Electronic Supplementary Information for Dalton Transactions

The geometric structures, vibrational frequencies and redox properties of the actinyl coordination complexes ($[AnO_2(L)_n]^m$; An= U, Pu, Np; L= H_2O, Cl^-, CO_3^{2-}, $CH_3CO_2^-$, OH^-) in aqueous solution, studied by density functional theory methods.

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Supplementary Information

Table S1.
Optimized Structures (Å) of micro-solvated structures, using BP86 and basis B1.

$[UO_2(H_2O)_5]^{2+}$

U	-0.025654	-0.004084	-0.002179
O	-0.027731	-0.010607	1.791440
O	2.392588	0.139831	-0.012969
O	-0.024380	-0.006565	-1.796155
O	0.582381	2.338809	0.009344
O	0.857734	-2.255634	0.008627
O	-2.060979	1.305232	-0.001213
O	-1.897205	-1.532113	-0.005523
H	2.739392	-0.290771	0.826610
H	2.728733	-0.297086	-0.856401
H	1.102587	2.519247	0.853422
H	1.102539	2.529715	-0.830490
H	0.548547	-2.709682	0.853309
H	0.552399	-2.717657	-0.831498
H	-2.073374	1.856949	0.840732
H	-2.073781	1.858058	-0.843003
H	-2.426446	-1.375783	0.837275
H	-2.425274	-1.373903	-0.848975
O	2.536320	-0.483135	2.608572
H	1.833381	-1.165632	2.772698
H	3.311287	-0.763668	3.140665
O	2.534153	-0.518949	-2.611339
H	1.830404	-1.203523	-2.767921
H	3.312521	-0.810362	-3.132311
O	1.258007	2.264039	2.605780
H	1.693491	1.383254	2.761954
H	1.775562	2.916123	3.124447
O	1.237933	2.280106	-2.602400
H	1.666728	1.399123	-2.766722
H	1.751586	2.930491	-3.127195
O	0.281450	-2.594171	2.610442
H	-0.584965	-2.133961	2.767697
H	0.241565	-3.425690	3.129266
O	0.297301	-2.595959	-2.603972
H	-0.566470	-2.133697	-2.767983
H	0.261164	-3.425031	-3.127067
O	-1.789430	1.910550	2.606734
H	-0.817437	2.040084	2.768151
H	-2.243525	2.604825	3.130110
O	-1.788718	1.920757	-2.603121
H	-0.816406	2.054865	-2.762037
H	-2.244420	2.617006	-3.122444

O	-2.402119	-1.091533	2.597633
H	-2.228307	-0.126721	2.761379
H	-3.206888	-1.310764	3.113845
O	-2.398968	-1.086131	-2.605975
H	-2.225970	-0.120969	-2.767479
H	-3.202696	-1.305300	-3.123793

$[UO_2(H_2O)_5]^{1+}$

U	0.012216	-0.303613	0.038875
O	0.158260	-0.369177	1.931851
O	2.441124	0.143283	-0.158886
O	-0.047543	-0.340784	-1.841052
O	0.431431	2.191998	0.013760
O	1.029908	-2.529546	0.042255
O	-2.084234	1.103943	0.140046
O	-1.981949	-1.707073	0.050217
H	2.942635	-0.082773	0.664883
H	2.852544	-0.265306	-0.990628
H	0.940963	2.436958	0.844654
H	0.967087	2.369443	-0.803258
H	0.546466	-3.044619	0.779855
H	0.979254	-2.988863	-0.837317
H	-1.969324	1.659714	0.962309
H	-2.013468	1.686506	-0.670942
H	-2.468329	-1.392816	0.881606
H	-2.494681	-1.376378	-0.771059
O	2.685630	0.160093	2.577735
H	1.769069	-0.258733	2.513500
H	3.140134	-0.253095	3.340208
O	2.992409	-0.656738	-2.607395
H	2.439483	-1.476980	-2.774102
H	3.883905	-0.864206	-2.953566
O	1.260403	2.452036	2.557975
H	1.927679	1.710477	2.702550
H	1.665354	3.263676	2.925692
O	0.977246	2.038764	-2.673398
H	1.181589	1.068681	-2.678128
H	1.560504	2.445016	-3.346832
O	-0.213084	-3.208348	2.250633
H	-0.151411	-2.237919	2.454015
H	-1.173691	-3.332243	2.094204
O	1.104820	-2.615106	-2.686641
H	0.474364	-1.839473	-2.557663
H	0.744558	-3.149842	-3.423588
O	-1.621460	1.746050	2.722909
H	-0.629050	1.727736	2.767261
H	-1.889408	2.512092	3.270523
O	-1.851636	1.882516	-2.442245
H	-0.873015	1.896615	-2.644533
H	-2.227973	2.661061	-2.900635

