1.185810
H	1.505072	0.292272	2.916297
H	2.347014	-4.779548	-0.301712
H	1.928639	-3.621517	-1.556685
H	3.301230	-3.304241	-0.505444

Cp2Pu(III)Me – Large core

E = -460.068003

G = -459.911939

C	-1.844011	-3.058210	1.600199
C	-1.661385	-3.544979	0.279374
C	-0.856702	-4.712143	0.348415
C	-0.527444	-4.933296	1.706078
C	-1.139169	-3.911942	2.480899
Pu	0.852444	-2.581258	0.967129
C	2.333859	-3.734207	-0.688446
C	0.498405	-0.063574	-0.154839
C	0.199702	0.142136	1.217549
C	1.404207	0.019239	1.949260
C	2.451155	-0.252498	1.028532
C	1.893950	-0.295849	-0.270486
H	-2.111349	-3.133907	-0.617500
H	-2.441193	-2.200166	1.885426
H	-1.113886	-3.828959	3.562241
H	0.053234	-5.764968	2.090038
H	-0.554251	-5.328918	-0.488437
H	-0.774437	0.379236	1.628622
H	-0.205565	0.009597	-0.976399
H	2.438113	-0.467713	-1.190618
H	3.502167	-0.364553	1.271166
H	1.515067	0.160676	3.019152
H	2.421611	-4.817171	-0.514389
H	1.960930	-3.629006	-1.719165
H	3.358063	-3.331902	-0.701958

Cp2Pu(III)Me – Small core

E = -980.929074
G = -980.772501

C	-1.760735	-2.946030	1.524648
C	-1.472343	-3.318340	0.183037
C	-0.726015	-4.521064	0.213786
C	-0.532761	-4.880234	1.570033
C	-1.184885	-3.913362	2.379603
Pu	0.929916	-2.605374	1.191190
C	2.347989	-3.691030	-0.431472
C	0.262424	-0.283429	-0.028879
C	0.194504	0.022749	1.357880
C	1.510350	-0.002331	1.874704
C	2.392333	-0.330922	0.812407
C	1.622440	-0.488474	-0.365630
H	-1.804039	-2.798284	-0.707337
H	-2.344354	-2.086893	1.832377
H	-1.249227	-3.925508	3.462569
H	-0.009138	-5.761236	1.925330
H	-0.355934	-5.067387	-0.644044
H	-0.705688	0.262562	1.911107
H	-0.574905	-0.309754	-0.715313
H	2.010242	-0.732080	-1.346348
H	3.470961	-0.416956	0.881382
H	1.797219	0.213925	2.898545
H	2.448500	-4.762270	-0.186356
H	2.024600	-3.644654	-1.480487
H	3.362063	-3.257958	-0.400887

Pyridine

E = -248.191331
G = -248.129589

N	0.027528	0.000000	0.012142
C	0.027566	0.000000	1.348816
C	1.185878	0.000000	2.125140
C	2.417820	0.000000	1.475869
C	2.436076	0.000000	0.083394
C	1.218099	0.000000	-0.595437
H	1.119493	0.000000	3.209020
H	3.344632	0.000000	2.043303
H	3.371271	0.000000	-0.468524
H	1.198637	0.000000	-1.684618
H	-0.951354	0.000000	1.826723

TS Pyridine Np IV – Large core

E = -753.233022
G = -752.958672

C	0.231055	1.684510	-1.852086
C	-0.484756	0.779821	-2.677566
C	-0.355789	-0.517522	-2.122707
C	0.446253	-0.418260	-0.960745
C	0.805265	0.942736	-0.791521
Np	2.153624	0.133506	-3.082807
C	1.384338	-1.912253	-4.257411
N	4.110061	-1.573650	-3.054946
C	4.853430	-2.523417	-3.624056
C	5.205638	-3.683849	-2.939574
C	4.727139	-3.861242	-1.641888
C	3.912468	-2.882759	-1.073043
C	3.620541	-1.729127	-1.804668
C	3.498142	0.748273	-5.442621
C	2.122668	0.838788	-5.770052
C	1.585137	1.957356	-5.087363
C	2.626047	2.550567	-4.328576
C	3.810459	1.802857	-4.554350
C	3.949332	0.948357	-1.172394
H	0.721476	-1.236186	-0.307128
H	-0.797403	-1.422938	-2.515307
H	-1.061106	1.036290	-3.557721
H	0.300865	2.756434	-1.989608
H	1.398548	1.347043	0.017800
H	4.188529	-0.001168	-5.807614
H	4.782696	2.007969	-4.123469
H	2.542163	3.439478	-3.714985
H	0.565501	2.314422	-5.155372
H	1.583283	0.178063	-6.435720
H	3.977172	0.844854	-0.080995
H	3.521575	1.941095	-1.372019
H	4.982221	0.945359	-1.536397
H	2.120256	-2.242173	-5.002889
H	1.230721	-2.753900	-3.568301
H	0.434948	-1.759452	-4.790028
H	5.834608	-4.428816	-3.416329
H	4.987602	-4.757270	-1.083329
H	3.517182	-3.008622	-0.068699
H	3.509380	-0.436416	-1.342722
H	5.176286	-2.350737	-4.648375

TS Pyridine Np IV – Small core

E = -1229.486246
G = -1229.212806

C	0.219265	1.529923	-1.884572
C	-0.448899	0.610515	-2.729749
C	-0.269785	-0.686201	-2.197352
C	0.522626	-0.572522	-1.029356
C	0.816785	0.800360	-0.833041
Np	2.207998	0.057784	-3.091020
C	1.252641	-1.680155	-4.520326
N	3.915177	-1.750354	-3.133525
C	4.543651	-2.811216	-3.649803
C	5.041565	-3.820302	-2.834784
C	4.862158	-3.715715	-1.452677
C	4.197356	-2.610986	-0.928238
C	3.722320	-1.634151	-1.808607
C	3.528907	0.748660	-5.384830
C	2.160293	0.909284	-5.712467
C	1.660429	2.001212	-4.968384
C	2.717984	2.517292	-4.179838
C	3.874808	1.746901	-4.443361
C	3.874074	1.098821	-1.215776
H	0.816460	-1.386705	-0.377939
H	-0.678060	-1.600681	-2.604021
H	-1.011461	0.855145	-3.621821
H	0.254970	2.604759	-2.013482
H	1.384258	1.217850	-0.012394
H	4.197768	0.002477	-5.795012
H	4.852071	1.897030	-4.001333
H	2.657249	3.365440	-3.508412
H	0.650735	2.389265	-5.009593
H	1.599933	0.310810	-6.416960
H	3.887404	0.981211	-0.125504
H	3.368720	2.048072	-1.430217
H	4.911079	1.181121	-1.561363
H	1.957374	-1.946962	-5.320295
H	1.135701	-2.571009	-3.880562
H	0.276940	-1.490189	-4.983912
H	5.550987	-4.672641	-3.272491
H	5.238346	-4.495438	-0.795156
H	4.048207	-2.504321	0.142240
H	3.584918	-0.377028	-1.419614
H	4.634603	-2.849336	-4.732030

Adduct of pyridine, Np IV – Large core

E = -753.278604
G = -753.001503

C	0.240141	1.926957	-1.833542
C	-0.547991	1.082912	-2.665466
C	-0.505327	-0.224275	-2.126736
C	0.317686	-0.193349	-0.973607
C	0.766342	1.137721	-0.784243
Np	2.041182	0.306611	-3.110958
C	1.270879	-1.823761	-4.195058
N	3.631387	-1.811067	-2.486271
C	4.373566	-2.439331	-3.410391
C	5.185694	-3.531114	-3.123797
C	5.216026	-4.020401	-1.821107
C	4.438858	-3.384705	-0.857263
C	3.677143	-2.282929	-1.231230
C	3.797919	0.865642	-5.212131
C	2.542926	0.631439	-5.827490
C	1.670781	1.678431	-5.446406
C	2.395518	2.570249	-4.606878
C	3.710845	2.069075	-4.469230
C	3.857872	0.936298	-1.495110
H	0.529011	-1.035803	-0.325178
H	-1.006454	-1.094554	-2.528278
H	-1.113277	1.393277	-3.535875
H	0.381439	2.993683	-1.958021
H	1.402461	1.489748	0.016715
H	4.687366	0.256249	-5.321529
H	4.507368	2.520043	-3.892897
H	2.018063	3.490620	-4.178300
H	0.643989	1.798927	-5.769826
H	2.289936	-0.200417	-6.471124
H	3.803054	0.445319	-0.513354
H	3.794431	2.017904	-1.298480
H	4.868759	0.744089	-1.880127
H	1.991254	-2.284823	-4.884840
H	0.992058	-2.605885	-3.475044
H	0.370073	-1.605948	-4.789826
H	5.772198	-3.988433	-3.913979
H	5.831254	-4.877511	-1.563108
H	4.424377	-3.725130	0.172967
H	3.082933	-1.747424	-0.497428
H	4.305617	-2.051591	-4.421756

Adduct of pyridine, Np IV – Small core

E = -1229.517606
G = -1229.243341

C	-0.019659	1.819025	-2.238381
C	-0.622404	0.694061	-2.854316
C	-0.400216	-0.429521	-2.027482
C	0.358531	-0.003957	-0.909705
C	0.583071	1.390335	-1.035439
Np	2.085210	0.212316	-3.024387
C	1.179611	-1.661468	-4.343850
N	3.758707	-1.849208	-2.519899
C	4.248011	-2.638255	-3.489024
C	5.037357	-3.753484	-3.231916
C	5.324428	-4.080596	-1.909267
C	4.817048	-3.270828	-0.897214
C	4.049069	-2.165542	-1.247793
C	3.788597	0.732759	-5.129966
C	2.499884	0.720753	-5.717732
C	1.782497	1.827259	-5.212738
C	2.634651	2.536657	-4.326968
C	3.875894	1.864839	-4.281099
C	3.592670	1.116885	-1.300028
H	0.673266	-0.625787	-0.078775
H	-0.750730	-1.435407	-2.217172
H	-1.165908	0.694438	-3.791016
H	-0.035865	2.834414	-2.614590
H	1.115199	2.015650	-0.331623
H	4.589520	0.030370	-5.331124
H	4.740319	2.165141	-3.704311
H	2.382175	3.440765	-3.786562
H	0.767448	2.098939	-5.474780
H	2.127202	-0.004330	-6.428104
H	3.376888	0.733847	-0.291421
H	3.568218	2.211695	-1.237446
H	4.622493	0.827716	-1.559964
H	1.872396	-2.051589	-5.101806
H	0.968671	-2.479126	-3.636006
H	0.238487	-1.426706	-4.855174
H	5.411245	-4.351346	-4.056572
H	5.932693	-4.948812	-1.672305
H	5.013231	-3.481581	0.148908
H	3.657670	-1.497207	-0.486921
H	3.987587	-2.362064	-4.505194

Product Pyridine Np IV – Large core

E = -712.792927
G = -712.561203

C	0.490502	1.008825	-1.817647
C	-0.502365	0.729260	-2.790299
C	-0.789947	-0.656683	-2.742040
C	0.036831	-1.240034	-1.750035
C	0.830053	-0.208260	-1.178037
Np	1.793965	-0.515429	-3.731680
C	2.751350	1.685591	-4.224273
N	2.094886	1.325748	-5.348569
C	2.039786	2.102130	-6.440924
C	2.669503	3.336618	-6.461836
C	3.363142	3.751017	-5.317522
C	3.406066	2.927464	-4.198033
C	0.480811	-1.466319	-5.601033
C	3.059554	-2.843887	-3.027762
C	3.861158	-1.808841	-2.473839
C	4.491066	-1.125003	-3.542549
C	4.071613	-1.728402	-4.754883
C	3.195824	-2.795220	-4.437303
H	4.378651	-1.433969	-5.751187
H	2.713735	-3.454690	-5.146693
H	2.477921	-3.567341	-2.469152
H	3.995529	-1.602157	-1.418894
H	5.175103	-0.291538	-3.449300
H	-0.972418	1.452743	-3.445314
H	0.911910	1.981362	-1.599066
H	1.542763	-0.325573	-0.370565
H	0.036507	-2.282107	-1.453404
H	-1.511448	-1.178417	-3.356643
H	-0.352125	-0.806979	-5.881559
H	1.095717	-1.595901	-6.502248
H	0.044785	-2.448848	-5.369753
H	2.621274	3.962056	-7.347707
H	3.864304	4.716615	-5.311401
H	3.942672	3.244137	-3.307182
H	1.484462	1.719754	-7.294083

Product Pyridine Np IV – Small core

E = -1189.041757
G = -1188.812055

C	0.019504	1.475234	-2.340689
C	-0.928188	0.682710	-3.035386
C	-0.948524	-0.602263	-2.442698
C	-0.004552	-0.608802	-1.387870
C	0.591943	0.675960	-1.323279
Np	1.488094	-0.407356	-3.661534
C	2.109488	1.348341	-5.176939
N	1.034819	0.739634	-5.713384
C	0.498264	1.095971	-6.890779
C	1.045352	2.137521	-7.621050
C	2.164246	2.805616	-7.102106
C	2.697877	2.413715	-5.880969
C	0.506341	-2.259120	-4.843205
C	4.193648	-0.392184	-3.351962
C	3.684918	-0.655786	-2.059709
C	3.093181	-1.945168	-2.075009
C	3.237645	-2.478079	-3.376903
C	3.906718	-1.514246	-4.169002

H	4.164181	-1.620186	-5.216425
H	2.896070	-3.448578	-3.710907
H	2.636746	-2.445311	-1.229947
H	3.757033	0.001376	-1.201748
H	4.711750	0.504973	-3.663828
H	-1.536941	1.007873	-3.869849
H	0.258644	2.510978	-2.549017
H	1.337681	0.996321	-0.606384
H	0.208439	-1.442549	-0.730487
H	-1.571927	-1.433472	-2.745370
H	-0.456125	-1.963285	-5.286732
H	1.148754	-2.600407	-5.668606
H	0.313908	-3.132005	-4.202065
H	0.613806	2.422786	-8.575340
H	2.609113	3.625310	-7.662101
H	3.566603	2.925508	-5.474623
H	-0.365842	0.534207	-7.237126

TS Pyridine Pu IV – Large core

E = -753.985923
G = -753.711245

C	0.233727	1.676956	-1.872517
C	-0.475521	0.762825	-2.693280
C	-0.339286	-0.530182	-2.130012
C	0.460715	-0.419030	-0.967945
C	0.811486	0.945177	-0.807087
Pu	2.151094	0.133022	-3.084156
C	1.399760	-1.906417	-4.250737
N	4.111502	-1.558351	-3.051288
C	4.859368	-2.507066	-3.615900
C	5.204895	-3.669378	-2.930896
C	4.712942	-3.850504	-1.638823
C	3.891435	-2.874118	-1.076036
C	3.608534	-1.717978	-1.807109
C	3.481391	0.727011	-5.436993
C	2.104742	0.836494	-5.754578
C	1.587035	1.960541	-5.066176
C	2.640138	2.536246	-4.310846
C	3.813365	1.773986	-4.547615
C	3.937367	0.959351	-1.187414
H	0.741327	-1.231412	-0.309922
H	-0.774811	-1.440623	-2.517538
H	-1.052152	1.009749	-3.575889
H	0.297901	2.748246	-2.016884
H	1.401777	1.358189	-0.000098
H	4.158344	-0.032174	-5.806627
H	4.790257	1.962837	-4.120103
H	2.572037	3.423507	-3.693051
H	0.571654	2.330714	-5.125517
H	1.552338	0.184557	-6.418175
H	3.958486	0.861166	-0.095368
H	3.514684	1.951974	-1.395613
H	4.971661	0.948414	-1.546637
H	2.138590	-2.231758	-4.995056
H	1.250382	-2.748091	-3.561070
H	0.450251	-1.758653	-4.784266
H	5.839454	-4.412668	-3.402876
H	4.968166	-4.747834	-1.079903
H	3.484483	-3.003661	-0.076816
H	3.495377	-0.421241	-1.350261
H	5.192659	-2.331802	-4.636499

TS Pyridine Pu IV – Small core

E = -1268.968953
G = -1268.696519

C	0.287001	1.464117	-1.849350
C	-0.416260	0.593753	-2.721468
C	-0.255497	-0.725745	-2.248570
C	0.560598	-0.678881	-1.090005
C	0.881839	0.678222	-0.838193
Pu	2.215453	0.019263	-3.142773
C	1.244779	-1.664326	-4.624601
N	3.904050	-1.801062	-3.125292
C	4.500222	-2.907897	-3.582180
C	4.993378	-3.872416	-2.711918
C	4.844594	-3.673609	-1.336214
C	4.215204	-2.521784	-0.873155
C	3.741939	-1.597448	-1.809263
C	3.481254	0.807269	-5.420916
C	2.104041	0.987478	-5.707429
C	1.630668	2.049468	-4.908481
C	2.712777	2.531420	-4.127113
C	3.858263	1.773136	-4.457351
C	3.888255	1.146913	-1.280986
H	0.845625	-1.525909	-0.477751
H	-0.686434	-1.614303	-2.688688
H	-0.987614	0.885992	-3.593418
H	0.341037	2.542593	-1.931835
H	1.469965	1.048431	-0.009621
H	4.135790	0.075377	-5.878664
H	4.848372	1.901696	-4.037723
H	2.675160	3.357404	-3.427622
H	0.622336	2.443174	-4.906334
H	1.522732	0.419209	-6.420173
H	3.935843	0.994252	-0.195973
H	3.349098	2.080278	-1.462303
H	4.909401	1.249621	-1.663612
H	1.982792	-1.891142	-5.405569
H	1.120132	-2.561321	-3.998085
H	0.283535	-1.441548	-5.099139
H	5.476118	-4.762500	-3.102020
H	5.216378	-4.417105	-0.635726
H	4.089593	-2.339908	0.190133
H	3.604095	-0.337223	-1.477119
H	4.571043	-3.016921	-4.661075

Adduct of pyridine, Pu IV – Large core

E = -754.032996
G = -753.755339

C	0.263449	1.923238	-1.842804
C	-0.527491	1.084837	-2.678103
C	-0.489621	-0.224160	-2.143933
C	0.332845	-0.200336	-0.990206
C	0.785866	1.128497	-0.795937
Pu	2.043499	0.306104	-3.114575
C	1.278149	-1.813563	-4.191163
N	3.620616	-1.800828	-2.483275
C	4.370947	-2.427135	-3.402116
C	5.182300	-3.518160	-3.110408
C	5.203145	-4.009134	-1.808201
C	4.417590	-3.375480	-0.849883
C	3.657434	-2.274230	-1.228538
C	3.794838	0.859114	-5.198430
C	2.542306	0.615752	-5.815093
C	1.663165	1.658409	-5.438484
C	2.381438	2.557349	-4.600754
C	3.699261	2.064369	-4.459446
C	3.852982	0.936091	-1.512813
H	0.540944	-1.046033	-0.345125
H	-0.993130	-1.091298	-2.549003
H	-1.090832	1.399968	-3.547907
H	0.408929	2.989711	-1.963381
H	1.423060	1.475572	0.006204
H	4.687827	0.254279	-5.303312
H	4.491908	2.521426	-3.882759
H	1.997963	3.476585	-4.175448
H	0.636205	1.771295	-5.763701
H	2.295053	-0.219694	-6.456128
H	3.800235	0.443733	-0.531818
H	3.789773	2.017359	-1.315311
H	4.862706	0.743773	-1.900481
H	2.001995	-2.276747	-4.875683
H	0.995998	-2.593160	-3.469905
H	0.380549	-1.597047	-4.790920
H	5.775627	-3.973605	-3.896579
H	5.817403	-4.865790	-1.546418
H	4.395300	-3.717071	0.179832
H	3.056720	-1.740549	-0.498891
H	4.310538	-2.038451	-4.413534

Adduct of pyridine, Pu IV – Small core

E = -1268.998780
G = -1268.726004

C	0.008224	1.812748	-2.286653
C	-0.603374	0.711547	-2.937522
C	-0.442020	-0.424873	-2.115751
C	0.290373	-0.033897	-0.968027
C	0.555410	1.355569	-1.068715
Pu	2.080471	0.163946	-3.019630
C	1.151173	-1.668467	-4.371800
N	3.791354	-1.859639	-2.510030
C	4.269320	-2.673021	-3.464671
C	5.066976	-3.778493	-3.189978
C	5.379346	-4.065951	-1.863896
C	4.886503	-3.229527	-0.866307
C	4.104703	-2.139491	-1.234582
C	3.741210	0.680321	-5.159514
C	2.425953	0.762787	-5.686403
C	1.802094	1.892346	-5.116818
C	2.732300	2.518297	-4.244276
C	3.932599	1.777837	-4.285824
C	3.511341	1.172581	-1.284694
H	0.559373	-0.674332	-0.134657
H	-0.810971	-1.419500	-2.329489
H	-1.115391	0.736574	-3.891339
H	0.035715	2.832064	-2.651094
H	1.070642	1.960899	-0.335984
H	4.489893	-0.058492	-5.422652
H	4.836817	2.004170	-3.735754
H	2.561107	3.416703	-3.664578
H	0.795590	2.233064	-5.324894
H	1.981803	0.087808	-6.405238
H	3.275154	0.760679	-0.293135
H	3.447601	2.262917	-1.220803
H	4.541649	0.897845	-1.553821
H	1.895225	-2.016911	-5.100122
H	0.953792	-2.479647	-3.654029
H	0.223093	-1.445190	-4.905932
H	5.428315	-4.398625	-4.003697
H	5.995772	-4.924421	-1.613113
H	5.102942	-3.408945	0.181643
H	3.719761	-1.454635	-0.484827
H	3.993948	-2.425940	-4.484671

Product Pyridine Pu IV – Large core

E = -713.547463
G = -713.315689

C	0.576775	0.800651	-1.587932
C	-0.440616	0.625477	-2.559805
C	-0.756294	-0.753619	-2.624924
C	0.078446	-1.436811	-1.706234
C	0.904786	-0.473906	-1.064621
Pu	1.794035	-0.574503	-3.640901
C	2.783386	1.626638	-3.957381
N	2.086058	1.387574	-5.088240
C	2.022421	2.260638	-6.104110
C	2.687299	3.474831	-6.032741
C	3.424571	3.765065	-4.877561
C	3.474712	2.842748	-3.838191
C	0.437411	-1.333736	-5.546020
C	3.024856	-2.957985	-3.161939
C	3.868530	-1.980383	-2.566657
C	4.469796	-1.231119	-3.607561
C	3.989246	-1.734461	-4.842452
C	3.105820	-2.807203	-4.568315
H	4.260660	-1.371193	-5.826100
H	2.582185	-3.403316	-5.303722
H	2.451393	-3.710713	-2.634616
H	4.048790	-1.854428	-1.505920
H	5.173594	-0.418714	-3.482140
H	-0.906662	1.411653	-3.141112
H	1.023790	1.742201	-1.296846
H	1.631107	-0.674659	-0.286286
H	0.062204	-2.500402	-1.501197
H	-1.500477	-1.206073	-3.266664
H	-0.385320	-0.637090	-5.757013
H	1.038233	-1.398909	-6.463314
H	-0.014795	-2.323479	-5.390042
H	2.633142	4.179260	-6.856812
H	3.954331	4.712144	-4.800223
H	4.045135	3.062179	-2.939124
H	1.432738	1.972107	-6.970990

Product Pyridine Pu IV – Small core

E = -1228.515981
G = -1228.286145

C	0.215274	1.243603	-2.019441
C	-0.712023	0.591670	-2.868417
C	-0.792329	-0.766234	-2.473494
C	0.097723	-0.956049	-1.395274
C	0.731059	0.285507	-1.119239
Pu	1.704294	-0.429758	-3.560320
C	0.487012	-1.731726	-5.132605
C	2.927384	0.947884	-5.091903
N	1.828291	1.644518	-4.772532
C	1.560511	2.859825	-5.275473
C	2.436488	3.453558	-6.170633
C	3.599688	2.759924	-6.531085
C	3.851072	1.503433	-5.990814
C	4.124079	-1.150623	-2.576000
C	3.196612	-1.846517	-1.770522
C	2.563298	-2.826343	-2.578375
C	3.114806	-2.744956	-3.875462
C	4.076138	-1.705997	-3.880555
H	4.686824	-1.406259	-4.721136
H	2.844085	-3.366259	-4.718747
H	1.803270	-3.527072	-2.256788
H	3.012716	-1.673028	-0.717968
H	4.768306	-0.340260	-2.253521
H	-1.272125	1.052586	-3.673290
H	0.492179	2.290150	-2.062627
H	1.451350	0.474392	-0.332384
H	0.260279	-1.883023	-0.861246
H	-1.422958	-1.522231	-2.921370
H	-0.335269	-1.094280	-5.498417
H	1.194445	-1.858868	-5.970890
H	0.067342	-2.716870	-4.903065
H	2.218241	4.434777	-6.580052
H	4.299169	3.208930	-7.232741
H	4.749619	0.956955	-6.264814
H	0.641043	3.344767	-4.955996

TS Pyridine Np III – Large core

E = -707.590856
G = -707.355132

C	0.977503	1.097989	-2.276521
N	-0.014547	0.462734	-2.917541
C	-0.782220	-0.452819	-2.282845
C	-0.539662	-0.743470	-0.934712
C	0.487415	-0.091589	-0.259918
C	1.263011	0.849071	-0.941752
Np	-1.510470	-0.160831	-4.872414
C	-3.040784	-1.895780	-3.426649
C	-4.011470	1.125341	-5.275583
C	-3.264642	1.389345	-6.449924
C	-2.212533	2.278423	-6.108461
C	-2.315666	2.565108	-4.724284
C	-3.422466	1.848840	-4.208694
C	-0.045881	-0.725222	-7.215957
C	0.864496	-1.013097	-6.169129
C	0.407411	-2.173547	-5.496340
C	-0.783483	-2.605447	-6.128500
C	-1.067862	-1.709190	-7.188917
H	0.898583	-2.661287	-4.662515
H	1.770511	-0.462104	-5.943940
H	0.043736	0.079424	-7.936487
H	-1.893085	-1.788283	-7.887485
H	-1.363840	-3.480583	-5.861471
H	-1.674757	3.234888	-4.162792
H	-3.776461	1.873029	-3.184641
H	-4.896445	0.503166	-5.209070
H	-3.481581	1.012559	-7.442803
H	-1.489614	2.702242	-6.796266
H	-2.732807	-2.903316	-3.120536
H	-3.561945	-2.033078	-4.389075
H	-3.812356	-1.555660	-2.724658
H	1.549709	1.819323	-2.855271
H	2.072550	1.377868	-0.448893
H	0.688468	-0.308366	0.786540
H	-1.156511	-1.478351	-0.423919
H	-1.882957	-1.152527	-2.889953

TS Pyridine Np III – Small core

E = -1189.635265

G = -1189.400017

C	1.042542	1.229264	-2.638205
N	0.002238	0.537759	-3.121462
C	-0.561195	-0.460769	-2.413388
C	-0.069121	-0.786161	-1.144703
C	1.014582	-0.079593	-0.633239
C	1.583731	0.947638	-1.391310
Np	-1.696127	-0.216065	-4.721974
C	-3.117471	-1.664688	-3.072505
C	-3.335401	1.194997	-6.442219
C	-2.173832	1.999667	-6.311564
C	-2.135442	2.503001	-4.990013
C	-3.270460	2.007225	-4.298814
C	-4.012439	1.204395	-5.199134
C	-0.527496	-0.926067	-7.086745
C	0.506559	-1.033631	-6.127347
C	0.203404	-2.126201	-5.275009
C	-1.020365	-2.688915	-5.707267
C	-1.478863	-1.944839	-6.823461
H	0.813039	-2.483858	-4.454410
H	1.389499	-0.408106	-6.070750
H	-0.575670	-0.206304	-7.894151
H	-2.374542	-2.143624	-7.400350
H	-1.513892	-3.547754	-5.268182
H	-3.540604	2.229817	-3.272648
H	-4.943256	0.694955	-4.976073
H	-3.662436	0.691158	-7.343712
H	-1.460216	2.218584	-7.096413
H	-1.386170	3.172057	-4.584099
H	-3.005882	-2.442203	-2.307587
H	-3.502728	-2.189453	-3.962852
H	-3.908094	-0.985808	-2.726080
H	1.443637	2.016792	-3.271355
H	2.429860	1.518221	-1.022300
H	1.418688	-0.321283	0.346728
H	-0.530449	-1.586262	-0.572223
H	-1.756285	-1.099144	-2.756557

Adduct of pyridine, Np III – Large core

E = -707.623684

G = -707.386531

C	0.697115	0.771572	-2.416171
N	-0.390998	0.016279	-2.628050
C	-0.901475	-0.669899	-1.592408
C	-0.347637	-0.626465	-0.316881
C	0.781542	0.159405	-0.104214
C	1.315083	0.872885	-1.175285
Np	-1.688087	-0.287148	-4.975117
C	-3.315927	-1.977014	-3.987069
C	-4.042380	1.267052	-5.318387
C	-3.248528	1.536338	-6.462339
C	-2.137268	2.315808	-6.051222
C	-2.241262	2.519827	-4.654378
C	-3.418022	1.870463	-4.202176
C	0.007247	-0.668994	-7.234945
C	0.861508	-0.927475	-6.136771
C	0.438569	-2.136898	-5.527309
C	-0.675808	-2.625654	-6.248270
C	-0.948345	-1.714840	-7.300083
H	0.909613	-2.622323	-4.679898
H	1.721007	-0.332550	-5.846787
H	0.087516	0.163966	-7.923651
H	-1.721709	-1.823862	-8.052447
H	-1.219265	-3.538888	-6.040151
H	-1.566141	3.110314	-4.044447
H	-3.792454	1.862997	-3.184866
H	-4.970302	0.708433	-5.301844
H	-3.475400	1.240316	-7.480433
H	-1.364320	2.712452	-6.699614
H	-2.838122	-2.878095	-3.569865
H	-4.003167	-2.351540	-4.762660
H	-3.969117	-1.571595	-3.197703
H	1.083080	1.312083	-3.276589
H	2.194122	1.497625	-1.056813
H	1.239175	0.215384	0.879247
H	-0.797621	-1.199632	0.486838
H	-1.781986	-1.271112	-1.808348

Adduct of pyridine, Np III – Small core

E = -1189.661225

G = -1189.424508

C	0.738955	1.118980	-2.667210
N	-0.234135	0.196955	-2.729046
C	-0.454487	-0.571130	-1.648935
C	0.286823	-0.450261	-0.478424
C	1.296239	0.507262	-0.421164
C	1.526752	1.307986	-1.538034
Np	-1.725919	-0.340584	-4.844284
C	-3.216526	-1.827053	-3.547197
C	-3.550875	1.111736	-6.271932
C	-2.355922	1.868125	-6.376300
C	-2.066711	2.406847	-5.100721
C	-3.085527	1.986753	-4.207118
C	-4.003740	1.191423	-4.930178
C	-0.008622	-0.829682	-6.944552
C	0.541591	-1.559112	-5.861734
C	-0.343399	-2.619094	-5.550255
C	-1.442634	-2.548718	-6.441117
C	-1.236101	-1.443263	-7.302214
H	-0.200311	-3.364294	-4.776532
H	1.488225	-1.357093	-5.372472
H	0.443462	0.023024	-7.437121
H	-1.886464	-1.136511	-8.112348
H	-2.285899	-3.228202	-6.462581
H	-3.161317	2.246246	-3.157078
H	-4.895074	0.725971	-4.528381
H	-4.050904	0.596646	-7.083595
H	-1.778102	2.022081	-7.279244
H	-1.237168	3.062769	-4.860183
H	-2.762189	-2.764799	-3.188321
H	-4.068650	-2.137682	-4.173813
H	-3.667594	-1.334631	-2.669394
H	0.883024	1.726715	-3.556564
H	2.300215	2.068902	-1.538418
H	1.892123	0.629889	0.478671
H	0.069995	-1.094721	0.367003
H	-1.258413	-1.297759	-1.740522

Product Pyridine Np III – Large core

E = -667.121134

G = -666.925993

C	1.020308	1.042685	-2.277774
C	-0.193252	0.613189	-2.870071
C	-0.843580	-0.255274	-1.954492
C	-0.032330	-0.362182	-0.799376
C	1.122145	0.434462	-1.000385
Np	1.441544	-1.703023	-2.829902
N	0.584206	-3.912588	-2.000931
C	-0.117147	-5.046466	-1.842136
C	0.185335	-5.951479	-0.837088
C	1.250312	-5.655875	0.020530
C	1.965857	-4.477389	-0.157553
C	1.629356	-3.583685	-1.189282
C	2.374672	-1.615725	-5.508599
C	3.247006	-0.754520	-4.798064
C	4.039567	-1.552114	-3.934055
C	3.666375	-2.907546	-4.120722
C	2.636009	-2.946964	-5.090086
H	-0.259529	-0.939735	0.088258
H	-1.813395	-0.719902	-2.094771
H	-0.579103	0.933158	-3.831797
H	1.727270	1.741190	-2.710147
H	1.920868	0.587793	-0.283087
H	2.160043	-3.841889	-5.474858
H	4.104667	-3.762989	-3.621745
H	4.828488	-1.193630	-3.281868
H	3.317670	0.320221	-4.917890
H	1.670063	-1.313778	-6.275997
H	-0.934965	-5.224531	-2.537992
H	-0.394765	-6.862348	-0.726667
H	1.511076	-6.347529	0.818991
H	2.794451	-4.241883	0.506016

Product Pyridine Np III – Small core

E = -1149.162563

G = -1148.967487

C	1.073449	1.297511	-2.847335
C	-0.190848	0.658213	-2.908254
C	-0.366193	-0.088930	-1.716837
C	0.791330	0.084263	-0.917549
C	1.682421	0.932824	-1.620386
Np	1.651641	-1.379931	-3.093580
C	2.150373	-3.037185	-1.426830
N	1.000299	-3.449888	-2.026969
C	0.364465	-4.578793	-1.676411
C	0.854450	-5.395109	-0.671222
C	2.036986	-5.012342	-0.023252
C	2.679703	-3.840288	-0.398963
C	2.510309	-2.842146	-5.265275
C	2.147086	-1.577601	-5.791773
C	3.079058	-0.619015	-5.319544
C	4.010840	-1.294494	-4.491876
C	3.666581	-2.668675	-4.465675
H	0.958659	-0.343972	0.062574
H	-1.241180	-0.670292	-1.449747
H	-0.911804	0.751456	-3.713503
H	1.488797	1.964246	-3.593386
H	2.650460	1.270606	-1.266152
H	4.200430	-3.449938	-3.939827
H	4.860213	-0.843072	-3.990712
H	3.092412	0.435169	-5.568189
H	1.319114	-1.381738	-6.464864
H	2.010035	-3.783485	-5.461294
H	-0.549285	-4.823862	-2.214745
H	0.329943	-6.305483	-0.398460
H	2.443925	-5.636110	0.770206
H	3.597074	-3.540706	0.102182

TS Pyridine Pu III – Large core

E = -708.259303

G = -708.023433

C	1.190859	1.073898	-2.557325
N	0.112261	0.467387	-3.073869
C	-0.697231	-0.294030	-2.303194
C	-0.407106	-0.454431	-0.942886
C	0.708807	0.170452	-0.395369
C	1.526159	0.950788	-1.216501
Pu	-1.538334	-0.209562	-4.854549
C	-3.034940	-1.770908	-3.218591
C	-3.546122	1.211862	-6.190339
C	-2.384964	2.016772	-6.326398
C	-2.073393	2.552029	-5.052066
C	-3.038616	2.079125	-4.129044
C	-3.950378	1.255046	-4.832835
C	-0.473426	-1.029300	-7.316083
C	0.613190	-1.142027	-6.413826
C	0.339786	-2.216589	-5.530021
C	-0.914599	-2.767094	-5.885355
C	-1.421345	-2.031622	-6.986263
H	0.990241	-2.571869	-4.739340
H	1.514009	-0.538806	-6.423861
H	-0.550130	-0.326811	-8.137576
H	-2.347664	-2.229352	-7.513688
H	-1.394934	-3.614713	-5.411616
H	-3.085941	2.325300	-3.074756
H	-4.816747	0.760604	-4.409957
H	-4.057918	0.693410	-6.993227
H	-1.856999	2.220846	-7.250653
H	-1.257750	3.229808	-4.827916
H	-2.715841	-2.767172	-2.888166
H	-3.627568	-1.941638	-4.132699
H	-3.747834	-1.386436	-2.478653
H	1.791853	1.668299	-3.241478
H	2.405407	1.452692	-0.825496
H	0.946950	0.055265	0.659390
H	-1.056132	-1.067604	-0.323031
H	-1.854260	-0.998812	-2.794137

TS Pyridine Pu III – Small core

E = -1229.130034

G = -1228.894987

C	1.079230	1.133959	-2.691206
N	0.008247	0.480074	-3.158767
C	-0.667805	-0.390120	-2.385717
C	-0.262443	-0.625039	-1.069080
C	0.851655	0.045447	-0.569761
C	1.536069	0.941822	-1.393220
Pu	-1.664167	-0.255211	-4.765479
C	-3.125643	-1.716652	-3.160448
C	-3.418497	1.169206	-6.296186
C	-2.228710	1.945136	-6.307557
C	-2.030967	2.462430	-5.006754
C	-3.091852	2.004641	-4.186580
C	-3.954324	1.213913	-4.985826
C	-0.502219	-0.924138	-7.155426
C	0.545026	-1.004407	-6.207333
C	0.269705	-2.093582	-5.343264
C	-0.945449	-2.689465	-5.760819
C	-1.427180	-1.963507	-6.879009
H	0.889092	-2.424210	-4.518055
H	1.413403	-0.357899	-6.161187
H	-0.575447	-0.209820	-7.966148
H	-2.326108	-2.181609	-7.444252
H	-1.418478	-3.553232	-5.308932
H	-3.231437	2.236357	-3.136815
H	-4.865697	0.731827	-4.651268
H	-3.855648	0.662959	-7.148825
H	-1.599718	2.131583	-7.169359
H	-1.217135	3.105129	-4.693016
H	-2.919807	-2.656581	-2.633559
H	-3.610843	-2.015310	-4.106339
H	-3.879546	-1.168430	-2.581831
H	1.573213	1.818541	-3.376228
H	2.407962	1.481229	-1.037313
H	1.188562	-0.125267	0.449664
H	-0.812681	-1.326622	-0.447939
H	-1.841018	-1.058348	-2.777538

Adduct of pyridine, Pu III – Large core

E = -708.292878

G = -708.055675

C	0.871042	0.796317	-2.703962
N	-0.272741	0.096523	-2.743854
C	-0.726186	-0.450090	-1.604022
C	-0.058328	-0.317242	-0.390789
C	1.127377	0.411183	-0.356015
C	1.602047	0.979439	-1.536156
Pu	-1.766326	-0.336398	-4.919228
C	-3.358051	-1.847468	-3.661567
C	-3.396630	1.419286	-6.380725
C	-2.200550	2.158022	-6.192481
C	-2.110808	2.499720	-4.821959
C	-3.252275	1.975864	-4.163110
C	-4.048837	1.313649	-5.125716
C	-0.423924	-1.022995	-7.314699
C	0.598538	-1.067628	-6.336937
C	0.342957	-2.173754	-5.485816
C	-0.837100	-2.811043	-5.936164
C	-1.315444	-2.096590	-7.063156
H	0.964407	-2.498520	-4.658897
H	1.455173	-0.404273	-6.283820
H	-0.495939	-0.312888	-8.130050
H	-2.186558	-2.353017	-7.655907
H	-1.290418	-3.694645	-5.504591
H	-3.490694	2.089329	-3.111677
H	-4.995185	0.821563	-4.937624
H	-3.770352	1.044756	-7.327127
H	-1.497091	2.438167	-6.968094
H	-1.329298	3.096038	-4.363813
H	-2.886278	-2.732707	-3.205926
H	-4.117496	-2.251184	-4.350478
H	-3.931396	-1.348696	-2.863913
H	1.208031	1.221301	-3.645926
H	2.521753	1.554553	-1.556832

H	1.673710	0.534295	0.574648
H	-0.465480	-0.778353	0.502829
H	-1.654383	-1.011491	-1.683413

Adduct of pyridine, Pu III – Small core

E = -1229.157524

G = -1228.922456

C	0.865554	0.797189	-2.807902
N	-0.273043	0.086958	-2.804929
C	-0.683587	-0.450022	-1.643758
C	0.021128	-0.298290	-0.454012
C	1.201092	0.440907	-0.464101
C	1.631382	0.999700	-1.665668
Pu	-1.811200	-0.373894	-4.868864
C	-3.335248	-1.842333	-3.613284
C	-3.332995	1.323689	-6.358972
C	-2.128445	2.044843	-6.154518
C	-2.051021	2.387214	-4.784246
C	-3.203601	1.876208	-4.138826
C	-3.999422	1.224092	-5.111719
C	-0.376543	-0.841619	-7.185838
C	0.544476	-1.096365	-6.143138
C	0.108147	-2.249279	-5.443786
C	-1.082932	-2.709473	-6.057116
C	-1.385324	-1.835288	-7.131540
H	0.608745	-2.711718	-4.600653
H	1.444184	-0.527076	-5.936971
H	-0.315041	-0.038086	-7.909520
H	-2.225506	-1.926654	-7.810440
H	-1.658282	-3.577118	-5.759030
H	-3.445316	1.979032	-3.086980
H	-4.949473	0.736219	-4.930765
H	-3.693688	0.944642	-7.308130
H	-1.407694	2.308241	-6.919000
H	-1.258687	2.957505	-4.312624
H	-2.846123	-2.729780	-3.177991
H	-4.115078	-2.237276	-4.285722
H	-3.879552	-1.344715	-2.793451
H	1.167445	1.214966	-3.764434
H	2.544233	1.583463	-1.722930
H	1.775641	0.579392	0.447179
H	-0.353887	-0.753168	0.456838
H	-1.609126	-1.019687	-1.685465

Product Pyridine Pu III – Large core

E = -667.789915

G = -667.594441

C	1.475706	1.230868	-2.785083
C	0.180110	0.766945	-3.123689
C	-0.354655	0.097218	-1.991923
C	0.609946	0.146033	-0.956860
C	1.743299	0.841217	-1.447815
Pu	1.735082	-1.568211	-2.899415
N	0.849778	-3.552569	-1.688510
C	0.097372	-4.595078	-1.302267
C	0.452583	-5.381664	-0.217961
C	1.625638	-5.062974	0.474378
C	2.392482	-3.979474	0.061051
C	2.000184	-3.204472	-1.044104
C	2.178857	-2.263161	-5.597963
C	3.005024	-1.133333	-5.375099
C	4.042629	-1.519634	-4.489545
C	3.864466	-2.892551	-4.175624
C	2.712872	-3.350270	-4.858951
H	0.497850	-0.264272	0.039173
H	-1.344643	-0.338946	-1.917606
H	-0.330400	0.938779	-4.064906
H	2.131642	1.810336	-3.424242
H	2.639837	1.073049	-0.883410
H	4.508269	-3.491362	-3.543082
H	4.860280	-0.890312	-4.155429
H	2.882516	-0.155336	-5.825639
H	1.320605	-2.301969	-6.260315
H	2.323428	-4.361381	-4.839967
H	-0.804113	-4.795838	-1.878110
H	-0.169414	-6.220583	0.078194
H	1.930064	-5.662989	1.329502
H	3.305232	-3.726977	0.595384

Product Pyridine Pu III – Small core

E = -1188.660081

G = -1188.465336

C	1.453520	1.275463	-2.787595
C	0.190421	0.728800	-3.126295
C	-0.287755	0.006239	-2.002651
C	0.681225	0.104844	-0.972905
C	1.757614	0.886889	-1.460758
Pu	1.824756	-1.445563	-2.887375
N	0.966269	-3.484678	-1.945260
C	0.227477	-4.579825	-1.698361
C	0.539386	-5.432973	-0.653181
C	1.649141	-5.128652	0.146454
C	2.399315	-3.991490	-0.125335
C	2.050630	-3.147939	-1.196104
C	2.992546	-2.904866	-4.860049
C	2.365911	-1.837488	-5.551459
C	3.045959	-0.641276	-5.220648
C	4.090951	-0.965374	-4.319534
C	4.061527	-2.366987	-4.100175
H	0.609901	-0.333591	0.014873
H	-1.237607	-0.511861	-1.932556
H	-0.330558	0.867623	-4.066887
H	2.072283	1.893225	-3.426645
H	2.651355	1.153868	-0.907391
H	4.742830	-2.931039	-3.474562
H	4.807504	-0.268214	-3.899979
H	2.814541	0.346772	-5.598857
H	1.525805	-1.923939	-6.232171
H	2.715205	-3.951036	-4.914731
H	-0.622104	-4.764399	-2.352825
H	-0.066860	-6.313669	-0.465662
H	1.915041	-5.783610	0.973464
H	3.261144	-3.749170	0.491724

Picoline

E = -287.500697

G = -287.414535

N	0.061151	-0.184386	0.009373
C	0.026778	-0.015100	1.340177
C	1.191187	0.155141	2.097701
C	2.426480	0.149343	1.456365
C	2.463680	-0.026217	0.076467
C	1.251435	-0.187918	-0.592636
H	1.124776	0.289779	3.173574
H	3.343200	0.279962	2.025413
H	3.401706	-0.037963	-0.469961
H	1.237017	-0.327642	-1.673261
C	-1.335877	-0.020317	1.976877
H	-1.967714	0.751262	1.525867
H	-1.832492	-0.980507	1.802812
H	-1.283275	0.154562	3.054476

TS Picoline sp2 Np IV – Large core

E = -792.542089

G = -792.241679

C	0.208791	1.578721	-1.680788
N	-0.432115	0.751482	-2.518430
C	-0.186338	-0.576075	-2.526150
C	0.729949	-1.138436	-1.636370
C	1.379284	-0.303297	-0.729628
C	1.119023	1.064876	-0.751520
Np	-1.251678	0.006789	-4.902938
C	1.000618	1.023602	-5.152867
C	-2.830724	-1.230132	-3.044906
C	-3.213408	1.150522	-6.516720
C	-2.053448	1.934363	-6.726775
C	-1.790245	2.656076	-5.533845
C	-2.779139	2.306956	-4.585224
C	-3.655605	1.369149	-5.189239
C	-1.079750	-1.383757	-7.271761
C	0.193571	-1.542124	-6.674139
C	0.041812	-2.369507	-5.532740
C	-1.323850	-2.720708	-5.425772
C	-2.022879	-2.103061	-6.494649
H	0.835777	-2.681649	-4.866462
H	1.122341	-1.118909	-7.031421
H	-1.292064	-0.825566	-8.174983
H	-3.080784	-2.203655	-6.704635
H	-1.761413	-3.353877	-4.665078
H	-2.859142	2.688509	-3.575558
H	-4.527340	0.923692	-4.725835
H	-3.686168	0.503760	-7.245158
H	-1.482021	1.998560	-7.644662
H	-0.976283	3.353241	-5.386060
H	-2.802448	-2.164569	-2.471249
H	-3.529892	-1.404831	-3.874086
H	-3.249639	-0.455877	-2.393178
H	1.105201	1.946238	-4.567180
H	1.796213	0.344917	-4.816516
H	1.223982	1.284565	-6.197344
H	1.616987	1.736560	-0.058785
H	2.085651	-0.709048	-0.008926
H	0.922901	-2.207518	-1.647179
H	-1.371831	-1.127953	-2.952004
C	-0.093630	3.045672	-1.775528
H	0.509904	3.625059	-1.072919
H	0.105310	3.410836	-2.787744
H	-1.150389	3.236270	-1.561307

TS Picoline sp2 Np IV – Small core

E = -1268.802286

G = -1268.503516

C	0.416389	1.439996	-1.697181
N	-0.316300	0.726854	-2.571614
C	-0.402080	-0.610109	-2.489293
C	0.247670	-1.322076	-1.479287
C	1.004144	-0.606275	-0.557545
C	1.086258	0.782643	-0.663792
Np	-1.202190	0.136418	-4.848585
C	0.742168	1.515057	-5.316064
C	-2.977695	-1.306576	-3.332023
C	-3.622424	0.811921	-5.962125
C	-2.656385	1.426267	-6.798404
C	-2.031846	2.457988	-6.063852
C	-2.609079	2.481953	-4.770467
C	-3.599605	1.472922	-4.713378
C	-0.628333	-1.159030	-7.176385
C	0.544535	-1.281242	-6.396704
C	0.256378	-2.136303	-5.306184
C	-1.092899	-2.552638	-5.422000
C	-1.640635	-1.947706	-6.575071
H	0.955620	-2.446243	-4.539659
H	1.497191	-0.814296	-6.605059
H	-0.722821	-0.586024	-8.089745
H	-2.649707	-2.080445	-6.944578
H	-1.609974	-3.229110	-4.755311
H	-2.356225	3.170444	-3.973499
H	-4.229577	1.245951	-3.863302
H	-4.284682	0.001825	-6.241090
H	-2.454090	1.170227	-7.830302
H	-1.257970	3.119374	-6.428527
H	-2.888252	-2.298703	-2.871368
H	-3.584120	-1.424694	-4.235728
H	-3.513710	-0.658285	-2.630147
H	0.632277	2.503356	-4.849151
H	1.625571	1.031677	-4.869676
H	0.959881	1.677903	-6.379602
H	1.668804	1.359091	0.048179
H	1.528503	-1.119594	0.244800
H	0.155637	-2.402144	-1.418637
H	-1.484861	-1.077885	-3.031669
C	0.488499	2.925445	-1.880083
H	0.897021	3.414643	-0.992711
H	1.127398	3.171461	-2.734800
H	-0.503392	3.335824	-2.086639

Adduct of picoline sp2, Np IV – Large core

E = -792.584008

G = -792.280488

C	0.008372	0.908762	-1.629554
N	0.001271	-0.052170	-2.575700
C	0.656742	-1.192892	-2.314891
C	1.337689	-1.443979	-1.130374
C	1.343409	-0.455431	-0.152139
C	0.670112	0.731629	-0.410617
Np	-1.307551	0.232906	-5.045195
C	0.984314	1.252827	-5.075975
C	-2.901850	-0.452918	-3.232067
C	-3.340841	1.329935	-6.508291
C	-2.147828	1.847638	-7.085803
C	-1.584427	2.768317	-6.171790
C	-2.419711	2.813110	-5.028898
C	-3.510120	1.934349	-5.240792
C	-1.566365	-1.532538	-7.139230
C	-0.166305	-1.379239	-6.979160
C	0.204964	-2.008161	-5.766606
C	-0.966229	-2.542207	-5.173278
C	-2.061577	-2.245401	-6.019225
H	1.214282	-2.071898	-5.379557
H	0.505960	-0.880918	-7.666584
H	-2.150931	-1.189230	-7.983425
H	-3.092488	-2.525183	-5.843055
H	-1.027224	-3.096788	-4.245202
H	-2.274351	3.445784	-4.162479
H	-4.326898	1.753868	-4.554858
H	-4.021025	0.624941	-6.970785
H	-1.755320	1.606075	-8.066116
H	-0.675605	3.335973	-6.319767
H	-2.555887	-1.331396	-2.671064
H	-3.852776	-0.738741	-3.708360
H	-3.159616	0.306657	-2.480429
H	1.115011	2.181269	-4.502270
H	1.763104	0.563854	-4.722984
H	1.235539	1.504196	-6.118118
H	0.650307	1.530482	0.324055
H	1.861236	-0.604341	0.791087
H	1.846585	-2.391579	-0.988208
H	0.634671	-1.942419	-3.097772
C	-0.715913	2.183118	-1.933236
H	-0.673921	2.879635	-1.092883
H	-0.272637	2.667820	-2.809227
H	-1.765918	1.975359	-2.162022

Adduct of picoline sp2, Np IV – Small core

E = -1268.830049

G = -1268.530127

C	0.232863	1.155795	-1.688330
N	-0.082661	0.133308	-2.508484
C	0.333124	-1.098553	-2.172772
C	1.098794	-1.378157	-1.049060
C	1.447348	-0.321371	-0.213766
C	1.002225	0.953741	-0.537794
Np	-1.316057	0.155753	-4.956673
C	0.884782	1.189848	-5.245549
C	-2.858848	-0.763184	-3.303595
C	-3.340619	1.176582	-6.476903
C	-2.178139	1.886582	-6.876309
C	-1.789427	2.726562	-5.809531
C	-2.701187	2.523483	-4.744484
C	-3.665672	1.573928	-5.161764
C	-1.190150	-1.284157	-7.286486
C	0.102957	-1.411888	-6.735278
C	-0.000567	-2.199959	-5.563329
C	-1.357966	-2.570402	-5.397583
C	-2.095405	-1.993333	-6.455463
H	0.830555	-2.500660	-4.936164
H	1.014205	-0.989050	-7.136436
H	-1.444067	-0.756357	-8.196780
H	-3.161894	-2.096073	-6.612819
H	-1.765782	-3.186356	-4.606513
H	-2.694145	3.037437	-3.791271
H	-4.502801	1.219068	-4.575906
H	-3.894457	0.470879	-7.083067
H	-1.686024	1.817027	-7.838383
H	-0.946494	3.404932	-5.812748
H	-2.432115	-1.592762	-2.722784
H	-3.775441	-1.139726	-3.779429
H	-3.160128	0.013213	-2.583779

H	1.068233	2.123019	-4.695503
H	1.666336	0.477911	-4.940546
H	1.051230	1.416234	-6.308719
H	1.240815	1.802532	0.095454
H	2.048091	-0.487412	0.675971
H	1.406714	-2.397383	-0.841309
H	0.029590	-1.898949	-2.840149
C	-0.307040	2.514786	-2.015509
H	-1.369980	2.566593	-1.753547
H	0.216078	3.294884	-1.457597
H	-0.216835	2.723923	-3.083361

Product Picoline sp2, Np IV – Large core

E = -752.102517

G = -751.845714

C	1.194376	1.493113	-2.008618
C	0.292966	1.031889	-3.006644
C	-0.680717	0.220163	-2.374303
C	-0.377615	0.171418	-0.991504
C	0.773577	0.966381	-0.762910
Np	1.693933	-1.198465	-2.229264
C	0.042462	-2.839660	-3.082397
N	1.820482	-2.779752	-0.328772
C	1.635798	-3.835111	0.489993
C	2.309139	-3.868209	1.707403
C	3.160839	-2.812525	2.051012
C	3.328187	-1.743467	1.179021
C	2.632120	-1.741528	-0.038488
C	0.714226	-4.926199	0.033379
C	2.998332	-0.805278	-4.609475
C	3.917748	-0.379512	-3.612115
C	4.362124	-1.526514	-2.909731
C	3.709593	-2.657000	-3.462512
C	2.875494	-2.213900	-4.517915
H	-0.938756	-0.366049	-0.236568
H	-1.508549	-0.277102	-2.861987
H	0.322680	1.287348	-4.059081
H	2.032877	2.160679	-2.166652
H	1.246210	1.141888	0.194679
H	3.839607	-3.684313	-3.144692
H	5.075601	-1.537900	-2.096034
H	4.248838	0.638206	-3.443177
H	2.505347	-0.168924	-5.334548
H	2.252772	-2.840633	-5.142397
H	0.477045	-3.842894	-3.187987
H	-0.822371	-2.939486	-2.412085
H	-0.354788	-2.561010	-4.069403
H	2.169473	-4.710309	2.378840
H	3.687424	-2.837318	3.002900
H	3.987845	-0.919331	1.437532
H	0.578611	-5.684790	0.808083
H	-0.262989	-4.516009	-0.237214
H	1.111587	-5.412813	-0.863526

Product Picoline sp2, Np IV – Small core

E = -1228.351593

G = -1228.096597

C	0.641945	1.465286	-1.861183
C	0.126776	0.904411	-3.058412
C	-0.352122	-0.393200	-2.763216
C	-0.122140	-0.638718	-1.388189
C	0.481977	0.514514	-0.827531
Np	2.353145	-0.570476	-2.486485
C	1.713212	-2.451691	-3.853733
N	3.467301	-2.235438	-1.169265
C	4.080828	-3.374715	-0.785437
C	4.478735	-3.501312	0.540625
C	4.237086	-2.453063	1.438215
C	3.600436	-1.298970	1.001921
C	3.210423	-1.204722	-0.343564
C	4.296823	-4.442459	-1.814882
C	4.830196	-0.384787	-3.606159
C	3.934222	-0.240382	-4.692342
C	3.254758	0.990786	-4.533746
C	3.739065	1.611678	-3.354257
C	4.715088	0.762594	-2.782060
H	-0.375518	-1.546702	-0.853371
H	-0.811739	-1.078435	-3.462704
H	0.083401	1.394353	-4.023207
H	1.061437	2.457973	-1.752795
H	0.765580	0.642595	0.208694
H	5.498558	-1.220460	-3.439420
H	5.277969	0.955881	-1.877223
H	3.432240	2.576900	-2.971128
H	2.511186	1.397506	-5.207924
H	3.790765	-0.947570	-5.498771
H	2.594466	-3.036282	-4.155773
H	1.034706	-3.139557	-3.326745
H	1.200759	-2.144970	-4.778051
H	4.971742	-4.410710	0.871278
H	4.549926	-2.554402	2.475393
H	3.405910	-0.481855	1.691535
H	4.777199	-5.322644	-1.380954
H	3.343793	-4.742889	-2.260664
H	4.926027	-4.069704	-2.629930

TS picoline sp2 Pu IV – Large core

E = -793.294941

G = -792.994002

C	0.200675	1.580438	-1.684988
N	-0.441234	0.755773	-2.524181
C	-0.186799	-0.569735	-2.543374
C	0.737854	-1.133740	-1.663359
C	1.386123	-0.301821	-0.752831
C	1.118167	1.064980	-0.763592
Pu	-1.251861	0.004662	-4.905841
C	0.988753	1.013243	-5.147065
C	-2.831512	-1.215926	-3.055305
C	-3.200210	1.140637	-6.516604
C	-2.038314	1.922188	-6.722766
C	-1.775500	2.640263	-5.527190
C	-2.766430	2.290924	-4.581251
C	-3.643255	1.355656	-5.188878
C	-1.082669	-1.376137	-7.260701
C	0.189892	-1.535326	-6.661942
C	0.036396	-2.361221	-5.519625
C	-1.329633	-2.710196	-5.413084
C	-2.027409	-2.092605	-6.482878
H	0.829301	-2.672345	-4.851802
H	1.119342	-1.113733	-7.019116
H	-1.293510	-0.818604	-8.164535
H	-3.085391	-2.191469	-6.692815
H	-1.768709	-3.341113	-4.651510
H	-2.845435	2.667575	-3.569846
H	-4.515896	0.909977	-4.727642
H	-3.672641	0.495956	-7.246953
H	-1.464976	1.987395	-7.639294
H	-0.959932	3.334692	-5.376119
H	-2.800266	-2.150353	-2.481661
H	-3.534039	-1.390078	-3.881062
H	-3.244738	-0.440664	-2.401570
H	1.091457	1.933489	-4.557744
H	1.782621	0.332682	-4.811200
H	1.213536	1.277590	-6.190211
H	1.615379	1.734341	-0.068037
H	2.097828	-0.708941	-0.038155
H	0.938020	-2.201368	-1.684191
H	-1.376252	-1.119344	-2.968109
C	-0.108607	3.046761	-1.768595
H	0.495055	3.624059	-1.064348
H	0.085253	3.419719	-2.778982
H	-1.165344	3.231586	-1.549305

TS picoline sp2 Pu IV – Small core

E = -1308.278227

G = -1307.981181

C	0.414729	1.467018	-1.694222
N	-0.323343	0.758611	-2.567576
C	-0.466586	-0.569737	-2.448000
C	0.128126	-1.279115	-1.403596
C	0.896731	-0.568333	-0.486663
C	1.036945	0.812324	-0.628902
Pu	-1.193509	0.110149	-4.826166
C	0.795714	1.406227	-5.403892
C	-3.011726	-1.314462	-3.339797
C	-3.438700	0.889772	-6.190411
C	-2.382516	1.641503	-6.771006
C	-1.933252	2.574910	-5.814189
C	-2.692550	2.391907	-4.632827
C	-3.635278	1.360851	-4.874743
C	-0.980571	-1.312905	-7.168907
C	0.337364	-1.213440	-6.669647
C	0.411645	-1.987072	-5.484625
C	-0.859969	-2.564414	-5.257612
C	-1.723603	-2.140967	-6.293865
H	1.292160	-2.123818	-4.867744
H	1.152139	-0.668226	-7.124496
H	-1.353193	-0.850618	-8.073625
H	-2.763530	-2.419957	-6.408639
H	-1.125803	-3.219905	-4.438570
H	-2.601040	2.965244	-3.718308
H	-4.379354	1.003300	-4.175454
H	-4.009603	0.110111	-6.679757
H	-2.004486	1.540334	-7.780234
H	-1.146476	3.301960	-5.960857
H	-2.915959	-2.313473	-2.897194
H	-3.598924	-1.414445	-4.256402
H	-3.552859	-0.672655	-2.636559
H	0.753537	2.349042	-4.843951
H	1.649186	0.818428	-5.031526
H	0.970983	1.636707	-6.459544
H	1.629623	1.384280	0.078389
H	1.385334	-1.080196	0.338748
H	-0.010918	-2.352188	-1.314651
H	-1.548895	-1.043136	-3.005905
C	0.550798	2.942389	-1.919224
H	0.913574	3.449226	-1.021838
H	1.257800	3.138292	-2.732857
H	-0.408652	3.376343	-2.211412

Adduct of picoline sp2, Pu IV – Large core

E = -793.338055

G = -793.034043

C	0.000944	0.914498	-1.626047
N	-0.003842	-0.041046	-2.577509
C	0.652556	-1.182195	-2.321174
C	1.330821	-1.439802	-1.136483
C	1.332942	-0.457242	-0.152316
C	0.659552	0.730652	-0.406162
Pu	-1.305998	0.228266	-5.053319
C	0.976129	1.230773	-5.080591
C	-2.888984	-0.449396	-3.247932
C	-3.331362	1.321126	-6.495650
C	-2.138822	1.826455	-7.085743
C	-1.560878	2.747136	-6.181253
C	-2.386543	2.805090	-5.032078
C	-3.485533	1.934080	-5.230401
C	-1.579122	-1.525165	-7.134436
C	-0.178684	-1.370662	-6.980104
C	0.197638	-1.997627	-5.767813
C	-0.970990	-2.529946	-5.168569
C	-2.070016	-2.234432	-6.010624
H	1.208366	-2.059566	-5.384437
H	0.490619	-0.872954	-7.670729
H	-2.167316	-1.182589	-7.976278
H	-3.100262	-2.512802	-5.829134
H	-1.028617	-3.081595	-4.238647
H	-2.228453	3.440617	-4.170214
H	-4.297846	1.763146	-4.536904
H	-4.020640	0.618709	-6.948268
H	-1.755699	1.576393	-8.067528
H	-0.648382	3.306009	-6.339057
H	-2.544130	-1.327746	-2.686358
H	-3.842871	-0.731956	-3.719798
H	-3.139720	0.313416	-2.497381
H	1.101032	2.160722	-4.508341
H	1.752068	0.543286	-4.719192
H	1.235130	1.479197	-6.121333
H	0.637310	1.525409	0.332890
H	1.848166	-0.611173	0.791541
H	1.840382	-2.387734	-0.998856
H	0.633954	-1.927308	-3.108225
C	-0.719969	2.192471	-1.922961
H	-0.687185	2.878384	-1.073486
H	-0.266427	2.687670	-2.787583
H	-1.766975	1.988287	-2.166944

Adduct of picoline sp2, Pu IV – Small core

E = -1308.304871

G = -1308.006336

C	0.273320	1.056359	-1.635910
N	-0.027769	0.040515	-2.469839
C	0.308011	-1.206976	-2.099920
C	0.961292	-1.509919	-0.913043
C	1.280775	-0.462632	-0.053823
C	0.926919	0.829356	-0.419940
Pu	-1.297362	0.231364	-4.909660
C	0.811452	1.370799	-5.436065
C	-3.017697	-0.728539	-3.449742
C	-3.300756	1.124736	-6.551205
C	-2.157920	1.887424	-6.906411
C	-1.864601	2.758746	-5.836593
C	-2.812333	2.521513	-4.809380
C	-3.708907	1.520291	-5.260671
C	-1.230112	-1.308720	-7.183992
C	0.112888	-1.270415	-6.753258
C	0.204115	-2.013237	-5.549057
C	-1.083252	-2.517512	-5.247843
C	-1.975868	-2.068370	-6.246739
H	1.114244	-2.190427	-4.987215
H	0.931982	-0.777678	-7.259031
H	-1.619680	-0.852465	-8.084857
H	-3.033720	-2.291677	-6.299926
H	-1.351048	-3.142290	-4.404014
H	-2.889643	3.061238	-3.871777
H	-4.562856	1.140282	-4.717426
H	-3.786934	0.378855	-7.167157
H	-1.609802	1.823591	-7.838104
H	-1.061222	3.482999	-5.811579
H	-2.534955	-1.541356	-2.890530
H	-3.924771	-1.113719	-3.923181
H	-3.295003	0.069230	-2.744553
H	0.845277	2.299882	-4.850747
H	1.603060	0.694860	-5.083584
H	0.991712	1.618975	-6.485669
H	1.149875	1.671364	0.227956
H	1.789689	-0.649339	0.887575
H	1.204519	-2.539715	-0.674149
H	0.033236	-1.995643	-2.792467
C	-0.095567	2.450750	-2.048456
H	-0.216057	3.098029	-1.176131
H	0.685538	2.883406	-2.682864
H	-1.028506	2.466135	-2.617916

Product Picoline sp2, Pu IV – Large core

E = -752.857228

G = -752.600169

C	1.222940	1.512063	-2.006165
C	0.324546	1.052398	-3.007924
C	-0.644376	0.230639	-2.381629
C	-0.342091	0.174679	-0.998768
C	0.803766	0.975352	-0.764138
Pu	1.726037	-1.158371	-2.241412
C	2.693075	-1.673285	-0.074561
N	1.884516	-2.718684	-0.343059
C	1.719661	-3.768017	0.487322
C	2.412702	-3.785615	1.694072
C	3.262396	-2.721194	2.014876
C	3.408648	-1.658525	1.131246
C	0.797766	-4.868902	0.055574
C	0.087941	-2.810538	-3.055715
C	2.978967	-0.773107	-4.628668
C	3.905198	-0.322100	-3.648672
C	4.375263	-1.453916	-2.938588
C	3.732084	-2.600366	-3.469122
C	2.878053	-2.182090	-4.518711
H	-0.899581	-0.372774	-0.248471
H	-1.468311	-0.269243	-2.873074
H	0.353663	1.314640	-4.058592
H	2.057749	2.185271	-2.158963

H	1.275183	1.146749	0.194673
H	3.879932	-3.621502	-3.139676
H	5.098694	-1.445097	-2.133832
H	4.223414	0.702141	-3.495974
H	2.467186	-0.152906	-5.354505
H	2.255797	-2.825026	-5.126801
H	0.529584	-3.811058	-3.156153
H	-0.766139	-2.909603	-2.371907
H	-0.324759	-2.545389	-4.039950
H	2.289809	-4.622651	2.375051
H	3.804197	-2.734196	2.958420
H	4.066505	-0.827542	1.371754
H	0.687920	-5.626525	0.835242
H	-0.189577	-4.468494	-0.192087
H	1.177740	-5.353834	-0.849648

Product Picoline sp2, Pu IV – Small core

E = -1267.825118

G = -1267.569488

C	-0.072385	1.433151	-1.647473
C	-0.220634	0.851029	-2.933470
C	0.123575	-0.515432	-2.836501
C	0.500872	-0.778495	-1.498893
C	0.379064	0.429199	-0.764222
Pu	2.458797	0.832771	-2.449502
C	2.678317	-0.369498	-4.493772
C	3.559168	-0.619807	-0.910187
N	4.546660	0.074707	-1.488738
C	5.851375	-0.091037	-1.186384
C	6.196260	-1.023656	-0.212452
C	5.193816	-1.766041	0.421835
C	3.862344	-1.570945	0.073442
C	6.866001	0.728124	-1.926336
C	3.799525	3.197477	-2.321802
C	2.433348	3.555321	-2.266165
C	1.864394	3.295157	-3.540795
C	2.871156	2.762403	-4.373708
C	4.066975	2.694089	-3.617771
H	0.811277	-1.735546	-1.101344
H	0.102813	-1.233306	-3.645257
H	-0.561253	1.355277	-3.828787
H	-0.281904	2.462900	-1.386975
H	0.592366	0.554725	0.291003
H	5.021745	2.329030	-3.975191
H	4.511765	3.284906	-1.509679
H	1.922882	3.990433	-1.415345
H	0.838067	3.484834	-3.826234
H	2.752608	2.458687	-5.405133
H	3.702873	-0.185401	-4.858147
H	2.624295	-1.433633	-4.205283
H	1.995539	-0.221053	-5.337108
H	7.240734	-1.169977	0.046185
H	5.466100	-2.493469	1.183583
H	3.072909	-2.142725	0.553419
H	7.872500	0.562327	-1.535068
H	6.864443	0.469206	-2.990645
H	6.633888	1.794662	-1.851094

TS Picoline sp2 Np III – Large core

E = -746.900650

G = -746.639439

C	-0.317420	0.931552	-2.257086
C	-0.249481	-0.050969	-3.278493
C	0.606637	-1.087180	-2.830163
C	1.069618	-0.745816	-1.535497
C	0.496083	0.499436	-1.180426
Np	2.309026	1.149918	-3.271366
N	4.137235	-0.542107	-3.748804
C	4.732360	-1.563965	-4.394500
C	5.999370	-1.990857	-4.003415
C	6.638399	-1.353150	-2.939127
C	6.000241	-0.303606	-2.287737
C	4.729413	0.095353	-2.715187
C	3.972690	-2.203145	-5.519350
C	3.609576	2.283980	-1.153825
C	1.572516	2.299635	-5.744112
C	1.310017	3.311186	-4.784158
C	2.553379	3.785708	-4.298730
C	3.583999	3.068208	-4.954833
C	2.978408	2.154682	-5.851155
H	1.723321	-1.345884	-0.913190
H	0.836864	-1.999531	-3.368403
H	-0.792493	-0.032463	-4.216368
H	-0.921574	1.831286	-2.279427
H	0.636491	1.018513	-0.239703
H	4.648762	3.215278	-4.816741
H	2.694319	4.577293	-3.572079
H	0.331076	3.683502	-4.505011
H	0.829024	1.769709	-6.328617
H	3.500660	1.485138	-6.524740
H	3.602037	1.805232	-0.166809
H	2.752207	2.977362	-1.154591
H	4.496414	2.928105	-1.205161
H	6.477480	-2.812366	-4.528285
H	7.628245	-1.679610	-2.628590
H	6.477795	0.208244	-1.456619
H	4.139249	1.182304	-1.977046
H	4.586512	-2.929380	-6.057037
H	3.085381	-2.720358	-5.137780
H	3.626062	-1.444958	-6.228465

TS Picoline sp2 Np III – Small core

E = -1228.946820

G = -1228.686128

C	-0.171805	0.923942	-2.221831
C	-0.130891	-0.038166	-3.262365
C	0.760560	-1.068476	-2.870538
C	1.268265	-0.741362	-1.588909
C	0.690408	0.485600	-1.185784
Np	2.336232	1.142923	-3.303283
N	4.077189	-0.503829	-3.763559
C	4.700612	-1.508332	-4.411254
C	5.918979	-1.984594	-3.933240
C	6.479405	-1.418139	-2.786273
C	5.812743	-0.384394	-2.137431
C	4.593883	0.058982	-2.655156
C	4.024503	-2.069526	-5.625938
C	3.493760	2.365206	-1.281654
C	1.487035	2.274319	-5.658604
C	1.333252	3.297805	-4.690182
C	2.626000	3.712559	-4.283384
C	3.575957	2.943025	-4.995663
C	2.874592	2.056594	-5.850162
H	1.963225	-1.337087	-1.008996
H	0.985213	-1.966332	-3.434176
H	-0.704536	-0.004699	-4.181201
H	-0.781738	1.819705	-2.209691
H	0.865462	0.991155	-0.244206
H	4.653351	3.032846	-4.917222
H	2.849924	4.491962	-3.565359
H	0.391860	3.710805	-4.347231
H	0.682758	1.771766	-6.183797
H	3.321676	1.366984	-6.556190
H	3.601545	1.974223	-0.261996
H	2.568497	2.965848	-1.269638
H	4.311693	3.075683	-1.454591
H	6.423244	-2.791522	-4.456304
H	7.430641	-1.786483	-2.410003
H	6.226677	0.076058	-1.244913
H	4.033836	1.151942	-1.988590
H	4.664123	-2.786165	-6.146040
H	3.094623	-2.577280	-5.346723
H	3.757149	-1.267265	-6.320549

Adduct of picoline sp2, Np III – Large core

E = -746.933324

G = -746.670070

C	-0.410573	0.666857	-2.631921
C	0.065040	-0.504635	-3.272616
C	0.956968	-1.155257	-2.384207
C	1.033664	-0.385806	-1.196932
C	0.187555	0.737300	-1.348009
Np	2.302649	1.273797	-3.164696
N	4.416170	-0.397003	-3.422090
C	4.609992	-1.376338	-4.328400
C	5.761462	-2.165550	-4.297789
C	6.724924	-1.941290	-3.319566
C	6.517812	-0.928464	-2.388113
C	5.348548	-0.183040	-2.479019
C	3.539778	-1.572557	-5.360289
C	3.340225	2.498054	-1.190950
C	2.005137	2.104135	-5.891732
C	1.195489	2.987503	-5.136372
C	2.052160	3.825291	-4.378165
C	3.388915	3.460860	-4.664896
C	3.361391	2.397020	-5.599527
H	1.617128	-0.626598	-0.316161
H	1.453565	-2.103832	-2.556892
H	-0.237860	-0.859514	-4.251507
H	-1.138095	1.361423	-3.035927
H	0.014206	1.505247	-0.603404
H	4.275462	3.929782	-4.255415
H	1.740966	4.623344	-3.714052
H	0.113514	3.040804	-5.166690
H	1.645859	1.368869	-6.603354
H	4.228842	1.927609	-6.050439
H	3.493092	1.887546	-0.287113
H	2.664605	3.310537	-0.877942
H	4.300623	2.993071	-1.406030
H	5.893194	-2.948008	-5.038242
H	7.624156	-2.549885	-3.286013
H	7.239170	-0.715210	-1.606790
H	5.133902	0.620874	-1.777157
H	3.777108	-2.399282	-6.032999
H	2.577562	-1.783160	-4.880277
H	3.414724	-0.663936	-5.959340

Adduct of picoline sp2, Np III – Small core

E = -1228.971488

G = -1228.707608

C	-0.331098	0.706315	-2.703328
C	0.125454	-0.472326	-3.343425
C	1.006207	-1.138987	-2.454763
C	1.097446	-0.366062	-1.271662
C	0.269907	0.770390	-1.419933
Np	2.314413	1.216985	-3.204445
N	4.371387	-0.359036	-3.406249
C	4.588158	-1.349276	-4.298814
C	5.757580	-2.109874	-4.258708
C	6.719778	-1.850470	-3.287608
C	6.489556	-0.827879	-2.370723
C	5.304327	-0.112033	-2.469121
C	3.520163	-1.585569	-5.323041
C	3.159879	2.491832	-1.266929
C	1.876091	2.089112	-5.799008
C	1.244918	3.035099	-4.954338
C	2.256608	3.752437	-4.265483
C	3.508473	3.246155	-4.683415
C	3.277879	2.222597	-5.634508
H	1.688624	-0.608787	-0.396421
H	1.487016	-2.095719	-2.624011
H	-0.178200	-0.817705	-4.325280
H	-1.041691	1.415033	-3.111707
H	0.117378	1.544648	-0.678535
H	4.477084	3.592944	-4.342920
H	2.102560	4.552277	-3.552050
H	0.177424	3.203960	-4.878318
H	1.371693	1.410779	-6.478038
H	4.042952	1.677032	-6.175108
H	3.330361	1.870985	-0.371233
H	2.452248	3.272357	-0.947186
H	4.105131	3.022868	-1.470321
H	5.904305	-2.899772	-4.988605
H	7.633036	-2.437154	-3.247885
H	7.207187	-0.585385	-1.594360
H	5.075377	0.696322	-1.776980
H	3.779699	-2.408016	-5.992940
H	2.567648	-1.821996	-4.835897
H	3.361403	-0.683841	-5.924727

Product Picoline sp2, Np III – Large core

E = -706.430718

G = -706.210515

C	-0.448378	0.422516	-2.708685
C	0.032717	-0.864069	-3.065432
C	1.051803	-1.220344	-2.147638
C	1.207070	-0.150017	-1.230848
C	0.275068	0.862733	-1.574842
Np	2.184736	0.886753	-3.675428
C	2.126987	3.380709	-3.470473
N	1.398473	3.085809	-4.582314
C	0.804790	4.023204	-5.348433
C	0.925633	5.367289	-5.012476
C	1.664681	5.721578	-3.879789
C	2.263513	4.731788	-3.110667
C	0.029134	3.553104	-6.545419
C	3.774391	-0.642116	-5.466697
C	4.280987	-0.961212	-4.182470
C	4.929109	0.191285	-3.670194
C	4.834374	1.218691	-4.643493
C	4.119039	0.705005	-5.751476
H	5.252759	2.214369	-4.562265
H	3.908345	1.236586	-6.672407
H	3.261839	-1.325617	-6.135177
H	4.213474	-1.925516	-3.692519
H	5.451662	0.259190	-2.722169
H	0.128179	1.798745	-1.050082
H	1.882413	-0.132154	-0.382313
H	1.592481	-2.159309	-2.129415
H	-0.348628	-1.489418	-3.865587
H	-1.253153	0.960830	-3.195923
H	0.448740	6.124990	-5.627241
H	1.764535	6.770998	-3.609542
H	2.839171	5.000061	-2.228367
H	-0.410679	4.390102	-7.093157
H	0.676478	2.996097	-7.231613
H	-0.779167	2.879077	-6.241325

Product Picoline sp2, Np III – Small core

E = -1188.471527

G = -1188.250928

C	-0.189030	0.759247	-2.211441
C	-0.113791	-0.211480	-3.242318
C	0.871033	-1.163030	-2.880373
C	1.413964	-0.772607	-1.629516
C	0.756316	0.412001	-1.215247
Np	2.266615	1.153729	-3.396914
C	2.875872	3.162790	-2.164059
N	1.842955	3.474317	-2.988891
C	1.290156	4.701361	-3.068147
C	1.787473	5.723849	-2.268474
C	2.852295	5.457554	-1.400315
C	3.396575	4.180203	-1.347785
C	0.157301	4.891960	-4.033960
C	2.483414	0.691431	-6.098501
C	3.324916	-0.276939	-5.498711
C	4.429141	0.402121	-4.922805
C	4.273615	1.787148	-5.176335
C	3.070700	1.967185	-5.902548
H	4.960851	2.570197	-4.879882
H	2.688331	2.911403	-6.271310
H	1.565283	0.486216	-6.637511
H	3.163348	-1.348345	-5.500598
H	5.266921	-0.060331	-4.411863
H	0.932281	0.948770	-0.291030
H	2.172439	-1.307793	-1.068100
H	1.143408	-2.044250	-3.448881
H	-0.724283	-0.241102	-4.137993
H	-0.869149	1.601629	-2.173828
H	1.348799	6.715906	-2.323791
H	3.245241	6.254798	-0.772601
H	4.224083	3.967642	-0.675293
H	-0.256842	5.901321	-3.974414
H	0.494306	4.718596	-5.062108
H	-0.645109	4.174382	-3.832229

TS picoline sp2 Pu III – Large core

E = -747.569139

G = -747.308305

C	-0.286726	0.931357	-2.252714
C	-0.223587	-0.043753	-3.281823
C	0.638034	-1.080978	-2.846944
C	1.109210	-0.747966	-1.552950
C	0.534792	0.492951	-1.184687
Pu	2.314030	1.152438	-3.274686
N	4.122305	-0.533161	-3.746846
C	4.715551	-1.555172	-4.393677
C	5.975667	-1.993729	-3.992985
C	6.609032	-1.367574	-2.918522
C	5.972430	-0.317478	-2.266313
C	4.708715	0.092864	-2.703425
C	3.961771	-2.182279	-5.529115
C	3.591731	2.306955	-1.175956
C	1.576870	2.281189	-5.735469
C	1.309607	3.293331	-4.777210
C	2.550573	3.772223	-4.290278
C	3.584648	3.057063	-4.943699
C	2.983381	2.140850	-5.840208
H	1.770464	-1.349951	-0.940739
H	0.868174	-1.987826	-3.394258
H	-0.772072	-0.019246	-4.216284
H	-0.892631	1.830047	-2.264577
H	0.681094	1.005822	-0.241588
H	4.648651	3.206924	-4.803155
H	2.687743	4.563669	-3.562871
H	0.329111	3.662281	-4.499330
H	0.836088	1.747612	-6.319969
H	3.508838	1.471745	-6.511607
H	3.643190	1.846974	-0.181388
H	2.704952	2.961406	-1.152082
H	4.448607	2.984876	-1.275645
H	6.452849	-2.815367	-4.518495
H	7.593444	-1.703336	-2.600696
H	6.445829	0.185567	-1.427490
H	4.118050	1.188961	-1.974579
H	4.577870	-2.904136	-6.070092
H	3.071650	-2.702073	-5.157697
H	3.619960	-1.416799	-6.232578

TS picoline sp2 Pu III – Small core

E = -1268.439800
G = -1268.179589

C	-0.159799	0.887571	-2.287529
C	-0.042135	-0.058471	-3.340432
C	0.863408	-1.062832	-2.926551
C	1.311854	-0.738988	-1.622034
C	0.671683	0.459891	-1.223308
Pu	2.379465	1.215532	-3.214685
N	4.085536	-0.442074	-3.735989
C	4.674912	-1.455302	-4.396720
C	5.862030	-2.000260	-3.906075
C	6.427566	-1.481755	-2.741492
C	5.799352	-0.427264	-2.084240
C	4.608423	0.075818	-2.610127
C	4.018978	-1.939055	-5.655476
C	3.593377	2.409883	-1.227665
C	1.404765	2.187957	-5.597173
C	1.274786	3.253792	-4.667429
C	2.576156	3.701042	-4.333091
C	3.508953	2.907268	-5.045514
C	2.783336	1.979624	-5.833264
H	2.004426	-1.319396	-1.024084
H	1.150231	-1.937863	-3.497438
H	-0.578090	-0.030268	-4.281325
H	-0.802612	1.760056	-2.286342
H	0.793549	0.956771	-0.268137
H	4.587686	3.009266	-5.012137
H	2.818844	4.510467	-3.654423
H	0.342594	3.671901	-4.306189
H	0.589295	1.652367	-6.067485
H	3.210424	1.251624	-6.512118
H	3.842977	2.061348	-0.217836
H	2.623359	2.926580	-1.125549
H	4.327230	3.175442	-1.508543
H	6.334346	-2.823073	-4.434215
H	7.351302	-1.904092	-2.353460
H	6.219231	-0.003899	-1.176171
H	4.090388	1.185843	-1.923326
H	4.372960	-2.934336	-5.934866
H	2.932933	-1.967009	-5.533833
H	4.236177	-1.257827	-6.486353

Adduct of picoline sp2, Pu III – Large core

E = -747.602366
G = -747.338193

C	-0.385801	0.688123	-2.619344
C	0.079642	-0.484265	-3.266222
C	0.977049	-1.139516	-2.386752
C	1.068092	-0.371672	-1.199492
C	0.224531	0.754667	-1.341087
Pu	2.308075	1.275219	-3.168787
N	4.401437	-0.388600	-3.418353
C	4.593793	-1.373807	-4.318824
C	5.743441	-2.165472	-4.282302
C	6.706933	-1.937687	-3.305039
C	6.501499	-0.918680	-2.380015
C	5.333995	-0.171287	-2.476000
C	3.525854	-1.573560	-5.352158
C	3.342610	2.509127	-1.222885
C	1.995296	2.068092	-5.885176
C	1.189880	2.958558	-5.133546
C	2.050571	3.802357	-4.386862
C	3.385855	3.435097	-4.677467
C	3.353199	2.363503	-5.602871
H	1.659968	-0.615170	-0.325158
H	1.468872	-2.089430	-2.565250
H	-0.233049	-0.836201	-4.243011
H	-1.113635	1.386470	-3.015950
H	0.062381	1.523129	-0.594603
H	4.274558	3.906524	-4.275794
H	1.743025	4.605184	-3.726889
H	0.107779	3.010955	-5.157732
H	1.631929	1.326428	-6.587917
H	4.218364	1.889583	-6.053365
H	3.496537	1.909918	-0.311863
H	2.664633	3.323454	-0.920078
H	4.301560	3.004005	-1.444006
H	5.873648	-2.952694	-5.017955
H	7.604661	-2.548250	-3.267234
H	7.222728	-0.702220	-1.599460
H	5.120380	0.637236	-1.779322
H	3.755431	-2.415095	-6.009029
H	2.558548	-1.761947	-4.873457
H	3.416209	-0.673936	-5.967430

Adduct of picoline sp2, Pu III – Small core

E = -1268.466111
G = -1268.203181

C	-0.253409	1.012148	-2.319043
C	-0.171123	0.026927	-3.336269
C	0.677448	-1.005558	-2.874688
C	1.128458	-0.658003	-1.577782
C	0.546853	0.586102	-1.230300
Pu	2.306534	1.227497	-3.203523
N	4.422413	-0.371595	-3.325405
C	4.693720	-1.335639	-4.229037
C	5.882487	-2.067067	-4.168729
C	6.802079	-1.808619	-3.158168
C	6.513719	-0.816370	-2.225393
C	5.315181	-0.125358	-2.350361
C	3.660883	-1.604075	-5.282516
C	3.294685	2.494304	-1.339025
C	1.898276	1.878755	-5.848768
C	1.102092	2.786611	-5.107102
C	1.969934	3.658787	-4.406859
C	3.301733	3.291563	-4.713236
C	3.259853	2.193830	-5.607504
H	1.783763	-1.250780	-0.949598
H	0.915031	-1.919200	-3.407630
H	-0.686952	0.050593	-4.288649
H	-0.848876	1.916944	-2.355928
H	0.688453	1.115778	-0.296700
H	4.194739	3.772231	-4.332627
H	1.670639	4.467428	-3.750450
H	0.019609	2.820356	-5.096577
H	1.524901	1.107998	-6.513706
H	4.120025	1.709895	-6.056350
H	3.441775	1.933105	-0.401820
H	2.585703	3.301669	-1.087431
H	4.246512	3.002037	-1.564506
H	6.075560	-2.832991	-4.913337
H	7.729368	-2.371739	-3.101665
H	7.198035	-0.574425	-1.419291
H	5.043271	0.665091	-1.655259
H	2.841232	-2.202988	-4.870247
H	3.230094	-0.667773	-5.650661
H	4.084807	-2.150402	-6.128360

Product picoline sp2, Pu III – Large core

E = -707.099386
G = -706.878938

C	-0.311097	0.744105	-2.319411
C	-0.193160	-0.476390	-3.032869
C	0.860601	-1.224612	-2.451178
C	1.400780	-0.461578	-1.385438
C	0.671788	0.753725	-1.301329
Pu	2.155243	0.952073	-3.685178
N	1.499702	3.271594	-4.288441
C	0.927698	4.328292	-4.899877
C	1.201431	5.615883	-4.451276
C	2.071099	5.788961	-3.370321
C	2.646122	4.679306	-2.763535
C	2.352859	3.388549	-3.233586
C	0.012254	4.049110	-6.057192
C	3.433758	-0.736192	-5.542519
C	4.179463	-0.888141	-4.347206
C	4.867073	0.328312	-4.103709
C	4.554940	1.227853	-5.153357
C	3.667855	0.572418	-6.040818
H	4.938863	2.234647	-5.262796
H	3.273800	0.983214	-6.963820
H	2.830663	-1.502434	-6.016970
H	4.239909	-1.786905	-3.744500
H	5.547873	0.522609	-3.282299
H	0.822890	1.539834	-0.571659
H	2.195351	-0.776104	-0.717633
H	1.177965	-2.216920	-2.749546
H	-0.831898	-0.804798	-3.845947
H	-1.042505	1.522490	-2.502285
H	0.741576	6.469714	-4.940146
H	2.290596	6.792983	-3.012530
H	3.323542	4.806961	-1.922998
H	-0.439741	4.966309	-6.442493
H	0.559806	3.568042	-6.875414
H	-0.791236	3.367415	-5.758395

Product picoline sp2, Pu III – Small core

E = -1227.969799
G = -1227.749982

C	-0.515504	0.658838	-3.025908
C	-0.270519	-0.619674	-3.590214
C	0.657030	-1.293293	-2.757666
C	0.990252	-0.431794	-1.684902
C	0.264262	0.774926	-1.847391
Pu	2.050933	0.794454	-3.890862
N	1.849079	3.148719	-4.302903
C	1.499580	4.333465	-4.846722
C	1.980880	5.509038	-4.283761
C	2.816807	5.439209	-3.162396
C	3.153408	4.202777	-2.627817
C	2.655132	3.027221	-3.216333
C	0.595674	4.309587	-6.044972
C	4.587156	0.432304	-4.763873
C	3.825581	0.642367	-5.941018
C	2.989736	-0.487379	-6.130135
C	3.235821	-1.395937	-5.073187
C	4.218017	-0.827365	-4.224941
H	5.329034	1.108921	-4.357533
H	3.887301	1.507182	-6.591165
H	2.301248	-0.641705	-6.953944
H	2.763964	-2.361923	-4.943355
H	4.635287	-1.289378	-3.337148
H	0.291910	1.629307	-1.182307
H	1.666955	-0.662712	-0.869467
H	1.035046	-2.296848	-2.907721
H	-0.733436	-1.024580	-4.483239
H	-1.197104	1.408471	-3.411477
H	1.706770	6.467660	-4.714304
H	3.196216	6.357344	-2.718470
H	3.800850	4.140962	-1.756809
H	0.392480	5.317533	-6.414632
H	1.046536	3.728188	-6.856503
H	-0.360075	3.834946	-5.796923

TS picoline sp3 Np IV – Large core

E = -792.547396
G = -792.245195

C	0.171073	1.645631	-1.881098
C	-0.400984	-2.162756	-5.617727
H	-0.181139	-3.222151	-5.595895
Np	0.329999	-0.725404	-3.340572
C	0.441232	-1.131855	-6.093642
H	1.433174	-1.251214	-6.511369
C	-0.244638	0.100492	-5.935362
H	0.121954	1.075797	-6.232237
C	-1.516466	-0.178330	-5.379253
H	-2.287967	0.549056	-5.163160
C	-1.608782	-1.572489	-5.168004
H	-2.458311	-2.103315	-4.757329
C	-1.803778	0.514292	-2.142394
H	-2.781496	0.215408	-2.499570
C	-1.017269	1.580573	-2.647161
H	-1.285733	2.246478	-3.457769
C	-1.103085	-0.072406	-1.058734
H	-1.447905	-0.901286	-0.455519
C	0.116172	0.626543	-0.898113
H	0.868307	0.430071	-0.145671
H	0.968968	2.365551	-2.006960
C	-0.407154	-2.865376	-2.303472
H	-0.052912	-3.041791	-1.278812
H	-1.505590	-2.893754	-2.255995
H	-0.091600	-3.729999	-2.900362
C	2.615473	0.724355	-3.722767
H	3.116950	1.456155	-3.080133
H	3.374318	0.239526	-4.345251
H	1.964715	1.305824	-4.391081
H	2.434382	-0.197598	-2.661353
C	2.580746	-1.316557	-1.732982
H	1.734440	-1.756605	-1.192962
H	3.291339	-0.920225	-1.005121
C	3.138043	-2.271256	-2.689775
C	4.394548	-2.895338	-2.617733
H	5.028033	-2.712189	-1.755402
C	4.789444	-3.754298	-3.630147
H	5.751087	-4.258249	-3.580164
C	3.929194	-3.976544	-4.710387
H	4.195222	-4.647803	-5.519947
C	2.720325	-3.299870	-4.735017
H	2.034692	-3.426662	-5.567512
N	2.336690	-2.449019	-3.771297

TS picoline sp3 Np IV – Small core

E = -1268.800851
G = -1268.501109

C	0.222901	1.500884	-1.740280
C	-0.455401	-2.152659	-5.538613
H	-0.317905	-3.225055	-5.485906
Np	0.355595	-0.761285	-3.314385
C	0.469483	-1.205013	-6.038425
H	1.451156	-1.416790	-6.443237
C	-0.115700	0.077667	-5.925689
H	0.334380	1.011076	-6.240209
C	-1.400927	-0.078649	-5.359236
H	-2.111379	0.715148	-5.169450
C	-1.609208	-1.455904	-5.113423
H	-2.498318	-1.902709	-4.686776
C	-1.782502	0.501907	-2.212738
H	-2.743430	0.281740	-2.660281