O	-2.788862	-0.943805	2.504608
H	-2.323299	-0.086423	2.689409
H	-3.734943	-0.755701	2.669297
O	-3.090977	-0.737120	-2.190694
H	-2.590248	0.098181	-2.391882
H	-4.011840	-0.438178	-2.046417

$[NpO_2(H_2O_5)]^{2+}$

Np	-0.030510	0.004021	-0.000056
O	-0.029606	0.006961	1.773632
O	2.372044	0.136603	-0.003544
O	-0.028968	0.006694	-1.773730
O	0.574674	2.329094	0.002901
O	0.849572	-2.238564	0.003422
O	-2.060401	1.295164	-0.000744
O	-1.886544	-1.529590	-0.001823
H	2.706966	-0.302687	0.837696
H	2.703470	-0.303218	-0.846766
H	1.098314	2.504023	0.846222
H	1.097738	2.507279	-0.839282
H	0.540934	-2.693913	0.845343
H	0.542440	-2.697112	-0.836740
H	-2.069414	1.846968	0.841029
H	-2.068372	1.846922	-0.842906
H	-2.415896	-1.375880	0.839274
H	-2.414469	-1.375206	-0.843871
O	2.508857	-0.506155	2.608103
H	1.805057	-1.191371	2.767960
H	3.286785	-0.792032	3.132812
O	2.507894	-0.514683	-2.608794
H	1.804789	-1.201626	-2.765994
H	3.287090	-0.802727	-3.130380
O	1.255499	2.257538	2.600010
H	1.689923	1.376344	2.756889
H	1.774442	2.909707	3.117253
O	1.245826	2.261933	-2.600764
H	1.679081	1.381142	-2.760549
H	1.761676	2.913963	-3.121334
O	0.286199	-2.558348	2.619648
H	-0.585316	-2.104206	2.774827
H	0.258160	-3.382565	3.150806
O	0.292915	-2.559947	-2.616876
H	-0.577728	-2.105269	-2.774322
H	0.266115	-3.383356	-3.149379
O	-1.784964	1.904640	2.607588
H	-0.813611	2.046313	2.764052
H	-2.245114	2.594117	3.132134
O	-1.781938	1.908690	-2.605956
H	-0.810224	2.051840	-2.760969
H	-2.242367	2.598932	-3.129221

O	-2.369520	-1.091991	2.614007
H	-2.208284	-0.123633	2.771973
H	-3.161374	-1.322356	3.145275
O	-2.367716	-1.090451	-2.616813
H	-2.205674	-0.122197	-2.773996
H	-3.159840	-1.319824	-3.148080

$[NpO_2(H_2O_5)]^{1+}$

Np	-0.314734	-0.078548	0.236787
O	-0.261371	-0.350402	2.063525
O	2.141017	0.124384	-0.159103
O	-0.369149	0.233200	-1.617342
O	0.469201	2.283840	0.769189
O	0.735910	-2.321566	0.083791
O	-2.381383	1.331129	0.445267
O	-2.150170	-1.696926	-0.109308
H	2.626892	-0.330256	0.585956
H	2.355146	-0.390860	-1.008517
H	1.344919	2.200063	1.302915
H	0.647812	2.717045	-0.113190
H	0.738328	-2.851761	0.918143
H	0.674516	-2.902475	-0.729608
H	-2.241117	1.993212	1.219865
H	-2.522717	1.920021	-0.385072
H	-3.071571	-1.375197	0.209666
H	-2.240474	-1.898771	-1.078386
O	3.143079	-0.726906	2.248532
H	2.497639	-1.430085	2.575950
H	4.040128	-1.062776	2.447662
O	2.625698	-1.177179	-2.464013
H	1.996160	-1.944483	-2.549849
H	3.517967	-1.570003	-2.543470
O	2.532059	2.000300	2.379653
H	2.738329	1.027532	2.469500
H	3.363285	2.397067	2.048473
O	0.187774	2.876956	-1.880922
H	0.116136	1.882447	-2.006066
H	0.777493	3.205568	-2.590244
O	1.158031	-2.490221	2.780156
H	0.484658	-1.743142	2.736362
H	0.989165	-2.971429	3.616009
O	0.691689	-3.207436	-2.434432
H	-0.177446	-2.797248	-2.749469
H	0.734896	-4.107941	-2.814714
O	-1.666283	3.091013	2.249906
H	-1.566565	2.710719	3.147176
H	-0.755702	3.016628	1.843468
O	-2.563317	2.906575	-1.675160
H	-1.601941	3.092870	-1.869474
H	-2.954301	3.772854	-1.439681