C	-0.901304	1.546094	-2.594686
H	-1.070640	2.266925	-3.384913
C	-1.201603	-0.185527	-1.123424
H	-1.634377	-1.025054	-0.596741
C	0.038923	0.429262	-0.834584
H	0.715614	0.152096	-0.036590
H	1.069539	2.174332	-1.765107
C	-0.415084	-2.863460	-2.364949
H	-0.071748	-3.027221	-1.332528
H	-1.513790	-2.903390	-2.337742
H	-0.073874	-3.721454	-2.958262
C	2.463825	0.759648	-3.854729
H	3.187216	1.380579	-3.313215
H	2.986652	0.284897	-4.691549
H	1.716538	1.452162	-4.266702
H	2.404449	-0.148342	-2.714626
C	2.619146	-1.193232	-1.794145
H	1.801468	-1.622607	-1.202242
H	3.337046	-0.737237	-1.109492
C	3.176591	-2.196832	-2.707448
C	4.453652	-2.772793	-2.652484
H	5.126618	-2.503697	-1.844278
C	4.823200	-3.694639	-3.620669
H	5.803428	-4.162796	-3.587851
C	3.916089	-4.024167	-4.631784
H	4.162260	-4.748496	-5.400989
C	2.683978	-3.387036	-4.641797
H	1.956482	-3.596631	-5.420603
N	2.326670	-2.480334	-3.722436

Adduct of picoline sp3, Np IV – Large core

E = -792.583953
G = -792.280536

C	0.143477	1.730495	-2.012714
C	-0.447011	-2.153184	-5.771034
H	-0.130383	-3.188714	-5.773697
Np	0.199546	-0.608743	-3.524394
C	0.271167	-1.045550	-6.286332
H	1.245845	-1.068538	-6.757477
C	-0.516695	0.114879	-6.092940
H	-0.246757	1.120814	-6.389052
C	-1.725919	-0.278154	-5.465636
H	-2.552710	0.374044	-5.214057
C	-1.679254	-1.679016	-5.260426
H	-2.451473	-2.285697	-4.804428
C	-1.838203	0.580498	-2.145406
H	-2.837928	0.280752	-2.435436
C	-1.089591	1.654866	-2.701693
H	-1.417649	2.320158	-3.491158
C	-1.065192	-0.002432	-1.113973
H	-1.360446	-0.838441	-0.494153
C	0.161573	0.701561	-1.039307
H	0.957531	0.514594	-0.329823
H	0.933355	2.445742	-2.199330
C	-0.251035	-2.809901	-2.414941
H	0.199528	-2.985203	-1.428241
H	-1.339245	-2.897451	-2.270790
H	0.051305	-3.657941	-3.043845
C	2.269163	0.662002	-4.142657
H	2.980242	0.873038	-3.331681
H	2.846756	0.166821	-4.934362
H	1.963011	1.641679	-4.541477
H	2.997346	-0.447244	-1.409804
C	2.984334	-1.515711	-1.171223
H	1.979731	-1.767667	-0.817419
H	3.693742	-1.696795	-0.360585
C	3.324326	-2.320457	-2.387291
C	4.459338	-3.136977	-2.410512
H	5.092401	-3.189291	-1.530242
C	4.766223	-3.867875	-3.551007
H	5.645174	-4.505507	-3.580480
C	3.921838	-3.759849	-4.650742
H	4.109262	-4.303304	-5.570887
C	2.813503	-2.928564	-4.549396
H	2.137735	-2.821085	-5.390425
N	2.503899	-2.220978	-3.452665

Adduct of picoline sp3, Np IV – Small core

E = -1268.830143
G = -1268.530438

C	0.186356	1.340929	-1.728760
C	-0.920414	-2.118877	-5.633353
H	-1.004485	-3.191299	-5.514865
Np	0.224479	-0.726653	-3.546503
C	0.159772	-1.418292	-6.224564
H	1.044714	-1.856591	-6.670920
C	-0.141677	-0.034847	-6.196899
H	0.482088	0.758033	-6.587091
C	-1.399759	0.121415	-5.576636
H	-1.918707	1.058302	-5.419243
C	-1.878579	-1.166421	-5.221355
H	-2.822370	-1.386144	-4.738145
C	-1.871923	0.498253	-2.281421
H	-2.848479	0.384151	-2.734670
C	-0.941822	1.534374	-2.556060
H	-1.078507	2.345986	-3.259903
C	-1.313858	-0.340164	-1.292263
H	-1.777713	-1.217856	-0.862701
C	-0.037816	0.174440	-0.956927
H	0.628091	-0.233410	-0.206803
H	1.061134	1.976855	-1.692849
C	-0.303455	-2.937726	-2.653569
H	0.122075	-3.047876	-1.643900
H	-1.386795	-3.101369	-2.566960
H	0.099691	-3.759319	-3.262355
C	2.070152	0.754310	-4.171582
H	2.797940	0.986703	-3.381637
H	2.634167	0.312818	-5.006781
H	1.672434	1.717345	-4.523097
H	2.864895	-0.185518	-1.577627
C	3.320085	-1.119335	-1.241089
H	2.647633	-1.573035	-0.504114
H	4.263799	-0.891391	-0.740102
C	3.526381	-2.058460	-2.390261
C	4.695032	-2.821320	-2.483882
H	5.470694	-2.695929	-1.734897
C	4.850982	-3.730056	-3.522389
H	5.755883	-4.325426	-3.604708
C	3.820007	-3.863882	-4.447307
H	3.879991	-4.564200	-5.273600
C	2.691160	-3.071702	-4.288005
H	1.860580	-3.157129	-4.981272
N	2.538346	-2.175538	-3.299993

Product picoline sp3, Np IV – Large core

E = -752.101481
G = -751.842269

N	0.392260	0.697441	-1.270526
C	0.405178	-0.037473	-2.424073
C	1.005548	-1.321168	-2.430410
C	1.686358	-1.751787	-1.309530
C	1.752701	-0.933788	-0.167524
C	1.068630	0.266900	-0.190704
C	-0.331591	0.593125	-3.485951
Np	-2.036351	1.418515	-1.707366
C	-1.618360	1.891690	0.698315
C	-4.474631	0.255322	-1.310979
C	-4.042975	-0.221947	-2.578192
C	-2.957288	-1.106276	-2.363664
C	-2.707692	-1.163980	-0.970081
C	-3.650347	-0.329421	-0.318910
C	-3.527790	3.713067	-1.768389
C	-3.497459	3.274158	-3.119616
C	-2.179571	3.442976	-3.604334
C	-1.393495	3.987599	-2.555179
C	-2.229564	4.166919	-1.427355
H	-1.938503	-1.753184	-0.485872
H	-2.417370	-1.646045	-3.130177
H	-4.487878	0.017613	-3.536382
H	-5.306111	0.926413	-1.132861
H	-3.727022	-0.168573	0.748005
H	-4.399235	3.738722	-1.125331
H	-4.341045	2.900308	-3.687037
H	-1.931081	4.574442	-0.470902
H	-0.342279	4.243763	-2.613531
H	-1.835273	3.207229	-4.603418
H	-0.786536	2.597540	0.834975
H	-2.500321	2.352247	1.167209
H	-1.380471	0.996189	1.286842
H	0.050950	1.588421	-3.724777
H	-0.507442	0.000578	-4.382162
H	0.960800	-1.925544	-3.331146
H	2.184598	-2.718284	-1.314496
H	2.296073	-1.241620	0.719021
H	1.022946	0.912028	0.682034

Product picoline sp3, Np IV – Small core

E = -1228.349990
G = -1228.091997

N	0.560603	0.685904	-1.550017
C	0.207273	-0.131954	-2.594341
C	-0.791595	-1.124298	-2.398018
C	-1.286583	-1.341407	-1.131364
C	-0.832034	-0.558866	-0.050427
C	0.066805	0.453372	-0.317470
C	0.828688	0.232319	-3.824688
Np	0.453415	2.664007	-3.060165
C	0.499515	3.674742	-0.865956
C	-2.233901	2.405044	-2.830298
C	-1.995577	3.794222	-2.689831
C	-1.547264	4.286525	-3.937166
C	-1.518450	3.203535	-4.853038
C	-1.948844	2.043173	-4.170635
C	3.116565	3.002806	-3.530395
C	2.547445	2.871367	-4.823349
C	1.754562	4.013575	-5.067184
C	1.831913	4.853314	-3.926455
C	2.684434	4.234813	-2.983637
H	-2.132706	4.375591	-1.788157
H	-2.583151	1.736323	-2.052588
H	-2.046861	1.053295	-4.596484
H	-1.237462	3.258431	-5.897382
H	-1.293266	5.315148	-4.160779
H	1.347865	5.814875	-3.808522
H	1.201750	4.222447	-5.974227
H	2.956393	4.632568	-2.015254
H	3.784866	2.295769	-3.052262
H	2.701759	2.046395	-5.507249
H	1.434358	3.401987	-0.351954
H	0.466072	4.772598	-0.913294
H	-0.334857	3.354728	-0.227311
H	1.910372	0.357843	-3.754339
H	0.509639	-0.276356	-4.731105
H	-1.109664	-1.730401	-3.240733
H	-2.019143	-2.126698	-0.961551
H	-1.192827	-0.723765	0.958812
H	0.408245	1.130712	0.460280

TS picoline sp3 Pu IV – Large core

E = -793.300061
G = -792.997549

C	0.179805	1.633995	-1.886930
C	-0.393453	-2.158212	-5.602268
H	-0.172626	-3.217257	-5.579517
Pu	0.328012	-0.725639	-3.339648
C	0.448416	-1.126441	-6.075963
H	1.441836	-1.244087	-6.490371
C	-0.238914	0.105287	-5.917510
H	0.127289	1.081151	-6.212729
C	-1.511880	-0.175466	-5.365461
H	-2.284170	0.551037	-5.149743
C	-1.602708	-1.569328	-5.153941
H	-2.452093	-2.101215	-4.744535
C	-1.795757	0.505313	-2.153519
H	-2.772975	0.207629	-2.512732
C	-1.006955	1.571116	-2.655619
H	-1.272311	2.237960	-3.466322
C	-1.097711	-0.083321	-1.069109
H	-1.444681	-0.912364	-0.467486
C	0.121413	0.614654	-0.904644
H	0.871923	0.416131	-0.151303
H	0.978893	2.352811	-2.010923
C	-0.401074	-2.855602	-2.313039
H	-0.046575	-3.030812	-1.288391
H	-1.499237	-2.887346	-2.266317
H	-0.082037	-3.718469	-2.910231
C	2.600254	0.717689	-3.734451
H	3.108837	1.445441	-3.092782
H	3.352925	0.228183	-4.360416
H	1.948857	1.302765	-4.397885
H	2.418023	-0.196905	-2.671347
C	2.570706	-1.311618	-1.734677
H	1.730075	-1.755901	-1.190289
H	3.280781	-0.905501	-1.011476
C	3.131393	-2.266049	-2.689633
C	4.386782	-2.891751	-2.614759
H	5.018929	-2.709098	-1.751335
C	4.782160	-3.752027	-3.625992
H	5.742920	-4.257483	-3.574204
C	3.923186	-3.973443	-4.707264
H	4.189452	-4.645412	-5.516179
C	2.715243	-3.294885	-4.734237
H	2.031262	-3.421350	-5.568116
N	2.331495	-2.442770	-3.771918

TS picoline sp3 Pu IV – Small core

E = -1308.275928
G = -1307.977099

C	0.250662	1.416095	-1.674032
C	-0.425376	-2.150612	-5.538342
H	-0.303312	-3.226050	-5.514190
Pu	0.379906	-0.820314	-3.283138
C	0.520195	-1.205516	-6.002769
H	1.504850	-1.424488	-6.397607
C	-0.047336	0.082797	-5.864499
H	0.416185	1.016465	-6.155341
C	-1.343745	-0.071584	-5.321921
H	-2.045448	0.728104	-5.124639
C	-1.575994	-1.450801	-5.110686
H	-2.477123	-1.895162	-4.709249
C	-1.766308	0.482797	-5.233685
H	-2.716260	0.305688	-2.718648
C	-0.837320	1.510631	-2.566996
H	-0.952383	2.249014	-3.350706
C	-1.248697	-0.235399	-1.140567
H	-1.730727	-1.063394	-0.639946
C	0.003509	0.331242	-0.798515
H	0.637900	0.021339	0.022889
H	1.120822	2.059069	-1.660577
C	-0.653148	-2.845494	-2.416842
H	-0.216138	-2.998521	-1.416265
H	-1.742114	-2.890281	-2.318680
H	-0.322854	-3.671446	-3.060237
C	2.403880	0.864534	-3.881601
H	3.133215	1.464569	-3.323886
H	2.919181	0.399994	-4.729806
H	1.650697	1.557442	-4.267368
H	2.410281	-0.092166	-2.757464
C	2.702578	-1.107740	-1.873940
H	1.926034	-1.493169	-1.201132
H	3.457253	-0.611305	-1.260324
C	3.226080	-2.169233	-2.749564
C	4.532858	-2.675856	-2.751266
H	5.253411	-2.303099	-2.030054
C	4.874272	-3.662230	-3.666245
H	5.878832	-4.076601	-3.675926
C	3.911946	-4.123065	-4.567981
H	4.137534	-4.898941	-5.291731
C	2.648734	-3.548965	-4.528568
H	1.873639	-3.855781	-5.224984
N	2.315536	-2.587902	-3.658186

Adduct of picoline sp3, Pu IV – Large core

E = -793.338029
G = -793.034061

C	0.148912	1.723104	-2.028665
C	-0.437813	-2.141283	-5.762193
H	-0.120545	-3.176507	-5.764533
Pu	0.196032	-0.603933	-3.529664
C	0.280919	-1.032740	-6.274021
H	1.257083	-1.054153	-6.741935

C	-0.507760	0.127286	-6.080314
H	-0.237066	1.133821	-6.373399
C	-1.718522	-0.267558	-5.457483
H	-2.545776	0.383918	-5.205983
C	-1.671478	-1.668281	-5.253427
H	-2.443893	-2.275802	-4.799111
C	-1.830997	0.569774	-2.158562
H	-2.830373	0.267900	-2.447242
C	-1.084846	1.645733	-2.715842
H	-1.414695	2.310408	-3.504934
C	-1.055533	-0.011594	-1.128276
H	-1.348273	-0.848494	-0.508616
C	0.170176	0.694276	-1.055340
H	0.967946	0.507930	-0.347981
H	0.937696	2.438963	-2.216979
C	-0.252449	-2.793545	-2.430884
H	0.200979	-2.966065	-1.445051
H	-1.339974	-2.883275	-2.284494
H	0.050902	-3.641217	-3.059441
C	2.258740	0.653868	-4.136161
H	2.961318	0.863476	-3.317542
H	2.843119	0.156417	-4.921120
H	1.958770	1.633731	-4.538768
H	2.994769	-0.455576	-1.395854
C	2.980275	-1.524316	-1.159508
H	1.975814	-1.774325	-0.804541
H	3.691144	-1.709183	-0.350991
C	3.316286	-2.326723	-2.378263
C	4.446037	-3.150830	-2.401138
H	5.076115	-3.210341	-1.519173
C	4.751612	-3.879813	-3.543117
H	5.626293	-4.523322	-3.572180
C	3.911473	-3.761605	-4.644982
H	4.098090	-4.302471	-5.566836
C	2.808475	-2.923172	-4.543644
H	2.136771	-2.807789	-5.386736
N	2.499390	-2.217912	-3.445359

Adduct of picoline sp3, Pu IV – Small core

E = -1308.305380
G = -1308.005917

C	0.162069	1.715072	-2.109321
C	-0.390878	-2.170197	-5.709248
H	-0.059915	-3.202003	-5.741796
Pu	0.307720	-0.668112	-3.475304
C	0.293724	-1.047509	-6.229619
H	1.253404	-1.052453	-6.733444
C	-0.497866	0.100470	-5.989835
H	-0.252512	1.113369	-6.281189
C	-1.682107	-0.321594	-5.338670
H	-2.507240	0.315748	-5.048809
C	-1.613066	-1.720723	-5.152090
H	-2.367424	-2.342935	-4.689283
C	-1.785575	0.511100	-2.179294
H	-2.771324	0.161373	-2.459529
C	-1.072585	1.582327	-2.778058
H	-1.417123	2.200938	-3.597230
C	-0.991406	-0.016367	-1.139893
H	-1.265671	-0.829250	-0.481179
C	0.221538	0.716148	-1.105315
H	1.024429	0.582856	-0.389724
H	0.922009	2.455485	-2.317708
C	-0.528536	-2.705028	-2.399305
H	-0.006606	-2.810033	-1.436136
H	-1.604133	-2.780842	-2.217552
H	-0.215970	-3.524496	-3.061015
C	2.067270	0.859875	-4.237006
H	2.741562	1.005851	-3.379268
H	2.607644	0.314410	-5.022595
H	1.772381	1.840858	-4.619062
H	3.059234	-0.544985	-1.329304
C	3.042700	-1.622430	-1.133984
H	2.038639	-1.883776	-0.784584
H	3.748752	-1.831089	-0.327242
C	3.392175	-2.386834	-2.375828
C	4.526179	-3.202147	-2.423160
H	5.155648	-3.289941	-1.543320
C	4.837012	-3.888322	-3.591310
H	5.715864	-4.524964	-3.639863
C	4.001287	-3.739548	-4.692864
H	4.196129	-4.248073	-5.631079
C	2.891221	-2.913075	-4.567835
H	2.215867	-2.770878	-5.403996
N	2.579337	-2.249195	-3.443811

Product picoline sp3, Pu IV – Large core

E = -752.855646
G = -752.595842

N	0.398464	0.678719	-1.264566
C	0.414590	-0.045813	-2.423608
C	1.002393	-1.334605	-2.436967
C	1.667435	-1.782703	-1.313021
C	1.730439	-0.976009	-0.163161
C	1.059182	0.232339	-0.182100
C	-0.307619	0.605851	-3.483945
Pu	-2.001035	1.443332	-1.723711
C	-1.594488	1.921669	0.668533
C	-4.441486	0.319374	-1.356116
C	-3.994982	-0.172757	-2.612503
C	-2.920872	-1.064933	-2.373693
C	-2.692346	-1.112202	-0.976286
C	-3.637114	-0.263244	-0.346779
C	-3.461049	3.735815	-1.792547
C	-3.435285	3.289855	-3.141648
C	-2.115626	3.440843	-3.626669
C	-1.323570	3.982357	-2.580123
C	-2.157853	4.177266	-1.453843
H	-1.934335	-1.701851	-0.475489
H	-2.373900	-1.615665	-3.127165
H	-4.421963	0.063400	-3.579529
H	-5.269040	0.999700	-1.196522
H	-3.727822	-0.091551	0.717266
H	-4.331908	3.773876	-1.149490
H	-4.282506	2.921704	-3.707188
H	-1.854999	4.586049	-0.499396
H	-0.269346	4.225461	-2.639138
H	-1.773384	3.194045	-4.623667
H	-0.749586	2.611675	0.805273
H	-2.470234	2.403208	1.127546
H	-1.378687	1.026168	1.265267
H	0.098583	1.593285	-3.715514
H	-0.490215	0.022743	-4.385179
H	0.960405	-1.930204	-3.343660
H	2.155725	-2.754243	-1.321786
H	2.261525	-1.297592	0.725967
H	1.011414	0.870124	0.695889

Product picoline sp3, Pu IV – Small core

E = -1267.819832
G = -1267.562370

N	0.420078	0.920057	-1.644075
C	0.175505	-0.014311	-2.615467
C	0.390771	-1.393568	-2.343051
C	1.005374	-1.758610	-1.165414
C	1.378311	-0.770250	-0.234100
C	1.035915	0.539446	-0.509768
C	-0.405323	0.528950	-3.794585
Pu	-1.814826	2.034925	-2.253076
C	-0.708168	4.134514	-2.467127
C	-2.046751	1.214179	0.337501
C	-1.496987	2.516787	0.415403
C	-2.491521	3.442451	0.021093
C	-3.654320	2.711136	-0.303146
C	-3.377194	1.331424	-0.126618
C	-3.950001	3.312916	-3.369306
C	-4.345401	1.951344	-3.274474
C	-3.562667	1.207750	-4.179543
C	-2.688773	2.107690	-4.844296
C	-2.936866	3.407178	-4.346639
H	-0.492613	2.770606	0.729549
H	-1.535841	0.290276	0.580989
H	-4.075028	0.515608	-0.274978
H	-4.601513	3.131076	-0.612946
H	-2.381505	4.517945	-0.013571
H	-4.368217	4.142002	-2.813806
H	-5.121247	1.555250	-2.631809
H	-2.442086	4.315389	-4.662109
H	-1.984171	1.849190	-5.623278
H	-3.619721	0.138441	-4.346119
H	-0.175214	4.110569	-3.432690
H	-1.257392	5.080783	-2.419906
H	0.058887	4.147618	-1.676798
H	0.079161	1.433104	-4.170587
H	-0.730723	-0.154454	-4.573629
H	0.120867	-2.130959	-3.092857
H	1.220693	-2.805024	-0.964321
H	1.895771	-1.023579	0.684720
H	1.246719	1.332082	0.203819

TS Picoline sp3 Np III – Large core

E = -746.903989
G = -746.641891

N	0.513213	1.812708	-2.815396
C	-0.269875	0.712413	-2.634406
C	0.177245	-0.337873	-1.804711
C	1.442473	-0.280070	-1.248155
C	2.264038	0.825448	-1.505481
C	1.742846	1.849320	-2.278442
C	-1.568873	0.734310	-3.310906
Np	-1.429201	3.569958	-2.863342
C	-3.868127	2.379541	-2.779172
C	-0.941897	5.734818	-4.590867
C	-2.305184	5.406105	-4.803803
C	-2.354332	4.164152	-5.486252
C	-1.025631	3.721659	-5.685991
C	-0.151737	4.690828	-5.130712
C	-2.529217	4.623378	-0.465365
C	-1.693649	3.570516	-0.014228
C	-0.350149	3.950449	-0.242328
C	-0.351752	5.231687	-0.848377
C	-1.701781	5.650232	-0.979011
H	0.526847	3.372180	0.023335
H	-2.025824	2.651664	0.454910
H	-3.610690	4.647737	-0.402445
H	-2.037401	6.603932	-1.369191
H	0.522905	5.815456	-1.112777
H	-0.570660	6.639956	-4.124836
H	-3.157338	6.020832	-4.536521
H	0.931580	4.655784	-5.151076
H	-0.723925	2.817939	-6.202536
H	-3.252728	3.654837	-5.813919
H	-4.409286	1.852782	-3.573808
H	-4.215371	1.988537	-1.815955
H	-4.209123	3.427531	-2.832352
H	-2.601467	1.595306	-2.967273
H	-1.444285	0.929708	-4.382750
H	-2.123476	-0.197510	-3.181943
H	-0.468827	-1.194415	-1.639430
H	1.802313	-1.096110	-0.626948
H	3.268176	0.895448	-1.102022
H	2.319651	2.750341	-2.475499

TS Picoline sp3 Np III – Small core

E = -1228.947198
G = -1228.682780

N	0.478273	1.832984	-2.756209
C	-0.338052	0.761490	-2.564972
C	0.046616	-0.275850	-1.692239
C	1.299219	-0.241087	-1.103514
C	2.160546	0.830521	-1.372453
C	1.693396	1.848803	-2.186655
C	-1.609815	0.810399	-3.296035
Np	-1.404042	3.554294	-2.892885
C	-3.840425	2.580400	-2.942135
C	-0.494547	5.510278	-4.575368
C	-1.908252	5.594246	-4.649848
C	-2.379969	4.444260	-5.330310
C	-1.260426	3.646303	-5.663793
C	-0.093594	4.304849	-5.201698
C	-2.390020	3.943388	-0.333376
C	-1.087268	3.425652	-0.140764
C	-0.157060	4.399208	-0.580567
C	-0.885075	5.521964	-1.046145
C	-2.265054	5.236036	-0.899426
H	0.922201	4.313694	-0.533868
H	-0.842140	2.459783	0.285604
H	-3.317369	3.446612	-0.078192
H	-3.081438	5.903353	-1.151192
H	-0.464024	6.447649	-1.419115
H	0.163668	6.254141	-4.142077
H	-2.515443	6.413759	-4.283395
H	0.924510	3.957142	-5.328996
H	-1.286707	2.711696	-6.211854
H	-3.413192	4.223061	-5.567442
H	-4.322784	2.219738	-3.858415
H	-4.316599	2.081419	-2.090368
H	-4.096139	3.651171	-2.855544
H	-2.604683	1.707017	-3.030412
H	-1.427036	0.958738	-4.366599
H	-2.211146	-0.090349	-3.157050
H	-0.632666	-1.104555	-1.518049
H	1.617354	-1.047949	-0.448569
H	3.155816	0.881254	-0.944460
H	2.302848	2.726003	-2.391596

Adduct of picoline sp3, Np III – Large core

E = -746.931744
G = -746.667993

N	0.114243	1.678580	-2.364007
C	-0.084875	0.392594	-2.719669
C	0.917563	-0.565624	-2.541579
C	2.142060	-0.193597	-1.999272
C	2.342756	1.136489	-1.640644
C	1.299102	2.030280	-1.839515
C	-1.408772	0.039831	-3.328271
Np	-1.688772	3.720335	-2.652259
C	-3.954093	2.571609	-2.647627
C	-0.460188	5.281850	-4.687124
C	-1.839888	5.609950	-4.734761
C	-2.539030	4.491826	-5.254321
C	-1.594684	3.473059	-5.520181
C	-0.309365	3.961409	-5.173134
C	-2.663211	5.475510	-0.656609
C	-2.444518	4.269182	0.051506
C	-1.047404	4.059692	0.136516
C	-0.400775	5.139400	-0.518355
C	-1.400462	6.015619	-1.007051
H	-0.558925	3.241001	0.653368
H	-3.213494	3.628537	0.465352
H	-3.628566	5.920113	-0.869985
H	-1.228117	6.952379	-1.523992
H	0.669392	5.306244	-0.580991
H	0.339239	5.941526	-4.369193
H	-2.276358	6.564984	-4.465358
H	0.628820	3.431777	-5.295697
H	-1.815290	2.506124	-5.958078
H	-3.606201	4.430566	-5.428532
H	-4.163872	1.968562	-3.544195
H	-4.131590	1.916400	-1.779096
H	-4.756214	3.325683	-2.604814
H	-2.240930	0.405584	-2.718392
H	-1.509140	0.504913	-4.315818
H	-1.514178	-1.040153	-3.450867
H	0.728040	-1.593996	-2.831976
H	2.927078	-0.930989	-1.857669
H	3.279031	1.477728	-1.212520
H	1.404410	3.075970	-1.560748

Adduct of picoline sp3, Np III – Small core

E = -1228.969885
G = -1228.707356

N	0.049808	1.718955	-2.425427
C	-0.263039	0.406188	-2.399409
C	0.724371	-0.566578	-2.223739
C	2.053210	-0.186457	-2.073409
C	2.369203	1.170652	-2.101967
C	1.336276	2.078921	-2.279633
C	-1.707952	0.045973	-2.569878
Np	-1.616716	3.722003	-2.739057
C	-3.890982	2.838809	-3.049000
C	-0.151320	5.257209	-4.500155

C	-1.495403	5.690991	-4.629834
C	-2.234113	4.654908	-5.254883
C	-1.347608	3.580798	-5.501680
C	-0.060121	3.952164	-5.043087
C	-2.928328	4.835528	-0.589922
C	-2.168003	3.790527	-0.014889
C	-0.797503	4.136301	-0.104545
C	-0.707614	5.395861	-0.746348
C	-2.024692	5.827353	-1.047587
H	0.031607	3.553116	0.279085
H	-2.569457	2.889889	0.436033
H	-4.007734	4.870352	-0.662022
H	-2.292710	6.768837	-1.512438
H	0.201766	5.952962	-0.940600
H	0.665893	5.839892	-4.090611
H	-1.879874	6.660529	-4.335816
H	0.840270	3.354406	-5.124309
H	-1.607421	2.642905	-5.979628
H	-3.287272	4.679402	-5.503449
H	-3.969203	2.180666	-3.931048
H	-4.243086	2.249050	-2.185812
H	-4.649295	3.622496	-3.199145
H	-2.324097	0.516098	-1.795680
H	-2.088895	0.397986	-3.534968
H	-1.857825	-1.034409	-2.517243
H	0.441047	-1.614253	-2.207392
H	2.828468	-0.934806	-1.936920
H	3.389537	1.521435	-1.990038
H	1.537943	3.147742	-2.309772

Product picoline sp3, Np III – Large core

E = -706.438489
G = -706.216053

C	1.092656	1.795292	-2.933864
C	0.105268	0.849491	-2.562885
C	0.659780	0.002838	-1.567713
C	1.990558	0.421059	-1.329640
C	2.261440	1.525720	-2.178167
Np	2.041619	-0.666566	-3.947118
C	1.552030	-3.184454	-3.332864
C	2.672007	-3.080348	-2.446382
N	3.722218	-2.308521	-2.891817
C	4.816991	-2.159289	-2.121415
C	4.943859	-2.708287	-0.861192
C	3.847604	-3.431496	-0.353712
C	2.721503	-3.608967	-1.126233
C	1.015652	0.078771	-6.470227
C	2.256766	0.758452	-6.381008
C	3.290404	-0.208172	-6.463134
C	2.689237	-1.483282	-6.605368
C	1.284126	-1.306840	-6.610467
H	2.673998	-0.013923	-0.609791
H	0.147266	-0.805525	-1.060637
H	-0.911516	0.810828	-2.938023
H	0.967345	2.600005	-3.648734
H	3.180845	2.100955	-2.202667
H	2.390763	1.831441	-6.306553
H	0.035996	0.543190	-6.478018
H	4.355654	-0.003815	-6.462575
H	3.214530	-2.424506	-6.717919
H	0.544842	-2.089676	-6.735177
H	1.816566	-3.464259	-4.356509
H	0.687850	-3.728771	-2.960494
H	1.876581	-4.185012	-0.761558
H	3.895908	-3.864152	0.642605
H	5.851475	-2.568918	-0.284602
H	5.617797	-1.559863	-2.551282

Product picoline sp3, Np III – Small core

E = -1188.478402
G = -1188.256366

C	0.978544	1.918962	-2.950190
C	-0.035035	0.929909	-2.974168
C	0.253313	-0.016244	-1.956412
C	1.446792	0.386403	-1.310119
C	1.897637	1.580931	-1.928104
Np	2.206131	-0.378332	-3.822716
C	1.887374	-2.901101	-3.430595
C	2.866472	-2.731757	-2.408656
N	3.879821	-1.844442	-2.705757
C	4.838910	-1.591626	-1.790855
C	4.854881	-2.153879	-0.531874
C	3.787580	-3.007109	-0.183031
C	2.798176	-3.284885	-1.097729
C	1.491979	0.727795	-6.226881
C	2.727493	1.345835	-5.905640
C	3.741005	0.360150	-5.987032
C	3.137096	-0.864898	-6.359162
C	1.744530	-0.637407	-6.505597
H	1.925756	-0.125460	-0.483689
H	-0.341727	-0.885919	-1.705661
H	-0.898765	0.920491	-3.628706
H	1.030210	2.791491	-3.589176
H	2.772972	2.154867	-1.643967
H	2.873847	2.394085	-5.675121
H	0.529392	1.221704	-6.278984
H	4.800003	0.517269	-5.813797
H	3.652645	-1.804013	-6.522434
H	1.006940	-1.374300	-6.803141
H	2.295862	-3.062437	-4.433570
H	1.031740	-3.532470	-3.206708
H	1.979128	-3.954359	-0.853462
H	3.753464	-3.456473	0.806433
H	5.655639	-1.930650	0.164290
H	5.619216	-0.900786	-2.105301

TS Picoline sp3 Pu III – Large core

E = -747.572180
G = -747.309469

N	0.497152	1.825980	-2.822819
C	-0.280790	0.725158	-2.625447
C	0.179099	-0.319156	-1.795359
C	1.451896	-0.255694	-1.256936
C	2.268052	0.849450	-1.532865
C	1.734241	1.868216	-2.303920
C	-1.586673	0.741729	-3.288289
Pu	-1.433284	3.566644	-2.862474
C	-3.872122	2.412625	-2.785821
C	-0.938115	5.722183	-4.568903
C	-2.298622	5.389357	-4.792850
C	-2.338406	4.146369	-5.474286
C	-1.006937	3.707125	-5.661659
C	-0.140514	4.679392	-5.099787
C	-2.530956	4.604702	-0.479313
C	-1.698628	3.547441	-0.032212
C	-0.354051	3.924253	-0.258702
C	-0.351608	5.207186	-0.861000
C	-1.700630	5.630480	-0.989867
H	0.521111	3.341801	0.003556
H	-2.033718	2.627589	0.432715
H	-3.612307	4.631708	-0.417179
H	-2.033509	6.586016	-1.377696
H	0.524759	5.788658	-1.124496
H	-0.573359	6.628119	-4.099506
H	-3.154750	6.001552	-4.532816
H	0.942953	4.646481	-5.109025
H	-0.698167	2.802404	-6.172083
H	-3.232630	3.633839	-5.808093
H	-4.408168	1.892184	-3.588031
H	-4.232512	2.022375	-1.827318
H	-4.202264	3.463681	-2.839988
H	-2.612562	1.617367	-2.955887
H	-1.471812	0.918973	-4.364241
H	-2.145097	-0.184568	-3.137758
H	-0.463181	-1.175716	-1.616006
H	1.821888	-1.067237	-0.635797
H	3.277726	0.923276	-1.144170
H	2.305974	2.769573	-2.513652

TS Picoline sp3 Pu III – Small core

E = -1268.439916
G = -1268.176981

N	0.481256	1.994337	-2.809319
C	-0.177163	0.816031	-2.645308
C	0.382012	-0.201007	-1.846221
C	1.643664	-0.024254	-1.303581
C	2.341160	1.166166	-1.545501
C	1.706259	2.149962	-2.286541
C	-1.480279	0.735574	-3.314285
Pu	-1.568019	3.483725	-2.860426
C	-3.863136	2.228632	-2.751252
C	-0.689753	5.508823	-4.470642
C	-2.108091	5.520071	-4.557873
C	-2.510696	4.358626	-5.262671
C	-1.345468	3.625857	-5.596379
C	-0.221664	4.340936	-5.113124
C	-2.582185	4.864274	-0.716520
C	-2.121587	3.635577	-0.181242
C	-0.708584	3.627343	-0.258798
C	-0.293894	4.845545	-0.850894
C	-1.454282	5.611963	-1.128704
H	-0.058120	2.830443	0.081786
H	-2.742301	2.848257	0.229290
H	-3.616526	5.181980	-0.783121
H	-1.473077	6.605610	-1.558891
H	0.729301	5.156067	-1.027188
H	-0.075433	6.274855	-4.013192
H	-2.762346	6.300648	-4.187567
H	0.813648	4.042445	-5.222197
H	-1.315569	2.698708	-6.156696
H	-3.528845	4.083787	-5.511917
H	-4.390613	1.728096	-3.571985
H	-4.211442	1.796374	-1.806650
H	-4.207506	3.279449	-2.762162
H	-2.567705	1.506794	-2.951682
H	-1.376476	0.941328	-4.385852
H	-1.966594	-0.233228	-3.180894
H	-0.171955	-1.121702	-1.691159
H	2.095313	-0.811221	-0.705302
H	3.338230	1.330955	-1.151775
H	2.177946	3.113687	-2.463545

Adduct of picoline sp3, Pu III – Large core

E = -747.600695
G = -747.337182

N	0.094665	1.692103	-2.357968
C	-0.106873	0.401440	-2.695190
C	0.899511	-0.552842	-2.517908
C	2.130120	-0.172589	-1.995710
C	2.333097	1.162173	-1.656306
C	1.285677	2.051859	-1.853090
C	-1.438128	0.038213	-3.280509
Pu	-1.688316	3.720682	-2.657474
C	-3.940150	2.584852	-2.657559
C	-0.449758	5.271533	-4.669548
C	-1.832555	5.583096	-4.739568
C	-2.511090	4.452466	-5.259155
C	-1.551361	3.442326	-5.501905
C	-0.276857	3.948833	-5.141299
C	-2.669116	5.469989	-0.685805
C	-2.444350	4.267232	0.026701
C	-1.046365	4.064183	0.111121
C	-0.405065	5.144025	-0.548970
C	-1.409204	6.014292	-1.039303
H	-0.553886	3.248980	0.629516
H	-3.210110	3.624325	0.442838
H	-3.636643	5.908817	-0.900930
H	-1.241409	6.949006	-1.561237
H	0.664215	5.315362	-0.613600
H	0.337324	5.942723	-4.345283
H	-2.284034	6.535027	-4.484551
H	0.668825	3.428713	-5.245035
H	-1.753922	2.469149	-5.934595
H	-3.574939	4.377013	-5.447047
H	-4.147846	1.975397	-3.550037
H	-4.123441	1.937603	-1.784417
H	-4.739486	3.342299	-2.624114
H	-2.261397	0.386417	-2.648999
H	-1.566280	0.514532	-4.259353
H	-1.531796	-1.041578	-3.413648
H	0.707960	-1.584908	-2.793436
H	2.918071	-0.907028	-1.855070
H	3.274181	1.510317	-1.244604
H	1.393027	3.101141	-1.589274

Adduct of picoline sp3, Pu III – Small core

E = -1268.465110
G = -1268.202470

N	0.014220	1.724977	-2.379350
C	-0.223638	0.422985	-2.639204
C	0.790111	-0.532658	-2.520995
C	2.066286	-0.143086	-2.131919
C	2.304895	1.202952	-1.866195
C	1.248968	2.093878	-2.002092
C	-1.613667	0.045291	-3.056305
Pu	-1.734030	3.702758	-2.669237
C	-3.972369	2.710608	-2.788946
C	-0.477205	5.425371	-4.414781
C	-1.866078	5.502379	-4.696391
C	-2.264401	4.272464	-5.276463
C	-1.124139	3.433831	-5.341889
C	-0.020263	4.149729	-4.815332
C	-2.746814	5.288409	-0.685329
C	-2.365630	4.098082	-0.021708
C	-0.951511	4.021920	-0.034709
C	-0.458298	5.163089	-0.714790
C	-1.570066	5.947920	-1.114723
H	-0.355252	3.239250	0.419907
H	-3.041225	3.376507	0.421715
H	-3.763569	5.631326	-0.837370
H	-1.524216	6.897674	-1.633447
H	0.583689	5.423290	-0.864485
H	0.128512	6.213600	-3.984046
H	-2.503657	6.362271	-4.525813
H	0.999057	3.787553	-4.748245
H	-1.093735	2.433323	-5.758889
H	-3.262569	4.018364	-5.610399
H	-4.144547	2.058492	-3.659915
H	-4.250087	2.126120	-1.896240
H	-4.723982	3.514534	-2.861883
H	-2.335998	0.256292	-2.260774
H	-1.928584	0.623192	-3.931917
H	-1.678057	-1.016164	-3.305145
H	0.568040	-1.573050	-2.736298
H	2.861149	-0.877472	-2.037697
H	3.282201	1.559675	-1.559106
H	1.384960	3.153165	-1.799980

Product picoline sp3, Pu III – Large core

E = -707.107050
G = -706.884572

C	1.126927	1.807979	-2.905112
C	0.080619	0.912996	-2.571736
C	0.572214	0.006077	-1.596655
C	1.922732	0.336790	-1.333265
C	2.268882	1.447269	-2.146239
Pu	1.931762	-0.664038	-3.965806
N	3.502892	-2.402074	-2.943972
C	2.411511	-3.137582	-2.539350
C	2.422045	-3.722827	-1.243126
C	3.548810	-3.635207	-0.455713
C	4.684456	-2.948121	-0.924527
C	4.596865	-2.340527	-2.161162
C	1.296392	-3.147924	-3.439750
C	1.002945	0.205132	-6.465361
C	2.273675	0.819169	-6.327085
C	3.260112	-0.194788	-6.416049
C	2.600639	-1.433612	-6.611796
C	1.206524	-1.187292	-6.643184
H	2.570947	-0.159427	-0.620585
H	0.006980	-0.785471	-1.120109
H	-0.932017	0.945658	-2.958373
H	1.058629	2.638221	-3.598029
H	3.221316	1.966485	-2.145599
H	2.458385	1.881237	-6.215101
H	0.047722	0.717686	-6.479581
H	4.333723	-0.044037	-6.383748
H	3.081547	-2.396239	-6.739992
H	0.432687	-1.928120	-6.808023
H	1.557111	-3.414055	-4.467997
H	0.399691	-3.655205	-3.092679

H	1.545971	-4.270283	-0.909274
H	3.566287	-4.111224	0.521664
H	5.592659	-2.878940	-0.336307
H	5.429830	-1.763663	-2.559339

Product picoline sp3, Pu III – Small core

E = -1227.968810

G = -1227.747698

C	0.583780	1.882926	-2.990181
C	-0.141529	0.753675	-2.540544
C	0.659200	0.067745	-1.591708
C	1.875373	0.779940	-1.449686
C	1.834556	1.896745	-2.318029
Pu	1.952320	-0.263199	-3.975141
N	4.054366	-1.096347	-2.965345
C	3.405635	-2.204901	-2.479378
C	3.722207	-2.670267	-1.173731
C	4.742563	-2.074283	-0.464719
C	5.454147	-0.993744	-1.021352
C	5.052102	-0.534545	-2.260216
C	2.363439	-2.711802	-3.322226
C	1.779966	-0.298430	-6.692548
C	1.489183	1.040800	-6.328873
C	2.684384	1.630777	-5.841700
C	3.708919	0.659224	-5.901318
C	3.151258	-0.535181	-6.420828
H	2.693737	0.510485	-0.793441
H	0.383706	-0.832437	-1.055708
H	-1.142964	0.473832	-2.850674
H	0.237053	2.621111	-3.703134
H	2.605299	2.650995	-2.425514
H	2.792926	2.653716	-5.502314
H	0.532616	1.538838	-6.438237
H	4.742296	0.798303	-5.608004
H	3.687708	-1.459555	-6.600390
H	1.085282	-1.007308	-7.130722
H	2.676762	-2.874294	-4.361347
H	1.771163	-3.535996	-2.932168
H	3.177083	-3.518080	-0.770122
H	5.009060	-2.449528	0.520392
H	6.275425	-0.520803	-0.494464
H	5.529775	0.327649	-2.721673

Lutidine

E = -326.809960

G = -326.699988

N	0.092455	-0.000686	0.009353
C	0.043036	0.057223	1.346644
C	1.197697	0.060825	2.136758
C	2.437249	0.002281	1.508787
C	2.487368	-0.057926	0.120198
C	1.285739	-0.057210	-0.596453
H	1.120462	0.108607	3.218972
H	3.353038	0.003526	2.094383
H	3.437360	-0.104777	-0.404001
C	-1.330531	0.118507	1.957888
C	1.264115	-0.120741	-2.099643
H	0.711211	-1.004451	-2.434237
H	0.745910	0.752436	-2.508849
H	2.271926	-0.158956	-2.520924
H	-1.871938	0.994854	1.587329
H	-1.914190	-0.761581	1.669129
H	-1.289544	0.168068	3.049000

TS Lutidine Np IV – Large core

E = -831.847976

G = -831.520195

Np	0.514149	-0.807677	-3.268193
C	2.620448	-1.030251	-1.478261
C	3.472905	-2.004700	-2.170186
C	4.789038	-2.316989	-1.799269
C	5.487496	-3.260213	-2.533085
C	4.852095	-3.883161	-3.606015
C	3.550044	-3.512733	-3.941962
N	2.888176	-2.552360	-3.262944
C	2.845416	-4.209262	-5.070636
C	-0.128802	-2.963570	-2.207888
C	2.681736	0.754583	-3.701663
C	0.151698	1.523456	-1.770283
C	-0.091245	0.490505	-0.834872
C	-1.267223	-0.191533	-1.225657
C	-1.756332	0.423749	-2.404512
C	-0.876475	1.485043	-2.743376
C	-1.136507	-0.325935	-5.504141
C	0.189157	-0.103850	-5.942935
C	0.859402	-1.355111	-5.956949
C	-0.050527	-2.341943	-5.510570
C	-1.282016	-1.702684	-5.219611
H	2.493108	-0.068052	-2.540643
H	3.197659	0.235587	-4.515763
H	3.443513	1.306940	-3.138435
H	2.016167	1.511714	-4.134324
H	-1.214171	-3.123487	-2.288155
H	0.114880	-3.038169	-1.139128
H	0.356440	-3.814970	-2.700435
H	3.139231	-0.419674	-0.735425
H	5.228287	-1.833229	-0.932619
H	6.506229	-3.528743	-2.265520
H	5.357081	-4.650254	-4.184389
H	3.483030	-4.980458	-5.508922
H	2.560217	-3.514338	-5.863804
H	1.931143	-4.688752	-4.707459
H	1.798925	-1.551668	-0.972404
H	0.513244	0.267199	0.034178
H	-1.721215	-1.026415	-0.709222
H	-2.662832	0.151794	-2.929881
H	-0.989924	2.167323	-3.576720
H	0.973526	2.227190	-1.742193
H	-1.905907	0.428945	-5.407107
H	0.610000	0.845150	-6.251749
H	1.883674	-1.511705	-6.270088
H	0.144637	-3.399964	-5.410892
H	-2.180637	-2.192396	-4.865603

TS Lutidine Np IV – Small core

E = -1308.097549

G = -1307.770528

Np	0.592614	-0.848503	-3.227653
C	2.710813	-0.907574	-1.563286
C	3.528260	-1.921912	-2.249566
C	4.886005	-2.149277	-1.994961
C	5.541688	-3.138679	-2.710852
C	4.824594	-3.884722	-3.643102
C	3.477594	-3.593705	-3.868444
N	2.853597	-2.597467	-3.208310
C	2.686945	-4.412888	-4.847392
C	-0.295432	-2.943011	-2.363946
C	2.520531	0.955626	-3.689441
C	0.132766	1.377581	-1.637050
C	-0.149234	0.279859	-0.789927
C	-1.303324	-0.372954	-1.280776
C	-1.730556	0.317128	-2.438053
C	-0.842437	1.401237	-2.657086
C	-0.896687	-0.223963	-5.485483
C	0.449917	-0.133619	-5.902514
C	0.999982	-1.437195	-5.887337
C	-0.012983	-2.332601	-5.468165
C	-1.181128	-1.582750	-5.210016
H	2.485014	0.041761	-2.537156
H	3.140741	0.522939	-4.483214
H	3.158185	1.623249	-3.097006
H	1.756265	1.589206	-4.153285
H	-1.381104	-3.084348	-2.427299
H	-0.020353	-3.044851	-1.301776
H	0.181774	-3.772958	-2.902109
H	3.264375	-0.290261	-0.852310
H	5.395470	-1.566603	-1.234137
H	6.593699	-3.345911	-2.532993
H	5.298443	-4.689321	-4.196211
H	3.260211	-5.283710	-5.174156
H	2.418974	-3.834392	-5.735785
H	1.758022	-4.762170	-4.388586
H	1.890773	-1.387266	-1.010990
H	0.401166	0.009417	0.102590
H	-1.785546	-1.232963	-0.838110
H	-2.601641	0.076289	-3.033664
H	-0.907376	2.130321	-3.455180
H	0.950380	2.077473	-1.522849
H	-1.596097	0.598759	-5.415838
H	0.967033	0.768474	-6.202494
H	2.015416	-1.691637	-6.164520
H	0.079619	-3.403198	-5.357345
H	-2.128026	-1.983979	-4.871926