O	-4.361873	-0.527476	0.649883
H	-4.605737	-0.695703	1.583101
H	-3.830630	0.321118	0.661895
O	-1.559488	-1.828015	-2.829776
H	-1.158985	-0.934118	-2.586205
H	-2.094363	-1.693638	-3.638859

$[PuO_2(H_2O)_5]^{2+}$

Pu	-0.024935	-0.000823	0.040202
O	-0.026882	-0.007848	1.800532
O	2.377250	0.154309	-0.011256
O	-0.024871	-0.002682	-1.719333
O	0.562365	2.329826	0.007953
O	0.872658	-2.232525	0.005003
O	-2.058843	1.281749	-0.004275
O	-1.870779	-1.536147	-0.005482
H	2.711276	-0.312016	0.813973
H	2.690905	-0.289955	-0.859545
H	1.108869	2.494472	0.837368
H	1.079579	2.503614	-0.837036
H	0.533943	-2.692293	0.833460
H	0.554608	-2.678061	-0.838798
H	-2.047111	1.856076	0.821375
H	-2.053983	1.827541	-0.850441
H	-2.413726	-1.351695	0.821028
H	-2.388278	-1.365371	-0.851796
O	2.510599	-0.491975	2.611004
H	1.825014	-1.190321	2.783879
H	3.300070	-0.755104	3.130493
O	2.492783	-0.496672	-2.611940
H	1.806061	-1.201064	-2.762652
H	3.278025	-0.767534	-3.133692
O	1.261093	2.240524	2.610701
H	1.704488	1.362897	2.763964
H	1.773954	2.900624	3.123184
O	1.212625	2.250688	-2.607665
H	1.657665	1.373409	-2.753070
H	1.713064	2.903916	-3.141000
O	0.265728	-2.582274	2.615408
H	-0.611509	-2.142012	2.771821
H	0.239055	-3.419418	3.125998
O	0.294609	-2.557786	-2.610261
H	-0.585154	-2.118538	-2.759225
H	0.275912	-3.383321	-3.139821
O	-1.762720	1.908742	2.608550
H	-0.791906	2.048261	2.769623
H	-2.228058	2.599726	3.125728
O	-1.767215	1.884606	-2.609219
H	-0.793994	2.035464	-2.752034
H	-2.231711	2.568392	-3.136681

O	-2.396071	-1.065047	2.605575
H	-2.225410	-0.101124	2.777455
H	-3.201534	-1.293742	3.115820
O	-2.362335	-1.075044	-2.613729
H	-2.200901	-0.106256	-2.770373
H	-3.155660	-1.308209	-3.140802

$[PuO_2(H_2O)_5]^{1+}$

Pu	-0.020974	-0.004914	0.030348
O	-0.030677	-0.012229	1.843175
O	2.479817	0.256179	-0.002582
O	-0.028499	-0.005361	-1.779712
O	0.472725	2.463133	0.014976
O	0.974908	-2.303813	0.012030
O	-2.206322	1.224865	0.005064
O	-1.884595	-1.671416	0.001721
H	2.750033	-0.254477	0.807567
H	2.725286	-0.237843	-0.831994
H	1.042488	2.547046	0.827738
H	1.022960	2.545078	-0.810276
H	0.582207	-2.721106	0.825639
H	0.592391	-2.706794	-0.812714
H	-2.113763	1.798205	0.813686
H	-2.111187	1.771644	-0.821845
H	-2.404989	-1.420411	0.811946
H	-2.380604	-1.422285	-0.824013
O	2.479645	-0.498705	2.663246
H	1.747157	-1.170510	2.728965
H	3.204694	-0.841104	3.225710
O	2.447789	-0.486694	-2.671145
H	1.722065	-1.169631	-2.728950
H	3.176888	-0.823605	-3.231642
O	1.230190	2.209164	2.661380
H	1.642221	1.303427	2.725493
H	1.789583	2.795898	3.211044
O	1.177913	2.203183	-2.662769
H	1.598232	1.300349	-2.723352
H	1.721436	2.789983	-3.228191
O	0.271727	-2.542745	2.671510
H	-0.545783	-1.977245	2.720268
H	0.092514	-3.318752	3.240634
O	0.297783	-2.508381	-2.671242
H	-0.532758	-1.959526	-2.722257
H	0.144640	-3.279327	-3.254770
O	-1.744606	1.875317	2.657200
H	-0.756036	1.975089	2.724885
H	-2.124539	2.589976	3.208379
O	-1.742662	1.838554	-2.660448
H	-0.753529	1.955630	-2.722188
H	-2.133414	2.542791	-3.217514