Adduct of lutidine, Np IV – Large core

E = -831.894793

G = -831.576794

Np	-0.541585	0.003754	-3.184613
C	4.203334	-2.104712	-1.319989
C	4.800904	-3.095669	-2.280183
C	5.899961	-3.884159	-1.923724
C	6.404947	-4.788448	-2.851339
C	5.803704	-4.877389	-4.101975
C	4.709438	-4.053059	-4.383964
N	4.222733	-3.184014	-3.486417
C	4.021233	-4.092467	-5.720653
C	-0.457490	-1.580451	-1.312588
C	1.410465	1.443619	-2.821353
C	-1.782160	2.444311	-2.723993
C	-2.039722	1.692620	-1.551570
C	-2.913916	0.630502	-1.888254
C	-3.189123	0.716041	-3.275626
C	-2.487683	1.838455	-3.793215
C	-0.463989	-0.514812	-5.872942
C	0.897518	-0.563742	-5.479662
C	1.079475	-1.704642	-4.658921
C	-0.167641	-2.370091	-4.554723
C	-1.124108	-1.635150	-5.299744
H	4.159679	-1.110702	-1.775257
H	2.341317	0.861071	-2.868026
H	1.371201	1.912100	-1.826974
H	1.516728	2.261371	-3.547272
H	-1.294248	-2.291702	-1.279133
H	-0.461239	-1.049263	-0.349463
H	0.461862	-2.181825	-1.347372
H	4.778849	-2.040245	-0.393140
H	6.344647	-3.786400	-0.937926
H	7.257256	-5.415624	-2.603038
H	6.171961	-5.570947	-4.851984
H	4.445080	-4.861172	-6.371683
H	4.110351	-3.124010	-6.223800
H	2.951719	-4.286931	-5.596427
H	3.175766	-2.387660	-1.068470
H	-1.645002	1.900823	-0.564301
H	-3.304926	-0.112153	-1.204671
H	-3.848167	0.064174	-3.836523
H	-2.518419	2.190852	-4.817443
H	-1.157895	3.326050	-2.790235
H	-0.914385	0.223729	-6.525761
H	1.666389	0.145615	-5.758991
H	2.014292	-2.026837	-4.208537
H	-0.355672	-3.282049	-4.002369
H	-2.165990	-1.899270	-5.438455

Adduct of lutidine, Np IV – Small core

E = -1308.122269

G = -1307.799355

Np	0.437319	-0.869596	-3.540135
C	3.294492	-0.831446	-0.915690
C	3.877950	-1.879885	-1.813412
C	5.121583	-2.436341	-1.506856
C	5.633125	-3.446846	-2.310011
C	4.881446	-3.868062	-3.396156
C	3.648836	-3.261024	-3.656114
N	3.150864	-2.278235	-2.879070
C	2.861562	-3.692283	-4.856191
C	-0.178358	-3.022166	-2.545792
C	2.149063	0.740125	-4.234332
C	0.266907	1.215660	-1.712488
C	-0.089652	0.070083	-0.961993
C	-1.326341	-0.412274	-1.449694
C	-1.729304	0.428142	-2.510879
C	-0.740601	1.431566	-2.679403
C	-1.256994	-0.235881	-5.583506
C	0.012982	-0.223027	-6.202221
C	0.485023	-1.555001	-6.247672
C	-0.496873	-2.393181	-5.667185
C	-1.570866	-1.577626	-5.245200
H	2.847699	-0.019764	-1.493582
H	2.761786	0.234130	-4.996082
H	2.813132	1.013307	-3.402015
H	1.774851	1.671116	-4.674054
H	-1.249660	-3.229226	-2.450157
H	0.251451	-3.014103	-1.531725
H	0.274717	-3.861261	-3.091865
H	4.055376	-0.409381	-0.254842
H	5.669118	-2.077811	-0.641066
H	6.596452	-3.898807	-2.090157
H	5.236069	-4.658122	-4.050679
H	3.049749	-4.743007	-5.092638
H	3.149647	-3.100545	-5.732239
H	1.791679	-3.557424	-4.695484
H	2.509665	-1.268020	-0.289284
H	0.460201	-0.344857	-0.126844
H	-1.870500	-1.264928	-1.067126
H	-2.649527	0.339662	-3.073222
H	-0.760316	2.235087	-3.405016
H	1.147953	1.828771	-1.571558
H	-1.890806	0.626571	-5.423415
H	0.528878	0.646729	-6.585463
H	1.421691	-1.873285	-6.686937
H	-0.449387	-3.470409	-5.570561
H	-2.478524	-1.922121	-4.765597

Product lutidine, Np IV – Large core

E = -791.406347

G = -791.120648

C	-0.747485	-0.597126	-5.654681
C	0.369688	0.267202	-5.510768
C	1.542625	-0.493579	-5.741973
C	1.153333	-1.827061	-6.011638
C	-0.262691	-1.891637	-5.961353
Np	0.482959	-1.404996	-3.340972
C	0.189070	-3.958413	-3.192791
C	1.354643	-3.996399	-2.351815
C	1.491743	-4.690499	-1.126544
C	2.708428	-4.654062	-0.475507
C	3.777636	-3.937724	-1.030386
C	3.566422	-3.193504	-2.185182
N	2.358885	-3.173358	-2.793207
C	4.681155	-2.399387	-2.804627
C	2.390697	0.011779	-2.615247
C	-1.272354	0.360544	-2.216044
C	-2.035674	-0.819958	-2.432047
C	-1.578778	-1.805836	-1.526250
C	-0.526750	-1.243939	-0.759371
C	-0.348739	0.098332	-1.176035
H	2.077623	1.065729	-2.651687
H	3.271654	-0.072062	-3.260437
H	2.720418	-0.184348	-1.585882
H	-0.686422	-4.497467	-2.836750
H	0.664466	-5.285960	-0.753589
H	2.851033	-5.212235	0.446738
H	4.758054	-3.947990	-0.565135
H	5.619552	-2.960358	-2.756269
H	4.831921	-1.451426	-2.279190
H	4.457347	-2.174771	-3.848762
H	0.416948	-4.186275	-4.236168
H	1.820344	-2.652948	-6.225980
H	2.556896	-0.118184	-5.711565
H	0.332502	1.328208	-5.295777
H	-1.788510	-0.309548	-5.575975
H	-0.868729	-2.771280	-6.139073
H	-2.849374	-0.934827	-3.137662
H	-1.969932	-2.809523	-1.431077
H	0.026794	-1.745195	0.025376
H	0.368044	0.799153	-0.770698
H	-1.399267	1.305064	-2.731278

Product lutidine, Np IV – Small core

E = -1267.655259

G = -1267.372025

C	-0.997216	-0.740005	-5.521195
C	-0.042347	0.304925	-5.422458
C	1.213707	-0.210850	-5.814302
C	1.042435	-1.579918	-6.131112
C	-0.328701	-1.902396	-5.961424
Np	0.644517	-1.428788	-3.436469
C	0.284659	-3.945159	-3.481060
C	1.303933	-4.019269	-2.482092
C	1.237741	-4.748306	-1.267514
C	2.325151	-4.730605	-0.422379
C	3.471379	-3.996627	-0.770149
C	3.460026	-3.227605	-1.925428
N	2.370734	-3.191498	-2.732716
C	4.662904	-2.429274	-2.337034
C	2.502688	0.063457	-3.033177
C	-1.078769	0.265960	-2.186565
C	-1.762103	-0.975852	-2.252106
C	-1.101645	-1.882756	-1.393474
C	-0.001476	-1.208368	-0.807833
C	0.003466	0.123713	-1.288815
H	2.208172	1.109186	-3.201375
H	3.346420	-0.146933	-3.704881
H	2.867122	-0.004262	-1.998660
H	-0.639498	-4.490816	-3.305664
H	0.361690	-5.353046	-1.055428
H	2.314039	-5.313352	0.495540
H	4.359067	-4.023014	-0.146683
H	5.565475	-2.822844	-1.862402
H	4.561158	-1.377430	-2.054911
H	4.789615	-2.463435	-3.421983
H	0.663880	-4.050094	-4.498928
H	1.819132	-2.256265	-6.469336
H	2.141258	0.343442	-5.861282
H	-0.244563	1.327555	-5.129254
H	-2.056832	-0.654736	-5.316647
H	-0.784988	-2.866405	-6.146506
H	-2.648353	-1.186461	-2.837570
H	-1.386258	-2.910591	-1.212160
H	0.703037	-1.635175	-0.103954
H	0.709005	0.896377	-1.015434
H	-1.353482	1.171654	-2.712456

TS Lutidine Pu IV – Large core

E = -832.600611

G = -832.272355

Pu	0.493565	-0.797998	-3.263766
C	2.589602	-1.062856	-1.486031
C	3.457174	-2.028308	-2.173556
C	4.769482	-2.335806	-1.784769
C	5.486518	-3.265518	-2.518315
C	4.873936	-3.879158	-3.609641
C	3.573697	-3.514867	-3.959971
N	2.892968	-2.570638	-3.278382
C	2.891570	-4.198048	-5.110773
C	-0.152478	-2.935548	-2.205803
C	2.675068	0.729474	-3.695986
C	0.165222	1.539007	-1.800747
C	-0.066703	0.518266	-0.848721
C	-1.247348	-0.168114	-1.216242
C	-1.750596	0.431695	-2.397428
C	-0.875110	1.489054	-2.760148
C	-1.167108	-0.350807	-5.484056
C	0.153453	-0.094970	-5.919832
C	0.855831	-1.328960	-5.932378
C	-0.029259	-2.338029	-5.487049
C	-1.277518	-1.730201	-5.198113
H	2.468701	-0.096398	-2.551800
H	3.296509	0.197574	-4.422947
H	3.339134	1.363043	-3.096081
H	2.013767	1.414111	-4.240873
H	-1.235172	-3.100466	-2.307527
H	0.070036	-3.005978	-1.132443
H	0.347229	-3.784583	-2.687397
H	3.098674	-0.448735	-0.739128
H	5.192385	-1.857981	-0.906723
H	6.503103	-3.529159	-2.237888
H	5.395296	-4.632946	-4.191037
H	3.548864	-4.941956	-5.566933
H	2.592948	-3.488227	-5.885735
H	1.987348	-4.709165	-4.765495
H	1.769584	-1.592213	-0.987452
H	0.549642	0.304055	0.014143
H	-1.694790	-0.996878	-0.684621
H	-2.663578	0.153114	-2.907744
H	-0.998697	2.160810	-3.600437
H	0.987438	2.242690	-1.792386
H	-1.955338	0.384484	-5.387725
H	0.548932	0.864069	-6.230963
H	1.885616	-1.458961	-6.239180
H	0.192793	-3.390367	-5.384854
H	-2.163447	-2.242677	-4.844774

TS Lutidine Pu IV – Small core

E = -1347.574658

G = -1347.249031

Pu	0.583912	-0.847636	-3.227834
C	2.709064	-0.913992	-1.567805
C	3.537813	-1.920239	-2.250425
C	4.901999	-2.119576	-2.006383
C	5.569767	-3.100929	-2.723526
C	4.860066	-3.863408	-3.647697
C	3.505591	-3.597602	-3.862994
N	2.867852	-2.614242	-3.198614
C	2.720511	-4.427567	-4.837420
C	-0.408882	-2.935913	-2.418345
C	2.542927	0.926209	-3.698948
C	0.171742	1.359740	-1.623258
C	-0.143926	0.267414	-0.774608
C	-1.321073	-0.342251	-1.260066
C	-1.728592	0.360721	-2.416646
C	-0.811587	1.422275	-2.632817
C	-0.917028	-0.252885	-5.463669
C	0.428345	-0.144004	-5.884450
C	0.993145	-1.440578	-5.874131
C	-0.007709	-2.350592	-5.454411
C	-1.185390	-1.617456	-5.196264
H	2.480949	0.024724	-2.560183
H	3.150574	0.471996	-4.488100
H	3.185754	1.581384	-3.099513
H	1.775034	1.559227	-4.153510
H	-1.486886	-3.080541	-2.532785
H	-0.158138	-3.006040	-1.349929
H	0.118155	-3.732165	-2.957673
H	3.251929	-0.280346	-0.863173
H	5.407706	-1.523043	-1.253794
H	6.626763	-3.287764	-2.553020
H	5.344618	-4.661305	-4.201236
H	3.300322	-5.294066	-5.164166
H	2.445808	-3.852239	-5.726066
H	1.795299	-4.783450	-4.376100
H	1.885321	-1.391120	-1.020669
H	0.399361	-0.020883	0.116872
H	-1.828677	-1.190064	-0.821386
H	-2.608900	0.146760	-3.009044
H	-0.858694	2.154307	-3.430183
H	1.007131	2.037688	-1.504460
H	-1.626960	0.560828	-5.391733
H	0.932382	0.765819	-6.183934
H	2.012495	-1.681931	-6.149907
H	0.098021	-3.420908	-5.352946
H	-2.128972	-2.029424	-4.862758

Adduct of lutidine, Pu IV – Large core

E = -832.650638

G = -832.333005

Pu	-0.516812	0.031592	-3.153686
C	4.210387	-2.152815	-1.373424
C	4.779551	-3.149666	-2.344669
C	5.878039	-3.948267	-2.009586
C	6.355989	-4.857834	-2.946326
C	5.729096	-4.941854	-4.184686
C	4.637225	-4.107424	-4.445390
N	4.176702	-3.233258	-3.539087
C	3.921655	-4.141406	-5.767800
C	-0.409243	-1.549212	-1.301147
C	1.456168	1.419974	-2.813223
C	-1.698174	2.482107	-2.698765
C	-1.911662	1.758280	-1.500332
C	-2.809891	0.698653	-1.775768
C	-3.144090	0.757355	-3.151579
C	-2.455605	1.861596	-3.723098
C	-0.495267	-0.453190	-5.831832
C	0.870265	-0.537664	-5.459274
C	1.037433	-1.689884	-4.651292
C	-0.223448	-2.326587	-4.534182
C	-1.173318	-1.562613	-5.258267
H	4.160141	-1.160133	-1.830792
H	2.374068	0.819270	-2.876590
H	1.439369	1.884974	-1.816922
H	1.566345	2.237836	-3.538341
H	-1.260507	-2.241519	-1.245300
H	-0.373273	-1.020317	-0.337622
H	0.495020	-2.170160	-1.365537
H	4.808620	-2.088301	-0.461062
H	6.343191	-3.853969	-1.032947
H	7.207198	-5.492789	-2.714585
H	6.075703	-5.639271	-4.941402
H	4.327160	-4.912205	-6.427986
H	4.006282	-3.173058	-6.271868
H	2.853743	-4.329596	-5.621727
H	3.187878	-2.429856	-1.095996
H	-1.470460	1.982135	-0.536555
H	-3.177065	-0.025869	-1.060387
H	-3.831919	0.099771	-3.669440
H	-2.527111	2.192167	-4.752417
H	-1.068193	3.355007	-2.811082
H	-0.937628	0.302391	-6.470320
H	1.651319	0.156026	-5.743657
H	1.970879	-2.037037	-4.217067
H	-0.425084	-3.238054	-3.985893
H	-2.223180	-1.800433	-5.382885

Adduct of lutidine, Pu IV – Small core

E = -1347.604220

G = -1347.280751

Pu	0.468599	-0.849843	-3.503381
C	3.251439	-0.956292	-0.899412
C	3.869367	-1.970871	-1.813149
C	5.109135	-2.528843	-1.496327
C	5.642950	-3.511081	-2.320576
C	4.916332	-3.904052	-3.434290
C	3.685795	-3.295869	-3.702352
N	3.168656	-2.338373	-2.907055
C	2.920744	-3.699859	-4.926823
C	-0.220407	-2.962324	-2.489495
C	2.127033	0.805215	-4.209524
C	0.218462	1.330913	-1.843236
C	-0.044874	0.214082	-1.012318
C	-1.274540	-0.359474	-1.419560
C	-1.758157	0.389122	-2.511270
C	-0.831335	1.430407	-2.780522
C	-1.281062	-0.260033	-5.539489
C	-0.008884	-0.193305	-6.143468
C	0.519527	-1.506998	-6.184733
C	-0.435867	-2.383350	-5.615594
C	-1.542273	-1.612099	-5.198158
H	2.861453	-0.102067	-1.458491
H	2.712817	0.296992	-4.989420
H	2.789373	1.010786	-3.356001
H	1.763311	1.759137	-4.600935
H	-1.282474	-3.215113	-2.436689
H	0.194316	-2.941448	-1.470459
H	0.303246	-3.742113	-3.061527
H	3.974351	-0.585032	-0.169209
H	5.635647	-2.195842	-0.607659
H	6.603853	-3.964906	-2.094422
H	5.288662	-4.673860	-4.102906
H	3.127857	-4.739870	-5.192753
H	3.210958	-3.077700	-5.780901
H	1.847016	-3.583866	-4.778645
H	2.417714	-1.405495	-0.349377
H	0.552314	-0.110263	-0.169532
H	-1.761200	-1.211219	-0.964762
H	-2.686869	0.210050	-3.036926
H	-0.919262	2.182632	-3.554186
H	1.071035	1.994367	-1.775798
H	-1.949824	0.575977	-5.382773
H	0.473324	0.697866	-6.521542
H	1.471464	-1.787241	-6.617322
H	-0.346690	-3.458067	-5.516159
H	-2.439845	-1.992588	-4.727767

Product lutidine, Pu IV – Large core

E = -792.160389

G = -791.874615

C	0.086761	-1.381851	-3.058380
C	1.237082	-0.784353	-2.472660
C	2.355801	-1.589625	-2.792151
C	1.900194	-2.690830	-3.559425
C	0.500733	-2.554013	-3.734983
Pu	0.804525	-3.063758	-1.054275
C	-0.557538	-4.889144	-2.014362
C	3.166616	-3.100511	-0.075589
C	3.361547	-4.377846	-0.706405
C	4.476583	-4.780273	-1.478576
C	4.512636	-6.069744	-1.969331
C	3.457361	-6.951007	-1.696645
C	2.341440	-6.481129	-1.014107
N	2.270638	-5.199175	-0.588057
C	1.184812	-7.391245	-0.712700
C	-1.526436	-2.261841	0.091331
C	-1.193187	-3.438162	0.808005
C	-0.038709	-3.168298	1.579637
C	0.336296	-1.818469	1.355302
C	-0.585015	-1.257034	0.438934
H	-1.465472	-4.446158	-2.450060
H	-0.894887	-5.624379	-1.275893
H	-0.055713	-5.439825	-2.820889
H	3.943996	-2.354932	-0.230457
H	5.305673	-4.094217	-1.620048
H	5.375813	-6.416220	-2.532669
H	3.497207	-7.986375	-2.019404
H	1.542400	-8.404095	-0.504894
H	0.492624	-7.447138	-1.558175
H	0.626919	-7.028420	0.152337
H	2.887489	-3.192518	0.975807
H	0.466425	-3.868455	2.233661
H	-1.726724	-4.378172	0.764620
H	-2.371089	-2.142598	-0.576038
H	-0.588141	-0.233031	0.086790
H	1.171804	-1.303683	1.812754
H	1.260843	0.142907	-1.913500
H	3.379995	-1.395110	-2.504970
H	2.517572	-3.486035	-3.959077
H	-0.138628	-3.227811	-4.288496
H	-0.922748	-0.990525	-3.022982

Product lutidine, Pu IV – Small core

E = -1307.128365

G = -1306.846245

C	0.201060	-1.518711	-2.971180
C	1.421279	-1.067959	-2.400536
C	2.424421	-2.004209	-2.724710
C	1.826416	-3.046853	-3.477376
C	0.454551	-2.730141	-3.648216
Pu	0.760148	-3.316779	-1.012206
C	-1.003439	-4.676230	-1.962565
C	3.081535	-3.141709	0.152374
C	3.360918	-4.346680	-0.549534
C	4.537310	-4.614443	-1.299646
C	4.666743	-5.830257	-1.931855
C	3.635425	-6.782565	-1.844094
C	2.471017	-6.454065	-1.166299
N	2.319825	-5.246305	-0.568104
C	1.330788	-7.421727	-1.034943
C	-1.542490	-2.289627	0.057916
C	-1.168939	-3.326833	0.944500
C	0.018804	-2.936506	1.603579
C	0.381222	-1.648837	1.131682
C	-0.589722	-1.248824	0.186391

H	-1.907311	-4.215184	-2.370204
H	-1.296548	-5.328901	-1.124705
H	-0.546327	-5.294334	-2.750341
H	3.807981	-2.335762	0.105878
H	5.335286	-3.878839	-1.315246
H	5.575898	-6.067301	-2.478746
H	3.740174	-7.760829	-2.301119
H	1.563577	-8.374134	-1.516581
H	0.417241	-7.022147	-1.485585
H	1.115196	-7.608342	0.022365
H	2.604063	-3.265632	1.121175
H	0.546500	-3.516813	2.351958
H	-1.699556	-4.259754	1.090547
H	-2.414907	-2.283019	-0.582337
H	-0.610458	-0.302530	-0.338413
H	1.233590	-1.065690	1.455840
H	1.563310	-0.159928	-1.827971
H	3.467919	-1.939871	-2.448227
H	2.339086	-3.911776	-3.882368
H	-0.268804	-3.310649	-4.203555
H	-0.755282	-1.014402	-2.913558

TS Lutidine Np III – Large core

E = -786.213363

G = -785.923377

C	-1.705935	5.631153	-0.948000
C	-2.473495	4.564906	-0.422239
C	-1.581775	3.543905	-0.008080
C	-0.262463	3.983384	-0.269244
C	-0.335884	5.270301	-0.858725
Np	-1.402475	3.580164	-2.864165
N	0.500442	1.768195	-2.821635
C	-0.325571	0.705625	-2.611881
C	0.072323	-0.341267	-1.755835
C	1.339745	-0.315884	-1.204101
C	2.204973	0.744560	-1.496994
C	1.744735	1.780795	-2.301284
C	-1.623058	0.760220	-3.290272
C	-3.875975	2.467788	-2.767029
C	-2.441029	5.243786	-4.893268
C	-1.183233	5.810568	-4.569341
C	-0.174902	4.926968	-5.027934
C	-0.810536	3.819607	-5.645601
C	-2.208885	4.014857	-5.561480
H	0.644173	3.440156	-0.030342
H	-1.860218	2.606429	0.459084
H	-3.552712	4.542000	-0.329871
H	-2.092719	6.573767	-1.317159
H	0.504373	5.897573	-1.134907
H	-1.021089	6.766263	-4.085160
H	-3.409702	5.691766	-4.702747
H	0.894314	5.092267	-4.961367
H	-0.309577	2.983862	-6.120061
H	-2.971009	3.354182	-5.957482
H	-4.427327	1.966034	-3.570843
H	-4.237532	2.074997	-1.809936
H	-4.184913	3.525768	-2.808807
H	-2.632936	1.649310	-2.951752
H	-1.493344	0.937743	-4.364633
H	-2.206322	-0.152055	-3.148813
H	-0.608299	-1.165589	-1.568511
H	1.671573	-1.125829	-0.559563
H	3.212856	0.772583	-1.096619
C	2.600957	2.967133	-2.637460
H	3.572591	2.913980	-2.141360
H	2.764471	3.025064	-3.718592
H	2.109391	3.897396	-2.332165

TS Lutidine Np III – Small core

E = -1268.256152

G = -1267.966342

C	-1.896752	5.489506	-0.997288
C	-2.557775	4.346238	-0.487505
C	-1.572762	3.404349	-0.105849
C	-0.300000	3.968924	-0.364590
C	-0.499726	5.255566	-0.922215
Np	-1.409076	3.541320	-2.874278
N	0.518984	1.847357	-2.797073
C	-0.288058	0.774147	-2.580849
C	0.112748	-0.256956	-1.710200
C	1.378445	-0.209552	-1.153805
C	2.229606	0.859376	-1.455808
C	1.760217	1.883739	-2.270453
C	-1.573848	0.809201	-3.288044
C	-3.831589	2.523915	-2.864771
C	-2.207097	5.442337	-4.672505
C	-0.811944	5.642388	-4.519380
C	-0.147285	4.540868	-5.112531
C	-1.131476	3.666500	-5.635904
C	-2.403928	4.224416	-5.369889
H	0.654198	3.507396	-0.142322
H	-1.759167	2.431960	0.335044
H	-3.628651	4.218454	-0.392170
H	-2.370020	6.396702	-1.353613
H	0.275938	5.958510	-1.204490
H	-0.340691	6.500944	-4.056139
H	-2.985171	6.121779	-4.343736
H	0.924907	4.403697	-5.182486
H	-0.938798	2.745875	-6.174302
H	-3.358515	3.804216	-5.660624
H	-4.342595	2.070637	-3.722747
H	-4.250329	2.087203	-1.950867
H	-4.117923	3.589629	-2.866530
H	-2.580652	1.681301	-2.995794
H	-1.414139	0.967236	-4.361039
H	-2.159135	-0.101060	-3.142633
H	-0.559970	-1.086206	-1.515794
H	1.718851	-1.007450	-0.498891
H	3.235745	0.904200	-1.052125
C	2.603586	3.077278	-2.612933
H	3.546436	3.072874	-2.061314
H	2.829930	3.089270	-3.684498
H	2.071481	4.006346	-2.383232

Adduct of lutidine, Np III – Large core

E = -786.238078

G = -785.947673

C	-1.546933	6.019959	-0.964786
C	-2.529156	5.140330	-0.446983
C	-1.864620	4.034887	0.133030
C	-0.470162	4.232579	-0.016318
C	-0.271730	5.458853	-0.698960
Np	-1.450576	3.795934	-2.703047
N	0.172241	1.518707	-2.549555
C	-0.381857	0.287587	-2.533006
C	0.382223	-0.855295	-2.285912
C	1.747502	-0.728108	-2.069813
C	2.317892	0.538079	-2.116859
C	1.504485	1.644944	-2.361411
C	-1.845728	0.171786	-2.838380
C	-3.865024	3.016142	-2.723140
C	-2.342646	4.849122	-5.183442
C	-1.414078	5.797348	-4.686647
C	-0.117128	5.229344	-4.775009
C	-0.248058	3.931036	-5.325534
C	-1.623319	3.695380	-5.571762
H	0.306413	3.581931	0.370915
H	-2.341011	3.198032	0.630431
H	-3.601288	5.288262	-0.482114
H	-1.732705	6.976882	-1.438502
H	0.682798	5.920655	-0.926234
H	-1.646984	6.799111	-4.345127
H	-3.414199	4.984759	-5.260706
H	0.810983	5.725546	-4.514070
H	0.562616	3.251061	-5.562739
H	-2.049053	2.801523	-6.012883
H	-4.129626	2.334795	-3.546549
H	-4.239564	2.557789	-1.795390
H	-4.483751	3.914497	-2.881808
H	-2.443939	0.952728	-2.357311
H	-2.014687	0.267782	-3.917663
H	-2.237883	-0.798920	-2.526783
H	-0.099610	-1.827357	-2.270247
H	2.360317	-1.603387	-1.873293
H	3.383025	0.678896	-1.965579
C	2.087529	3.024044	-2.441891
H	3.163602	3.011435	-2.256256
H	1.914102	3.456036	-3.433222
H	1.621221	3.690262	-1.708281

Adduct of lutidine, Np III – Small core

E = -1268.276297

G = -1267.984992

C	-2.021607	5.829801	-1.121930
C	-2.912682	4.818846	-0.683895
C	-2.147895	3.811242	-0.052358
C	-0.786760	4.199770	-0.085045
C	-0.707256	5.447505	-0.752911
Np	-1.482685	3.700552	-2.755882
N	0.283180	1.678835	-2.428043
C	-0.162886	0.402882	-2.433228
C	0.698736	-0.678578	-2.251199
C	2.054744	-0.444380	-2.057831
C	2.510419	0.868052	-2.054873
C	1.602546	1.910384	-2.245267
C	-1.631823	0.193249	-2.645223
C	-3.764111	2.811494	-3.026939
C	-1.520887	5.673970	-4.650768
C	-0.165985	5.257778	-4.622210
C	-0.097492	3.956025	-5.177820
C	-1.410847	3.567880	-5.537606
C	-2.289788	4.628842	-5.220604
H	0.037422	3.656939	0.363343
H	-2.540994	2.907850	0.400197
H	-3.987823	4.816382	-0.805952
H	-2.297430	6.752898	-1.617387
H	0.189856	6.034648	-0.913905
H	0.670965	5.853956	-4.276681
H	-1.894228	6.638473	-4.328383
H	0.800870	3.371768	-5.340609
H	-1.693391	2.627693	-5.997637
H	-3.358687	4.638829	-5.388718
H	-3.880481	2.158180	-3.907810
H	-4.117986	2.231336	-2.158033
H	-4.503712	3.616316	-3.160591
H	-2.223551	0.691853	-1.869433
H	-1.957623	0.603516	-3.607621
H	-1.887585	-0.868392	-2.630217
H	0.299821	-1.687652	-2.261301
H	2.744592	-1.270744	-1.911801
H	3.561260	1.095647	-1.908081
C	2.064881	3.335535	-2.267891
H	3.115893	3.417468	-1.982211
H	1.946587	3.762269	-3.269165
H	1.470833	3.947706	-1.581815

Product lutidine, Np III – Large core

E = -745.747576

G = -745.499741

C	-1.418030	5.404046	-0.805141
C	-2.390528	4.380581	-0.675055
C	-1.744100	3.226952	-0.164508
C	-0.374540	3.537797	0.023725
C	-0.172663	4.882801	-0.370920
Np	-0.735601	3.533980	-2.809766
C	1.869054	3.297105	-3.101027
C	1.589924	2.019629	-3.688007
N	0.539470	1.321662	-3.137384
C	0.197565	0.101329	-3.609615
C	0.850264	-0.473045	-4.687840
C	1.868538	0.260737	-5.323030
C	2.233776	1.497652	-4.842716
C	-0.937271	-0.590672	-2.906642
C	-0.827674	4.377651	-5.510393
C	-1.683355	5.273749	-4.817635
C	-2.833392	4.554492	-4.409350
C	-2.684180	3.211836	-4.839573
C	-1.446456	3.104965	-5.524932
H	-1.050718	2.211851	-5.994048
H	0.120376	4.628982	-5.970249
H	-1.511148	6.334184	-4.670023
H	-3.689051	4.965402	-3.886767
H	-3.416757	2.420846	-4.718889
H	-2.222569	2.285515	0.083046
H	-3.448679	4.477842	-0.888546
H	0.379347	2.871298	0.426285
H	0.762294	5.428520	-0.317604
H	-1.605014	6.420565	-1.132482
H	1.968163	3.276836	-2.011803
H	2.646005	3.888417	-3.579134
H	3.035824	2.067461	-5.301085
H	2.379944	-0.160578	-6.185199
H	0.566918	-1.459559	-5.038551
H	-1.131262	-1.576555	-3.335329
H	-0.714116	-0.711070	-1.841461
H	-1.863141	-0.007250	-2.981628

Product lutidine, Np III – Small core

E = -1227.787863

G = -1227.540843

C	-1.676833	5.266198	-0.991204
C	-2.436466	4.078858	-0.832780
C	-1.586569	3.089009	-0.282087
C	-0.304163	3.660085	-0.098389
C	-0.360205	5.007211	-0.539404
Np	-0.617777	3.513154	-2.824434
C	1.922837	3.262775	-3.129886
C	1.597962	1.994224	-3.695068
N	0.546600	1.336426	-3.094564
C	0.121884	0.136544	-3.559475
C	0.697884	-0.457400	-4.668039
C	1.724788	0.231998	-5.343336
C	2.167502	1.448282	-4.879470
C	-1.005488	-0.504311	-2.799484
C	-0.688381	4.459633	-5.379360
C	-1.550803	5.320090	-4.650204
C	-2.695393	4.575762	-4.275832
C	-2.538596	3.254910	-4.761643
C	-1.299789	3.184993	-5.449223
H	-0.891304	2.311147	-5.943271
H	0.262735	4.732205	-5.820150
H	-1.381452	6.371276	-4.447178
H	-3.548616	4.954570	-3.727184
H	-3.259414	2.450841	-4.660992
H	-1.871103	2.075116	-0.023291
H	-3.489235	3.961890	-1.059823
H	0.559347	3.161306	0.325873
H	0.455472	5.721032	-0.509627
H	-2.047841	6.212786	-1.365066
H	2.001964	3.270842	-2.037417
H	2.695688	3.847450	-3.621548
H	2.970753	1.984489	-5.374757
H	2.176841	-0.208971	-6.228540
H	0.352817	-1.426117	-5.013151
H	-1.344073	-1.422598	-3.284442
H	-0.691828	-0.744566	-1.777782
H	-1.862530	0.174815	-2.721045

TS Lutidine Pu III – Large core

E = -786.881497

G = -786.591222

C	-1.713428	5.610460	-0.957917
C	-2.475889	4.539981	-0.433796
C	-1.579719	3.520957	-0.024211
C	-0.262512	3.966625	-0.285496
C	-0.341600	5.254621	-0.871556
Pu	-1.403460	3.576866	-2.861790
N	0.488909	1.779996	-2.819805
C	-0.333661	0.716473	-2.602668
C	0.071947	-0.328995	-1.748684
C	1.344088	-0.301949	-1.208006
C	2.205863	0.758810	-1.509903
C	1.737786	1.794315	-2.310595
C	-1.634922	0.769519	-3.273435
C	-3.875440	2.498263	-2.777333
C	-2.428455	5.232744	-4.877716
C	-1.171030	5.796800	-4.548053
C	-0.162404	4.910534	-5.000815
C	-0.797562	3.804417	-5.621392
C	-2.195747	4.002919	-5.544333
H	0.646437	3.425732	-0.050507

H	-1.853824	2.580639	0.439647
H	-3.554830	4.512172	-0.340941
H	-2.104421	6.552173	-1.324742
H	0.495811	5.885563	-1.147719
H	-1.009097	6.751700	-4.062413
H	-3.397007	5.682514	-4.691262
H	0.906731	5.073210	-4.928471
H	-0.296242	2.966468	-6.091416
H	-2.957405	3.343268	-5.942768
H	-4.419105	2.006126	-3.592247
H	-4.251705	2.101441	-1.827763
H	-4.174597	3.558766	-2.815409
H	-2.638885	1.671062	-2.944792
H	-1.510667	0.933623	-4.350450
H	-2.222764	-0.137394	-3.117150
H	-0.606488	-1.153596	-1.554798
H	1.682285	-1.110858	-0.565476
H	3.217251	0.787985	-1.118542
C	2.589972	2.981343	-2.653965
H	3.563876	2.931513	-2.161985
H	2.748710	3.036495	-3.735964
H	2.097199	3.911130	-2.349532

TS Lutidine Pu III – Small core

E = -1307.748472
G = -1307.459303

C	-1.767910	5.577539	-1.093885
C	-2.554658	4.536950	-0.548899
C	-1.681860	3.508331	-0.114871
C	-0.352990	3.924551	-0.370321
C	-0.402891	5.197229	-0.985520
Pu	-1.484677	3.504007	-2.855661
N	0.480901	1.860570	-2.807577
C	-0.289944	0.754350	-2.630307
C	0.144894	-0.294806	-1.798431
C	1.408400	-0.226195	-1.238819
C	2.224327	0.878640	-1.503391
C	1.722380	1.915674	-2.283136
C	-1.579662	0.774415	-3.328476
C	-3.860211	2.408883	-2.767884
C	-2.210434	5.414299	-4.644184
C	-0.824433	5.642763	-4.439328
C	-0.114404	4.561599	-5.008025
C	-1.057491	3.662331	-5.565574
C	-2.352261	4.193404	-5.349289
H	0.541692	3.365967	-0.124382
H	-1.979512	2.578263	0.355587
H	-3.635345	4.525960	-0.473448
H	-2.136997	6.515014	-1.491729
H	0.447722	5.802857	-1.275567
H	-0.389190	6.508034	-3.954608
H	-3.014754	6.078282	-4.348660
H	0.961903	4.446456	-5.031980
H	-0.822894	2.746679	-6.095365
H	-3.286289	3.748785	-5.671584
H	-4.419302	1.888450	-3.554567
H	-4.215010	2.044151	-1.797324
H	-4.152318	3.471742	-2.840052
H	-2.612954	1.610571	-2.979733
H	-1.438308	0.969863	-4.397198
H	-2.140858	-0.154091	-3.203133
H	-0.500724	-1.151891	-1.635177
H	1.774198	-1.035056	-0.611572
H	3.229178	0.941326	-1.098813
C	2.537417	3.137204	-2.592789
H	3.437505	3.184770	-1.975441
H	2.843552	3.132190	-3.644929
H	1.948213	4.044370	-2.430132

Adduct of lutidine, Pu III – Large core

E = -786.906905
G = -786.616119

C	-1.597361	6.007428	-1.004673
C	-2.583417	5.126160	-0.496635
C	-1.922476	4.025814	0.096796
C	-0.526468	4.228937	-0.033729
C	-0.323511	5.452591	-0.718361
Pu	-1.462515	3.793242	-2.715932
N	0.163869	1.543374	-2.473805
C	-0.394809	0.313788	-2.454629
C	0.379534	-0.841952	-2.340588
C	1.760317	-0.729113	-2.244737
C	2.330741	0.536905	-2.266166
C	1.506714	1.657893	-2.382099
C	-1.888040	0.227846	-2.563820
C	-3.859211	3.038836	-2.817918
C	-2.275975	4.792373	-5.225487
C	-1.385162	5.762818	-4.704346
C	-0.075417	5.217943	-4.734755
C	-0.161207	3.911179	-5.274489
C	-1.521404	3.647166	-5.570536
H	0.246727	3.581831	0.365806
H	-2.402243	3.190593	0.593873
H	-3.655390	5.269559	-0.547715
H	-1.780392	6.961300	-1.485487
H	0.632145	5.915296	-0.938165
H	-1.648998	6.763736	-4.383485
H	-3.346206	4.906273	-5.343225
H	0.832341	5.735521	-4.445397
H	0.669833	3.243216	-5.472443
H	-1.913096	2.740014	-6.016218
H	-4.107209	2.395808	-3.676582
H	-4.214665	2.515371	-1.916780
H	-4.505877	3.924979	-2.916989
H	-2.381759	0.770530	-1.750735
H	-2.245551	0.667622	-3.501093
H	-2.226196	-0.809913	-2.529421
H	-0.105819	-1.812186	-2.328842
H	2.382924	-1.614907	-2.155509
H	3.405391	0.668338	-2.195035
C	2.093400	3.037389	-2.409442
H	3.182951	3.004987	-2.343073
H	1.819912	3.556959	-3.333650
H	1.714849	3.636221	-1.574862

Adduct of lutidine, Pu III – Small core

E = -1307.769789
G = -1307.480825

C	-2.105607	5.747506	-1.131240
C	-2.898080	4.686376	-0.629833
C	-2.027932	3.719800	-0.069963
C	-0.699661	4.189002	-0.209867
C	-0.744200	5.438946	-0.871864
Pu	-1.596400	3.661056	-2.795584
N	0.294523	1.697645	-2.444338
C	-0.156984	0.424034	-2.398629
C	0.695796	-0.654115	-2.164925
C	2.051356	-0.417881	-1.968724
C	2.512422	0.889889	-2.016487
C	1.611783	1.930156	-2.262436
C	-1.626353	0.210099	-2.607754
C	-3.849626	2.738560	-3.109535
C	-1.433911	5.718260	-4.572446
C	-0.108760	5.214834	-4.503369
C	-0.096072	3.937050	-5.112493
C	-1.411893	3.645859	-5.545412
C	-2.237593	4.747852	-5.218260
H	0.189828	3.684386	0.148410
H	-2.330851	2.794388	0.407176
H	-3.977897	4.620291	-0.670043
H	-2.474821	6.653948	-1.595440
H	0.103236	6.074019	-1.102561
H	0.746188	5.739636	-4.094376
H	-1.762558	6.689345	-4.223100
H	0.767226	3.295755	-5.245420
H	-1.732058	2.744113	-6.054978
H	-3.297472	4.828520	-5.424914
H	-3.968417	2.113513	-4.009599
H	-4.242735	2.151742	-2.263647
H	-4.551536	3.579521	-3.238558
H	-2.219884	0.732880	-1.848868
H	-1.951229	0.585887	-3.584413
H	-1.883822	-0.850131	-2.556825
H	0.291424	-1.660587	-2.134496
H	2.735447	-1.240370	-1.779495
H	3.562919	1.118857	-1.867807
C	2.111051	3.341506	-2.358440
H	3.008187	3.478884	-1.748808
H	2.372550	3.584321	-3.394194
H	1.351285	4.056263	-2.035225

Product lutidine, Pu III – Large core

E = -746.416124
G = -746.168365

C	-1.045170	5.593119	-1.056796
C	-2.152804	4.720920	-0.902785
C	-1.667094	3.475543	-0.429767
C	-0.259687	3.579171	-0.294603
C	0.123679	4.886855	-0.681510
Pu	-0.746944	3.644492	-3.080062
N	1.626568	3.174715	-3.897098
C	1.506948	4.191272	-4.815982
C	2.021937	3.999317	-6.126041
C	2.720592	2.850075	-6.419209
C	2.905651	1.863646	-5.434132
C	2.325662	2.055298	-4.190623
C	0.753282	5.334872	-4.388094
C	2.424686	1.026159	-3.099157
C	-2.004437	3.078957	-5.534176
C	-3.065522	3.341466	-4.628567
C	-3.121775	2.275627	-3.697439
C	-2.087568	1.360478	-4.018138
C	-1.401790	1.855126	-5.158144
H	-0.576556	1.371821	-5.667908
H	-1.720067	3.694411	-6.378826
H	-3.744467	4.186053	-4.670634
H	-3.843016	2.166527	-2.896305
H	-1.895208	0.418361	-3.516120
H	-2.271258	2.612178	-0.176069
H	-3.193167	4.974724	-1.071455
H	0.403555	2.806671	0.078755
H	1.131895	5.283915	-0.666816
H	-1.089321	6.629039	-1.372887
H	1.085379	5.752186	-3.432854
H	0.579916	6.103728	-5.137099
H	1.892967	4.785372	-6.863274
H	3.147402	2.710479	-7.409527
H	3.473872	0.963116	-5.640960
H	3.035193	0.174370	-3.407492
H	2.864760	1.463202	-2.196881
H	1.433231	0.644112	-2.826486

Product lutidine, Pu III – Small core

E = -1267.283466
G = -1267.035475

C	-1.157836	5.586140	-1.200296
C	-2.224906	4.661169	-1.091162
C	-1.701531	3.446892	-0.574482
C	-0.312541	3.625734	-0.364251
C	0.023461	4.945446	-0.752688
Pu	-0.656496	3.663629	-3.080580
N	1.638950	3.168261	-3.874940
C	1.536729	4.213877	-4.764809
C	1.977660	4.026873	-6.104861
C	2.600227	2.851329	-6.453048
C	2.776571	1.830722	-5.497522
C	2.263790	2.018802	-4.226379
C	0.858088	5.367138	-4.268187
C	2.355215	0.962701	-3.161154
C	-1.893507	3.097682	-5.415147
C	-2.953547	3.347095	-4.505875
C	-2.984337	2.287146	-3.568171
C	-1.940721	1.385826	-3.890493
C	-1.267798	1.883833	-5.034768
H	-0.429280	1.418289	-5.538963
H	-1.617282	3.716520	-6.260351
H	-3.636794	4.188395	-4.536865
H	-3.689234	2.178895	-2.753366
H	-1.718806	0.460097	-3.370660
H	-2.271177	2.553543	-0.348383
H	-3.263665	4.854449	-1.331166
H	0.373544	2.888788	0.038552
H	1.010796	5.389569	-0.703039
H	-1.232317	6.609269	-1.550389
H	1.191830	5.706516	-3.284475
H	0.678968	6.180232	-4.967282
H	1.856732	4.836381	-6.817843
H	2.974684	2.712751	-7.464414
H	3.288660	0.908666	-5.751169
H	2.892485	0.080637	-3.517202
H	2.868851	1.352655	-2.276216
H	1.355852	0.641428	-2.843118

Pyridine N-oxide

E = -323.325931
G = -323.261160

C	0.034827	0.000000	0.016670
C	0.020202	0.000000	1.397982
C	1.212436	0.000000	2.120803
C	2.404669	0.000000	1.397982
C	2.390045	0.000000	0.016670
H	-0.942001	0.000000	1.900493
H	1.212436	0.000000	3.204924
H	3.366872	0.000000	1.900493
H	3.269832	0.000000	-0.613179
N	1.212436	0.000000	-0.687369
H	-0.844960	0.000000	-0.613179
O	1.212436	0.000000	-1.953288

TS Pyridine N-oxide Np IV – Large core

E = -828.395014
G = -828.116786

C	0.686201	1.705400	-1.481775
C	-0.118808	0.964132	-2.389211
C	0.315208	-0.379267	-2.362263
C	1.381042	-0.475279	-1.431242
C	1.622064	0.818176	-0.907227
Np	-0.857168	0.025227	0.123332
C	-0.045439	-1.406586	2.359245
C	1.005323	-0.497454	2.073356
C	0.543165	0.811948	2.362127
C	-0.792753	0.708737	2.826599
C	-1.151487	-0.659283	2.827067
O	-3.202499	-0.354421	0.843751
N	-3.891298	-0.371961	-0.275877
C	-3.293556	0.197095	-1.358943
C	-3.995841	0.172008	-2.563111
C	-5.246168	-0.432712	-2.653489
C	-5.807909	-0.995824	-1.504719
C	-5.109936	-0.955274	-0.312258
C	-2.139798	2.405327	-0.092864
C	-1.349611	-2.326055	-0.517384
H	-0.907072	1.369854	-3.010667
H	-0.094451	-1.196510	-2.940729
H	1.934114	-1.375537	-1.193025
H	2.388883	1.082477	-0.190235
H	0.613501	2.768643	-1.291211
H	-1.426834	1.531878	3.132628
H	1.118903	1.725522	2.272314
H	1.997214	-0.762250	1.729388
H	-0.004683	-2.482297	2.248050
H	-2.117511	-1.059928	3.102439
H	-2.118901	3.081060	-0.954798
H	-1.334026	2.737618	0.578687
H	-3.081056	2.553967	0.447148
H	-1.989430	-2.805361	0.233868
H	-1.852296	-2.433246	-1.487340
H	-0.423877	-2.915377	-0.580524
H	-5.450560	-1.372122	0.627028
H	-6.782083	-1.472014	-1.525377
H	-5.781217	-0.465609	-3.597495
H	-3.544647	0.635218	-3.435773
H	-2.564938	1.177274	-0.914403