O	-2.347971	-1.062042	2.660152
H	-2.070530	-0.107840	2.711321
H	-3.143567	-1.137183	3.225466
O	-2.300472	-1.068014	-2.674603
H	-2.047145	-0.105488	-2.724592
H	-3.084061	-1.168094	-3.252773

$UO_2Cl_4^{2-}$

U	-0.008134	0.003543	-0.000036
O	0.661821	0.587193	1.591726
O	-0.679093	-0.580614	-1.591591
Cl	-0.091410	2.532610	-0.897866
Cl	0.076893	-2.526086	0.896237
Cl	-2.499083	0.243591	0.967397
Cl	2.484166	-0.238294	-0.964574
O	0.008203	1.666900	4.257522
H	0.130204	1.701404	3.279654
H	-0.809182	1.063920	4.335887
O	0.219514	2.161648	-4.203585
H	0.221614	2.377455	-3.238118
H	-0.583729	1.549402	-4.279573
O	-0.258393	-2.162880	4.197593
H	-0.264485	-2.374499	3.231164
H	0.558612	-1.569427	4.274298
O	0.041635	-1.671547	-4.246485
H	-0.084896	-1.701242	-3.269120
H	0.845551	-1.051093	-4.326338
O	-2.028669	-0.104888	4.267316
H	-2.262954	-0.010467	3.310832
H	-1.435086	-0.929086	4.272626
O	-1.792894	0.318899	-4.207959
H	-1.844574	0.280381	-3.225171
H	-1.170089	-0.464548	-4.380359
O	1.795611	-0.365772	4.197712
H	1.843419	-0.330215	3.214869
H	1.191738	0.431776	4.373562
O	2.038703	0.145995	-4.261807
H	2.268898	0.059804	-3.303509
H	1.426080	0.956126	-4.272324

$UO_2Cl_4^{3-}$

U	0.001264	-0.000260	-0.000661
O	0.720348	0.572452	1.635771
O	-0.717931	-0.572847	-1.636851
Cl	0.001585	2.664434	-0.974077
Cl	0.000419	-2.664552	0.972940
Cl	-2.598922	0.321719	1.078397
Cl	2.601409	-0.325279	-1.078621
O	-0.044799	1.680336	4.155061

H	0.126333	1.568541	3.178702
H	-0.839432	1.060933	4.273730
O	0.193012	2.177365	-4.186198
H	0.226750	2.386819	-3.211776
H	-0.592451	1.538280	-4.216631
O	-0.208957	-2.176849	4.184370
H	-0.242094	-2.387150	3.210163
H	0.581375	-1.543802	4.215337
O	0.059429	-1.680398	-4.153342
H	-0.114115	-1.569811	-3.177377
H	0.850172	-1.055652	-4.270325
O	-2.062984	-0.159089	4.268811
H	-2.279955	-0.027515	3.304654
H	-1.430554	-0.951783	4.242877
O	-1.799369	0.297426	-4.098190
H	-1.706642	0.223055	-3.108095
H	-1.181648	-0.466734	-4.342074
O	1.797750	-0.312680	4.095447
H	1.704442	-0.237203	3.105525
H	1.187454	0.456949	4.340631
O	2.063288	0.174120	-4.265353
H	2.280593	0.047626	-3.300581
H	1.424218	0.961538	-4.242285