TS Pyridine N-oxide Np IV – Small core

E = -1304.647292
G = -1304.369769

C	0.389896	1.623388	-1.711910
C	-0.194828	0.585678	-2.478845

C	0.481924	-0.619423	-2.177671
C	1.471633	-0.330818	-1.212723
C	1.417183	1.057426	-0.926463
Np	-0.891215	0.002417	0.118948
C	-0.025655	-1.454076	2.272101
C	1.010088	-0.523635	2.015020
C	0.527565	0.769511	2.335377
C	-0.804882	0.637207	2.790952
C	-1.145008	-0.735106	2.750803
O	-3.182367	-0.354094	0.844563
N	-3.873801	-0.328395	-0.273847
C	-3.289698	0.311411	-1.321982
C	-3.990039	0.346111	-2.525498
C	-5.229901	-0.274653	-2.649467
C	-5.774430	-0.924645	-1.539195
C	-5.073767	-0.944548	-0.347250
C	-2.011322	2.393237	0.049391
C	-1.401015	-2.279221	-0.563989
H	-0.991007	0.700067	-3.203123
H	0.283686	-1.587618	-2.615349
H	2.167107	-1.043797	-0.788321
H	2.065573	1.592628	-0.244214
H	0.111049	2.668171	-1.737386
H	-1.454768	1.444090	3.106349
H	1.087934	1.693903	2.262305
H	2.007575	-0.761294	1.669293
H	0.029524	-2.525869	2.131492
H	-2.105938	-1.156391	3.012992
H	-2.146706	3.130855	-0.749652
H	-1.075293	2.665693	0.563883
H	-2.829562	2.503197	0.769267
H	-2.088130	-2.726138	0.167453
H	-1.861247	-2.375311	-1.557069
H	-0.490852	-2.896560	-0.579165
H	-5.400077	-1.430303	0.563518
H	-6.737348	-1.421031	-1.589347
H	-5.768736	-0.255203	-3.591699
H	-3.549727	0.870932	-3.368140
H	-2.533653	1.229398	-0.856315

Adduct of pyridine N-oxide, Np IV – Large core

E = -828.415993
G = -828.138153

C	1.010793	1.791477	-1.427410
C	0.366585	0.943032	-2.365424
C	0.882001	-0.364090	-2.203006
C	1.824103	-0.333769	-1.146145
C	1.913282	1.005573	-0.678185
Np	-0.565277	0.105242	0.128095
C	-0.212702	-1.453206	2.407807
C	0.946822	-0.646932	2.283702
C	0.575127	0.698305	2.548099
C	-0.812275	0.720890	2.834028
C	-1.295281	-0.606994	2.744097
O	-3.118197	-0.302948	0.352959
N	-4.028276	-0.364794	-0.555813
C	-3.871505	0.235336	-1.767811
C	-4.862977	0.158515	-2.729498
C	-6.042282	-0.534871	-2.472493
C	-6.186972	-1.137450	-1.223236
C	-5.177800	-1.044800	-0.285600
C	-1.739939	2.324217	-0.024297
C	-1.247569	-2.123787	-0.790970
H	-0.362603	1.255461	-3.103874
H	0.601730	-1.237354	-2.776154
H	2.406244	-1.175201	-0.790514
H	2.571694	1.364192	0.103375
H	0.838421	2.852846	-1.309280
H	-1.398228	1.598377	3.075019
H	1.239935	1.553664	2.555483
H	1.946996	-0.998995	2.062644
H	-0.260911	-2.525468	2.267437
H	-2.322377	-0.917194	2.883128
H	-1.971485	2.697952	-1.033448
H	-1.072874	3.082164	0.415336
H	-2.674207	2.356207	0.550829
H	-1.926260	-2.642253	-0.101539
H	-1.768040	-2.070554	-1.760227
H	-0.383212	-2.784205	-0.951071
H	-5.205077	-1.487103	0.701065
H	-7.082840	-1.690972	-0.962984
H	-6.824822	-0.603132	-3.219879
H	-4.694841	0.654220	-3.679661
H	-2.948660	0.788822	-1.884430

Adduct of pyridine N-oxide, Np IV – Small core

E = -1304.666761
G = -1304.390157

C	0.588647	1.542433	-1.749592
C	0.545850	0.301553	-2.431659
C	1.452147	-0.583347	-1.796281
C	2.034769	0.102003	-0.708363
C	1.498878	1.416192	-0.677304
Np	-0.591740	-0.216705	0.004963
C	-0.379514	-1.503584	2.426881
C	0.751365	-0.662127	2.350651
C	0.305808	0.683527	2.429874
C	-1.100549	0.671955	2.556216
C	-1.526685	-0.679447	2.537773
O	-2.679171	-1.012513	-0.987614
N	-3.834961	-0.485517	-1.257566
C	-4.049679	0.091468	-2.465885
C	-5.289733	0.612089	-2.787561
C	-6.332239	0.551747	-1.865653
C	-6.087065	-0.041433	-0.629031
C	-4.834682	-0.552318	-0.343004
C	-2.047477	1.763813	-0.170183
C	-0.391860	-2.610504	-0.436674
H	-0.048056	0.075497	-3.310273
H	1.658842	-1.603012	-2.091024
H	2.778788	-0.298577	-0.031614
H	1.760431	2.195627	0.027320
H	0.022930	2.429903	-1.999918
H	-1.737329	1.541573	2.647545
H	0.935171	1.564582	2.423157
H	1.780184	-0.989537	2.268626
H	-0.370484	-2.584657	2.399347
H	-2.549289	-1.026891	2.634034
H	-2.328031	1.990909	-1.210997
H	-1.536047	2.656932	0.215081
H	-2.981293	1.664615	0.405681
H	-1.187328	-3.157366	0.089473
H	-0.519814	-2.801031	-1.512203
H	0.570867	-3.042639	-0.132041
H	-4.557285	-1.028834	0.587588
H	-6.860746	-0.113398	0.127606
H	-7.309445	0.957340	-2.103679
H	-5.423246	1.065822	-3.763514
H	-3.186697	0.098156	-3.117816

Product pyridine N-oxide, Np IV – Large core

E = -787.950001
G = -787.715393

C	1.068338	1.360744	-1.065209
N	0.077820	1.289607	-1.978894
C	-0.160577	0.243154	-2.815382
C	0.718657	-0.833441	-2.687355
C	1.764231	-0.825648	-1.762798
C	1.937192	0.290046	-0.942650
O	-0.772562	2.309565	-2.114139
Np	-2.187071	1.406913	-3.903071
C	-2.153361	-0.734149	-5.132697
C	-2.657391	2.795744	-6.230179
C	-1.509989	2.019412	-6.517535
C	-0.436051	2.520968	-5.738184
C	-0.917051	3.623575	-4.987071
C	-2.289373	3.791111	-5.281794
C	-4.922185	1.437751	-3.628716
C	-4.444834	2.316786	-2.616645
C	-3.790426	1.534839	-1.636451
C	-3.843160	0.179506	-2.046025
C	-4.553785	0.118774	-3.272798
H	-3.306885	1.912237	-0.744760
H	-3.437623	-0.666207	-1.504327
H	-4.778363	-0.778322	-3.833672
H	-5.496580	1.724281	-4.501717
H	-4.588241	3.390168	-2.583057
H	-0.341085	4.216462	-4.288332
H	-2.937636	4.560908	-4.880500
H	-3.635464	2.676144	-6.681107
H	-1.461492	1.189398	-7.209140
H	0.580994	2.148493	-5.742238
H	-1.191611	-0.891967	-5.639182
H	-2.304630	-1.589184	-4.460129
H	-2.934311	-0.792688	-5.905622
H	1.110444	2.272424	-0.482108
H	2.735900	0.340281	-0.210432
H	2.437881	-1.673625	-1.678275
H	0.570217	-1.694078	-3.333736

Product pyridine N-oxide, Np IV – Small core

E = -1264.194400
G = -1263.959300

C	0.197626	0.809202	-2.122011
N	-0.099778	-0.363914	-2.714692
C	0.522630	-1.553413	-2.504333
C	1.554308	-1.515087	-1.563975
C	1.906638	-0.339911	-0.897103
C	1.219002	0.838412	-1.187279
O	-1.102514	-0.423865	-3.599560
Np	-0.893698	-2.677263	-4.323387
C	-0.133705	-1.723632	-6.366418
C	-3.508827	-2.337434	-3.660346
C	-3.374220	-3.726937	-3.891119
C	-3.163086	-3.917354	-5.280269
C	-3.159156	-2.649375	-5.902988
C	-3.367639	-1.672860	-4.901216
C	-0.158764	-5.125000	-5.306421
C	1.017680	-4.344335	-5.378553
C	1.444458	-4.079044	-4.059273
C	0.535987	-4.705755	-3.168267
C	-0.448931	-5.359711	-3.938842
H	2.318421	-3.505599	-3.778519
H	1.507110	-4.015034	-6.284808
H	-0.717698	-5.504232	-6.152084
H	-1.274216	-5.945270	-3.554138
H	0.593190	-4.691513	-2.086394
H	-3.676394	-1.860285	-2.702220
H	-3.456740	-4.508480	-3.145194
H	-3.050374	-4.871056	-5.778409
H	-3.017983	-2.457812	-6.958599
H	-3.389955	-0.600850	-5.048376
H	-0.703682	-0.797241	-6.527391
H	0.919631	-1.435639	-6.209450
H	-0.176882	-2.314498	-7.288828
H	-0.400892	1.659410	-2.425373
H	1.463709	1.776255	-0.700481
H	2.708209	-0.336403	-0.163804
H	2.094518	-2.434351	-1.351220

TS Pyridine N-oxide Pu IV – Large core

E = -829.147966
G = -828.869295

C	0.669560	1.700906	-1.476557
C	-0.131666	0.952568	-2.381776
C	0.308694	-0.388389	-2.349874
C	1.374834	-0.476042	-1.418184
C	1.609977	0.820586	-0.899524
Pu	-0.854394	0.021072	0.121476
C	-0.040667	-1.403890	2.340330
C	1.003310	-0.486599	2.056052
C	0.530434	0.819110	2.344131
C	-0.804982	0.705017	2.807970
C	-1.152481	-0.665636	2.808769
O	-3.189773	-0.359329	0.842196
N	-3.881040	-0.372898	-0.275569
C	-3.279917	0.191472	-1.358914
C	-3.983564	0.171208	-2.562436
C	-5.238461	-0.424334	-2.651379
C	-5.803654	-0.982385	-1.501764
C	-5.104454	-0.946324	-0.309883
C	-2.131259	2.391543	-0.082546
C	-1.344636	-2.317136	-0.510451
H	-0.922261	1.352077	-3.004112
H	-0.097319	-1.209693	-2.925016
H	1.931867	-1.372815	-1.176368
H	2.374751	1.091199	-0.182853
H	0.591548	2.764242	-1.289135
H	-1.446405	1.523094	3.111912
H	1.098479	1.737381	2.254111
H	1.997235	-0.743767	1.712583
H	0.008540	-2.479115	2.228588
H	-2.115897	-1.073845	3.081669
H	-2.115654	3.069191	-0.943045
H	-1.325314	2.724508	0.587413
H	-3.072156	2.532495	0.459918
H	-1.981179	-2.795458	0.243805
H	-1.851565	-2.423584	-1.478072
H	-0.418812	-2.905471	-0.577746
H	-5.447647	-1.359683	0.630027
H	-6.781447	-1.451153	-1.521393
H	-5.774468	-0.453938	-3.594966
H	-3.530097	0.630609	-3.435973
H	-2.548295	1.170397	-0.908328

TS Pyridine N-oxide Pu IV – Small core

E = -1344.120719
G = -1343.844350

C	0.173415	1.405586	-1.876463
C	-0.332364	0.254137	-2.531442
C	0.447069	-0.858484	-2.128412
C	1.415250	-0.399872	-1.212420
C	1.246421	1.000563	-1.054955
Pu	-0.968378	-0.122160	0.103743
C	0.219056	-1.363144	2.227335
C	1.034442	-0.237735	1.973433
C	0.294818	0.928277	2.297561
C	-0.975234	0.519411	2.761596
C	-1.027437	-0.893297	2.708588
O	-3.260405	-0.517245	0.781734
N	-3.922498	-0.316358	-0.340601
C	-3.340196	0.505614	-1.254500
C	-4.012421	0.727383	-2.453367
C	-5.235362	0.113436	-2.708716
C	-5.782466	-0.728521	-1.737745
C	-5.104545	-0.938923	-0.551135
C	-1.863877	2.423486	0.196287
C	-1.133940	-2.519769	-0.268497
H	-1.134034	0.232219	-3.259090
H	0.329470	-1.876020	-2.473946
H	2.163832	-1.013271	-0.727843
H	1.846255	1.649176	-0.428863
H	-0.189251	2.417668	-1.993519
H	-1.780648	1.171572	3.074994
H	0.653830	1.947714	2.231254
H	2.057851	-0.260154	1.622759
H	0.499151	-2.398411	2.086650
H	-1.879339	-1.505562	2.975840
H	-2.123678	3.149366	-0.585040
H	-0.867347	2.695093	0.558979
H	-2.576284	2.535999	1.021317
H	-1.719893	-2.922722	0.566789
H	-1.748967	-2.575212	-1.183896
H	-0.243461	-3.136016	-0.420093
H	-5.434928	-1.581957	0.254632
H	-6.731754	-1.229345	-1.893247
H	-5.758235	0.284520	-3.644393
H	-3.563338	1.396701	-3.181075
H	-2.540816	1.313450	-0.719149

Adduct of pyridine N-oxide, Pu IV – Large core

E = -829.170120
G = -828.892505

C	0.974618	1.797637	-1.426896
C	0.331891	0.939406	-2.357017
C	0.859522	-0.362617	-2.191675
C	1.807339	-0.319575	-1.140740

C	1.887461	1.022932	-0.678951
Pu	-0.560479	0.105670	0.138059
C	-0.196405	-1.462801	2.383793
C	0.957282	-0.647891	2.264483
C	0.576369	0.693193	2.538007
C	-0.810767	0.703995	2.825919
C	-1.284745	-0.626505	2.726972
O	-3.111085	-0.293344	0.336594
N	-4.018098	-0.357622	-0.573653
C	-3.839487	0.195904	-1.804920
C	-4.829509	0.117059	-2.767912
C	-6.030485	-0.530828	-2.493487
C	-6.197416	-1.086689	-1.225389
C	-5.189456	-0.993237	-0.286788
C	-1.735566	2.306833	0.022401
C	-1.238508	-2.117269	-0.761637
H	-0.403161	1.242444	-3.093568
H	0.582938	-1.241009	-2.758629
H	2.398850	-1.154317	-0.785129
H	2.547330	1.390947	0.096884
H	0.793771	2.857836	-1.312193
H	-1.402562	1.575955	3.071885
H	1.234634	1.553428	2.549549
H	1.959437	-0.991552	2.039628
H	-0.237780	-2.534034	2.234790
H	-2.309663	-0.944795	2.863593
H	-2.002243	2.663197	-0.984165
H	-1.065094	3.077048	0.433726
H	-2.653518	2.332360	0.622929
H	-1.918415	-2.631429	-0.070624
H	-1.753579	-2.074783	-1.733955
H	-0.370018	-2.774956	-0.910509
H	-5.234145	-1.400697	0.714145
H	-7.110639	-1.603657	-0.950602
H	-6.812208	-0.600049	-3.241602
H	-4.642573	0.574779	-3.733508
H	-2.898750	0.713099	-1.939609

Adduct of pyridine N-oxide, Pu IV – Small core

E = -1344.142154

G = -1343.866023

C	0.303415	1.156536	-1.694643
C	-0.612965	0.254978	-2.293933
C	-0.124112	-1.057929	-2.101537
C	1.077644	-0.976331	-1.363327
C	1.346288	0.395647	-1.124111
Pu	-0.843316	-0.167798	0.433684
C	0.256742	-1.127571	2.761251
C	1.295981	-0.402577	2.140711
C	0.950387	0.972930	2.167950
C	-0.301233	1.096506	2.807955
C	-0.742660	-0.203752	3.158773
O	-3.199315	-0.505121	-0.050111
N	-3.998068	-0.223657	-1.037972
C	-4.694656	0.940095	-1.033437
C	-5.563360	1.239406	-2.068350
C	-5.728756	0.344371	-3.122608
C	-5.003333	-0.845643	-3.102161
C	-4.144082	-1.113056	-2.052731
C	-1.681679	2.156010	0.365646
C	-0.979479	-2.622938	0.534619
H	-1.509804	0.531583	-2.837379
H	-0.587374	-1.973154	-2.449402
H	1.693806	-1.812599	-1.058621
H	2.210946	0.791868	-0.607109
H	0.224166	2.235088	-1.688518
H	-0.828598	2.021742	2.997235
H	1.544186	1.789703	1.776673
H	2.203778	-0.824617	1.727212
H	0.230807	-2.197275	2.914871
H	-1.663863	-0.447014	3.677471
H	-2.161260	2.311001	-0.611976
H	-0.949618	2.954175	0.521742
H	-2.444141	2.225711	1.157357
H	-1.644109	-2.847426	1.381629
H	-1.471908	-2.948463	-0.391923
H	-0.045867	-3.179852	0.654347
H	-3.543585	-2.007482	-1.951262
H	-5.094264	-1.577898	-3.896981
H	-6.405857	0.567733	-3.939850
H	-6.101476	2.180421	-2.035090
H	-4.494983	1.579584	-0.184064

Product pyridine N-oxide, Pu IV – Large core

E = -788.704563

G = -788.469689

C	1.136484	1.211520	-1.265534
N	0.161309	1.071127	-2.187778
C	-0.056036	-0.031508	-2.954702
C	0.826557	-1.091118	-2.739580
C	1.856472	-1.012731	-1.800842
C	2.009480	0.157695	-1.056533
O	-0.694384	2.070530	-2.406325
Pu	-2.055963	1.024054	-4.149592
C	-2.006099	-1.201114	-5.188211
C	-4.780716	1.098316	-3.945995
C	-4.315680	2.049091	-2.994495
C	-3.687737	1.339980	-1.944279
C	-3.742839	-0.042323	-2.250281
C	-4.430708	-0.191823	-3.482802
C	-2.479433	2.258197	-6.545497
C	-1.364231	1.419938	-6.780409
C	-0.268931	1.930343	-6.037001
C	-0.704090	3.098862	-5.361917
C	-2.070320	3.298746	-5.664371
H	-3.216588	1.781622	-1.075901
H	-3.354950	-0.846859	-1.637685
H	-4.650905	-1.127596	-3.978284
H	-5.336110	1.320984	-4.849295
H	-4.449903	3.122817	-3.046441
H	-0.104768	3.712335	-4.701940
H	-2.687119	4.116948	-5.313043
H	-3.462411	2.147717	-6.987680
H	-1.349616	0.544400	-7.414988
H	0.732036	1.517577	-6.015336
H	-1.039596	-1.399948	-5.670125
H	-2.159362	-1.991131	-4.440655
H	-2.780600	-1.334974	-5.957931
H	1.163643	2.161035	-0.745326
H	2.795897	0.263226	-0.316905
H	2.533247	-1.848405	-1.647249
H	0.693136	-1.994933	-3.327569

Product pyridine N-oxide, Pu IV – Small core

E = -1303.669850

G = -1303.437278

C	-0.281888	1.040555	-2.005800
N	-0.007895	-0.161455	-2.551842
C	0.999878	-0.996751	-2.191925
C	1.814397	-0.522762	-1.160001
C	1.594597	0.714368	-0.553307
C	0.527191	1.504064	-0.983229
O	-0.771593	-0.622838	-3.555646
Pu	0.316781	-2.704658	-3.951547
C	2.456725	-2.472879	-4.954840
C	-0.910703	-1.807166	-6.187267
C	0.031030	-2.747674	-6.666888
C	-0.379220	-4.028905	-6.239618
C	-1.591860	-3.884033	-5.514980
C	-1.916312	-2.511939	-5.478335
C	-0.521080	-4.816878	-2.452197
C	0.293258	-4.059727	-1.580708
C	1.629341	-4.155337	-2.040097
C	1.648253	-4.990420	-3.182955
C	0.321368	-5.401248	-3.434999
H	2.490355	-3.675636	-1.591841
H	2.523341	-5.268239	-3.755238
H	0.002161	-6.067311	-4.225220
H	-1.591726	-4.959017	-2.364114
H	-0.043627	-3.492019	-0.721890
H	-2.771469	-2.066290	-4.985528
H	-2.169043	-4.686593	-5.073160
H	0.132504	-4.959166	-6.451030
H	0.909596	-2.526474	-7.256927
H	-0.870644	-0.734017	-6.322759
H	2.444893	-1.478356	-5.432883
H	3.121439	-2.407885	-4.076937
H	2.896681	-3.181642	-5.663296
H	-1.132022	1.566973	-2.422131
H	0.317476	2.470854	-0.538721
H	2.242947	1.062990	0.245675
H	2.642557	-1.142981	-0.827267

TS Pyridine N-oxide Np III – Large core

E = -782.745931

G = -782.506868

C	1.334581	1.192108	-1.862980
N	0.245413	0.732856	-2.524885
C	-0.382609	-0.433651	-2.217612
C	0.153720	-1.172725	-1.164371
C	1.271283	-0.743596	-0.453043
C	1.864887	0.466132	-0.813786
O	-0.213413	1.464118	-3.532236
Np	-1.694740	0.100076	-4.930388
C	-3.042536	-1.177890	-2.966665
C	-3.608631	1.072562	-6.765134
C	-2.581498	2.051559	-6.762741
C	-2.618249	2.720681	-5.514470
C	-3.661178	2.153540	-4.743405
C	-4.275479	1.137001	-5.516916
C	-0.655304	-1.147432	-7.230570
C	0.483794	-0.905242	-6.422038
C	0.421987	-1.777805	-5.306390
C	-0.756473	-2.554850	-5.422691
C	-1.422773	-2.165280	-6.610861
H	1.163311	-1.859656	-4.520757
H	1.281876	-0.204068	-6.639223
H	-0.882588	-0.663243	-8.172906
H	-2.338312	-2.597214	-6.999251
H	-1.078236	-3.330204	-4.737755
H	-3.954398	2.460792	-3.746170
H	-5.126891	0.536486	-5.217583
H	-3.863888	0.419679	-7.591716
H	-1.915606	2.276853	-7.588117
H	-1.967923	3.530484	-5.205418
H	-2.960197	-2.061562	-2.321244
H	-3.602900	-1.540823	-3.849084
H	-3.702958	-0.466452	-2.454212
H	1.726089	2.133635	-2.226827
H	2.735569	0.852534	-0.295229
H	1.672761	-1.331532	0.366805
H	-0.336379	-2.106993	-0.902674
H	-1.636176	-0.771955	-2.701067

TS Pyridine N-oxide Np III – Small core

E = -1264.787137

G = -1264.547523

C	1.101638	1.159473	-1.707635
N	0.055613	0.713027	-2.441201
C	-0.491076	-0.523650	-2.290645
C	0.073150	-1.349262	-1.321038
C	1.143832	-0.931016	-0.534929
C	1.660435	0.349226	-0.737051
O	-0.446739	1.513630	-3.371080
Np	-1.710465	0.084489	-4.841580
C	-3.120720	-1.288164	-3.135980
C	-3.549979	1.014923	-6.628876
C	-2.410245	1.834562	-6.839523
C	-2.243517	2.655329	-5.700610
C	-3.281144	2.349592	-4.784327
C	-4.091328	1.343095	-5.360051
C	-1.027193	-1.272165	-7.126960
C	0.159986	-0.633753	-6.686442
C	0.575475	-1.268698	-5.488716
C	-0.357016	-2.290939	-5.188183
C	-1.347498	-2.292220	-6.201538
H	1.464890	-1.030169	-4.917012
H	0.678541	0.169938	-7.195656
H	-1.580537	-1.031767	-8.025899
H	-2.190337	-2.970619	-6.266175
H	-0.310980	-2.966213	-4.342614
H	-3.428928	2.812294	-3.815736
H	-4.976593	0.905482	-4.912874
H	-3.961621	0.301981	-7.333223
H	-1.790745	1.844550	-7.727991
H	-1.462704	3.391179	-5.550831
H	-3.089310	-2.161948	-2.474086
H	-3.571469	-1.663032	-4.075822
H	-3.837842	-0.579801	-2.698923
H	1.435560	2.160013	-1.951845
H	2.492943	0.727089	-0.153625
H	1.568276	-1.582962	0.222389
H	-0.356569	-2.338033	-1.184751
H	-1.699848	-0.866538	-2.772571

Adduct of pyridine N-oxide, Np III – Large core

E = -782.767704

G = -782.526575

C	1.465637	1.057150	-1.833150
N	0.321094	0.490375	-2.294626
C	-0.355075	-0.413165	-1.537936
C	0.119783	-0.767631	-0.287626
C	1.291520	-0.200762	0.207831
C	1.964272	0.724946	-0.587576
O	-0.117080	0.837041	-3.467590
Np	-1.742420	-0.044259	-5.155067
C	-3.027492	-1.465185	-3.445794
C	-3.890814	1.139474	-6.576727
C	-2.793757	2.000491	-6.836152
C	-2.482547	2.683830	-5.636066
C	-3.386634	2.246725	-4.635645
C	-4.258660	1.295848	-5.217004
C	-0.555719	-1.004669	-7.555964
C	0.499485	-1.074377	-6.615619
C	0.190883	-2.099473	-5.685948
C	-1.052814	-2.665946	-6.053631
C	-1.518337	-1.986306	-7.206305
H	0.816470	-2.419818	-4.860073
H	1.400607	-0.470909	-6.624293
H	-0.605362	-0.340995	-8.411335
H	-2.429047	-2.206638	-7.751885
H	-1.555721	-3.481821	-5.549487
H	-3.422967	2.600092	-3.611338
H	-5.071882	0.787195	-4.713955
H	-4.388002	0.506577	-7.303173
H	-2.303799	2.136372	-7.793418
H	-1.708608	3.433389	-5.512033
H	-2.520048	-2.338507	-3.004583
H	-3.872195	-1.896056	-4.009387
H	-3.501264	-0.917530	-2.614487
H	1.919395	1.762598	-2.516541
H	2.881086	1.198663	-0.253962
H	1.670907	-0.471996	1.186936
H	-0.445215	-1.493494	0.287042
H	-1.256762	-0.807638	-2.000700

Adduct of pyridine N-oxide, Np III – Small core

E = -1264.805685

G = -1264.565218

C	1.266803	0.966980	-1.567775
N	0.230825	0.345973	-2.188159
C	-0.334443	-0.767140	-1.651674
C	0.146667	-1.283150	-0.461733
C	1.211740	-0.668585	0.193443
C	1.769502	0.474447	-0.378712
O	-0.213205	0.836548	-3.308846
Np	-1.707287	0.122721	-5.084794
C	-3.102549	-1.306834	-3.600571
C	-3.689867	1.149899	-6.709568
C	-2.566851	1.981334	-6.950277
C	-2.320573	2.734438	-5.778587
C	-3.291447	2.368352	-4.810926
C	-4.138813	1.393034	-5.388515
C	-1.215528	-1.247650	-7.400340
C	0.022957	-0.643231	-7.067531
C	0.524199	-1.290302	-5.909337

C	-0.406317	-2.283131	-5.524809
C	-1.484293	-2.255582	-6.444093
H	1.464829	-1.072349	-5.416460
H	0.517538	0.144349	-7.623918
H	-1.838340	-0.993046	-8.248950
H	-2.352987	-2.902080	-6.422644
H	-0.311664	-2.956166	-4.680935
H	-3.384595	2.779761	-3.812001
H	-4.983704	0.919001	-4.904363
H	-4.142842	0.469758	-7.421101
H	-2.006891	2.042086	-7.875544
H	-1.539947	3.476089	-5.650011
H	-2.732227	-2.267751	-3.209201
H	-3.921222	-1.588406	-4.287248
H	-3.597703	-0.787479	-2.763610
H	1.635632	1.843467	-2.083943
H	2.598717	0.994788	0.088181
H	1.596992	-1.067621	1.125399
H	-0.327747	-2.171798	-0.059591
H	-1.167108	-1.165663	-2.228601

Product pyridine N-oxide, Np III – Large core

E = -742.288067
G = -742.089395

C	1.750694	1.473244	-2.167836
C	0.812053	1.040429	-3.138571
C	-0.066546	0.115664	-2.516479
C	0.335168	-0.030467	-1.168107
C	1.462360	0.805175	-0.953361
Np	2.424102	-1.240588	-2.668516
O	1.261862	-3.360083	-3.016710
N	1.462261	-3.899892	-1.804886
C	0.951599	-5.129984	-1.574861
C	1.133801	-5.721206	-0.338765
C	1.843052	-5.029536	0.643204
C	2.345852	-3.763831	0.345226
C	2.168002	-3.155596	-0.901661
C	5.169575	-0.544240	-2.642062
C	4.720458	-0.162223	-3.930569
C	4.437422	-1.343592	-4.662635
C	4.720124	-2.454718	-3.829669
C	5.171381	-1.961694	-2.581469
H	-0.146232	-0.653089	-0.423724
H	-0.913136	-0.374295	-2.983971
H	0.742978	1.398987	-4.159957
H	2.534379	2.205675	-2.322388
H	1.981490	0.943605	-0.011448
H	5.489231	-2.563533	-1.738629
H	5.498309	0.128845	-1.858101
H	4.641619	0.852674	-4.302847
H	4.111024	-1.388996	-5.696249
H	4.625992	-3.498315	-4.105738
H	0.418961	-5.574688	-2.406281
H	0.721915	-6.708405	-0.159083
H	1.998447	-5.474031	1.622214
H	2.899673	-3.217815	1.104643

Product pyridine N-oxide, Np III – Small core

E = -1224.328628
G = -1224.129430

C	1.629074	1.407400	-1.711321
C	0.858928	1.172747	-2.875360
C	-0.173960	0.260045	-2.539983
C	-0.044696	-0.059910	-1.165867
C	1.067851	0.649368	-0.652015
Np	2.138235	-1.209232	-2.381672
O	1.500305	-3.292463	-1.456629
N	2.207121	-3.209050	-0.312257
C	2.128866	-4.228959	0.566311
C	2.848317	-4.156818	1.745195
C	3.633165	-3.027458	1.986671
C	3.669952	-2.008214	1.037125
C	2.945430	-2.071739	-0.159494
C	3.443580	-1.870806	-4.703455
C	3.689434	-0.484190	-4.530955
C	4.530680	-0.327449	-3.403574
C	4.816286	-1.616177	-2.884516
C	4.142831	-2.567970	-3.687569
H	-0.692035	-0.722323	-0.603297
H	-0.950961	-0.098362	-3.206680
H	1.019083	1.626961	-3.846135
H	2.481240	2.073223	-1.638470
H	1.412891	0.631929	0.373859
H	4.165444	-3.643038	-3.554169
H	5.454129	-1.837116	-2.038356
H	4.912794	0.612903	-3.023340
H	3.316018	0.313867	-5.161768
H	2.857100	-2.321570	-5.496926
H	1.488850	-5.051951	0.272724
H	2.788336	-4.974814	2.454676
H	4.206651	-2.949139	2.906285
H	4.279555	-1.127314	1.222108

TS Pyridine N-oxide Pu III – Large core

E = -783.414273
G = -783.175105

C	1.329109	1.189303	-1.881106
N	0.239962	0.726300	-2.540254
C	-0.391651	-0.435625	-2.224493
C	0.141437	-1.166608	-1.163814
C	1.258680	-0.733580	-0.454265
C	1.855974	0.471479	-0.824626
O	-0.216486	1.450230	-3.554355
Pu	-1.695525	0.094828	-4.931153
C	-3.044326	-1.185972	-2.991957
C	-3.596342	1.062432	-6.751275
C	-2.563733	2.035990	-6.752022
C	-2.593300	2.705425	-5.503839
C	-3.636737	2.143797	-4.729402
C	-4.259163	1.130804	-5.501199
C	-0.669795	-1.137182	-7.221720
C	0.470431	-0.886571	-6.417454
C	0.417340	-1.757303	-5.299764
C	-0.757003	-2.541308	-5.410587
C	-1.429627	-2.157899	-6.597233
H	1.161147	-1.832408	-4.515896
H	1.262711	-0.179928	-6.637720
H	-0.903736	-0.655182	-8.163427
H	-2.344651	-2.594912	-6.980967
H	-1.072733	-3.316104	-4.722335
H	-3.924301	2.451751	-3.730801
H	-5.112175	0.534210	-5.198838
H	-3.857064	0.410218	-7.576595
H	-1.898254	2.256807	-7.578838
H	-1.936029	3.509862	-5.195806
H	-2.957015	-2.082418	-2.365121
H	-3.605307	-1.532259	-3.880433
H	-3.705367	-0.486456	-2.464622
H	1.723341	2.126646	-2.252752
H	2.726756	0.860277	-0.308038
H	1.657298	-1.315084	0.371575
H	-0.350667	-2.097696	-0.894582
H	-1.647264	-0.776943	-2.717892

TS Pyridine N-oxide Pu III – Small core

E = -1304.281523
G = -1304.042951

C	1.128221	1.212659	-1.726597
N	0.093451	0.737959	-2.457311
C	-0.417748	-0.512319	-2.311659
C	0.171223	-1.327485	-1.347836
C	1.238155	-0.884804	-0.569256
C	1.717197	0.410894	-0.766375
O	-0.443079	1.524187	-3.382422
Pu	-1.671477	0.098461	-4.884116
C	-3.105534	-1.122121	-3.065644
C	-3.544102	0.935161	-6.662924
C	-2.459941	1.838741	-6.820232
C	-2.374380	2.626111	-5.648416
C	-3.402470	2.211924	-4.766485
C	-4.131155	1.174413	-5.396122
C	-0.862429	-1.165095	-7.180441
C	0.324360	-0.725108	-6.545069
C	0.491762	-1.482580	-5.358911
C	-0.596907	-2.386708	-5.259570
C	-1.431945	-2.188521	-6.385920
H	1.319927	-1.403549	-4.664827
H	0.998776	0.039890	-6.913033
H	-1.257611	-0.792267	-8.116893
H	-2.341719	-2.734714	-6.608002
H	-0.753333	-3.114020	-4.472194
H	-3.594107	2.619337	-3.780776
H	-4.988096	0.656793	-4.981716
H	-3.884260	0.215090	-7.397541
H	-1.825340	1.925108	-7.694112
H	-1.646567	3.404179	-5.451097
H	-3.056224	-2.021225	-2.437914
H	-3.615881	-1.452493	-3.991922
H	-3.780724	-0.413504	-2.570633
H	1.430247	2.225145	-1.963267
H	2.543014	0.807697	-0.186039
H	1.687908	-1.529702	0.179553
H	-0.232148	-2.327238	-1.211224
H	-1.651128	-0.791371	-2.766664

Adduct of pyridine N-oxide, Pu III – Large core

E = -783.436569
G = -783.195483

C	1.377027	1.063024	-1.794305
N	0.256600	0.479576	-2.292329
C	-0.344761	-0.540559	-1.626525
C	0.183220	-0.999060	-0.432474
C	1.331714	-0.417679	0.098953
C	1.926740	0.629356	-0.602597
O	-0.233969	0.925039	-3.410617
Pu	-1.778359	0.003190	-5.128221
C	-3.129302	-1.386299	-3.472739
C	-3.848799	1.165650	-6.646423
C	-2.736718	2.017224	-6.871289
C	-2.468838	2.712002	-5.667393
C	-3.414737	2.291528	-4.698938
C	-4.269490	1.339991	-5.304292
C	-0.693122	-1.088104	-7.495773
C	0.437304	-0.892230	-6.667171
C	0.363602	-1.823546	-5.599617
C	-0.811349	-2.593920	-5.768935
C	-1.469351	-2.135262	-6.936650
H	1.102078	-1.951505	-4.815862
H	1.236390	-0.179356	-6.838553
H	-0.912952	-0.551063	-8.410981
H	-2.383817	-2.542617	-7.352941
H	-1.145355	-3.400499	-5.128376
H	-3.488009	2.654512	-3.680095
H	-5.105008	0.841587	-4.828223
H	-4.320810	0.527475	-7.385055
H	-2.208060	2.139226	-7.809597
H	-1.694278	3.456584	-5.520321
H	-2.679292	-2.275437	-3.002280
H	-3.962722	-1.790123	-4.072347
H	-3.616453	-0.813128	-2.667472
H	1.769550	1.865463	-2.404742
H	2.821815	1.120414	-0.236593
H	1.752166	-0.769015	1.034880
H	-0.322739	-1.816025	0.070424
H	-1.238044	-0.932342	-2.109160

Adduct of pyridine N-oxide, Pu III – Small core

E = -1304.301365
G = -1304.062250

C	-1.427929	-2.203452	-6.567841
C	-0.915008	-1.133418	-7.338702
C	0.231265	-0.626225	-6.678223
C	0.431052	-1.392131	-5.501995
C	-0.595629	-2.366237	-5.434132
Pu	-1.860498	0.042851	-5.044496
O	-0.538619	0.999983	-3.231731
N	0.086510	0.445753	-2.231894
C	1.213237	1.033503	-1.754755
C	1.892782	0.483660	-0.683947
C	1.422344	-0.684453	-0.085478
C	0.264131	-1.267341	-0.594446
C	-0.394620	-0.691667	-1.666579
C	-3.225792	-1.349675	-3.513796
C	-3.723125	1.127898	-6.718010
C	-2.562760	1.909037	-6.954891
C	-2.304706	2.672873	-5.793326
C	-3.301584	2.365452	-4.835265
C	-4.182884	1.414891	-5.408220
H	1.243823	-1.270852	-4.794562
H	0.858259	0.186458	-7.026903
H	-1.321757	-0.772042	-8.275152
H	-2.299628	-2.802241	-6.805486
H	-0.720128	-3.114425	-4.661190
H	-3.381002	2.789368	-3.840812
H	-5.055620	0.987370	-4.929441
H	-4.192377	0.453922	-7.425541
H	-1.985724	1.929549	-7.871517
H	-1.486558	3.371382	-5.658220
H	-2.852448	-2.279036	-3.055281
H	-4.016540	-1.687257	-4.210620
H	-3.758504	-0.792476	-2.725493
H	1.503570	1.934001	-2.279823
H	2.789900	0.979896	-0.330007
H	1.945305	-1.126774	0.755411
H	-0.146447	-2.176061	-0.167736
H	-1.301984	-1.072027	-2.132161

Product pyridine N-oxide, Pu III – Large core

E = -742.956921
G = -742.757474

C	1.724528	1.446051	-2.196584
C	0.786867	1.007559	-3.166036
C	-0.097240	0.092550	-2.537427
C	0.300157	-0.042273	-1.186486
C	1.429828	0.791256	-0.976515
Pu	2.373774	-1.259165	-2.665870
O	1.202770	-3.361426	-2.971985
N	1.421775	-3.884301	-1.755972
C	0.908676	-5.107616	-1.497508
C	1.110614	-5.680433	-0.255770
C	1.841864	-4.977653	0.701937
C	2.345895	-3.719528	0.375195
C	2.147890	-3.130143	-0.877515
C	5.112520	-0.619006	-2.694611
C	4.634967	-0.196274	-3.959871
C	4.305316	-1.353109	-4.711384
C	4.588958	-2.490206	-3.914009
C	5.086257	-2.037506	-2.668195
H	-0.185207	-0.656438	-0.437749
H	-0.943401	-0.399901	-3.002932
H	0.723061	1.355437	-4.191366
H	2.511967	2.173264	-2.356069
H	1.947587	0.935712	-0.034808
H	5.414595	-2.666123	-1.849402
H	5.476986	0.027808	-1.904354
H	4.565072	0.828841	-4.304586
H	3.947335	-1.366187	-5.735339
H	4.463186	-3.524435	-4.211541
H	0.358318	-5.562167	-2.311886
H	0.696702	-6.662278	-0.052966
H	2.013071	-5.407788	1.684701
H	2.916598	-3.164847	1.115553

Product pyridine N-oxide, Pu III – Small core

E = -1263.822896
G = -1263.624987

C	1.716070	1.288589	-1.672476
C	0.891337	1.082168	-2.808759
C	-0.114612	0.151159	-2.453222
C	0.085810	-0.217985	-1.100664
C	1.215034	0.487211	-0.616795
Pu	2.207414	-1.282254	-2.445253

O	1.151353	-3.394872	-2.331883
N	1.677287	-3.821541	-1.165563
C	1.318830	-5.041967	-0.717254
C	1.842238	-5.500052	0.478785
C	2.726092	-4.683580	1.184312
C	3.056052	-3.432234	0.663526
C	2.532284	-2.958675	-0.544409
C	3.926790	-2.265510	-4.296357
C	3.472386	-1.044313	-4.856026
C	4.001387	0.015542	-4.080603
C	4.776403	-0.547808	-3.038602
C	4.734733	-1.959327	-3.172628
H	-0.519906	-0.916341	-0.535514
H	-0.906129	-0.213212	-3.099047
H	0.999649	1.568891	-3.770748
H	2.562747	1.962574	-1.616066
H	1.615877	0.428662	0.388485
H	3.702674	-3.259069	-4.666973
H	5.243002	-2.675883	-2.539159
H	5.324305	0.004679	-2.283335
H	3.846315	1.072605	-4.257902
H	2.851245	-0.939177	-5.738748
H	0.626415	-5.587536	-1.346483
H	1.554754	-6.480822	0.841686
H	3.149019	-5.022111	2.126116
H	3.744669	-2.792068	1.209096

Picoline N-oxide

E = -362.638142

G = -362.547471

N	0.096418	0.134653	0.027941
C	0.056022	0.145530	1.396178
C	1.200182	0.012574	2.156614
C	2.437350	-0.137609	1.532972
C	2.467470	-0.147848	0.140865
C	1.310076	-0.013449	-0.613238
H	1.108375	0.028324	3.237854
H	3.348822	-0.243505	2.110922
H	3.406405	-0.262464	-0.392388
C	1.239387	-0.012364	-2.099407
H	0.581772	-0.814730	-2.450255
H	0.792803	0.920583	-2.459260
H	2.234095	-0.135625	-2.532263
O	-0.971134	0.259395	-0.649837
H	-0.942806	0.266535	1.794329

TS Picoline N-oxide sp2 Np IV – Large core

E = -867.707069

G = -867.403403

C	-5.105403	-0.994966	-0.321766
N	-3.884991	-0.395513	-0.290809
C	-3.279152	0.183068	-1.363880
C	-3.959990	0.162927	-2.577537
C	-5.205090	-0.450995	-2.678621
C	-5.773430	-1.021459	-1.540109
O	-3.198217	-0.375053	0.835033
Np	-0.857174	0.025382	0.116949
C	-1.322964	-2.330372	-0.531899
C	-2.153919	2.399750	-0.084849
C	1.366436	-0.467406	-1.463684
C	0.295361	-0.335451	-2.384608
C	-0.120899	1.013581	-2.376797
C	0.699260	1.722388	-1.456954
C	1.628047	0.809738	-0.911268
C	1.008766	-0.506848	2.065529
C	-0.048123	-1.407215	2.355946
C	-1.147151	-0.650273	2.824852
C	-0.777998	0.714929	2.820248
C	0.557476	0.806638	2.352308
H	-0.909012	1.444096	-2.981509
H	-0.129671	-1.133401	-2.978725
H	1.908324	-1.380559	-1.250310
H	2.402944	1.047051	-0.193580
H	0.641505	2.781729	-1.240813
H	-1.404698	1.543735	3.126230
H	1.139851	1.715564	2.258642
H	1.997510	-0.780166	1.719089
H	-0.015549	-2.483404	2.246858
H	-2.115436	-1.042664	3.103941
H	-2.137946	3.078006	-0.944874
H	-1.349560	2.734663	0.586945
H	-3.096026	2.540048	0.455804
H	-1.961652	-2.820004	0.213826
H	-1.819028	-2.438358	-1.505101
H	-0.391135	-2.910378	-0.592023
C	-5.606156	-1.583458	0.951558
H	-6.744870	-1.503003	-1.581467
H	-5.733651	-0.485410	-3.626563
H	-3.501934	0.633806	-3.442199
H	-2.566450	1.171986	-0.906690
H	-6.590603	-2.030969	0.802729
H	-4.910748	-2.345575	1.317073
H	-5.668597	-0.818045	1.731439

TS Picoline N-oxide sp2 Np IV – Small core

E = -1343.959491

G = -1343.655871

C	-5.083080	-0.949364	-0.345923
N	-3.874644	-0.329661	-0.282052
C	-3.281774	0.316851	-1.320793
C	-3.966538	0.366520	-2.529935
C	-5.207302	-0.251202	-2.660677
C	-5.759485	-0.904258	-1.559471
O	-3.180315	-0.361685	0.839330
Np	-0.892091	-0.000252	0.114733
C	-1.385404	-2.291301	-0.554187
C	-2.007272	2.394867	0.060988
C	1.472960	-0.325355	-1.217788
C	0.483827	-0.624818	-2.179995
C	-0.200650	0.574503	-2.486516
C	0.378096	1.619481	-1.725056
C	1.409909	1.063745	-0.938010
C	1.014005	-0.521139	2.010145
C	-0.023475	-1.447317	2.274634
C	-1.139502	-0.722482	2.752469
C	-0.795459	0.648912	2.784746
C	0.535925	0.775071	2.324698
H	-0.998478	0.679800	-3.210141
H	0.290774	-1.596373	-2.612562
H	2.173222	-1.031960	-0.790674
H	2.055735	1.606366	-0.259209
H	0.092785	2.662402	-1.755361
H	-1.442018	1.459403	3.097619
H	1.098647	1.697476	2.245424
H	2.009819	-0.763451	1.662859
H	0.028791	-2.519914	2.139475
H	-2.100841	-1.139465	3.019873
H	-2.153735	3.133400	-0.735278
H	-1.065414	2.667179	0.564327
H	-2.817509	2.501732	0.790239
H	-2.061965	-2.745271	0.182598
H	-1.857197	-2.384461	-1.542378
H	-0.473175	-2.904869	-0.582608
C	-5.565406	-1.628271	0.888919
H	-6.725355	-1.393995	-1.626462
H	-5.743941	-0.226048	-3.604351
H	-3.519578	0.897763	-3.364694
H	-2.530088	1.234962	-0.843414
H	-6.543266	-2.081518	0.716095
H	-4.855701	-2.401354	1.199308
H	-5.635580	-0.916511	1.717423

Adduct of picoline N-oxide sp2, Np IV – Large core

E = -867.728091

G = -867.424031

C	-5.222161	-1.019471	-0.338760
N	-4.049849	-0.355573	-0.598158
C	-3.846547	0.247043	-1.800991
C	-4.804580	0.201166	-2.794582
C	-6.003094	-0.469640	-2.568282
C	-6.194922	-1.071669	-1.328554
O	-3.151222	-0.312303	0.329600
Np	-0.601867	0.093343	0.131711
C	-1.269748	-2.145467	-0.778662
C	-1.768836	2.319152	-0.000801
C	1.785210	-0.338823	-1.149234
C	0.840076	-0.372968	-2.203196
C	0.320012	0.932513	-2.365057
C	0.964430	1.783727	-1.429671
C	1.871504	1.001206	-0.682548
C	0.920002	-0.657840	2.281309
C	-0.235920	-1.468444	2.407985
C	-1.320432	-0.626412	2.748988
C	-0.841910	0.703015	2.839911
C	0.544350	0.685763	2.548942
H	-0.411363	1.242139	-3.102512
H	0.560866	-1.247484	-2.774939
H	2.370951	-1.178218	-0.794727
H	2.531235	1.362687	0.096593
H	0.789199	2.844623	-1.311720
H	-1.430029	1.578250	3.083679
H	1.205915	1.543609	2.554916
H	1.920589	-1.006005	2.055976
H	-0.280226	-2.540639	2.266017
H	-2.345369	-0.940842	2.894499
H	-1.995448	2.707911	-1.005024
H	-1.100632	3.067961	0.453088
H	-2.705549	2.345799	0.570700
H	-1.938459	-2.665209	-0.080188
H	-1.800246	-2.100057	-1.742600
H	-0.402305	-2.800873	-0.943092
C	-5.343285	-1.638751	1.008545
H	-7.113628	-1.604110	-1.105115
H	-6.768803	-0.521206	-3.334612
H	-4.598382	0.698109	-3.736256
H	-2.909568	0.782967	-1.883492
H	-6.306528	-2.141999	1.108733
H	-4.534532	-2.358234	1.170717
H	-5.245802	-0.878399	1.790153

Adduct of picoline N-oxide sp2, Np IV – Small core

E = -1343.978900

G = -1343.675983

C	-5.079209	-0.659697	-0.570202
N	-3.905671	-0.469485	-1.243201
C	-3.859749	0.246419	-2.394303
C	-5.001951	0.807787	-2.927886
C	-6.218862	0.638839	-2.270687
C	-6.239893	-0.098602	-1.092684
O	-2.818780	-1.024995	-0.787259
Np	-0.702497	-0.250670	0.144662
C	-0.540806	-2.659323	-0.223193
C	-2.160583	1.738938	0.111309
C	1.837222	0.077249	-0.824056
C	1.177024	-0.669415	-1.823282
C	0.202221	0.169667	-2.418322
C	0.275368	1.441614	-1.798382
C	1.277005	1.381294	-0.804845
C	0.912723	-0.581128	2.339378
C	-0.164554	-1.465071	2.562115
C	-1.326690	-0.685868	2.785086
C	-0.959670	0.681524	2.724771
C	0.421320	0.746791	2.438259
H	-0.450109	-0.109957	-3.238130
H	1.379326	-1.697938	-2.089109
H	2.648089	-0.276413	-0.200180
H	1.581091	2.197410	-0.161479
H	-0.327139	2.308033	-2.037039
H	-1.619038	1.526475	2.870754
H	1.006852	1.652135	2.338940
H	1.939324	-0.869271	2.152335
H	-0.111573	-2.545183	2.561755
H	-2.314117	-1.072340	3.011364
H	-2.525628	2.020707	-0.887526
H	-1.623440	2.614447	0.502519
H	-3.045139	1.598850	0.753631
H	-1.296374	-3.170409	0.392207
H	-0.760495	-2.893639	-1.274380
H	0.437604	-3.093082	0.022482
C	-5.011208	-1.468940	0.675971
H	-7.166241	-0.254764	-0.550017
H	-7.130846	1.071938	-2.667455
H	-4.924295	1.374663	-3.848900
H	-2.870371	0.327896	-2.823725
H	-6.008286	-1.592233	1.101842
H	-4.572120	-2.450120	0.471449
H	-4.361078	-0.983293	1.410812

Product picoline N-oxide sp2, Np IV – Large core

E = -827.261464

G = -827.000866

C	-4.780302	-0.900294	0.435601
C	-3.369461	-1.029867	0.310406
C	-3.105586	-2.046403	-0.637330
C	-4.350128	-2.540264	-1.107690
C	-5.381518	-1.840984	-0.432295
Np	-4.197765	0.040533	-2.102312
C	-2.094240	-0.584500	-3.232167
C	-5.073658	-0.615899	-4.431074
N	-6.376565	-0.495618	-4.056936
C	-7.467671	-0.695394	-4.839520
C	-7.232062	-1.062103	-6.160632
C	-5.928360	-1.210386	-6.628315
C	-4.861055	-0.985590	-5.757727
C	-8.809741	-0.506924	-4.218814
O	-6.547630	-0.145010	-2.775764
C	-3.158066	2.369440	-1.102068
C	-2.813285	2.407131	-2.474157
C	-4.007453	2.575415	-3.220263
C	-5.087344	2.663275	-2.306264
C	-4.569059	2.526812	-0.997883
H	-6.131126	2.786977	-2.564322
H	-4.078233	2.650347	-4.298090
H	-1.815031	2.321580	-2.881544
H	-2.465576	2.274315	-0.274175
H	-5.140428	2.567614	-0.078280
H	-6.444716	-1.980436	-0.577995
H	-5.302785	-0.224808	1.102372
H	-2.626603	-0.471583	0.867763
H	-2.127618	-2.390343	-0.945687
H	-4.486427	-3.336794	-1.829295
H	-2.095775	-1.649186	-3.503427
H	-1.944597	-0.019174	-4.161636
H	-1.203721	-0.416348	-2.608338
H	-8.085385	-1.228784	-6.810198
H	-5.752844	-1.498998	-7.661082
H	-3.837645	-1.098026	-6.104164
H	-9.598271	-0.698043	-4.949516
H	-8.936419	-1.179505	-3.364642
H	-8.915160	0.510694	-3.829721

Product picoline N-oxide sp2, Np IV – Small core

E = -1303.506157

G = -1303.245672

C	-5.056269	-0.893287	-0.158832
C	-3.643539	-0.777147	-0.121655
C	-3.246380	0.099906	-1.155282
C	-4.411461	0.526645	-1.834234
C	-5.528139	-0.091828	-1.224828
Np	-4.634551	1.686203	0.634730
C	-2.767016	3.035835	0.039533
C	-6.482482	3.395172	1.098824
N	-6.595203	3.683137	-0.224377
C	-7.373266	4.635657	-0.794662
C	-8.164868	5.390824	0.065770
C	-8.128188	5.156985	1.437808
C	-7.281748	4.166880	1.940723
C	-7.316540	4.784501	-2.276708
O	-5.834741	2.902846	-1.009967
C	-5.263398	1.326591	3.276030
C	-4.448759	2.487537	3.250638
C	-3.137998	2.095382	2.903188
C	-3.141023	0.695799	2.703303
C	-4.453055	0.218544	2.948321
H	-4.770767	3.497262	3.469355

H	-2.281055	2.748614	2.811466
H	-2.280802	0.093458	2.441201
H	-4.774758	-0.814098	2.900648
H	-6.320025	1.295725	3.513940
H	-6.562843	0.042433	-1.515537
H	-5.663028	-1.514296	0.489524
H	-2.984256	-1.292358	0.564157
H	-2.231161	0.395297	-1.386099
H	-4.450030	1.224919	-2.660263
H	-2.828222	3.229296	-1.041206
H	-2.902705	4.002790	0.553384
H	-1.752559	2.686580	0.264831
H	-8.804251	6.158097	-0.358632
H	-8.751812	5.746388	2.104618
H	-7.239112	3.986398	3.011744
H	-7.981737	5.585834	-2.604751
H	-6.294798	5.005143	-2.601159
H	-7.604164	3.850046	-2.768644

TS Picoline N-oxide sp2 Pu IV – Large core

E = -868.460002
G = -868.155284

C	-5.096317	-0.999711	-0.322462
N	-3.873293	-0.405661	-0.292073
C	-3.263364	0.167280	-1.365540
C	-3.942088	0.145566	-2.580450
C	-5.189293	-0.464181	-2.681541
C	-5.762133	-1.028165	-1.541944
O	-3.186889	-0.383416	0.833581
Pu	-0.855768	0.024146	0.116765
C	-1.308946	-2.321322	-0.520176
C	-2.154077	2.383790	-0.078873
C	1.335416	-0.479806	-1.478284
C	0.258885	-0.311396	-2.387551
C	-0.132886	1.043941	-2.350982
C	0.706381	1.720442	-1.423678
C	1.624570	0.781842	-0.905307
C	1.000923	-0.500906	2.051625
C	-0.058940	-1.395749	2.348053
C	-1.154771	-0.632337	2.813551
C	-0.781572	0.731507	2.798958
C	0.553989	0.815986	2.329678
H	-0.919543	1.499510	-2.938839
H	-0.186198	-1.090468	-2.991874
H	1.861915	-1.406449	-1.286300
H	2.408753	0.992085	-0.189481
H	0.668522	2.776130	-1.186353
H	-1.405859	1.564272	3.098727
H	1.138789	1.722481	2.228981
H	1.988435	-0.780252	1.706841
H	-0.029995	-2.472576	2.245404
H	-2.124595	-1.019628	3.093919
H	-2.144701	3.061864	-0.939084
H	-1.350442	2.723114	0.590542
H	-3.096265	2.515101	0.463587
H	-1.952105	-2.809557	0.222180
H	-1.796108	-2.433627	-1.497114
H	-0.374389	-2.897493	-0.570370
C	-5.601683	-1.580952	0.952413
H	-6.735375	-1.506063	-1.583423
H	-5.716163	-0.500281	-3.630379
H	-3.480842	0.611539	-3.446115
H	-2.553515	1.159066	-0.903454
H	-6.587816	-2.024842	0.803850
H	-4.910203	-2.344571	1.322270
H	-5.662188	-0.812109	1.729090

TS Picoline N-oxide sp2 Pu IV – Small core

E = -1383.432331
G = -1383.130691

C	-5.097983	-0.912393	-0.323466
N	-3.872535	-0.329224	-0.249533
C	-3.254414	0.299276	-1.284806
C	-3.929421	0.374264	-2.497555
C	-5.188711	-0.203411	-2.636347
C	-5.766613	-0.842422	-1.540770
O	-3.183632	-0.386712	0.876731
Pu	-0.901926	-0.087136	0.110563
C	-1.484657	-2.294603	-0.739441
C	-1.930236	2.353735	0.068682
C	1.450296	-0.422333	-1.192212
C	0.474321	-0.711531	-2.171224
C	-0.199148	0.493180	-2.481132
C	0.378907	1.532913	-1.712754
C	1.394832	0.969581	-0.913531
C	1.072846	-0.252940	2.041458
C	0.209819	-1.348654	2.274937
C	-1.026622	-0.836364	2.734651
C	-0.920428	0.576191	2.799122
C	0.373500	0.937514	2.370476
H	-0.988870	0.604471	-3.212644
H	0.287974	-1.676805	-2.619187
H	2.141263	-1.134023	-0.757034
H	2.032936	1.508811	-0.225188
H	0.101452	2.577491	-1.743713
H	-1.706653	1.255287	3.103923
H	0.771138	1.943658	2.314671
H	2.100956	-0.314553	1.709080
H	0.451834	-2.394627	2.126582
H	-1.904021	-1.417082	2.987450
H	-2.089365	3.068208	-0.747199
H	-0.994957	2.642581	0.565841
H	-2.744608	2.460799	0.793686
H	-2.231873	-2.658076	-0.019460
H	-1.870515	-2.424858	-1.754907
H	-0.582900	-2.916538	-0.637077
C	-5.611797	-1.578898	0.905547
H	-6.747225	-1.300848	-1.614042
H	-5.720121	-0.155992	-3.582108
H	-3.461172	0.894180	-3.327528
H	-2.473806	1.190132	-0.820936
H	-6.606133	-1.991581	0.725307
H	-4.936602	-2.382697	1.215446
H	-5.656873	-0.869834	1.738007

Adduct of picoline N-oxide sp2, Pu IV – Large core

E = -868.482224
G = -868.177640

C	-5.244528	-0.946911	-0.343144
N	-4.021704	-0.398152	-0.641191
C	-3.772689	0.101603	-1.882232
C	-4.733932	0.068151	-2.873355
C	-5.983298	-0.483946	-2.606531
C	-6.220156	-0.985299	-1.330056
O	-3.124149	-0.366353	0.285471
Pu	-0.591882	0.079881	0.147832
C	-1.193134	-2.165005	-0.757808
C	-1.819751	2.254109	0.093363
C	1.774032	-0.260588	-1.157946
C	0.819240	-0.317223	-2.201642
C	0.254613	0.972152	-2.346708
C	0.881228	1.836379	-1.411126
C	1.820536	1.077839	-0.679677
C	0.955631	-0.681602	2.249480
C	-0.185313	-1.513603	2.367844
C	-1.282245	-0.696473	2.730716
C	-0.825298	0.638839	2.844618
C	0.558923	0.650747	2.543942
H	-0.490181	1.266081	-3.077261
H	0.563327	-1.195942	-2.777695
H	2.390831	-1.083147	-0.817259
H	2.476939	1.454850	0.094786
H	0.672468	2.889761	-1.282196
H	-1.426168	1.499723	3.106779
H	1.205344	1.519772	2.561169
H	1.960017	-1.008451	2.009793
H	-0.213155	-2.583041	2.204102
H	-2.300609	-1.031706	2.876558
H	-2.130040	2.604732	-0.902139
H	-1.160726	3.041784	0.489661
H	-2.720019	2.247360	0.720600
H	-1.856803	-2.700676	-0.067158
H	-1.704748	-2.148584	-1.732218
H	-0.298608	-2.789635	-0.896963
C	-5.411637	-1.463659	1.041968
H	-7.178938	-1.424337	-1.074202
H	-6.752896	-0.522300	-3.369669
H	-4.488987	0.480474	-3.846080
H	-2.791489	0.539729	-2.007213
H	-6.413279	-1.876410	1.173978
H	-4.665802	-2.236794	1.252466
H	-5.245846	-0.664624	1.771712

Adduct of picoline N-oxide sp2, Pu IV – Small core

E = -1383.453799
G = -1383.152818

C	-5.077364	-1.116783	-1.046995
N	-4.118579	-0.146172	-0.962203
C	-4.120586	0.929137	-1.789995
C	-5.089846	1.071517	-2.762347
C	-6.080060	0.099544	-2.890109
C	-6.061443	-0.986087	-2.022013
O	-3.192903	-0.257487	-0.052048
Pu	-0.835106	-0.004767	0.428894
C	-1.074682	-2.460625	0.361850
C	-1.527218	2.373909	0.483402
C	1.261822	-0.679866	-1.207901
C	0.127538	-0.894264	-2.017994
C	-0.462261	0.363849	-2.290779
C	0.333654	1.363310	-1.672800
C	1.391694	0.719258	-0.999618
C	1.245866	-0.336191	2.202907
C	0.217561	-1.172183	2.687754
C	-0.842187	-0.343939	3.136011
C	-0.451943	1.005231	2.950189
C	0.831123	1.010369	2.362117
H	-1.327894	0.534886	-2.921112
H	-0.232189	-1.855548	-2.361222
H	1.925395	-1.447608	-0.830362
H	2.176944	1.209572	-0.438175
H	0.167623	2.431006	-1.716232
H	-1.035142	1.879353	3.208208
H	1.399446	1.891184	2.090219
H	2.193508	-0.667028	1.796515
H	0.238893	-2.252435	2.722441
H	-1.772859	-0.683645	3.577603
H	-1.911206	2.716357	-0.488055
H	-0.747172	3.074643	0.797498
H	-2.348135	2.414875	1.215401
H	-1.728093	-2.729461	1.204234
H	-1.592646	-2.685423	-0.580993
H	-0.161777	-3.061383	0.412807
C	-4.984628	-2.238555	-0.074165
H	-6.816410	-1.762633	-2.085296
H	-6.852003	0.187371	-3.647174
H	-5.057874	1.942985	-3.406753
H	-3.317745	1.630090	-1.603187
H	-5.791044	-2.953399	-0.245852
H	-4.018196	-2.745414	-0.157531
H	-5.046513	-1.859777	0.951295

Product picoline N-oxide sp2, Pu IV – Large core

E = -828.017382
G = -827.755248

C	-5.208535	-0.554154	0.027033
C	-3.860228	-0.716465	-0.389967
C	-3.799726	-0.468630	-1.784886
C	-5.105735	-0.146175	-2.227339
C	-5.977568	-0.208729	-1.111185
Pu	-4.331001	1.953713	-0.616885
C	-2.448230	2.389884	-2.126989
O	-5.106994	3.472294	-2.343803
N	-6.368480	3.647275	-1.931799
C	-7.191691	4.454117	-2.648616
C	-8.492363	4.602356	-2.178218
C	-8.900194	3.939936	-1.023199
C	-7.991075	3.127068	-0.344371
C	-6.682540	2.964019	-0.797450
C	-6.630879	5.103063	-3.867417
C	-4.591962	3.534759	1.635048
C	-3.507208	4.093717	0.914019
C	-2.434377	3.169396	0.945913
C	-2.860605	2.030778	1.675199
C	-4.197719	2.255825	2.099030
H	-3.495786	5.063289	0.431317
H	-1.461136	3.309401	0.495435
H	-2.259180	1.158358	1.900136
H	-4.796671	1.584264	2.702039
H	-5.551645	4.004699	1.805176
H	-7.044387	-0.028426	-1.127179
H	-5.587649	-0.702801	1.030793
H	-3.030174	-1.014803	0.238983
H	-2.912855	-0.517270	-2.402035
H	-5.389434	0.096766	-3.243948
H	-2.704095	2.107399	-3.156496
H	-2.217505	3.463293	-2.142826
H	-1.521497	1.860478	-1.862569
H	-9.172815	5.241782	-2.731149
H	-9.917426	4.059143	-0.660225
H	-8.300235	2.605470	0.557710
H	-7.387627	5.723454	-4.351941
H	-5.763983	5.719664	-3.610149
H	-6.271970	4.347986	-4.573850

Product picoline N-oxide sp2, Pu IV – Small core

E = -1342.981129
G = -1342.721042

C	-5.028508	-0.737251	-0.489009
C	-3.612471	-0.632448	-0.451797
C	-3.171259	-0.151918	-1.702371
C	-4.312306	0.030837	-2.521838
C	-5.454684	-0.346166	-1.778472
Pu	-4.582853	1.947784	-0.607820
C	-2.722337	2.941698	-1.687693
O	-5.979602	2.432845	-2.466357
N	-6.606617	3.525845	-2.003229
C	-7.458973	4.195440	-2.818802
C	-8.106861	5.298866	-2.272527
C	-7.866441	5.670186	-0.952295
C	-6.959733	4.932957	-0.188488
C	-6.296281	3.824799	-0.714338
C	-7.629131	3.693426	-4.211837
C	-5.032184	2.467244	2.027088
C	-4.241702	3.552066	1.567301
C	-2.942671	3.064162	1.294748
C	-2.931835	1.681453	1.567743
C	-4.223750	1.312217	2.030045
H	-4.564156	4.579578	1.465802
H	-2.104565	3.649139	0.941954
H	-2.077034	1.025938	1.466093
H	-4.529011	0.322246	2.344480
H	-6.073823	2.519333	2.322192
H	-6.478047	-0.301936	-2.129092
H	-5.662695	-1.101201	0.310818
H	-2.982159	-0.897452	0.386073
H	-2.145027	0.037261	-1.987632
H	-4.316433	0.411297	-3.535315
H	-2.860952	2.749508	-2.762559
H	-2.903391	4.019086	-1.518025
H	-1.678214	2.737042	-1.432404
H	-8.799047	5.854320	-2.896995
H	-8.380511	6.528676	-0.528580
H	-6.763043	5.221536	0.840562
H	-8.334666	4.322274	-4.758606
H	-6.668909	3.684937	-4.737120
H	-7.991300	2.660567	-4.208355

TS Picoline N-oxide sp2 Np III – Large core

E = -822.057512
G = -821.792432

C	-1.425675	-2.173270	-6.605177
C	-0.662465	-1.155108	-7.229226
C	0.479828	-0.910557	-6.425792
C	0.424079	-1.781919	-5.308912

C	-0.753906	-2.560452	-5.419306
Np	-1.694228	0.093807	-4.924145
O	-0.217236	1.473127	-3.535915
N	0.245136	0.739036	-2.527916
C	1.340137	1.208184	-1.863638
C	1.845378	0.444863	-0.817898
C	1.249133	-0.764542	-0.473733
C	0.132691	-1.186348	-1.191625
C	-0.388846	-0.428807	-2.234945
C	-3.051083	-1.181898	-2.965690
C	-2.587204	2.038324	-6.764955
C	-3.614252	1.059415	-6.759614
C	-4.277184	1.129492	-5.509704
C	-3.660643	2.149576	-4.742733
C	-2.620245	2.713171	-5.519683
H	1.168018	-1.861585	-4.525574
H	1.276467	-0.209345	-6.648204
H	-0.894528	-0.672232	-8.171058
H	-2.342407	-2.606715	-6.989042
H	-1.071773	-3.335135	-4.731801
H	-3.950789	2.461158	-3.745943
H	-5.127317	0.530025	-5.204751
H	-3.871691	0.402392	-7.582213
H	-1.924056	2.259890	-7.593537
H	-1.969237	3.524694	-5.216666
H	-2.962535	-2.062800	-2.317469
H	-3.610902	-1.549237	-3.846332
H	-3.712940	-0.471342	-2.454060
C	1.910766	2.506660	-2.320470
H	2.714741	0.816221	-0.285338
H	1.648470	-1.359588	0.342416
H	-0.363625	-2.120635	-0.942951
H	-1.646346	-0.766210	-2.708743
H	2.772441	2.778928	-1.707610
H	2.215705	2.445080	-3.369851
H	1.157488	3.298406	-2.264083

TS Picoline N-oxide sp2 Np III – Small core

E = -1304.099105
G = -1303.833589

C	-1.394185	-2.320222	-6.204529
C	-1.058864	-1.312287	-7.137991
C	0.144548	-0.696842	-6.709326
C	0.554919	-1.333858	-5.510805
C	-0.396654	-2.334589	-5.198218
Np	-1.697907	0.070484	-4.854645
O	-0.390845	1.506601	-3.434051
N	0.115365	0.712821	-2.495154
C	1.184617	1.167340	-1.783739
C	1.721494	0.330879	-0.811774
C	1.184127	-0.934259	-0.591487
C	0.095928	-1.343147	-1.358662
C	-0.455515	-0.510787	-2.325727
C	-3.111872	-1.246965	-3.108087
C	-2.397068	1.815645	-6.860819
C	-3.542201	1.006467	-6.639289
C	-4.073890	1.345824	-5.369551
C	-3.252846	2.349239	-4.803925
C	-2.218018	2.641705	-5.727647
H	1.452439	-1.111313	-4.945501
H	0.675659	0.093521	-7.226550
H	-1.613445	-1.064954	-8.034262
H	-2.251575	-2.981025	-6.259698
H	-0.359262	-3.005078	-4.348439
H	-3.392195	2.818557	-3.837248
H	-4.959783	0.917337	-4.914854
H	-3.963004	0.292387	-7.337000
H	-1.782410	1.815611	-7.752732
H	-1.430815	3.372438	-5.586666
H	-3.082102	-2.102489	-2.422780
H	-3.577656	-1.641074	-4.032255
H	-3.814493	-0.518082	-2.681688
C	1.691112	2.528855	-2.115350
H	2.567744	0.690611	-0.235805
H	1.607120	-1.583946	0.169005
H	-0.354057	-2.320458	-1.207717
H	-1.681297	-0.837926	-2.778177
H	2.538724	2.784648	-1.476584
H	1.997693	2.578876	-3.164917
H	0.899835	3.274179	-1.989246

Adduct of picoline N-oxide sp2, Np III – Large core

E = -822.080163
G = -821.813075

C	-1.427598	-2.113507	-6.943464
C	-0.660498	-1.057889	-7.498867
C	0.469166	-0.856644	-6.670271
C	0.403766	-1.792791	-5.606482
C	-0.765295	-2.571590	-5.778084
Np	-1.764146	0.029565	-5.114675
O	-0.234416	0.946747	-3.356247
N	0.254357	0.499645	-2.233157
C	1.341546	1.134146	-1.699911
C	1.859607	0.662649	-0.498445
C	1.293374	-0.427456	0.152826
C	0.184502	-1.043205	-0.423163
C	-0.321915	-0.564391	-1.615276
C	-3.124448	-1.400420	-3.475749
C	-2.770865	2.038198	-6.870370
C	-3.871833	1.176023	-6.632741
C	-4.285756	1.354020	-5.289080
C	-3.438062	2.319177	-4.695380
C	-2.503162	2.743818	-5.672574
H	1.144090	-1.918850	-4.824060
H	1.263946	-0.138793	-6.841568
H	-0.884634	-0.519832	-8.412538
H	-2.339102	-2.526560	-7.360745
H	-1.092278	-3.383699	-5.140766
H	-3.510547	2.689146	-3.678890
H	-5.112718	0.849488	-4.804483
H	-4.341344	0.527757	-7.364251
H	-2.250116	2.160489	-7.813154
H	-1.738212	3.500583	-5.536786
H	-2.669883	-2.291738	-3.013961
H	-3.958159	-1.800999	-4.077062
H	-3.609751	-0.835851	-2.663278
C	1.878725	2.292314	-2.464631
H	2.722520	1.173312	-0.084071
H	1.706762	-0.786460	1.089300
H	-0.301151	-1.894888	0.039984
H	-1.186558	-0.972016	-2.135469
H	2.733699	2.725952	-1.943469
H	2.183176	1.982150	-3.469217
H	1.105403	3.055441	-2.597012

Adduct of picoline N-oxide sp2, Np III – Small core

E = -1304.118268
G = -1303.851647

C	-1.493468	-2.249544	-6.429832
C	-1.218534	-1.244031	-7.386835
C	0.021737	-0.644254	-7.052300
C	0.517651	-1.292019	-5.892139
C	-0.417606	-2.280539	-5.508201
Np	-1.710602	0.131287	-5.072223
O	-0.207749	0.872397	-3.312609
N	0.261335	0.385817	-2.195793
C	1.300825	1.034338	-1.589904
C	1.802378	0.511286	-0.403467
C	1.264530	-0.640916	0.160718
C	0.201105	-1.266010	-0.487402
C	-0.287793	-0.738130	-1.665859
C	-3.100242	-1.289175	-3.575809
C	-2.566599	1.986810	-6.944914
C	-3.689313	1.154889	-6.704610
C	-4.141278	1.400743	-5.385087
C	-3.296071	2.378241	-4.807969
C	-2.323617	2.742956	-5.774607
H	1.458443	-1.078307	-5.397575
H	0.520751	0.140223	-7.609165
H	-1.838519	-0.987927	-8.237042
H	-2.364913	-2.892377	-6.409242
H	-0.327653	-2.952775	-4.663199
H	-3.392327	2.791912	-3.810265
H	-4.986437	0.926742	-4.901319
H	-4.140058	0.472656	-7.415546
H	-2.004579	2.045597	-7.869078
H	-1.544396	3.486268	-5.646976
H	-2.726132	-2.245566	-3.177373
H	-3.923937	-1.577148	-4.253697
H	-3.588052	-0.761387	-2.739838
C	1.807946	2.259593	-2.266014
H	2.628868	1.030432	0.070373
H	1.665083	-1.040394	1.086366
H	-0.260920	-2.163342	-0.090932
H	-1.120907	-1.136956	-2.241714
H	2.629262	2.694426	-1.694201
H	2.151509	2.025945	-3.278680
H	1.006824	2.997695	-2.373161

Product picoline N-oxide sp2, Np III – Large core

E = -781.599352
G = -781.375684

C	-1.153043	-1.493459	-6.712863
C	-0.356557	-0.799596	-7.658648
C	0.961997	-0.724783	-7.148146
C	0.985088	-1.386592	-5.892471
C	-0.320108	-1.861621	-5.624643
Np	-0.544389	0.966539	-5.441024
C	1.374460	1.487193	-3.747777
N	0.562486	1.151330	-2.700518
C	0.902406	1.170084	-1.383306
C	2.194129	1.568959	-1.060954
C	3.086874	1.929478	-2.066218
C	2.665142	1.882950	-3.394308
O	-0.688845	0.766288	-3.009611
C	-0.136765	0.761623	-0.395903
C	-0.710924	3.119469	-7.275865
C	-2.034654	2.619856	-7.195720
C	-2.541231	2.930100	-5.907530
C	-1.532709	3.624004	-5.194496
C	-0.401713	3.740423	-6.039084
H	-1.618694	4.015214	-4.187682
H	-3.542024	2.715690	-5.547796
H	-2.577279	2.123561	-7.992150
H	-0.065405	3.071906	-8.145653
H	0.525768	4.243022	-5.792041
H	-0.623484	-2.428840	-4.752155
H	1.854458	-1.523123	-5.260909
H	1.815110	-0.282323	-7.650514
H	-0.692496	-0.416983	-8.615353
H	-2.200726	-1.749219	-6.829850
H	2.482299	1.590244	-0.014934
H	4.096438	2.241070	-1.812172
H	3.353832	2.160700	-4.187873
H	0.260070	0.821000	0.619771
H	-1.020274	1.402034	-0.479745
H	-0.476012	-0.259765	-0.594811

Product picoline N-oxide sp2, Np III – Small core

E = -1263.640269
G = -1263.414741

C	-1.131060	-1.570966	-6.416438
C	-0.616825	-0.827662	-7.509913
C	0.742199	-0.539683	-7.239851
C	1.075154	-1.116033	-5.987227
C	-0.083761	-1.750930	-5.479388
Np	-0.668237	0.938860	-5.404752
C	1.236729	1.417223	-3.837637
N	0.461898	1.107814	-2.757815
C	0.830204	1.145538	-1.452154
C	2.134774	1.536741	-1.173994
C	2.999632	1.869285	-2.214943
C	2.542971	1.806734	-3.530055
O	-0.801702	0.729278	-3.050805
C	-0.190396	0.767503	-0.433231
C	-0.419987	3.078919	-7.112022
C	-1.757091	2.642296	-7.269635
C	-2.453545	2.921106	-6.065778
C	-1.546162	3.538672	-5.169901
C	-0.289682	3.637992	-5.815174
H	-1.776999	3.886412	-4.169834
H	-3.505464	2.733790	-5.878514
H	-2.178846	2.193754	-8.161438
H	0.358979	3.020533	-7.863384
H	0.604392	4.083447	-5.398114
H	-0.154575	-2.289290	-4.541660
H	2.047395	-1.094205	-5.512147
H	1.417256	0.003080	-7.891526
H	-1.161567	-0.546491	-8.403396
H	-2.136785	-1.968691	-6.331807
H	2.455360	1.575394	-0.138096
H	4.019408	2.174528	-1.995312
H	3.212441	2.066234	-4.346055
H	0.230206	0.842346	0.571704
H	-1.068223	1.416739	-0.509065
H	-0.544870	-0.253833	-0.603596

TS Picoline N-oxide sp2 Pu III – Large core

E = -822.725839
G = -822.460739

C	-1.428262	-2.164838	-6.588021
C	-0.676610	-1.142380	-7.219105
C	0.467359	-0.885349	-6.422080
C	0.424587	-1.753821	-5.302206
C	-0.747187	-2.542734	-5.404434
Pu	-1.693960	0.090563	-4.922953
O	-0.219578	1.460670	-3.554565
N	0.238658	0.732761	-2.539889
C	1.332961	1.204282	-1.876338
C	1.832836	0.447645	-0.823206
C	1.231787	-0.757279	-0.471563
C	0.116434	-1.181613	-1.189745
C	-0.399847	-0.430634	-2.240501
C	-3.053364	-1.192219	-2.993016
C	-2.570969	2.022731	-6.753270
C	-3.603643	1.049460	-6.741755
C	-4.260510	1.125361	-5.489058
C	-3.634355	2.142733	-4.726208
C	-2.594620	2.699539	-5.508980
H	1.172379	-1.823703	-4.521682
H	1.255757	-0.176614	-6.649559
H	-0.918228	-0.663354	-8.160377
H	-2.343883	-2.606257	-6.965245
H	-1.055743	-3.316961	-4.712303
H	-3.917128	2.456435	-3.728025
H	-5.111747	0.530329	-5.178797
H	-3.868004	0.392020	-7.561747
H	-1.909566	2.238553	-7.584654
H	-1.936051	3.506019	-5.209179
H	-2.959069	-2.086172	-2.363784
H	-3.612061	-1.543286	-3.880714
H	-3.717682	-0.495082	-2.466826
C	1.908514	2.497566	-2.341578
H	2.701737	0.820479	-0.290925
H	1.626801	-1.347057	0.350520
H	-0.382770	-2.112825	-0.935314
H	-1.658377	-0.771306	-2.725474
H	2.769158	2.772225	-1.728322
H	2.216309	2.427015	-3.389555
H	1.157304	3.291823	-2.293457

TS Picoline N-oxide sp2 Pu III – Small core

E = -1343.590241
G = -1343.324568

C	-1.442326	-2.179059	-6.392964
C	-0.841747	-1.157364	-7.169726
C	0.350940	-0.753106	-6.520065
C	0.482745	-1.521235	-5.337433
C	-0.626451	-2.402776	-5.259370
Pu	-1.657916	0.115543	-4.874054
O	-0.292371	1.549963	-3.498688
N	0.179903	0.766010	-2.535540
C	1.265096	1.195047	-1.832287
C	1.763642	0.363237	-0.835414

C	1.175045	-0.871842	-0.582133
C	0.072071	-1.256469	-1.341993
C	-0.440974	-0.426966	-2.330914
C	-3.074786	-1.193035	-3.119308
C	-2.528592	1.812404	-6.833041
C	-3.607885	0.911520	-6.618781
C	-4.152494	1.180712	-5.340836
C	-3.400201	2.228341	-4.756251
C	-2.404781	2.626271	-5.683842
H	1.301618	-1.466075	-4.629950
H	1.048636	-0.003379	-6.875978
H	-1.213965	-0.773322	-8.111320
H	-2.358395	-2.705953	-6.634254
H	-0.809163	-3.129758	-4.477456
H	-3.563824	2.661688	-3.776341
H	-4.992846	0.670780	-4.885113
H	-3.971034	0.175256	-7.325897
H	-1.926101	1.880342	-7.731035
H	-1.673352	3.410890	-5.530316
H	-2.966553	-2.108824	-2.523819
H	-3.601574	-1.510850	-4.037195
H	-3.757050	-0.526874	-2.576128
C	1.830087	2.524668	-2.196153
H	2.622881	0.703301	-0.266728
H	1.568914	-1.517170	0.197354
H	-0.418867	-2.209809	-1.168003
H	-1.658877	-0.748770	-2.795981
H	2.683568	2.761023	-1.557744
H	2.145942	2.534500	-3.244203
H	1.070402	3.305868	-2.094988

Adduct of picoline N-oxide sp2, Pu III – Large core

E = -822.749107
G = -822.481856

C	-1.408192	-2.102208	-6.899540
C	-0.639575	-1.042564	-7.445134
C	0.472617	-0.828180	-6.596693
C	0.395340	-1.760618	-5.530290
C	-0.763671	-2.550074	-5.720295
Pu	-1.785510	0.031812	-5.096473
O	-0.293939	0.975297	-3.345926
N	0.227472	0.504279	-2.247260
C	1.333196	1.124542	-1.735787
C	1.885253	0.628971	-0.559446
C	1.334292	-0.470950	0.088420
C	0.205628	-1.071409	-0.464645
C	-0.334965	-0.568277	-1.631546
C	-3.155564	-1.380376	-3.480000
C	-2.747678	2.018887	-6.870987
C	-3.855203	1.162998	-6.640990
C	-4.284063	1.351370	-5.303390
C	-3.438619	2.315889	-4.705616
C	-2.490384	2.730240	-5.674460
H	1.121595	-1.876989	-4.733380
H	1.263697	-0.103562	-6.755816
H	-0.851939	-0.509224	-8.364244
H	-2.308881	-2.523777	-7.331392
H	-1.095978	-3.362018	-5.085653
H	-3.519694	2.690781	-3.691671
H	-5.118387	0.852981	-4.825290
H	-4.318668	0.511791	-7.373651
H	-2.214752	2.132209	-7.807959
H	-1.722030	3.482485	-5.533679
H	-2.705613	-2.270132	-3.010952
H	-3.986288	-1.781945	-4.084481
H	-3.644109	-0.810176	-2.673550
C	1.852075	2.294563	-2.495076
H	2.762653	1.128453	-0.162230
H	1.774364	-0.848921	1.005060
H	-0.269529	-1.929554	-0.002538
H	-1.216983	-0.962743	-2.131758
H	2.723790	2.715740	-1.991728
H	2.125507	2.001724	-3.513681
H	1.078044	3.062410	-2.590693

Adduct of picoline N-oxide sp2, Pu III – Small core

E = -1343.613804
G = -1343.348273

C	-1.389708	-2.185564	-6.535486
C	-0.870686	-1.113955	-7.299916
C	0.264602	-0.601987	-6.624180
C	0.451320	-1.366615	-5.444923
C	-0.572496	-2.344476	-5.390403
Pu	-1.853617	0.059704	-5.017849
O	-0.565073	1.025798	-3.191256
N	0.088773	0.459917	-2.210821
C	1.235011	1.052061	-1.760611
C	1.914707	0.455260	-0.704047
C	1.447620	-0.714674	-0.114643
C	0.274193	-1.284455	-0.604404
C	-0.392228	-0.681110	-1.652638
C	-3.243929	-1.337138	-3.515539
C	-2.535183	1.924832	-6.940309
C	-3.700018	1.149467	-6.707678
C	-4.166289	1.442522	-5.401492
C	-3.284469	2.391339	-4.826472
C	-2.280654	2.691320	-5.779659
H	1.253663	-1.243063	-4.726031
H	0.893785	0.211921	-6.966118
H	-1.266038	-0.754695	-8.242043
H	-2.256148	-2.787424	-6.784254
H	-0.704991	-3.092163	-4.618316
H	-3.367917	2.818162	-3.833596
H	-5.043263	1.019754	-4.926322
H	-4.167537	0.474519	-7.415468
H	-1.952825	1.940021	-7.853702
H	-1.461489	3.388422	-5.643358
H	-2.865182	-2.261250	-3.050975
H	-4.028318	-1.682424	-4.215345
H	-3.783527	-0.780225	-2.731757
C	1.658108	2.301495	-2.449808
H	2.824357	0.931496	-0.353437
H	1.986835	-1.170409	0.709010
H	-0.137196	-2.195247	-0.183606
H	-1.311760	-1.042894	-2.108047
H	2.570809	2.692309	-1.996889
H	1.832063	2.114902	-3.514423
H	0.867851	3.056525	-2.392907

Product picoline N-oxide sp2, Pu III – Large core

E = -782.268208
G = -782.043073

C	-1.253382	-1.856796	-6.741971
C	-0.797322	-0.990444	-7.769285
C	0.559369	-0.674378	-7.503589
C	0.936001	-1.335359	-6.309065
C	-0.183931	-2.068642	-5.840207
Pu	-0.898642	0.641363	-5.479875
O	-2.375804	0.045038	-3.647251
N	-1.458099	-0.003936	-2.665140
C	-1.895297	-0.325742	-1.417702
C	-0.948683	-0.377210	-0.401453
C	0.388659	-0.105397	-0.675773
C	0.760098	0.217180	-1.980301
C	-0.168208	0.275695	-3.020623
C	-3.350802	-0.596013	-1.244422
C	-0.529273	3.362649	-4.826103
C	0.323493	3.137258	-5.938439
C	-0.489844	2.928442	-7.078733
C	-1.845204	3.010550	-6.670015
C	-1.867599	3.285625	-5.278379
H	-2.753517	3.431164	-4.671314
H	-2.710575	2.933207	-7.319485
H	-0.139420	2.760525	-8.090358
H	1.407393	3.167644	-5.926393
H	-0.211196	3.578501	-3.813498
H	-0.209407	-2.694786	-4.956522
H	1.918638	-1.316123	-5.851653
H	1.202060	-0.059335	-8.122716
H	-1.367350	-0.668558	-8.633763
H	-2.239375	-2.303104	-6.673971
H	-1.279429	-0.632432	0.600112
H	1.127002	-0.146113	0.120468
H	1.801308	0.431073	-2.206643
H	-3.570702	-0.839494	-0.202811
H	-3.942297	0.273430	-1.547772
H	-3.667530	-1.423907	-1.886431

Product picoline N-oxide sp2, Pu III – Small core

E = -1303.134126
G = -1302.910154

C	-1.242685	-1.712026	-6.669754
C	-0.807980	-0.828247	-7.688863
C	0.554592	-0.516942	-7.443212
C	0.956709	-1.205491	-6.273808
C	-0.153561	-1.943287	-5.794478
Pu	-0.850018	0.665660	-5.410520
O	-2.339578	0.038117	-3.683826
N	-1.457310	-0.019487	-2.661761
C	-1.931752	-0.357332	-1.435572
C	-1.011152	-0.414496	-0.394309
C	0.330827	-0.131830	-0.632106
C	0.737151	0.208271	-1.922773
C	-0.164310	0.272522	-2.986708
C	-3.390160	-0.637456	-1.305718
C	-0.349563	3.296215	-4.956191
C	0.352645	3.006891	-6.154498
C	-0.600133	2.766296	-7.174569
C	-1.890577	2.897012	-6.608416
C	-1.737035	3.225251	-5.237718
H	-2.539596	3.400339	-4.530668
H	-2.831675	2.786539	-7.136026
H	-0.380199	2.528939	-8.208175
H	1.430101	2.997059	-6.275849
H	0.094255	3.544750	-3.999835
H	-0.165647	-2.574420	-4.914081
H	1.943267	-1.181426	-5.824720
H	1.182213	0.118901	-8.055803
H	-1.399614	-0.477261	-8.526395
H	-2.233895	-2.141283	-6.574371
H	-1.365641	-0.682436	0.595676
H	1.048024	-0.177293	0.183160
H	1.783062	0.430917	-2.117112
H	-3.635589	-0.898790	-0.274224
H	-3.978594	0.234088	-1.609236
H	-3.685451	-1.456691	-1.968619

TS Picoline N-oxide sp3 Np IV – Large core

E = -867.694582
G = -867.390156

C	0.341381	1.651757	-1.850672
C	-0.007855	0.768874	-2.897888
C	0.581265	-0.492349	-2.624331
C	1.293136	-0.387202	-1.407427
C	1.138535	0.934456	-0.922805
Np	-1.376033	-0.155770	-0.646453
C	-3.399043	1.265732	0.627203
C	-2.483452	2.250615	0.174299
C	-1.301375	2.130855	0.945886
C	-1.479339	1.065823	1.861333
C	-2.778950	0.537734	1.667200
O	-3.246453	-1.717666	-0.078721
N	-3.811091	-2.660696	-0.801092
C	-5.040691	-3.091154	-0.431709
C	-5.705187	-4.059680	-1.155185
C	-5.088484	-4.597301	-2.287957
C	-3.823770	-4.153266	-2.639667
C	-3.151595	-3.180628	-1.887061
H	-5.430365	-2.602814	0.451835
C	-1.868496	-2.572584	-2.187248
C	-3.043478	-0.034003	-2.797784
C	-0.272677	-1.827020	0.832278
H	0.520994	-1.371089	-3.252690
H	1.860795	-1.173968	-0.929808
H	1.582028	1.330639	-0.017952
H	0.062498	2.695668	-1.782009
H	-0.598354	1.019227	-3.769040
H	-4.394031	1.094092	0.236430
H	-2.669132	2.988587	-0.597170
H	-0.423737	2.758652	0.864374
H	-0.757183	0.723757	2.591556
H	-3.206943	-0.303875	2.194380
H	-2.859691	-0.139816	-3.873212
H	-2.997092	1.045800	-2.590999
H	-4.074275	-0.352008	-2.599433
H	-1.008668	-2.215071	1.548883
H	0.175316	-2.699632	0.335010
H	0.537288	-1.364217	1.414333
H	-6.689599	-4.377586	-0.831666
H	-5.587163	-5.357992	-2.880126
H	-3.310714	-4.558701	-3.505213
H	-2.293272	-1.253608	-2.456526
H	-1.158326	-2.728565	-1.364077
H	-1.436624	-2.950569	-3.113981

TS Picoline N-oxide sp3 Np IV – Small core

E = -1343.950523
G = -1343.647437

C	0.271044	1.526803	-1.909312
C	-0.013391	0.553011	-2.890620
C	0.616972	-0.654568	-2.502002
C	1.297682	-0.424176	-1.284439
C	1.079467	0.920898	-0.914304
Np	-1.372696	-0.245113	-0.611751
C	-3.386761	1.267845	0.486266
C	-2.427304	2.217118	0.064890
C	-1.288791	2.082512	0.895647
C	-1.540284	1.046145	1.823364
C	-2.838291	0.544753	1.570484
O	-3.124229	-1.837023	-0.056478
N	-3.735693	-2.735109	-0.794149
C	-4.903043	-3.250828	-0.340176
C	-5.607183	-4.171285	-1.087640
C	-5.099032	-4.570191	-2.327536
C	-3.893759	-4.041958	-2.762606
C	-3.182081	-3.119947	-1.986212
H	-5.211811	-2.865883	0.622866
C	-1.943395	-2.440342	-2.331430
C	-3.065651	0.164792	-2.662865
C	-0.239808	-1.725129	0.944286
H	0.621364	-1.579264	-3.064737
H	1.891324	-1.144866	-0.739127
H	1.484342	1.405987	-0.035509
H	-0.054502	2.559148	-1.924768
H	-0.594014	0.706470	-3.790068
H	-4.363824	1.112455	0.046517
H	-2.551092	2.938436	-0.733680
H	-0.393958	2.688652	0.846702
H	-0.864128	0.700753	2.594664
H	-3.316457	-0.271686	2.094884
H	-3.043983	-0.014931	-3.745275
H	-2.855117	1.232929	-2.527281
H	-4.088342	-0.021829	-2.311892
H	-0.978975	-2.051637	1.688594
H	0.144477	-2.630517	0.448158
H	0.604487	-1.268298	1.475990
H	-6.541669	-4.560413	-0.699990
H	-5.635524	-5.289112	-2.938325
H	-3.463443	-4.339072	-3.713069
H	-2.336037	-1.147485	-2.458476
H	-1.167228	-2.653374	-1.581257
H	-1.569566	-2.731237	-3.313243