$NpO_2Cl_4^{2-}$

Np	-0.009454	0.003512	0.000161
O	0.644077	0.594407	1.576161
O	-0.663680	-0.587939	-1.575619
Cl	-0.120307	2.516813	-0.896268
Cl	0.103914	-2.510367	0.894763
Cl	-2.493292	0.215330	0.952648
Cl	2.475892	-0.208937	-0.949161
O	0.016157	1.665855	4.242868
H	0.128992	1.711313	3.264520
H	-0.803346	1.065445	4.321890
O	0.225559	2.162251	-4.196482
H	0.228829	2.374585	-3.230122
H	-0.579261	1.552311	-4.270836
O	-0.266629	-2.163305	4.190051
H	-0.273782	-2.371770	3.222799
H	0.552950	-1.573509	4.265367
O	0.037780	-1.670665	-4.230801
H	-0.078873	-1.710083	-3.252714
H	0.842835	-1.051628	-4.312616
O	-2.026950	-0.096634	4.254962
H	-2.257900	-0.005907	3.297091
H	-1.437436	-0.923644	4.264468
O	-1.793043	0.325152	-4.187142

H	-1.846721	0.299287	-3.204319
H	-1.171988	-0.461403	-4.351659
O	1.795411	-0.375419	4.176095
H	1.843747	-0.352397	3.193125
H	1.195075	0.426351	4.345082
O	2.038783	0.140602	-4.249458
H	2.264185	0.058145	-3.289520
H	1.428466	0.952238	-4.265355

$NpO_2Cl_4^{3-}$

Np	0.001940	-0.000069	-0.000125
O	0.710859	0.586210	1.611454
O	-0.707003	-0.586369	-1.611594
Cl	-0.047447	2.658968	-1.021006
Cl	0.050533	-2.659143	1.020813
Cl	-2.600293	0.300149	1.111671
Cl	2.603480	-0.300607	-1.112851
O	-0.043873	1.671559	4.164432
H	0.106525	1.587668	3.184451
H	-0.841820	1.052518	4.282834
O	0.209587	2.185669	-4.212774
H	0.234647	2.398284	-3.237390
H	-0.580574	1.555298	-4.246696
O	-0.225312	-2.185151	4.211333
H	-0.248898	-2.398130	3.236056
H	0.569309	-1.560465	4.246673
O	0.057321	-1.672195	-4.162721
H	-0.093965	-1.588972	-3.182899
H	0.851219	-1.047938	-4.280863
O	-2.061345	-0.150213	4.285024
H	-2.284381	-0.026898	3.319533
H	-1.438703	-0.950665	4.262138
O	-1.796740	0.310901	-4.105095
H	-1.719821	0.268335	-3.115213
H	-1.176625	-0.459585	-4.325144
O	1.794779	-0.325738	4.104904
H	1.718419	-0.282871	3.115066
H	1.180822	0.449679	4.324969
O	2.060970	0.164468	-4.284450
H	2.284372	0.045270	-3.318582
H	1.432012	0.960025	-4.263969

$PuO_2Cl_4^{2-}$

Pu	-0.005601	-0.010515	0.003315
O	0.674694	0.551097	1.560044

O	-0.684200	-0.571523	-1.553871
Cl	-0.035615	2.527023	-0.846313
Cl	0.023896	-2.548117	0.851024
Cl	-2.494178	0.268258	0.941097
Cl	2.482432	-0.291196	-0.935430
O	-0.016188	1.664444	4.255353
H	0.079489	1.744930	3.278699
H	-0.826167	1.047330	4.330238
O	0.218983	2.162115	-4.162172
H	0.163950	2.369783	-3.195957
H	-0.579310	1.556799	-4.292609
O	-0.229303	-2.155920	4.166761
H	-0.193382	-2.376437	3.202635
H	0.577524	-1.556473	4.275142
O	0.035666	-1.658106	-4.248431
H	-0.068860	-1.735515	-3.272312
H	0.842608	-1.036284	-4.318181
O	-2.023282	-0.117340	4.217357
H	-2.228391	0.017324	3.257728
H	-1.428182	-0.939759	4.209985
O	-1.810146	0.320517	-4.239902
H	-1.895121	0.309816	-3.259955
H	-1.178967	-0.463124	-4.378389
O	1.810804	-0.330794	4.216739
H	1.883219	-0.313783	3.235636
H	1.188533	0.457532	4.368103
O	2.029928	0.137445	-4.211489
H	2.256411	0.015351	-3.255160
H	1.428746	0.955110	-4.199706