Adduct of picoline N-oxide sp3, Np IV – Large core

E = -867.729611
G = -867.425047

C	0.144396	1.933031	-1.947340
C	-0.113944	0.921806	-2.901800
C	0.621621	-0.230003	-2.526709
C	1.350853	0.073285	-1.350993
C	1.051384	1.407044	-0.985974
Np	-1.308698	0.080738	-0.532958
C	-3.560037	1.261094	0.613435
C	-2.626729	2.299595	0.376267

C	-1.540821	2.125772	1.276104
C	-1.798452	0.973740	2.056726
C	-3.042434	0.438021	1.643399
O	-2.208561	-2.293886	-0.632685
N	-3.251728	-2.860401	-1.161908
C	-4.484974	-2.614541	-0.650500
C	-5.605703	-3.242648	-1.154704
C	-5.471080	-4.141488	-2.210598
C	-4.199137	-4.377751	-2.719045
C	-3.080649	-3.736989	-2.197015
H	-4.491167	-1.900514	0.161645
C	-1.686134	-3.938214	-2.673505
C	-3.056373	-0.053843	-2.347818
C	-0.093983	-1.545427	0.926137
H	0.648690	-1.170664	-3.063947
H	2.012206	-0.597367	-0.819692
H	1.468962	1.941565	-0.141514
H	-0.254777	2.939978	-1.963826
H	-0.762343	1.011193	-3.762910
H	-4.499623	1.128388	0.093362
H	-2.739523	3.102961	-0.341487
H	-0.680084	2.776611	1.368178
H	-1.158702	0.568803	2.829498
H	-3.515653	-0.440928	2.064873
H	-2.776426	-0.705645	-3.190035
H	-3.169164	0.955548	-2.773454
H	-4.067822	-0.360574	-2.047312
H	-0.763790	-2.017826	1.656569
H	0.371138	-2.361780	0.356562
H	0.709692	-1.050633	1.492848
H	-6.572007	-3.017353	-0.717220
H	-6.335999	-4.646737	-2.626789
H	-4.047930	-5.070193	-3.540535
H	-1.276977	-2.997636	-3.056048
H	-1.040210	-4.245757	-1.845601
H	-1.660198	-4.691091	-3.463130

Adduct of picoline N-oxide sp3, Np IV – Small core

E = -1343.978990
G = -1343.676832

C	0.021319	1.891401	-1.934332
C	-0.242451	0.874120	-2.877206
C	0.516705	-0.264901	-2.510701
C	1.268331	0.058288	-1.354073
C	0.956170	1.386427	-0.992988
Np	-1.357722	-0.015308	-0.521731
C	-3.443789	1.435764	0.550190
C	-2.358643	2.334573	0.456733
C	-1.373880	1.934234	1.397546
C	-1.848567	0.786615	2.067863
C	-3.123135	0.469801	1.535873
O	-2.182369	-2.306445	-0.705238
N	-3.226620	-2.888063	-1.224129
C	-4.452990	-2.662229	-0.689985
C	-5.572305	-3.299831	-1.184830
C	-5.439680	-4.185554	-2.252234
C	-4.173140	-4.399126	-2.783206
C	-3.055026	-3.749588	-2.270267
H	-4.454917	-1.954268	0.127832
C	-1.665589	-3.925709	-2.771273
C	-3.138664	0.073048	-2.221245
C	-0.043460	-1.435853	0.968192
H	0.552897	-1.206513	-3.046655
H	1.958070	-0.595297	-0.837778
H	1.376941	1.930325	-0.156687
H	-0.397177	2.889978	-1.943893
H	-0.906011	0.952213	-3.727864
H	-4.355755	1.482496	-0.029882
H	-2.302683	3.193805	-0.199710
H	-0.433468	2.435618	1.587474
H	-1.332732	0.246246	2.849655
H	-3.759064	-0.342448	1.870384
H	-2.897667	-0.563987	-3.087700
H	-3.253196	1.096304	-2.605406
H	-4.131278	-0.233741	-1.859134
H	-0.709701	-1.936311	1.684914
H	0.452385	-2.220088	0.377173
H	0.731405	-0.906371	1.538271
H	-6.535127	-3.091966	-0.731608
H	-6.303805	-4.697927	-2.661461
H	-4.025442	-5.080379	-3.614507
H	-1.273261	-2.975604	-3.147838
H	-1.002159	-4.237832	-1.959008
H	-1.643409	-4.667438	-3.571321

Product picoline N-oxide sp3, Np IV – Large core

E = -827.253727
G = -826.990914

C	0.629616	1.007267	-1.589471
N	0.554052	-0.112632	-2.385110
C	1.174582	-1.274445	-2.090719
C	1.987474	-1.378465	-0.980757
C	2.156583	-0.251001	-0.167673
C	1.478872	0.917463	-0.469566
O	-0.138743	-0.029750	-3.515825
Np	-0.224503	2.129541	-4.650193
C	-1.140477	0.386588	-6.147723
C	-0.135944	2.134937	-2.040390
C	1.683303	3.078832	-6.350597
C	2.105762	3.504208	-5.063535
C	2.534104	2.359220	-4.345229
C	2.369675	1.230814	-5.184154
C	1.847185	1.672068	-6.422983
C	-1.684840	4.009034	-6.070139
C	-1.203126	4.717987	-4.940040
C	-1.858843	4.209680	-3.794513
C	-2.747766	3.185376	-4.215470
C	-2.645851	3.069774	-5.622861
H	0.994727	-2.066600	-2.806420
H	-3.415460	2.617285	-3.577998
H	-3.204083	2.386219	-6.247782
H	-1.394901	4.175788	-7.100354
H	-0.478408	5.522676	-4.952334
H	-1.721547	4.555559	-2.778013
H	2.926054	2.352472	-3.335939
H	2.131626	4.526109	-4.705354
H	1.330429	3.720097	-7.148710
H	1.616276	1.047080	-7.275382
H	2.596126	0.204976	-4.922765
H	-0.465244	-0.477411	-6.175748
H	-2.110588	0.016588	-5.787322
H	-1.290073	0.726077	-7.182507
H	2.484939	-2.318154	-0.771831
H	2.797787	-0.298017	0.707359
H	1.564361	1.791920	0.166786
H	-1.204670	1.876173	-2.087479
H	0.006157	3.020333	-1.421111

Product picoline N-oxide sp3, Np IV – Small core

E = -1303.497630
G = -1303.236888

C	0.672311	1.117792	-1.584672
N	0.501809	-0.045326	-2.307492
C	1.094295	-1.217941	-1.998649
C	1.986466	-1.297741	-0.953134
C	2.267990	-0.128497	-0.225592
C	1.620688	1.049585	-0.535877
O	-0.264400	0.020774	-3.398941
Np	-0.294586	1.994559	-4.638427
C	-1.060751	0.511142	-6.382362
C	-0.073287	2.243811	-2.022014
C	1.649056	3.147382	-6.135081
C	2.060493	3.357409	-4.794740
C	2.437185	2.105451	-4.253686
C	2.239716	1.122447	-5.249282
C	1.755906	1.764262	-6.415812
C	-1.695889	3.866126	-6.094408
C	-1.172429	4.577499	-4.987572
C	-1.827367	4.116930	-3.823468
C	-2.756600	3.116322	-4.211610
C	-2.680365	2.972551	-5.617390
H	0.828466	-2.037569	-2.654315
H	-3.435644	2.585478	-3.553475
H	-3.271457	2.298293	-6.222188
H	-1.401097	3.986767	-7.129452
H	-0.413620	5.348851	-5.026229
H	-1.668257	4.482019	-2.817327
H	2.813354	1.933984	-3.253394
H	2.100188	4.309570	-4.280034
H	1.327420	3.913946	-6.828662
H	1.525039	1.283898	-7.356913
H	2.424762	0.060635	-5.141337
H	-0.363165	-0.339048	-6.400068
H	-2.042528	0.121790	-6.068730
H	-1.162995	0.887055	-7.406714
H	2.461237	-2.244631	-0.726229
H	2.979850	-0.155975	0.594053
H	1.800353	1.953788	0.035860
H	-1.140057	2.015616	-2.148082
H	0.082537	3.146663	-1.436405

TS Picoline N-oxide sp3 Pu IV – Large core

E = -868.446918
G = -868.142115

C	0.325046	1.640569	-1.856657
C	-0.017059	0.745667	-2.896070
C	0.579981	-0.508988	-2.610213
C	1.288932	-0.388240	-1.393228
C	1.125598	0.936912	-0.921165
Pu	-1.367775	-0.157622	-0.643700
C	-3.392906	1.240095	0.613346
C	-2.488014	2.231241	0.152139
C	-1.303612	2.128516	0.922342
C	-1.468179	1.066314	1.843282
C	-2.763364	0.524631	1.655978
O	-3.229033	-1.727457	-0.064036
N	-3.801010	-2.658867	-0.794523
C	-5.033255	-3.085327	-0.429030
C	-5.703519	-4.043574	-1.161030
C	-5.090513	-4.574680	-2.298789
C	-3.823357	-4.134567	-2.647102
C	-3.145498	-3.172827	-1.885858
H	-5.419966	-2.602956	0.459094
C	-1.860495	-2.566924	-2.180693
C	-3.048025	-0.030066	-2.769169
C	-0.276522	-1.814691	0.833603
H	0.525737	-1.394196	-3.229727
H	1.860338	-1.167133	-0.907400
H	1.565937	1.344054	-0.019716
H	0.039246	2.683167	-1.798235
H	-0.608216	0.984188	-3.770026
H	-4.386030	1.054829	0.224483
H	-2.682376	2.962196	-0.623735
H	-0.432253	2.764087	0.834622
H	-0.740746	0.735098	2.573160
H	-3.180968	-0.319151	2.187707
H	-2.878043	-0.146686	-3.845783
H	-2.993618	1.050405	-2.571808
H	-4.076653	-0.343445	-2.554261
H	-1.014409	-2.201295	1.548549
H	0.170120	-2.687570	0.335789
H	0.533657	-1.353020	1.415970
H	-6.689635	-4.358698	-0.839914
H	-5.593777	-5.327253	-2.897417
H	-3.312955	-4.535016	-3.516556
H	-2.291434	-1.242845	-2.437630
H	-1.150530	-2.729685	-1.359417
H	-1.430748	-2.935753	-3.112081

TS Picoline N-oxide sp3 Pu IV – Small core

E = -1383.426950
G = -1383.124373

C	0.293736	1.484297	-1.873688
C	0.021171	0.514156	-2.859919
C	0.637463	-0.697890	-2.460396
C	1.305206	-0.468487	-1.233213
C	1.086015	0.875035	-0.866016
Pu	-1.376365	-0.291673	-0.615524
C	-3.402246	1.174606	0.494560
C	-2.504233	2.153138	0.011242
C	-1.335353	2.100462	0.810736
C	-1.502992	1.082595	1.774150
C	-2.782515	0.509628	1.578432
O	-3.080189	-1.936460	-0.021903
N	-3.726191	-2.788836	-0.782706
C	-4.874372	-3.332432	-0.310972
C	-5.613302	-4.203243	-1.083597
C	-5.162513	-4.524234	-2.367586
C	-3.975510	-3.970659	-2.820874
C	-3.228057	-3.100402	-2.019441
H	-5.139831	-3.007665	0.686544
C	-1.998579	-2.407898	-2.380470
C	-3.036046	0.217728	-2.694052
C	-0.175964	-1.599388	1.055818
H	0.649685	-1.621425	-3.025848
H	1.891408	-1.190439	-0.681703
H	1.472208	1.355516	0.023571
H	-0.029850	2.517179	-1.893425
H	-0.545520	0.670571	-3.767651
H	-4.384166	0.956927	0.092816
H	-2.689558	2.845712	-0.800398
H	-0.471720	2.744783	0.711329
H	-0.787628	0.798476	2.534264
H	-3.204585	-0.311541	2.142830
H	-3.004663	0.021493	-3.773083
H	-2.799225	1.276258	-2.557654
H	-4.061115	0.044202	-2.343209
H	-0.930167	-1.879487	1.802280
H	0.156512	-2.517652	0.544887
H	0.688179	-1.154046	1.557094
H	-6.531388	-4.615041	-0.680415
H	-5.728307	-5.202336	-2.998127
H	-3.588113	-4.207604	-3.806095
H	-2.353781	-1.112048	-2.476987
H	-1.194254	-2.657990	-1.673495
H	-1.663188	-2.660452	-3.387014

Adduct of picoline N-oxide sp3, Pu IV – Large core

E = -868.483658
G = -868.178128

C	0.135922	1.924544	-1.932397
C	-0.124163	0.915339	-2.888265
C	0.607442	-0.239238	-2.513870
C	1.336202	0.060477	-1.337117
C	1.040296	1.394520	-0.970502
Pu	-1.309352	0.082909	-0.531823
C	-3.557400	1.239343	0.601177
C	-2.637198	2.285766	0.347698
C	-1.544834	2.133834	1.243595
C	-1.784511	0.986568	2.036604
C	-3.024955	0.432703	1.636217
O	-2.197901	-2.289706	-0.635372
N	-3.242352	-2.855557	-1.162167
C	-4.473958	-2.611944	-0.645505
C	-5.596203	-3.239806	-1.146633
C	-5.465086	-4.136270	-2.205005
C	-4.194907	-4.370476	-2.718824
C	-3.074890	-3.729921	-2.199849
H	-4.477108	-1.899716	0.168230
C	-1.682067	-3.929404	-2.681993
C	-3.044961	-0.054714	-2.336958
C	-0.109754	-1.530935	0.928782
H	0.631220	-1.179692	-3.051359
H	1.994451	-0.612886	-0.805591
H	1.458404	1.926227	-0.124653
H	-0.260575	2.932459	-1.948048
H	-0.771798	1.007544	-3.749540
H	-4.497959	1.090774	0.087383
H	-2.762980	3.079427	-0.378482
H	-0.690964	2.794973	1.323935
H	-1.135402	0.596109	2.808911
H	-3.484366	-0.448669	2.067541
H	-2.761978	-0.705375	-3.178837
H	-3.161377	0.954404	-2.761770
H	-4.055002	-0.365411	-2.036426
H	-0.783160	-1.998504	1.658832
H	0.354939	-2.350537	0.363925
H	0.692982	-1.035248	1.495787

H	-6.560964	-3.016268	-0.704835
H	-6.331226	-4.641323	-2.618891
H	-4.046378	-5.061102	-3.542346
H	-1.274560	-2.987633	-3.063191
H	-1.033135	-4.239012	-1.857223
H	-1.658732	-4.680167	-3.473724

Adduct of picoline N-oxide sp3, Pu IV – Small core

E = -1383.454899
G = -1383.152910

C	0.160029	1.941415	-1.678965
C	-0.095656	1.048763	-2.741461
C	0.630906	-0.143323	-2.491831
C	1.356829	0.028956	-1.287186
C	1.056809	1.310429	-0.779420
Pu	-1.284540	-0.102600	-0.545108
C	-3.562766	1.016603	0.598025
C	-2.697097	2.097909	0.321486
C	-1.588392	2.002432	1.200872
C	-1.756967	0.853129	2.001707
C	-2.977638	0.236662	1.623913
O	-2.175200	-2.344662	-0.825360
N	-3.272020	-2.884652	-1.280803
C	-4.460032	-2.579044	-0.701324
C	-5.634242	-3.151591	-1.146224
C	-5.596403	-4.053531	-2.207700
C	-4.366862	-4.349286	-2.784245
C	-3.191913	-3.764532	-2.322314
H	-4.386778	-1.865083	0.108609
C	-1.836474	-4.025184	-2.877332
C	-2.923676	0.202763	-2.369576
C	0.077616	-1.384977	1.037656
H	0.664774	-1.015215	-3.136319
H	2.024091	-0.692263	-0.834998
H	1.452799	1.736507	0.134053
H	-0.249134	2.938915	-1.576516
H	-0.726250	1.242665	-3.598042
H	-4.507743	0.827466	0.103611
H	-2.865703	2.873616	-0.414660
H	-0.759816	2.697152	1.255076
H	-1.084134	0.509993	2.775722
H	-3.399611	-0.651951	2.081090
H	-2.581237	-0.392617	-3.229521
H	-3.071224	1.234750	-2.703077
H	-3.897168	-0.188566	-2.039400
H	-0.638862	-1.842775	1.732855
H	0.534832	-2.178254	0.427967
H	0.860647	-0.871573	1.602841
H	-6.564368	-2.881122	-0.659037
H	-6.505352	-4.515108	-2.578395
H	-4.293995	-5.045381	-3.613100
H	-1.399639	-3.101141	-3.269664
H	-1.162185	-4.381353	-2.092428
H	-1.892256	-4.765382	-3.677108

Product picoline N-oxide sp3, Pu IV – Large core

E = -828.007726
G = -827.744675

C	0.351381	1.000680	-1.751935
N	0.223132	-0.180786	-2.444616
C	0.879985	-1.311223	-2.110050
C	1.784688	-1.318856	-1.068142
C	2.008288	-0.127574	-0.367589
C	1.292965	1.008690	-0.705368
O	-0.560765	-0.193782	-3.516498
C	-0.466971	2.080375	-2.229140
Pu	-0.779672	1.863309	-4.795648
C	-1.734351	-0.005873	-6.077686
C	1.112587	1.424077	-6.735849
C	0.953256	2.829900	-6.640898
C	1.482193	3.247824	-5.391342
C	1.974392	2.099407	-4.720602
C	1.742074	0.976384	-5.549735
C	-3.259394	2.892459	-4.175120
C	-2.361556	3.975641	-3.977231
C	-1.864093	4.367364	-5.241256
C	-2.445928	3.523578	-6.221284
C	-3.317333	2.621138	-5.562712
H	0.650793	-2.160451	-2.741200
H	-3.827921	2.385710	-3.403972
H	-3.919557	1.859430	-6.038508
H	-2.280454	3.577007	-7.290419
H	-1.170712	5.178186	-5.427857
H	-2.117621	4.435194	-3.028021
H	2.450091	2.087593	-3.748207
H	1.532091	4.266906	-5.027679
H	0.530382	3.475202	-7.400650
H	0.809824	0.802804	-7.568342
H	1.989235	-0.050982	-5.314451
H	-1.015308	-0.832725	-6.126474
H	-2.637795	-0.402461	-5.593754
H	-2.010313	0.256466	-7.108678
H	2.309244	-2.235587	-0.826029
H	2.721905	-0.098824	0.450297
H	1.421387	1.933248	-0.152524
H	-1.530876	1.812285	-2.147216
H	-0.278924	3.018055	-1.706135

Product picoline N-oxide sp3, Pu IV – Small core

E = -1342.974849
G = -1342.715347

C	0.301115	0.944691	-1.831403
N	0.263634	-0.232880	-2.545375
C	0.992848	-1.323530	-2.228743
C	1.895762	-1.286293	-1.188192
C	2.039512	-0.088463	-0.470924
C	1.252010	1.001168	-0.788051
O	-0.524624	-0.272317	-3.618195
C	-0.582931	1.969640	-2.278907
Pu	-0.817452	1.723771	-4.844529
C	-2.078512	0.041515	-6.032573
C	1.257318	1.445254	-6.574836
C	1.011643	2.837203	-6.530330
C	1.410552	3.310860	-5.252149
C	1.898862	2.213871	-4.511713
C	1.793822	1.056249	-5.321987
C	-3.135844	2.972855	-4.150570
C	-2.149403	3.990468	-4.081061
C	-1.719437	4.264991	-5.397057
C	-2.420257	3.405750	-6.277443
C	-3.311528	2.619840	-5.508042
H	0.820012	-2.177114	-2.872077
H	-3.683055	2.557433	-3.311950
H	-4.016010	1.895748	-5.891588
H	-2.317499	3.376159	-7.355816
H	-0.985201	5.006520	-5.683630
H	-1.806028	4.486042	-3.182709
H	2.289592	2.251185	-3.503244
H	1.364076	4.336483	-4.908514
H	0.617372	3.439410	-7.339287
H	1.063420	0.789523	-7.416070
H	2.089108	0.052653	-5.042585
H	-1.300552	-0.738916	-6.055557
H	-2.968683	-0.368559	-5.545712
H	-2.330991	0.335001	-7.059025
H	2.481108	-2.168331	-0.957516
H	2.752772	-0.023912	0.345338
H	1.321681	1.924280	-0.222386
H	-1.621620	1.615984	-2.335367
H	-0.506242	2.895557	-1.712748

TS Picoline N-oxide sp3 Np III – Large core

E = -822.055627
G = -821.790435

C	0.524814	1.540007	-2.052692
N	-0.617793	0.932282	-2.522306
C	-0.834559	-0.399290	-2.412612
C	0.106238	-1.231698	-1.846602
C	1.303228	-0.671439	-1.382420
C	1.496897	0.693163	-1.486472
O	-1.549378	1.674401	-3.099218
Np	-0.955269	3.308517	-4.829330
C	0.652935	2.967787	-2.234589
C	1.615896	4.182643	-4.641290
C	-3.103331	5.059386	-5.288081
C	-1.951777	5.872767	-5.449292
C	-1.364587	6.056616	-4.173709
C	-2.151621	5.358409	-3.224895
C	-3.225529	4.742423	-3.912268
C	-0.769157	0.877795	-6.310004
C	0.349813	1.628562	-6.738939
C	-0.125903	2.736347	-7.486411
C	-1.539524	2.667264	-7.518858
C	-1.939685	1.523651	-6.782163
H	-1.787095	-0.721991	-2.812634
H	-1.985535	5.332281	-2.154180
H	-4.015096	4.152471	-3.461085
H	-3.792287	4.768283	-6.072266
H	-1.604861	6.306616	-6.380333
H	-0.483053	6.648668	-3.958764
H	1.390069	1.384400	-6.558351
H	0.487126	3.481435	-7.980389
H	-2.198377	3.352158	-8.039094
H	-2.958422	1.179441	-6.643123
H	-0.737996	-0.042220	-5.738193
H	2.029264	4.997959	-4.036487
H	1.285368	4.654317	-5.584915
H	2.439052	3.510503	-4.910751
H	-0.096975	-2.293866	-1.777935
H	2.066930	-1.298762	-0.933526
H	2.406078	1.155404	-1.116826
H	1.026657	3.448581	-3.467860
H	-0.266581	3.500527	-1.969259
H	1.490214	3.368291	-1.659982

TS Picoline N-oxide sp3 Np III – Small core

E = -1304.094496
G = -1303.827822

C	0.381366	1.471745	-2.164286
N	-0.828187	0.971065	-2.584305
C	-1.154536	-0.335465	-2.462652
C	-0.262997	-1.246954	-1.934479
C	0.994576	-0.795274	-1.523101
C	1.299704	0.551424	-1.636051
O	-1.707701	1.796776	-3.120455
Np	-0.873235	3.367684	-4.798278
C	0.604331	2.899104	-2.333255
C	1.601284	4.267520	-4.634342
C	-3.072028	4.951154	-5.151946
C	-1.983660	5.731419	-5.620336
C	-1.197451	6.101564	-4.502025
C	-1.798959	5.547688	-3.345858
C	-2.959473	4.840676	-3.744211
C	-0.084549	1.062734	-6.122433
C	0.528212	2.117923	-6.841405
C	-0.494884	2.862900	-7.475445
C	-1.739395	2.261331	-7.157486
C	-1.483674	1.147187	-6.321937
H	-2.145478	-0.575730	-2.825333
H	-1.450578	5.674519	-2.327203
H	-3.641715	4.314042	-3.087887
H	-3.869333	4.542013	-5.761443
H	-1.805581	6.017786	-6.650294
H	-0.306632	6.716804	-4.523578
H	1.591347	2.310389	-6.908049
H	-0.352287	3.724613	-8.117400
H	-2.710141	2.580708	-7.517415
H	-2.228613	0.476143	-5.911635
H	0.432225	0.304911	-5.544193
H	1.908988	5.110172	-4.003055
H	1.301742	4.703426	-5.605087
H	2.489517	3.656755	-4.836439
H	-0.552579	-2.288638	-1.859555
H	1.720710	-1.487474	-1.108689
H	2.259612	0.933858	-1.305375
H	1.006157	3.416649	-3.505247
H	-0.274465	3.474952	-2.016284
H	1.474549	3.225992	-1.759657

Adduct of picoline N-oxide sp3, Np III – Large core

E = -822.078413
G = -821.811900

C	0.702871	1.322099	-1.616330
N	-0.358335	1.157165	-2.463102
C	-0.828872	-0.077140	-2.777287
C	-0.245393	-1.214171	-2.256864
C	0.842121	-1.090206	-1.394260
C	1.301830	0.183911	-1.083949
O	-0.950427	2.208439	-2.955402
Np	-0.910019	3.533575	-5.057160
C	1.128715	2.718524	-1.333100
C	1.461871	4.412092	-4.756274
C	-3.360799	4.983357	-5.253687
C	-2.397771	5.799837	-5.900025
C	-1.523245	6.313263	-4.909853
C	-1.942015	5.810301	-3.655074
C	-3.078961	4.991277	-3.866390
C	-0.172128	1.031446	-6.294305
C	0.455994	2.031840	-7.072464
C	-0.554968	2.750869	-7.756366
C	-1.808502	2.186469	-7.408956
C	-1.572404	1.125856	-6.503072
H	-1.671408	-0.069173	-3.455735
H	-1.487044	6.035742	-2.697243
H	-3.650255	4.483292	-3.097291
H	-4.188680	4.473930	-5.733548
H	-2.364409	6.026578	-6.959807
H	-0.688808	6.982590	-5.079955
H	1.521330	2.213015	-7.139246
H	-0.394868	3.563089	-8.456532
H	-2.774325	2.493516	-7.792984
H	-2.331472	0.472747	-6.085277
H	0.336069	0.292911	-5.683616
H	1.584327	5.096266	-3.901620
H	1.774763	4.992503	-5.638804
H	2.227448	3.626524	-4.644768
H	-0.647954	-2.182027	-2.533929
H	1.320320	-1.967601	-0.972238
H	2.144821	0.323429	-0.415629
H	1.444467	3.224197	-2.252754
H	0.292053	3.297388	-0.929564
H	1.952660	2.721604	-0.617750

Adduct of picoline N-oxide sp3, Np III – Small core

E = -1304.115251
G = -1303.848958

C	0.854851	1.320309	-1.671036
N	-0.279516	1.254365	-2.434024
C	-0.913695	0.074910	-2.666156
C	-0.429760	-1.104141	-2.138469
C	0.725382	-1.083041	-1.357810
C	1.353983	0.138448	-1.135188
O	-0.776918	2.356210	-2.926220
Np	-0.968482	3.494604	-5.020724
C	1.455535	2.667675	-1.481639
C	1.290342	4.474036	-4.889860
C	-3.279800	4.942534	-5.475642
C	-2.224155	5.789318	-5.896014
C	-1.503344	6.198835	-4.747470
C	-2.108659	5.595851	-3.618947
C	-3.208908	4.822997	-4.065781
C	-0.134268	1.103025	-6.188398
C	0.423408	2.128800	-6.988367
C	-0.640838	2.788217	-7.649912
C	-1.854197	2.163535	-7.269903
C	-1.540830	1.121047	-6.363649
H	-1.794660	0.160671	-3.287935
H	-1.795543	5.718016	-2.588187
H	-3.889619	4.259870	-3.437069
H	-4.024940	4.487803	-6.117736
H	-2.020635	6.092031	-6.916769
H	-0.645110	6.858088	-4.734263
H	1.475049	2.366484	-7.079687
H	-0.542396	3.615553	-8.343308

H	-2.843531	2.421847	-7.627478
H	-2.252779	0.431232	-5.923004
H	0.423996	0.401962	-5.577447
H	1.433030	5.160780	-4.039658
H	1.491067	5.075885	-5.791791
H	2.109984	3.737144	-4.845819
H	-0.961007	-2.026204	-2.347029
H	1.127010	-1.996725	-0.933251
H	2.255266	0.198308	-0.534296
H	1.689052	3.128996	-2.447214
H	0.744111	3.335971	-0.985243
H	2.362779	2.593924	-0.879932

Product picoline N-oxide sp3, Np III – Large core

E = -781.597087
G = -781.371541

C	0.370087	1.426545	-2.613528
C	-1.019587	1.170407	-2.499469
C	-1.183151	-0.159281	-2.042306
C	0.105694	-0.726954	-1.873045
C	1.065540	0.252140	-2.231124
Np	-0.064719	1.218336	0.181973
C	-2.491466	1.045593	1.271025
C	-3.198370	1.989786	0.473815
N	-2.549064	3.155343	0.102228
C	-3.138069	4.134660	-0.620525
C	-4.421324	3.997464	-1.097445
C	-5.108338	2.804099	-0.818277
C	-4.506286	1.831285	-0.050385
O	-1.266191	3.314163	0.451800
C	0.838562	0.316514	2.723288
C	1.708731	-0.307865	1.792601
C	2.526802	0.694809	1.218077
C	2.159749	1.939937	1.789414
C	1.119993	1.704924	2.723128
H	-2.500594	4.991888	-0.796479
H	0.641235	2.453994	3.342969
H	2.625026	2.897905	1.583842
H	3.318040	0.533489	0.495241
H	1.766286	-1.370933	1.587239
H	0.115216	-0.186139	3.355010
H	-2.128084	-0.663749	-1.879341
H	0.319820	-1.745312	-1.568410
H	2.140416	0.114649	-2.243581
H	0.820919	2.344631	-2.974539
H	-1.817669	1.861698	-2.743942
H	-4.864867	4.796467	-1.679185
H	-6.118401	2.655312	-1.188295
H	-5.031841	0.916260	0.201305
H	-1.977808	1.495163	2.128158
H	-3.079444	0.174504	1.549993

Product picoline N-oxide sp3, Np III – Small core

E = -1263.636035
G = -1263.411469

C	0.205814	1.308595	-2.544213
C	-1.099540	0.786512	-2.363669
C	-0.975755	-0.517272	-1.823790
C	0.403204	-0.802809	-1.672251
C	1.133646	0.327333	-2.119010
Np	-0.139548	1.160471	0.174813
C	-2.524969	1.118151	1.207187
C	-3.200676	2.106091	0.439191
N	-2.488321	3.222544	0.038408
C	-3.033557	4.250361	-0.648234
C	-4.344507	4.211158	-1.063706
C	-5.101090	3.065450	-0.762031
C	-4.538050	2.043822	-0.028627
O	-1.175471	3.272352	0.311978
C	0.828237	0.097927	2.507640
C	1.777306	-0.285256	1.529097
C	2.448061	0.882623	1.088475
C	1.912918	1.986650	1.796723
C	0.916476	1.504076	2.678900
H	-2.341898	5.057870	-0.852675
H	0.339761	2.102682	3.374203
H	2.222763	3.020999	1.695940
H	3.250646	0.920024	0.362233
H	1.975624	-1.296226	1.195321
H	0.170264	-0.569159	3.053409
H	-1.795957	-1.183219	-1.581320
H	0.826798	-1.731724	-1.310607
H	2.212668	0.412131	-2.157764
H	0.451002	2.280619	-2.957570
H	-2.028217	1.288215	-2.609911
H	-4.755915	5.044832	-1.619742
H	-6.134396	2.992378	-1.088139
H	-5.116359	1.166107	0.239635
H	-1.949773	1.540094	2.043399
H	-3.154349	0.287328	1.517936

TS Picoline N-oxide sp3 Pu III – Large core

E = -822.723864
G = -822.457302

C	0.284560	1.437371	-2.038373
N	-0.822862	0.887082	-2.643279
C	-1.076565	-0.442104	-2.632181
C	-0.209648	-1.329163	-2.031847
C	0.950283	-0.827149	-1.428104
C	1.181875	0.535615	-1.434951
O	-1.681322	1.686873	-3.255839
Pu	-0.872864	3.357153	-4.838907
C	0.459091	2.868326	-2.132732
C	1.664023	4.174100	-4.374158
C	-3.236953	4.836150	-4.766184
C	-2.397072	5.548264	-5.662084
C	-1.355066	6.139073	-4.907546
C	-1.551349	5.795937	-3.545903
C	-2.716465	4.997276	-3.458108
C	-0.084463	1.078389	-6.336712
C	0.625850	2.152323	-6.925668
C	-0.310377	2.999243	-7.566991
C	-1.602540	2.440962	-7.382987
C	-1.461120	1.254796	-6.623728
H	-1.994067	-0.717460	-3.135836
H	-0.933776	6.118240	-2.715691
H	-3.144470	4.587753	-2.550746
H	-4.142221	4.301052	-5.030039
H	-2.546773	5.650051	-6.730314
H	-0.562772	6.767801	-5.297088
H	1.699742	2.292405	-6.905360
H	-0.077694	3.891813	-8.136619
H	-2.529298	2.833341	-7.785072
H	-2.264756	0.591253	-6.326567
H	0.352538	0.248631	-5.792768
H	1.973840	4.995048	-3.717256
H	1.450463	4.640036	-5.353413
H	2.530384	3.521732	-4.534264
H	-0.440163	-2.387900	-2.044358
H	1.655496	-1.498505	-0.948227
H	2.062755	0.952266	-0.958143
H	0.957608	3.394423	-3.306267
H	-0.468256	3.413240	-1.926363
H	1.250591	3.218353	-1.467430

TS Picoline N-oxide sp3 Pu III – Small core

E = -1343.589768
G = -1343.323819

C	0.281578	1.434066	-2.014173
N	-0.704968	0.736871	-2.668484
C	-0.859124	-0.601616	-2.542154
C	0.004844	-1.346546	-1.768796
C	1.052363	-0.691398	-1.109862
C	1.177010	0.680592	-1.235675
O	-1.542052	1.392299	-3.454812
Pu	-0.944162	3.253316	-4.845619
C	0.334781	2.865156	-2.228640
C	1.558983	4.061468	-4.515604
C	-3.121007	4.866365	-4.926365
C	-2.149223	5.582077	-5.672965
C	-1.149991	6.028059	-4.779387
C	-1.497685	5.589048	-3.479409
C	-2.721101	4.877920	-3.566940
C	-0.265427	1.162215	-6.487675
C	0.479615	2.255334	-6.988824
C	-0.429963	3.190687	-7.536220
C	-1.740696	2.664276	-7.389593
C	-1.637315	1.411808	-6.742181
H	-1.691018	-1.003680	-3.105769
H	-0.941035	5.794326	-2.572727
H	-3.264401	4.434018	-2.740227
H	-4.027033	4.420571	-5.321215
H	-2.179112	5.768514	-6.739253
H	-0.273701	6.608652	-5.039791
H	1.556855	2.358442	-6.957321
H	-0.170247	4.127088	-8.015493
H	-2.656082	3.129431	-7.734788
H	-2.461335	0.759191	-6.477529
H	0.141930	0.281332	-6.004779
H	1.905833	4.870247	-3.861200
H	1.337113	4.527468	-5.489463
H	2.395731	3.371967	-4.682064
H	-0.140135	-2.417913	-1.694314
H	1.752727	-1.250129	-0.497148
H	1.966097	1.217896	-0.720357
H	0.846307	3.323143	-3.391197
H	-0.651902	3.327360	-2.100213
H	1.043134	3.344172	-1.549875

Adduct of picoline N-oxide sp3, Pu III – Large core

E = -822.747352
G = -822.480685

C	0.643430	1.324761	-1.609757
N	-0.398929	1.166524	-2.480751
C	-0.862318	-0.065121	-2.815003
C	-0.289877	-1.206301	-2.291368
C	0.778739	-1.089221	-1.404542
C	1.231180	0.182362	-1.073873
O	-0.981630	2.222107	-2.975924
Pu	-0.885005	3.535103	-5.061943
C	1.062354	2.718803	-1.305285
C	1.471101	4.388441	-4.719530
C	-3.326156	4.963937	-5.261974
C	-2.367665	5.773944	-5.923167
C	-1.487018	6.297953	-4.944049
C	-1.897600	5.808325	-3.681245
C	-3.035534	4.986858	-3.876629
C	-0.149490	1.043727	-6.279892
C	0.493003	2.042157	-7.048669
C	-0.506019	2.768455	-7.742534
C	-1.766507	2.210196	-7.410835
C	-1.546864	1.146620	-6.504477
H	-1.689779	-0.051720	-3.511650
H	-1.435212	6.042619	-2.729237
H	-3.600617	4.485277	-3.098912
H	-4.156179	4.448194	-5.731165
H	-2.340560	5.988614	-6.985563
H	-0.653441	6.965068	-5.126580
H	1.559954	2.217905	-7.102151
H	-0.333466	3.581837	-8.438299
H	-2.726255	2.524673	-7.803763
H	-2.314809	0.497647	-6.096655
H	0.347720	0.301765	-5.664438
H	1.582640	5.076745	-3.866927
H	1.805741	4.960532	-5.599434
H	2.227174	3.596777	-4.588753
H	-0.686123	-2.171915	-2.584866
H	1.247995	-1.969968	-0.979456
H	2.059393	0.316593	-0.386275
H	1.399375	3.231422	-2.213346
H	0.216389	3.294473	-0.916949
H	1.869380	2.715900	-0.570885

Adduct of picoline N-oxide sp3, Pu III – Small core

E = -1343.612284
G = -1343.346602

C	0.672029	1.379193	-1.633206
N	-0.396388	1.270717	-2.479525
C	-0.928254	0.063681	-2.800508
C	-0.401766	-1.103458	-2.285920
C	0.692656	-1.038305	-1.425122
C	1.215887	0.210011	-1.109248
O	-0.939254	2.356479	-2.962554
Pu	-0.812720	3.545824	-5.061595
C	1.162886	2.751855	-1.339716
C	1.475966	4.397115	-4.731024
C	-3.264385	4.769645	-5.370199
C	-2.319735	5.631420	-5.986352
C	-1.505834	6.186071	-4.967761
C	-1.943974	5.662166	-3.726609
C	-3.034221	4.793732	-3.975169
C	-0.177827	1.101675	-6.158783
C	0.490085	2.064812	-6.954989
C	-0.491117	2.790765	-7.673652
C	-1.763170	2.272474	-7.327127
C	-1.570703	1.229292	-6.392377
H	-1.768834	0.117916	-3.479127
H	-1.522597	5.895009	-2.755371
H	-3.589486	4.240230	-3.226778
H	-4.039816	4.208408	-5.877730
H	-2.254252	5.850218	-7.045849
H	-0.694900	6.890318	-5.109063
H	1.560724	2.216888	-7.006900
H	-0.300695	3.590010	-8.380735
H	-2.715245	2.607958	-7.719230
H	-2.356943	0.620916	-5.958406
H	0.301159	0.371650	-5.515447
H	1.598239	5.097188	-3.888681
H	1.750210	4.971242	-5.633122
H	2.259420	3.628292	-4.626646
H	-0.852520	-2.048816	-2.566625
H	1.127282	-1.940577	-1.008387
H	2.065932	0.304038	-0.441820
H	1.474103	3.258045	-2.260090
H	0.360526	3.358572	-0.907734
H	2.002865	2.709686	-0.644435

Product picoline N-oxide sp3, Pu III – Large core

E = -782.265867
G = -782.040054

C	-0.163299	1.033183	-2.425888
C	-1.484440	0.544659	-2.558608
C	-1.484375	-0.824533	-2.188184
C	-0.160626	-1.182946	-1.833740
C	0.656226	-0.032739	-1.972308
Pu	-0.989588	0.543364	0.230371
O	-1.561878	2.874210	0.475761
N	-2.676194	3.147906	-0.214812
C	-3.706832	2.222725	-0.204691
C	-4.791480	2.514507	-1.069965
C	-4.841296	3.673887	-1.813349
C	-3.795907	4.607913	-1.720518
C	-2.725229	4.305851	-0.911150
C	-3.560134	1.056054	0.598811
C	-0.490136	0.549734	3.011433
C	0.791848	0.482073	2.410679
C	0.927180	-0.794203	1.807424
C	-0.274353	-1.510682	2.026288
C	-1.150761	-0.679825	2.771374
H	-1.849372	4.929543	-0.784666
H	-2.136582	-0.953767	3.129096
H	-0.886069	1.389460	3.570380
H	1.552813	1.254044	2.447373
H	1.805921	-1.167220	1.294486
H	-0.473234	-2.530214	1.715570
H	-2.340804	-1.488784	-2.211872
H	0.175515	-2.168331	-1.532780
H	1.727412	0.009893	-1.810479
H	0.170658	2.037723	-2.660055
H	-2.341823	1.110115	-2.903977
H	-3.804570	5.540582	-2.271512
H	-5.696645	3.872209	-2.452365
H	-5.602778	1.795244	-1.105059
H	-3.223646	1.269980	1.619299

H	-4.421841	0.393185	0.577224

Product picoline N-oxide sp3, Pu III – Small core

E = -1303.132254
G = -1302.907716

C	-0.098754	1.022454	-2.259414
C	-1.414588	0.543824	-2.467574
C	-1.441717	-0.829901	-2.120255
C	-0.143475	-1.200146	-1.696101
C	0.687699	-0.052615	-1.776446
Pu	-1.054867	0.501617	0.239254
O	-1.608848	2.783535	0.447264
N	-2.721253	3.105719	-0.227333
C	-3.752580	2.184238	-0.259431
C	-4.835658	2.517748	-1.111331
C	-4.881121	3.713079	-1.795987
C	-3.834668	4.640873	-1.655341
C	-2.764587	4.297890	-0.861205
C	-3.597753	0.986706	0.492278
C	-0.392196	0.629490	2.873411
C	0.849069	0.475147	2.208265
C	0.894305	-0.829625	1.660409
C	-0.320943	-1.482427	1.979646
C	-1.117164	-0.581670	2.732716
H	-1.886774	4.912073	-0.704575
H	-2.094257	-0.791251	3.152832
H	-0.725070	1.516150	3.399965
H	1.633909	1.220923	2.146030
H	1.718778	-1.258472	1.104203
H	-0.583841	-2.500904	1.717665
H	-2.305805	-1.481941	-2.179450
H	0.167184	-2.188727	-1.380102
H	1.745348	-0.014856	-1.544090
H	0.246118	2.033851	-2.441950
H	-2.253627	1.122866	-2.834834
H	-3.842053	5.599598	-2.159638
H	-5.734462	3.944303	-2.426622
H	-5.648620	1.803004	-1.182919
H	-3.259320	1.164131	1.522186
H	-4.454728	0.318116	0.448068

Lutidine N-oxide

E = -401.950185
G = -401.833516

N	0.109805	-0.092490	0.028790
C	0.041076	-0.006040	1.402263
C	1.204105	0.168785	2.137149
C	2.442669	0.258705	1.508903
C	2.483426	0.168569	0.120734
C	1.323143	-0.006124	-0.618487
H	1.119378	0.233070	3.217520
H	3.351404	0.395127	2.085307
H	3.424722	0.233052	-0.416215
C	-1.330322	-0.115731	1.970223
C	1.252407	-0.114221	-2.101280
H	0.607094	0.670028	-2.510898
H	2.249199	-0.037230	-2.540200
H	0.792403	-1.064127	-2.393296
H	-1.976915	0.667928	1.561569
H	-1.789194	-1.066097	1.678039
H	-1.302327	-0.039483	3.059073
O	-0.958705	-0.253721	-0.649160

TS Lutidine N-oxide Np IV – Large core

E = -907.005503
G = -906.675479

C	-3.146032	-3.179417	-1.889123
N	-3.814636	-2.667722	-0.804556
C	-5.042699	-3.113082	-0.411895
C	-5.669370	-4.101853	-1.156640
C	-5.047882	-4.626488	-2.288333
C	-3.791602	-4.162687	-2.645108
O	-3.256235	-1.708243	-0.093731
Np	-1.381620	-0.153277	-0.658534
C	-0.282083	-1.813828	0.836260
C	-1.866831	-2.555999	-2.184894
C	-3.049573	-0.025386	-2.812050
C	1.153505	0.893471	-0.925056
C	0.366792	1.653114	-1.827097
C	-0.012658	0.806799	-2.893472
C	0.551833	-0.474048	-2.659815
C	1.275376	-0.417900	-1.447152
C	-3.388049	1.336036	0.570517
C	-2.419887	2.287497	0.156855
C	-1.269087	2.113645	0.964106
C	-1.518582	1.049133	1.863104
C	-2.831284	0.575888	1.623296
C	-5.624431	-2.481413	0.805389
H	0.466231	-1.333447	-3.311360
H	1.828991	-1.229526	-0.995147
H	1.611210	1.254305	-0.012471
H	0.111307	2.700397	-1.727454
H	-0.605638	1.093149	-3.751818
H	-4.377137	1.212318	0.147671
H	-2.551843	3.038774	-0.612779
H	-0.364717	2.705994	0.916845
H	-0.834241	0.672015	2.612115
H	-3.307912	-0.251798	2.130021
H	-2.848919	-0.116888	-3.885740
H	-3.020089	1.052322	-2.591393
H	-4.079033	-0.358211	-2.632015
H	-1.016311	-2.187815	1.562227
H	0.156621	-2.696217	0.348129
H	0.534396	-1.348941	1.407547
H	-6.646538	-4.446636	-0.837415
H	-5.537114	-5.396669	-2.876481
H	-3.269531	-4.559108	-3.509144
H	-2.300169	-1.239584	-2.461378
H	-1.155398	-2.720412	-1.364295
H	-1.433710	-2.929478	-3.113081
H	-6.597798	-2.921767	1.029190
H	-4.957486	-2.615177	1.662656
H	-5.737636	-1.402215	0.664588

TS Lutidine N-oxide Np IV – Small core

E = -1383.262005
G = -1382.932900

C	-3.212343	-3.085969	-2.009073
N	-3.784508	-2.698389	-0.826547
C	-4.962526	-3.210009	-0.365881
C	-5.634878	-4.138291	-1.146987
C	-5.111453	-4.536155	-2.376694
C	-3.901443	-4.008296	-2.799486
O	-3.175172	-1.792232	-0.091547
Np	-1.390136	-0.231678	-0.628181
C	-0.306068	-1.706527	0.969940
C	-1.962292	-2.411924	-2.332010
C	-3.044125	0.201950	-2.711299
C	1.088653	0.884519	-0.890149
C	0.312709	1.503068	-1.903015
C	0.027044	0.531628	-2.886208
C	0.624922	-0.687053	-2.481223
C	1.286738	-0.466058	-1.251701
C	-3.389206	1.338838	0.417412
C	-2.400595	2.262362	0.006105
C	-1.282326	2.111661	0.860928
C	-1.574644	1.090525	1.793126
C	-2.878160	0.615082	1.519232
C	-5.439103	-2.708925	0.953354
H	0.621596	-1.613519	-3.040914
H	1.855125	-1.196482	-0.692584
H	1.484783	1.364014	-0.004344
H	0.007810	2.541473	-1.927986
H	-0.534020	0.693228	-3.796630
H	-4.360201	1.202065	-0.041626
H	-2.492066	2.977410	-0.802392
H	-0.373434	2.697300	0.823672
H	-0.921931	0.738526	2.581373
H	-3.383440	-0.184496	2.044177
H	-3.001059	0.012537	-3.791439
H	-2.821733	1.267784	-2.579185
H	-4.077036	0.032500	-2.382381
H	-1.059169	-2.015945	1.707471
H	0.071099	-2.621924	0.486598
H	0.538173	-1.257953	1.508662
H	-6.573732	-4.537144	-0.779211
H	-5.640940	-5.258047	-2.990468
H	-3.454253	-4.305772	-3.741736
H	-2.341053	-1.115198	-2.476766
H	-1.199953	-2.640126	-1.571788
H	-1.576380	-2.707670	-3.307871
H	-6.376011	-3.198298	1.225193
H	-4.690029	-2.897169	1.728632
H	-5.590734	-1.625593	0.922538