$PuO_2Cl_4^{3-}$

Pu	0.000536	-0.000003	0.000067
O	0.719478	0.589886	1.585360
O	-0.718355	-0.589889	-1.585222
Cl	0.028378	2.653982	-1.036678
Cl	-0.027510	-2.654038	1.036486
Cl	-2.599174	0.321841	1.118166
Cl	2.600107	-0.321779	-1.118322
O	-0.063724	1.665388	4.152543
H	0.074133	1.603622	3.171048
H	-0.856898	1.037202	4.269787
O	0.207476	2.192004	-4.220646
H	0.244222	2.403518	-3.244059
H	-0.580927	1.560747	-4.247457
O	-0.209647	-2.191959	4.220273
H	-0.245748	-2.404206	3.243837
H	0.579458	-1.561571	4.247180
O	0.065339	-1.665551	-4.152282
H	-0.072331	-1.604042	-3.170756

H	0.857953	-1.036657	-4.269583
O	-2.057925	-0.168388	4.277008
H	-2.281763	-0.056343	3.309355
H	-1.431368	-0.966167	4.265372
O	-1.799879	0.308741	-4.096934
H	-1.736435	0.284441	-3.107225
H	-1.172555	-0.461070	-4.300798
O	1.799549	-0.310743	4.097239
H	1.736395	-0.286177	3.107523
H	1.172989	0.459667	4.301149
O	2.057665	0.170203	-4.276774
H	2.280256	0.059947	-3.308626
H	1.430295	0.967380	-4.267053

$[UO_2(CH_3COO)_3]^{1-}$

U	0.039882	-0.000032	4.401025
O	0.039824	1.793678	4.397827
O	0.039912	-1.793728	4.397803
O	1.112498	-0.000213	2.124457
O	-1.098817	0.000213	2.146805
C	-0.000833	0.000041	1.485444
C	-0.004127	0.000150	-0.029082
H	-1.032517	0.000310	-0.420036
H	0.535373	0.889655	-0.398395
H	0.535148	-0.889435	-0.398527
O	-1.335959	0.000332	6.518526
O	-2.471614	-0.000336	4.620329
C	-2.461193	0.000044	5.904068
C	-3.767094	0.000167	6.671306
H	-3.586227	0.000483	7.756575
H	-4.358452	0.889615	6.392146
H	-4.358336	-0.889512	6.392643
O	1.467843	-0.000390	6.473936
C	2.581778	-0.000091	5.835298
O	2.566098	0.000236	4.553535
C	3.890037	-0.000081	6.598601
H	4.748150	-0.000012	5.910013
H	3.935482	0.889331	7.250967
H	3.935559	-0.889523	7.250915
O	3.499741	1.711761	2.338598
H	2.748697	1.235389	1.924031
H	3.520972	1.256387	3.207257
O	3.499839	-1.711676	2.338659
H	2.748135	-1.236276	1.924175
H	3.521476	-1.255310	3.206787
O	0.101996	1.712701	8.440930

H	0.837157	1.237410	7.997644
H	-0.659258	1.256390	8.022920
O	0.102204	-1.712888	8.440836
H	-0.659077	-1.254884	8.024747
H	0.837308	-1.239161	7.995773
O	-3.482083	1.714055	2.452212
H	-3.466655	1.236308	3.309171
H	-2.740649	1.258446	1.999295
O	-3.482115	-1.714369	2.452489
H	-3.465564	-1.237839	3.310107
H	-2.741935	-1.257426	1.998873

$[UO_2(CH_3COO)_3]^{2-}$

U	0.037844	-0.000150	4.399822
O	0.037262	1.849605	4.398410
O	0.037455	-1.849898	4.398298
O	1.123299	-0.000219	1.964771
O	-1.112720	0.000059	1.982892
C	-0.000652	0.000010	1.356850
C	0.001500	0.000296	-0.175229
H	-1.025487	0.000067	-0.573721
H	0.542621	0.890029	-0.544041
H	0.543201	-0.888928	-0.544409
O	-1.455024	0.000281	6.604159
O	-2.617467	-0.000341	4.693662
C	-2.563571	0.000132	5.970308
C	-3.879868	0.000464	6.754046
H	-3.696208	0.001539	7.840232
H	-4.474651	0.889460	6.477547
H	-4.474026	-0.889491	6.479272
O	1.588517	-0.000615	6.555643
C	2.683275	-0.000153	5.894970
O	2.707580	0.000214	4.618829
C	4.001505	0.000121	6.675543
H	4.867316	-0.000490	5.994389
H	4.043907	0.889976	7.328860
H	4.043582	-0.888753	7.330201
O	3.485736	1.665976	2.343470
H	2.695766	1.226214	1.952976
H	3.469153	1.239234	3.230259
O	3.485589	-1.666029	2.343212
H	2.694652	-1.227546	1.953229
H	3.469956	-1.237947	3.229366
O	0.102958	1.666709	8.423792
H	0.836615	1.225908	7.936624
H	-0.654245	1.239864	7.961577
O	0.103531	-1.667428	8.423464
H	-0.653805	-1.238083	7.963818

H	0.837002	-1.228990	7.933866
O	-3.469824	1.666610	2.455412
H	-3.419579	1.226292	3.334673
H	-2.690220	1.240639	2.031249
O	-3.469902	-1.667002	2.455760
H	-3.418747	-1.227841	3.335552
H	-2.691220	-1.239877	2.031076

$[NpO_2(CH_3COO)_3]^{1-}$

Np	0.040283	-0.000061	4.403989
O	0.039814	1.787302	4.398869
O	0.039869	-1.787431	4.398857
O	1.112240	-0.000276	2.133514
O	-1.098908	0.000273	2.155871
C	-0.001020	0.000036	1.495844
C	-0.004022	0.000154	-0.019907
H	-1.032098	0.000328	-0.411696
H	0.535726	0.889532	-0.389175
H	0.535483	-0.889311	-0.389318
O	-1.330432	0.000428	6.514552
O	-2.465636	-0.000407	4.615700
C	-2.454462	0.000058	5.898908
C	-3.761750	0.000199	6.666038
H	-3.582215	0.000566	7.751532
H	-4.353076	0.889499	6.386333
H	-4.352933	-0.889379	6.386913
O	1.461788	-0.000503	6.470287
C	2.574615	-0.000118	5.830361
O	2.559763	0.000285	4.549100
C	3.883880	-0.000092	6.594157
H	4.742348	-0.000011	5.906017
H	3.929286	0.889200	7.246703
H	3.929384	-0.889412	7.246653
O	3.488306	1.712872	2.344003
H	2.740080	1.231733	1.929142
H	3.513009	1.253097	3.210524
O	3.488490	-1.712713	2.344029
H	2.739441	-1.232752	1.929290
H	3.513624	-1.251826	3.209947
O	0.102428	1.714400	8.427375
H	0.836474	1.233711	7.987426
H	-0.659088	1.254738	8.012918
O	0.102664	-1.714572	8.427340
H	-0.658787	-1.252888	8.015035
H	0.836749	-1.235836	7.985313
O	-3.470324	1.716229	2.459713
H	-3.457226	1.232658	3.313762
H	-2.731651	1.257160	2.005233

O	-3.470370	-1.716553	2.459937
H	-3.456083	-1.234436	3.314793
H	-2.733057	-1.255962	2.004797

$[NpO_2(CH_3COO)_3]^{2-}$

Np	0.038133	-0.000071	4.401549
O	0.036682	1.827141	4.395469
O	0.036891	-1.827281	4.395172
O	1.126804	-0.000029	1.968267
O	-1.109895	0.000035	1.991242
C	0.001532	0.000025	1.364429
C	-0.000144	0.000090	-0.168559
H	-1.027998	0.000083	-0.564956
H	0.540475	0.889567	-0.538838
H	0.540522	-0.889326	-0.538915
O	-1.449519	0.000088	6.610699
O	-2.596854	-0.000216	4.691387
C	-2.552001	0.000033	5.968972
C	-3.875768	0.000276	6.740898
H	-3.702009	0.000495	7.828781
H	-4.467835	0.889710	6.459831
H	-4.467951	-0.889198	6.460201
O	1.578598	-0.000240	6.555712
C	2.669908	-0.000067	5.890974
O	2.688507	0.000089	4.614533
C	3.992572	-0.000017	6.664707
H	4.854842	-0.000034	5.979042
H	4.038468	0.889371	7.318498
H	4.038494	-0.889323	7.318606
O	3.482218	1.664150	2.347231
H	2.693775	1.222236	1.955355
H	3.465148	1.234043	3.232523
O	3.482247	-1.664048	2.347136
H	2.693480	-1.222585	1.955406
H	3.465449	-1.233498	3.232216
O	0.104617	1.666008	8.425287
H	0.836040	1.222415	7.936868
H	-0.653688	1.235539	7.967849
O	0.104826	-1.666316	8.425149
H	-0.653494	-1.234717	7.968810
H	0.836209	-1.223766	7.935719
O	-3.462644	1.664415	2.463473
H	-3.410308	1.220952	3.341269
H	-2.685404	1.236079	2.036841
O	-3.462610	-1.664661	2.463518
H	-3.409888	-1.221845	3.341616
H	-2.685822	-1.235684	2.036707