Adduct of lutidine N-oxide, Np IV – Large core

E = -907.038405
G = -906.705166

C	-3.106170	-3.514229	-2.423600
N	-3.370398	-2.917962	-1.220704
C	-4.618100	-2.960004	-0.660055
C	-5.648806	-3.586551	-1.347564
C	-5.423573	-4.176377	-2.585098
C	-4.137765	-4.140787	-3.109808
O	-2.396116	-2.355520	-0.559889
Np	-1.435643	0.033622	-0.416715
C	-0.391205	-1.594922	1.157586
C	-1.699804	-3.459666	-2.902291
C	-3.311750	-0.009328	-2.101839
C	0.852191	1.366918	-1.168202
C	-0.034956	1.490416	-2.270790
C	-0.149400	0.217669	-2.882214
C	0.649046	-0.692001	-2.146250
C	1.269686	0.017472	-1.089927
C	-3.499573	1.497200	0.755194
C	-2.514539	2.436287	0.362117
C	-1.385832	2.264384	1.206855
C	-1.667163	1.208972	2.105619
C	-2.971731	0.734565	1.825617
C	-4.769695	-2.333707	0.679621
H	0.785486	-1.745237	-2.356369
H	1.943159	-0.401512	-0.354201
H	1.182686	2.171330	-0.523656
H	-0.511838	2.402460	-2.608450
H	-0.742731	-0.007400	-3.758918
H	-4.480905	1.391953	0.311056
H	-2.622106	3.179045	-0.418877
H	-0.482048	2.859912	1.190684
H	-1.005963	0.829141	2.873102
H	-3.475542	-0.061198	2.359845
H	-3.166019	-0.671540	-2.967540
H	-3.395712	1.007894	-2.516598
H	-4.308270	-0.250298	-1.703180
H	-1.118119	-2.000461	1.874719
H	0.044087	-2.456273	0.633639
H	0.416075	-1.133278	1.746047
H	-6.631500	-3.602752	-0.888556
H	-6.229969	-4.663067	-3.123566
H	-3.908423	-4.601874	-4.064510
H	-1.400534	-2.423882	-3.087872
H	-1.022489	-3.851775	-2.137512
H	-1.592266	-4.036423	-3.822643
H	-5.779142	-2.498586	1.060625
H	-4.036552	-2.747605	1.378564
H	-4.577776	-1.257991	0.622439

Adduct of lutidine N-oxide, Np IV – Small core

E = -1383.287871
G = -1382.956474

C	-3.137573	-3.539010	-2.419893
N	-3.397531	-2.935724	-1.220308
C	-4.638629	-2.977573	-0.646470
C	-5.671123	-3.617006	-1.319521
C	-5.451862	-4.218046	-2.552593
C	-4.171825	-4.178254	-3.090536
O	-2.419098	-2.354835	-0.574745
Np	-1.459027	-0.083318	-0.434987
C	-0.292747	-1.471384	1.195217
C	-1.738992	-3.472334	-2.917394
C	-3.207882	0.055544	-2.163577
C	0.920374	1.187756	-0.929157
C	0.044202	1.612718	-1.962494
C	-0.195292	0.510269	-2.812295
C	0.517593	-0.599379	-2.293432
C	1.215684	-0.175638	-1.136737
C	-3.513484	1.407275	0.667113
C	-2.540966	2.346551	0.255509
C	-1.415256	2.210132	1.105509
C	-1.682218	1.175453	2.027815
C	-2.978983	0.676466	1.755692
C	-4.786129	-2.333874	0.684750
H	0.574947	-1.587876	-2.731977
H	1.862842	-0.787815	-0.523453
H	1.317516	1.804289	-0.133310
H	-0.352358	2.612103	-2.091690
H	-0.811481	0.518163	-3.701618
H	-4.493716	1.281658	0.225062
H	-2.650540	3.059594	-0.552085
H	-0.516946	2.812261	1.069712
H	-1.021141	0.829981	2.811146
H	-3.477291	-0.107769	2.312760
H	-3.024108	-0.593956	-3.032859
H	-3.280470	1.082211	-2.549372
H	-4.204842	-0.201997	-1.773301
H	-1.031529	-1.841407	1.921799
H	0.137941	-2.346307	0.686456
H	0.511408	-0.978238	1.755457
H	-6.649835	-3.633894	-0.852339
H	-6.259979	-4.714816	-3.079245
H	-3.948659	-4.645393	-4.043597
H	-1.452265	-2.432888	-3.101834
H	-1.045530	-3.862683	-2.166287
H	-1.640844	-4.043694	-3.841928
H	-5.797649	-2.484524	1.065589
H	-4.059720	-2.746018	1.391902
H	-4.582800	-1.261235	0.615179

Product lutidine N-oxide, Np IV – Large core

E = -866.564891
G = -866.277118

C	-3.620635	-3.032357	-1.512741
C	-3.296457	-3.241119	-0.150717
C	-4.368522	-3.948136	0.449586
C	-5.357540	-4.169036	-0.545193
C	-4.892256	-3.602829	-1.759169
Np	-3.284736	-5.794219	-1.255579
C	-0.919888	-5.805795	-0.172552
C	-0.115504	-4.771678	-0.765368
N	-0.374037	-4.515774	-2.092663
C	0.312655	-3.615714	-2.844638
C	1.294130	-2.849591	-2.232413
C	1.552568	-3.012621	-0.869653
C	0.859850	-3.970516	-0.148889
O	-1.381005	-5.175504	-2.660828
C	-0.077630	-3.505079	-4.279258
C	-3.894868	-6.094969	-3.636731
C	-3.102039	-8.538042	-0.898658
C	-3.171788	-8.013683	0.418882
C	-4.468610	-7.482094	0.610154
C	-5.202575	-7.678411	-0.587854
C	-4.360802	-8.338995	-1.515515
H	-2.247779	-9.035055	-1.343720
H	-4.632985	-8.639906	-2.517865
H	-6.236375	-7.402373	-0.756351
H	-4.841103	-7.027780	1.520016
H	-2.377932	-8.032814	1.154568
H	-2.393215	-2.912728	0.347597
H	-4.434608	-4.238418	1.491061
H	-6.312779	-4.656865	-0.395342
H	-5.418716	-3.601691	-2.704346
H	-3.000635	-2.528076	-2.242900
H	-3.645310	-5.194307	-4.211302
H	-3.330544	-6.923161	-4.088167
H	-4.961088	-6.307103	-3.799882
H	1.834008	-2.123097	-2.828977
H	2.311414	-2.406819	-0.383202
H	1.071743	-4.147121	0.900080

H	-0.755304	-6.760344	-0.695199
H	-0.729471	-5.928635	0.893764
H	0.554998	-2.773957	-4.785992
H	0.009918	-4.474917	-4.778171
H	-1.126313	-3.207509	-4.374219

Product lutidine N-oxide, Np IV – Small core

E = -1342.814548

G = -1342.527847

C	-3.585179	-3.088420	-1.434484
C	-3.311056	-3.342344	-0.069127
C	-4.402618	-4.065104	0.465734
C	-5.358453	-4.243784	-0.566874
C	-4.853564	-3.640114	-1.741003
Np	-3.230950	-5.782823	-1.293875
C	-0.941202	-5.725059	-0.111694
C	-0.138524	-4.722138	-0.735338
N	-0.370056	-4.525209	-2.079757
C	0.331882	-3.665954	-2.864787
C	1.298107	-2.868922	-2.272097
C	1.523526	-2.960760	-0.893721
C	0.819288	-3.878996	-0.138583
O	-1.373101	-5.212836	-2.632302
C	-0.030068	-3.628349	-4.310892
C	-3.978143	-6.028639	-3.575846
C	-3.082721	-8.484072	-0.970563
C	-3.130555	-7.975379	0.353692
C	-4.418186	-7.436651	0.566551
C	-5.170006	-7.617513	-0.621416
C	-4.349593	-8.272697	-1.566200
H	-2.237441	-8.981148	-1.433365
H	-4.639564	-8.565022	-2.565950
H	-6.201946	-7.327395	-0.773825
H	-4.774757	-6.986285	1.484127
H	-2.327005	-8.009413	1.078325
H	-2.424082	-3.037108	0.470702
H	-4.500720	-4.399238	1.491062
H	-6.317188	-4.736595	-0.467678
H	-5.350186	-3.601139	-2.701137
H	-2.941366	-2.556803	-2.124274
H	-3.714362	-5.120046	-4.133991
H	-3.428805	-6.863834	-4.037030
H	-5.049898	-6.218285	-3.720517
H	1.851370	-2.172789	-2.891868
H	2.269062	-2.326706	-0.422780
H	1.007311	-3.997986	0.922931
H	-0.858101	-6.687002	-0.641913
H	-0.748274	-5.847749	0.952756
H	0.618494	-2.928894	-4.841487
H	0.060578	-4.622915	-4.757799
H	-1.073715	-3.326722	-4.442054

TS Lutidine N-oxide Pu IV – Large core

E = -907.757801

G = -907.426974

C	-3.142628	-3.169139	-1.889899
N	-3.807245	-2.664373	-0.799597
C	-5.037931	-3.106579	-0.411310
C	-5.670563	-4.084266	-1.165724
C	-5.052801	-4.601134	-2.302958
C	-3.793976	-4.140794	-2.655669
O	-3.241798	-1.716837	-0.079580
Pu	-1.373149	-0.155301	-0.656206
C	-0.288226	-1.803733	0.836803
C	-1.860999	-2.548160	-2.179304
C	-3.054096	-0.017683	-2.783131
C	1.137702	0.902987	-0.922949
C	0.346928	1.640446	-1.839930
C	-0.018456	0.773697	-2.894914
C	0.558172	-0.497237	-2.638974
C	1.274893	-0.415015	-1.423830
C	-3.382912	1.306818	0.557563
C	-2.428191	2.267474	0.133669
C	-1.272881	2.114212	0.938336
C	-1.504800	1.051479	1.843881
C	-2.812864	0.560709	1.612904
C	-5.615272	-2.484187	0.812837
H	0.484240	-1.367839	-3.276697
H	1.834261	-1.214008	-0.956848
H	1.588540	1.282484	-0.014663
H	0.080190	2.686374	-1.757954
H	-0.610323	1.040787	-3.760128
H	-4.370879	1.166550	0.137720
H	-2.572228	3.011415	-0.640759
H	-0.376146	2.717205	0.883194
H	-0.812634	0.687105	2.591919
H	-3.276295	-0.270844	2.125221
H	-2.872790	-0.125945	-3.858763
H	-3.009223	1.061619	-2.576939
H	-4.082463	-0.339761	-2.580267
H	-1.025683	-2.177036	1.559374
H	0.149752	-2.685820	0.347652
H	0.527695	-1.341168	1.410473
H	-6.649510	-4.426707	-0.849348
H	-5.546719	-5.362607	-2.898478
H	-3.274525	-4.531386	-3.523957
H	-2.299494	-1.226471	-2.443078
H	-1.150187	-2.721232	-1.360716
H	-1.430073	-2.911795	-3.112394
H	-6.591414	-2.920578	1.032365
H	-4.948942	-2.631279	1.668426
H	-5.721556	-1.402819	0.683719

TS Lutidine N-oxide Pu IV – Small core

E = -1422.738438

G = -1422.409631

C	-3.267724	-3.049503	-2.046483
N	-3.797478	-2.721066	-0.827050
C	-4.958207	-3.259338	-0.351360
C	-5.656363	-4.148527	-1.154800
C	-5.177577	-4.482638	-2.421078
C	-3.983298	-3.931319	-2.858649
O	-3.164795	-1.848378	-0.073417
Pu	-1.400329	-0.264138	-0.638841
C	-0.280360	-1.594245	1.075404
C	-2.022614	-2.367763	-2.381222
C	-3.000295	0.272020	-2.758001
C	1.094949	0.834888	-0.833362
C	0.348444	1.453034	-1.870262
C	0.078562	0.479045	-2.853434
C	0.650762	-0.743897	-2.422888
C	1.289276	-0.517993	-1.179763
C	-3.407252	1.267482	0.420600
C	-2.479668	2.218388	-0.062233
C	-1.325295	2.151529	0.756559
C	-1.530589	1.151389	1.731095
C	-2.819551	0.604616	1.523358
C	-5.389714	-2.826669	1.006844
H	0.654493	-1.673800	-2.977753
H	1.840204	-1.248706	-0.604028
H	1.466287	1.314692	0.062839
H	0.052011	2.493438	-1.910502
H	-0.458984	0.639454	-3.778146
H	-4.386811	1.066769	0.004508
H	-2.636751	2.902603	-0.886778
H	-0.446128	2.775162	0.661808
H	-0.833762	0.862143	2.506401
H	-3.267480	-0.198290	2.094146
H	-2.957126	0.056541	-3.832959
H	-2.734565	1.325303	-2.634871
H	-4.035534	0.133987	-2.421836
H	-1.058369	-1.837187	1.810297
H	0.030991	-2.531454	0.585984
H	0.587910	-1.170903	1.588626
H	-6.581207	-4.568086	-0.774676
H	-5.728254	-5.173502	-3.051521
H	-3.568912	-4.180288	-3.829556
H	-2.356682	-1.065100	-2.505406
H	-1.237323	-2.629971	-1.656728
H	-1.667443	-2.633391	-3.377781
H	-6.315264	-3.333422	1.285723
H	-4.614098	-3.049450	1.746085
H	-5.545588	-1.743832	1.036197

Adduct of lutidine N-oxide, Pu IV – Large core

E = -907.792285

G = -907.458601

C	-3.105066	-3.510939	-2.424302
N	-3.366673	-2.913057	-1.221431
C	-4.613522	-2.955728	-0.658469
C	-5.645566	-3.582521	-1.343732
C	-5.422895	-4.172811	-2.581517
C	-4.137892	-4.137871	-3.108267
O	-2.391502	-2.349970	-0.563214
Pu	-1.434595	0.039584	-0.416931
C	-0.403059	-1.582799	1.148588
C	-1.699334	-3.458212	-2.904911
C	-3.298360	-0.006457	-2.092171
C	0.841281	1.363542	-1.158230
C	-0.045828	1.485610	-2.261148
C	-0.161539	0.211369	-2.869485
C	0.635299	-0.697481	-2.131136
C	1.256353	0.013808	-1.076269
C	-3.492925	1.487020	0.742516
C	-2.510634	2.427689	0.346148
C	-1.380991	2.260767	1.190632
C	-1.658352	1.206134	2.091134
C	-2.962149	0.727850	1.813613
C	-4.762256	-2.330303	0.681848
H	0.768464	-1.751910	-2.336753
H	1.928334	-0.404416	-0.338880
H	1.173304	2.168832	-0.515820
H	-0.521533	2.397263	-2.601177
H	-0.755780	-0.015163	-3.745076
H	-4.474096	1.378100	0.299195
H	-2.620855	3.168192	-0.436458
H	-0.478904	2.858566	1.172600
H	-0.995155	0.829114	2.858158
H	-3.462432	-0.069264	2.348887
H	-3.150324	-0.671307	-2.955210
H	-3.384426	1.009179	-2.509793
H	-4.294031	-0.249071	-1.692791
H	-1.131964	-1.986809	1.864288
H	0.030377	-2.444461	0.624093
H	0.404371	-1.123092	1.738070
H	-6.627299	-3.598704	-0.882631
H	-6.230337	-4.659641	-3.118288
H	-3.910124	-4.599898	-4.062909
H	-1.399703	-2.423036	-3.091961
H	-1.021578	-3.849667	-2.140221
H	-1.593276	-4.036468	-3.824489
H	-5.770980	-2.494962	1.064886
H	-4.027639	-2.745071	1.378765
H	-4.569312	-1.254893	0.625038

Adduct of lutidine N-oxide, Pu IV – Small core

E = -1422.764245

G = -1422.435401

C	-3.222018	-3.495216	-2.481704
N	-3.453169	-2.938781	-1.253949
C	-4.677952	-3.000043	-0.648097
C	-5.730563	-3.604077	-1.322817
C	-5.544071	-4.152429	-2.585804
C	-4.276878	-4.099482	-3.152816
O	-2.461357	-2.368552	-0.618463
Pu	-1.440189	-0.144480	-0.418440
C	-0.206019	-1.392539	1.287798
C	-1.831826	-3.425156	-3.004468
C	-3.093493	0.205896	-2.225066
C	0.931702	1.152728	-0.879497
C	0.082023	1.535779	-1.949884
C	-0.122522	0.405840	-2.770244
C	0.580684	-0.682466	-2.194373
C	1.245141	-0.212671	-1.034140
C	-3.545439	1.217475	0.790172
C	-2.742817	2.221936	0.201294
C	-1.525152	2.277113	0.920331
C	-1.561652	1.293269	1.933695
C	-2.815151	0.637451	1.853648
C	-4.783109	-2.420162	0.717060
H	0.655554	-1.685254	-2.598260
H	1.885926	-0.795832	-0.387396
H	1.292313	1.795319	-0.086561
H	-0.330423	2.522997	-2.117391
H	-0.709469	0.382132	-3.678682
H	-4.550337	0.956152	0.479560
H	-3.024167	2.852736	-0.631766
H	-0.711950	2.966319	0.733555
H	-0.782987	1.089485	2.656151
H	-3.155791	-0.153732	2.511626
H	-2.920503	-0.495536	-3.053738
H	-3.125852	1.218521	-2.639134
H	-4.078032	-0.015024	-1.784936
H	-0.985495	-1.711659	1.994555
H	0.186236	-2.279452	0.769679
H	0.604844	-0.907956	1.837830
H	-6.697719	-3.637531	-0.833103
H	-6.367991	-4.621269	-3.113495
H	-4.080357	-4.529346	-4.128963
H	-1.523556	-2.385187	-3.147618
H	-1.131402	-3.865380	-2.287810
H	-1.762569	-3.954631	-3.956172
H	-5.788877	-2.571521	1.112437
H	-4.051586	-2.883959	1.386332
H	-4.558418	-1.349434	0.703987

Product lutidine N-oxide, Pu IV – Large core

E = -867.318944

G = -867.029869

C	-3.647002	-2.995264	-1.579037
C	-3.257500	-3.202556	-0.234408
C	-4.287233	-3.932865	0.411093
C	-5.316812	-4.167568	-0.538196
C	-4.917532	-3.589770	-1.769719
Pu	-3.257036	-5.733480	-1.345816
O	-1.337862	-5.093206	-2.706088
N	-0.339326	-4.447952	-2.108116
C	-0.108779	-4.724971	-0.780197
C	0.856769	-3.938632	-0.131081
C	1.568609	-2.972862	-0.822675
C	1.339105	-2.788257	-2.187562
C	0.366848	-3.539966	-2.831915
C	-0.929988	-5.766842	-0.223379
C	0.006968	-3.405863	-4.272342
C	-3.829971	-5.947515	-3.730913
C	-3.054340	-8.470775	-1.074425
C	-3.161210	-7.987432	0.256349
C	-4.465764	-7.470055	0.430697
C	-5.167760	-7.633569	-0.791315
C	-4.298168	-8.260723	-1.716696
H	-2.185263	-8.947265	-1.512968
H	-4.542764	-8.531724	-2.734502
H	-6.198319	-7.357328	-0.977953
H	-4.863826	-7.044891	1.343866
H	-2.385997	-8.023825	1.010912
H	-2.338547	-2.860008	0.223926
H	-4.297847	-4.231252	1.452323
H	-6.254688	-4.674247	-0.347632
H	-5.485414	-3.595691	-2.690589
H	-3.070799	-2.478264	-2.335560
H	-3.589455	-5.020302	-4.265550
H	-3.244994	-6.746724	-4.207055
H	-4.890162	-6.171243	-3.915695
H	1.894767	-2.055406	-2.761495
H	2.319904	-2.378068	-0.311549
H	1.046097	-4.132481	0.919170
H	-0.744510	-6.713847	-0.751988
H	-0.769588	-5.902025	0.846537
H	0.652452	-2.669525	-4.754693
H	0.101531	-4.368382	-4.784009
H	-1.038574	-3.103326	-4.384135

Product lutidine N-oxide, Pu IV – Small core

E = -1382.288491

G = -1382.002261

C	-3.679319	-3.076686	-1.646149

C	-3.117694	-3.264610	-0.363461
C	-4.028450	-4.025253	0.406486
C	-5.170759	-4.276555	-0.395507
C	-4.954261	-3.700453	-1.666168
Pu	-3.166684	-5.751066	-1.508679
O	-1.234302	-5.176212	-2.690873
N	-0.282975	-4.471815	-2.072195
C	-0.137986	-4.680261	-0.715626
C	0.749944	-3.811653	-0.046744
C	1.480234	-2.870722	-0.744751
C	1.350155	-2.772841	-2.136045
C	0.448870	-3.587670	-2.800592
C	-0.945736	-5.705174	-0.145494
C	0.186664	-3.543412	-4.267794
C	-4.225120	-5.868614	-3.679955
C	-3.013973	-8.436865	-1.124278
C	-3.169828	-7.906704	0.184305
C	-4.478835	-7.389504	0.287971
C	-5.134678	-7.595450	-0.950903
C	-4.234831	-8.252942	-1.817637
H	-2.129812	-8.931315	-1.512138
H	-4.443713	-8.563466	-2.832597
H	-6.150673	-7.309755	-1.192492
H	-4.907416	-6.923144	1.166015
H	-2.426201	-7.919469	0.970585
H	-2.157452	-2.894519	-0.028702
H	-3.887369	-4.333448	1.435026
H	-6.057684	-4.815761	-0.088330
H	-5.644354	-3.714481	-2.498656
H	-3.221642	-2.541534	-2.469760
H	-4.006956	-4.908361	-4.168559
H	-3.652731	-6.655035	-4.198617
H	-5.291736	-6.087582	-3.782283
H	1.928211	-2.057631	-2.709673
H	2.172725	-2.220220	-0.218632
H	0.863084	-3.931585	1.025206
H	-0.861580	-6.658431	-0.683985
H	-0.823761	-5.829480	0.927920
H	0.854690	-2.824672	-4.745610
H	0.331434	-4.530642	-4.716859
H	-0.851479	-3.260953	-4.468148

TS Lutidine N-oxide Np III – Large core

E = -861.366555
G = -861.074193

C	-1.416771	1.376481	-6.866653
C	-0.110933	1.012843	-6.449273
C	0.780750	2.027862	-6.866955
C	0.029189	3.020406	-7.545092
C	-1.327595	2.613471	-7.551532
Np	-0.823591	3.272755	-4.848265
O	-1.355211	1.476609	-3.257792
N	-0.378046	0.774452	-2.700642
C	0.695605	1.453741	-2.168796
C	1.734689	0.677405	-1.631109
C	1.660905	-0.703306	-1.611482
C	0.527684	-1.337759	-2.124897
C	-0.498094	-0.583191	-2.672226
C	0.688281	2.899816	-2.254190
C	1.622103	4.410902	-4.497365
C	-3.247675	4.656687	-5.169393
C	-2.252425	5.616277	-5.492790
C	-1.582669	5.970592	-4.297026
C	-2.161403	5.231086	-3.235349
C	-3.191994	4.423130	-3.773157
C	-1.748135	-1.154302	-3.249189
H	-1.892194	5.305183	-2.188069
H	-3.835940	3.755426	-3.212672
H	-3.955239	4.215215	-5.861803
H	-2.065486	6.031821	-6.476398
H	-0.785342	6.698488	-4.205356
H	1.853740	2.035596	-6.717269
H	0.429211	3.911731	-8.014960
H	-2.148506	3.140649	-8.022910
H	-2.319549	0.793407	-6.723264
H	0.162747	0.102440	-5.928407
H	1.855553	5.254988	-3.838102
H	1.313916	4.855190	-5.461025
H	2.555547	3.873513	-4.702191
H	0.427605	-2.417103	-2.111645
H	2.470150	-1.288537	-1.185635
H	2.590128	1.199127	-1.215889
H	1.067097	3.518825	-3.423468
H	-0.284121	3.320608	-1.974875
H	1.466529	3.332460	-1.622085
H	-1.745651	-2.241012	-3.147280
H	-2.626962	-0.741474	-2.744600
H	-1.844812	-0.889623	-4.306319

TS Lutidine N-oxide Np III – Small core

E = -1343.404692
G = -1343.111693

C	-1.421541	1.427307	-6.864036
C	-0.037051	1.226729	-6.641139
C	0.655709	2.365822	-7.111556
C	-0.303553	3.278400	-7.621225
C	-1.584285	2.693091	-7.475108
Np	-0.747092	3.263140	-4.907989
O	-1.175182	1.246217	-3.649290
N	-0.359640	0.660250	-2.791441
C	0.541050	1.432921	-2.097720
C	1.436192	0.767652	-1.248029
C	1.387738	-0.606367	-1.094430
C	0.423776	-1.338938	-1.790932
C	-0.455065	-0.693296	-2.645367
C	0.498977	2.861149	-2.335501
C	1.680500	4.216660	-4.562908
C	-3.165414	4.589724	-4.950710
C	-2.258027	5.492372	-5.560168
C	-1.374162	5.964255	-4.561664
C	-1.736924	5.357765	-3.333960
C	-2.844070	4.506320	-3.574407
C	-1.509098	-1.376267	-3.447643
H	-1.274068	5.546713	-2.372559
H	-3.369515	3.915096	-2.833471
H	-3.978458	4.072182	-5.446628
H	-2.257300	5.786132	-6.602611
H	-0.575221	6.682109	-4.704583
H	1.729209	2.507713	-7.103716
H	-0.092032	4.239932	-8.074942
H	-2.523023	3.131270	-7.791379
H	-2.215193	0.731747	-6.618963
H	0.416456	0.349740	-6.194497
H	1.981956	5.022877	-3.883575
H	1.379081	4.710802	-5.505529
H	2.570151	3.622262	-4.800318
H	0.347145	-2.415407	-1.686618
H	2.082188	-1.108685	-0.428116
H	2.155590	1.368785	-0.702427
H	1.036969	3.386431	-3.492587
H	-0.525625	3.244906	-2.232798
H	1.139567	3.397869	-1.632761
H	-1.504144	-2.447689	-3.239188
H	-2.496345	-0.963844	-3.217593
H	-1.347142	-1.212971	-4.517309

Adduct of lutidine N-oxide, Np III – Large core

E = -861.389462
G = -861.095769

C	-1.198904	1.240824	-6.856791
C	0.107400	1.035759	-6.342106
C	0.935380	2.079405	-6.818864
C	0.143846	2.930141	-7.627456
C	-1.173860	2.410282	-7.654701
Np	-0.852678	3.421369	-5.012985
O	-0.658895	2.029433	-2.957609
N	0.000184	0.987664	-2.524181
C	1.222625	1.175673	-1.937976
C	1.914444	0.064024	-1.473336
C	1.374812	-1.211249	-1.588996
C	0.119223	-1.355095	-2.167754
C	-0.576451	-0.248237	-2.635088
C	1.710899	2.576344	-1.827458
C	1.210104	4.876068	-4.661043
C	-3.540772	4.319026	-5.336458
C	-2.733074	5.401838	-5.769615
C	-2.095622	5.956121	-4.631855
C	-2.502232	5.212534	-3.498716
C	-3.397690	4.203370	-3.932989
C	-1.930626	-0.302728	-3.250150
H	-2.202163	5.400151	-2.473946
H	-3.908804	3.489477	-3.296485
H	-4.181431	3.711475	-5.965534
H	-2.651615	5.767708	-6.787064
H	-1.423156	6.804905	-4.628082
H	1.992334	2.201794	-6.616638
H	0.493091	3.811430	-8.153022
H	-2.008750	2.816896	-8.213078
H	-2.054764	0.588640	-6.719798
H	0.430786	0.196934	-5.734895
H	1.193802	5.442666	-3.716677
H	1.254452	5.636993	-5.457075
H	2.184174	4.362954	-4.704400
H	-0.345569	-2.330038	-2.266788
H	1.919314	-2.077206	-1.227386
H	2.885386	0.222977	-1.017080
H	1.802449	3.053709	-2.809327
H	0.998010	3.183090	-1.259661
H	2.680262	2.594577	-1.326571
H	-2.309086	-1.326108	-3.234428
H	-2.622374	0.352024	-2.711479
H	-1.900107	0.051878	-4.285765

Adduct of lutidine N-oxide, Np III – Small core

E = -1343.426958
G = -1343.133187

C	-1.515785	1.261455	-6.937868
C	-0.107512	1.165078	-6.786876
C	0.472679	2.336244	-7.328219
C	-0.574350	3.160449	-7.807804
C	-1.801554	2.493553	-7.568536
Np	-0.844914	3.237081	-5.076828
O	-0.897372	1.721570	-3.180301
N	-0.148377	0.888960	-2.502020
C	0.756142	1.388745	-1.604553
C	1.546281	0.495172	-0.892443
C	1.412462	-0.876199	-1.073099
C	0.460146	-1.341730	-1.972929
C	-0.330844	-0.454178	-2.688962
C	0.813422	2.866527	-1.456863
C	1.439952	4.153531	-4.754798
C	-3.242217	4.588989	-5.077680
C	-2.343651	5.416189	-5.799584
C	-1.386869	5.925830	-4.890513
C	-1.695226	5.417509	-3.603984
C	-2.841535	4.597204	-3.718988
C	-1.388202	-0.856056	-3.655087
H	-1.153393	5.635323	-2.690885
H	-3.331367	4.069777	-2.907979
H	-4.103688	4.073843	-5.485750
H	-2.395999	5.637116	-6.858533
H	-0.567765	6.592143	-5.130245
H	1.530932	2.560149	-7.370684
H	-0.455554	4.119637	-8.297302
H	-2.786469	2.855217	-7.836659
H	-2.247745	0.512531	-6.656113
H	0.439704	0.325036	-6.372303
H	1.616915	4.865095	-3.933962
H	1.642615	4.722902	-5.677774
H	2.240031	3.396156	-4.699859
H	0.311611	-2.403827	-2.134960
H	2.033507	-1.570434	-0.516699
H	2.266899	0.901268	-0.191014
H	1.043791	3.347373	-2.415698
H	-0.158952	3.254591	-1.136090
H	1.571811	3.140088	-0.721502
H	-1.448534	-1.943818	-3.716414
H	-2.358832	-0.453391	-3.347845
H	-1.182114	-0.444514	-4.647470

Product lutidine N-oxide, Np III – Large core

E = -820.907743
G = -820.655652

C	-1.191453	1.119452	-7.097686
C	0.039840	0.830543	-6.455911
C	0.859767	1.981325	-6.545290
C	0.137543	2.980773	-7.247503
C	-1.128498	2.446548	-7.591080
Np	-1.223846	2.731323	-4.761060
C	-1.501483	5.366684	-4.928298
C	-2.688795	5.560278	-4.161464
N	-3.705872	4.626443	-4.280791
C	-4.906848	4.720163	-3.644991
C	-5.122395	5.764285	-2.763096
C	-4.102346	6.697378	-2.536651
C	-2.912675	6.595899	-3.225154
O	-3.489395	3.556876	-5.059966
C	-5.902159	3.648912	-3.938468
C	-1.845819	2.458479	-1.995922
C	-1.552873	1.141809	-2.435850
C	-0.165552	1.072485	-2.716640
C	0.395832	2.348264	-2.463593
C	-0.642901	3.203160	-2.013064
H	-1.905386	2.954236	-8.150696
H	-2.018377	0.430101	-7.230087
H	0.317088	-0.115371	-6.005469
H	1.876768	2.068041	-6.179262
H	0.506264	3.965310	-7.511251
H	-0.531051	4.237030	-1.709643
H	1.444152	2.611105	-2.552027
H	0.375549	0.192133	-3.042606
H	-2.255886	0.317992	-2.496404
H	-2.814211	2.822279	-1.672463
H	-6.077568	5.831819	-2.255473
H	-4.257506	7.513417	-1.836854
H	-2.123271	7.327773	-3.092443
H	-1.699590	5.144089	-5.983140
H	-0.770170	6.162655	-4.807367
H	-6.839594	3.857158	-3.419421
H	-6.086522	3.577776	-5.014396
H	-5.525975	2.670723	-3.622597

Product lutidine N-oxide, Np III – Small core

E = -1302.947024
G = -1302.695590

C	-1.196194	1.331567	-7.044927
C	-0.044010	0.892787	-6.348554
C	0.881041	1.965353	-6.314442
C	0.300233	3.065223	-6.992199
C	-0.983771	2.671942	-7.450195
Np	-1.210931	2.801370	-4.722598
C	-1.588733	5.358213	-4.854693
C	-2.811360	5.537805	-4.144185
N	-3.778087	4.552994	-4.255762
C	-5.009678	4.615724	-3.680393
C	-5.313327	5.691048	-2.864403
C	-4.346975	6.681083	-2.640866
C	-3.123003	6.604710	-3.270241
O	-3.464970	3.447634	-4.951915
C	-5.933633	3.477017	-3.953249
C	-1.421703	2.801241	-1.990692
C	-1.656506	1.455851	-2.370036
C	-0.442684	0.920785	-2.865236
C	0.545637	1.934683	-2.791697
C	-0.060798	3.095351	-2.252844
H	-1.673060	3.280029	-8.024239
H	-2.080771	0.739197	-7.251982
H	0.114261	-0.096867	-5.938390
H	1.869627	1.939170	-5.872467
H	0.766388	4.029684	-7.159588
H	0.431007	4.042137	-2.061506
H	1.586489	1.829336	-3.072209
H	-0.287181	-0.095352	-3.206542
H	-2.595014	0.921124	-2.274310
H	-2.147637	3.480843	-1.559635
H	-6.291629	5.736455	-2.400283
H	-4.570666	7.520512	-1.988826
H	-2.374273	7.378176	-3.138075
H	-1.742619	5.087389	-5.909275
H	-0.891184	6.186085	-4.745820

H	-6.900514	3.658856	-3.480471
H	-6.072457	3.340363	-5.029758
H	-5.516531	2.539830	-3.571576

TS Lutidine N-oxide Pu III – Large core

E = -862.034646

G = -861.742011

C	-1.389322	1.365271	-6.821040
C	-0.082951	1.014804	-6.393732
C	0.803986	2.030765	-6.818962
C	0.049102	3.010794	-7.511503
C	-1.304933	2.594861	-7.519574
Pu	-0.815643	3.277187	-4.839996
O	-1.363906	1.507876	-3.248510
N	-0.386576	0.792186	-2.708278
C	0.699615	1.458694	-2.185985
C	1.738525	0.670102	-1.666188
C	1.652530	-0.710079	-1.654279
C	0.507285	-1.331291	-2.156968
C	-0.518608	-0.564181	-2.686823
C	0.701716	2.905049	-2.262423
C	1.600691	4.441017	-4.500605
C	-3.236320	4.620106	-5.186280
C	-2.247328	5.587844	-5.505282
C	-1.589722	5.951646	-4.305557
C	-2.168891	5.209337	-3.246185
C	-3.188203	4.390448	-3.789258
C	-1.780985	-1.120707	-3.251080
H	-1.906627	5.286973	-2.197450
H	-3.827847	3.716101	-3.232031
H	-3.933592	4.168844	-5.882699
H	-2.056605	6.002044	-6.488674
H	-0.799088	6.686230	-4.210326
H	1.875921	2.047902	-6.663228
H	0.445211	3.899969	-7.988548
H	-2.127247	3.112086	-7.999302
H	-2.289399	0.779108	-6.673943
H	0.194296	0.112976	-5.860073
H	1.815916	5.288593	-3.839668
H	1.285588	4.879138	-5.464582
H	2.544283	3.921218	-4.703631
H	0.397773	-2.409765	-2.148944
H	2.461817	-1.305147	-1.242348
H	2.603690	1.181583	-1.258454
H	1.064301	3.533556	-3.433322
H	-0.263476	3.331230	-1.967294
H	1.493219	3.328470	-1.640591
H	-1.786720	-2.208020	-3.155972
H	-2.649555	-0.703395	-2.732628
H	-1.888839	-0.848545	-4.305182

TS Lutidine N-oxide Pu III – Small core

E = -1382.900796

G = -1382.607594

C	-1.372946	1.413547	-6.864321
C	0.008686	1.256767	-6.587317
C	0.677159	2.426937	-7.016804
C	-0.290309	3.315735	-7.542373
C	-1.558382	2.683856	-7.455869
Pu	-0.862071	3.206523	-4.859307
O	-1.279577	1.239403	-3.552258
N	-0.390430	0.636879	-2.777134
C	0.520235	1.412795	-2.100854
C	1.487744	0.744701	-1.337297
C	1.495578	-0.636054	-1.246196
C	0.517822	-1.372747	-1.917562
C	-0.433150	-0.722697	-2.688788
C	0.420964	2.849310	-2.273871
C	1.548667	4.247891	-4.492122
C	-3.167740	4.629264	-4.976611
C	-2.220109	5.478048	-5.606401
C	-1.323455	5.943578	-4.619114
C	-1.711486	5.385158	-3.377492
C	-2.855999	4.577874	-3.595201
C	-1.510110	-1.410077	-3.455966
H	-1.234651	5.573836	-2.422964
H	-3.407154	4.031459	-2.838007
H	-4.004574	4.138687	-5.460685
H	-2.200028	5.737517	-6.657573
H	-0.489203	6.615039	-4.779544
H	1.742094	2.610660	-6.952926
H	-0.093612	4.291066	-7.971352
H	-2.498934	3.093022	-7.804061
H	-2.150960	0.687554	-6.657228
H	0.474420	0.386818	-6.138729
H	1.824559	5.050348	-3.797273
H	1.289170	4.739102	-5.443006
H	2.440830	3.639433	-4.685079
H	0.484873	-2.454777	-1.858438
H	2.246403	-1.141317	-0.646596
H	2.217735	1.347026	-0.807505
H	0.898593	3.407416	-3.410664
H	-0.609861	3.197604	-2.130402
H	1.071714	3.376744	-1.573361
H	-1.455893	-2.488019	-3.293446
H	-2.494930	-1.043775	-3.150008
H	-1.418596	-1.199261	-4.525697

Adduct of lutidine N-oxide, Pu III – Large core

E = -862.058348

G = -861.764828

C	-1.196216	1.289486	-6.854636
C	0.061246	1.008319	-6.261512
C	0.975807	2.004363	-6.678230
C	0.287848	2.900400	-7.530960
C	-1.053203	2.457965	-7.643141
Pu	-0.850523	3.430785	-5.001882
O	-0.650310	2.073857	-2.946437
N	0.004969	1.019434	-2.537550
C	1.251211	1.183607	-1.996254
C	1.938199	0.058471	-1.557550
C	1.370430	-1.206111	-1.654177
C	0.091718	-1.325305	-2.186174
C	-0.599326	-0.204782	-2.627110
C	1.770050	2.574562	-1.902793
C	1.156764	4.933076	-4.665510
C	-3.546367	4.234624	-5.362824
C	-2.765471	5.340610	-5.786671
C	-2.158064	5.913207	-4.641546
C	-2.555605	5.157686	-3.513148
C	-3.416196	4.122883	-3.957939
C	-1.976472	-0.232373	-3.191196
H	-2.271586	5.352477	-2.485215
H	-3.912857	3.393821	-3.327368
H	-4.161095	3.608376	-5.999270
H	-2.682979	5.708987	-6.803074
H	-1.509604	6.780375	-4.630376
H	2.023759	2.064089	-6.410631
H	0.719352	3.763140	-8.024670
H	-1.827329	2.913438	-8.249385
H	-2.095810	0.689397	-6.771280
H	0.297370	0.151059	-5.640170
H	1.130215	5.502799	-3.723508
H	1.171296	5.690759	-5.465686
H	2.145304	4.449567	-4.714756
H	-0.394984	-2.291078	-2.268295
H	1.911263	-2.082732	-1.313338
H	2.928002	0.198418	-1.137013
H	1.840885	3.049436	-2.887570
H	1.086910	3.196027	-1.314913
H	2.754559	2.574069	-1.432009
H	-2.375238	-1.247611	-3.158242
H	-2.633515	0.438287	-2.629342
H	-1.977368	0.119150	-4.228374

Adduct of lutidine N-oxide, Pu III – Small core

E = -1382.923220

G = -1382.630553

C	-1.166913	1.363895	-6.754346
C	0.029499	1.030978	-6.071577
C	1.021913	1.969719	-6.443833
C	0.444238	2.876584	-7.363817
C	-0.907580	2.504797	-7.556033
Pu	-0.798610	3.449641	-4.986851
O	-0.592369	2.232271	-2.906172
N	0.010913	1.133805	-2.526719
C	1.295908	1.212003	-2.063116
C	1.928669	0.042238	-1.661704
C	1.268966	-1.179816	-1.716455
C	-0.046030	-1.209905	-2.166717
C	-0.683751	-0.044218	-2.569348
C	1.913099	2.564330	-2.008784
C	1.099389	4.982166	-4.656287
C	-3.417730	4.052593	-5.644289
C	-2.667403	5.231903	-5.882865
C	-2.235152	5.736571	-4.631127
C	-2.714212	4.865093	-3.621165
C	-3.448528	3.829011	-4.248352
C	-2.093863	0.024718	-3.040154
H	-2.555486	4.978313	-2.554758
H	-3.954787	3.013241	-3.744899
H	-3.897650	3.440768	-6.398748
H	-2.479511	5.682496	-6.850790
H	-1.646130	6.631615	-4.473344
H	2.049482	1.986823	-6.100965
H	0.951878	3.710733	-7.833344
H	-1.615701	2.992143	-8.214995
H	-2.105161	0.822629	-6.709262
H	0.175060	0.181690	-5.413171
H	1.047084	5.563049	-3.721125
H	1.032883	5.724083	-5.471829
H	2.118996	4.571351	-4.722319
H	-0.603193	-2.139408	-2.211699
H	1.767614	-2.091763	-1.405164
H	2.949847	0.112647	-1.303128
H	1.924246	3.043792	-2.993364
H	1.326718	3.223765	-1.360269
H	2.932733	2.494201	-1.626180
H	-2.549420	-0.966449	-3.006794
H	-2.671028	0.714122	-2.416127
H	-2.144976	0.412079	-4.063202

Product lutidine N-oxide, Pu III – Large core

E = -821.576542

G = -821.324143

C	-0.690677	0.799897	-6.672954
C	0.602749	1.105505	-6.177285
C	0.908199	2.441352	-6.541275
C	-0.199834	2.965398	-7.249713
C	-1.187135	1.949254	-7.333989
Pu	-1.126282	2.664941	-4.597573
O	-2.380490	0.916859	-3.497213
N	-3.454026	1.442145	-2.888862
C	-4.157830	2.433476	-3.554035
C	-5.193453	3.052375	-2.816731
C	-5.517172	2.635351	-1.543631
C	-4.817164	1.572687	-0.957709
C	-3.773610	0.981240	-1.647513
C	-3.743732	2.786233	-4.872826
C	-2.934432	-0.128805	-1.111003
C	0.812237	4.179492	-3.230101
C	0.066993	3.554487	-2.198616
C	-1.226220	4.133000	-2.178758
C	-1.281995	5.114226	-3.198957
C	-0.022423	5.143481	-3.849195
H	-2.137632	2.027317	-7.848645
H	-1.199694	-0.152357	-6.580512
H	1.263146	0.420755	-5.656219
H	1.836058	2.961813	-6.335512
H	-0.264138	3.954001	-7.690676
H	-2.130309	5.750291	-3.422519
H	0.265984	5.811727	-4.652762
H	1.849031	3.982821	-3.477263
H	0.436710	2.795964	-1.517325
H	-2.025540	3.886221	-1.489905
H	-5.064200	1.206236	0.031908
H	-6.329068	3.114546	-1.004275
H	-5.744383	3.850141	-3.302946
H	-3.590216	1.919123	-5.524924
H	-4.368182	3.545485	-5.337998
H	-3.316638	-0.450669	-0.140492
H	-2.927837	-0.976762	-1.802093
H	-1.893047	0.189207	-0.999476

Product lutidine N-oxide, Pu III – Small core

E = -1342.442743

G = -1342.192380

C	-0.889867	0.969388	-6.648712
C	0.394741	1.081626	-6.062879
C	0.894526	2.375910	-6.344944
C	-0.082552	3.068220	-7.102349
C	-1.186192	2.197840	-7.292246
Pu	-1.220522	2.772041	-4.632018
O	-2.288677	1.004868	-3.495435
N	-3.389489	1.407017	-2.840360
C	-4.175795	2.372663	-3.445651
C	-5.239791	2.876498	-2.662517
C	-5.507880	2.369390	-1.408773
C	-4.722338	1.331039	-0.890131
C	-3.650122	0.855544	-1.623937
C	-3.803406	2.810574	-4.749811
C	-2.720716	-0.214683	-1.160009
C	0.698557	3.948064	-3.096879
C	-0.399170	3.742565	-2.223682
C	-1.445446	4.609207	-2.623070
C	-0.992668	5.355359	-3.739702
C	0.331846	4.951839	-4.029454
H	-2.086576	2.420650	-7.853509
H	-1.529878	0.095708	-6.613142
H	0.909511	0.305217	-5.507740
H	1.860383	2.764539	-6.046118
H	0.010143	4.075584	-7.491668
H	-1.561477	6.110534	-4.270683
H	0.960429	5.346789	-4.818222
H	1.661606	3.454187	-3.039185
H	-0.429393	3.051527	-1.389171
H	-2.418888	4.692527	-2.154853
H	-4.924763	0.896981	0.082086
H	-6.341962	2.758930	-0.832249
H	-5.857190	3.654452	-3.098493
H	-3.605705	1.980368	-5.441878
H	-4.479247	3.548783	-5.176729
H	-3.055360	-0.609008	-0.198690
H	-2.670615	-1.026949	-1.891270
H	-1.702311	0.172664	-1.055503