$[PuO_2(CH_3COO)_3]^{1-}$

Pu	0.042823	-0.000086	4.404074
O	0.038036	1.772337	4.402744
O	0.038164	-1.772506	4.402726
O	1.121637	-0.000317	2.132690
O	-1.088601	0.000308	2.169255
C	0.006427	0.000042	1.502362
C	-0.009070	0.000171	-0.013600
H	-1.040339	0.000351	-0.397042
H	0.527339	0.889654	-0.387464
H	0.527096	-0.889391	-0.387622
O	-1.334519	0.000463	6.517617
O	-2.467381	-0.000446	4.616242
C	-2.455741	0.000072	5.898590
C	-3.764806	0.000233	6.664588
H	-3.586558	0.000625	7.750415
H	-4.355924	0.889631	6.384696
H	-4.355788	-0.889447	6.385312
O	1.457272	-0.000570	6.456564
C	2.574380	-0.000140	5.821808
O	2.566004	0.000276	4.542468
C	3.878216	-0.000077	6.595054
H	4.741208	0.000021	5.912417
H	3.919651	0.889360	7.247656
H	3.919796	-0.889528	7.247623
O	3.493671	1.707127	2.339883
H	2.744106	1.226482	1.926294
H	3.518383	1.248306	3.207128
O	3.493831	-1.706990	2.339888
H	2.743406	-1.227563	1.926447
H	3.519019	-1.247015	3.206508
O	0.099567	1.709005	8.418764
H	0.832145	1.228634	7.975979
H	-0.663214	1.250044	8.004867
O	0.099914	-1.709192	8.418715
H	-0.662804	-1.248116	8.007081
H	0.832516	-1.230891	7.973717
O	-3.463752	1.712988	2.467248
H	-3.451064	1.228610	3.321320
H	-2.723688	1.254852	2.014090
O	-3.463748	-1.713344	2.467493
H	-3.449903	-1.230473	3.322404
H	-2.725101	-1.253578	2.013682

$[PuO_2(CH_3COO)_3]^{2-}$

Pu	0.039012	-0.000083	4.404154
O	0.038742	1.807563	4.403156
O	0.038853	-1.807705	4.403112
O	1.122902	-0.000099	1.986776

O	-1.112938	0.000012	2.005810
C	-0.001243	0.000008	1.380880
C	0.000669	0.000157	-0.152418
H	-1.026283	0.000085	-0.551283
H	0.541961	0.889706	-0.521593
H	0.542174	-0.889181	-0.521781
O	-1.445368	0.000119	6.598122
O	-2.599836	-0.000201	4.682899
C	-2.549800	0.000047	5.958981
C	-3.870581	0.000263	6.737468
H	-3.692207	0.000556	7.824635
H	-4.464006	0.889640	6.459039
H	-4.464008	-0.889266	6.459528
O	1.579256	-0.000280	6.550852
C	2.670010	-0.000086	5.885407
O	2.690909	0.000089	4.609907
C	3.992224	-0.000008	6.661540
H	4.855859	-0.000124	5.977491
H	4.037020	0.889428	7.315361
H	4.036983	-0.889223	7.315660
O	3.475710	1.666326	2.350738
H	2.687244	1.222233	1.961143
H	3.462058	1.233370	3.234976
O	3.475689	-1.666306	2.350608
H	2.686851	-1.222709	1.961200
H	3.462408	-1.232811	3.234585
O	0.103138	1.668238	8.410164
H	0.835654	1.223371	7.924213
H	-0.653407	1.235163	7.951975
O	0.103665	-1.668581	8.410023
H	-0.653066	-1.234259	7.953349
H	0.835952	-1.224835	7.922688
O	-3.460502	1.667369	2.463197
H	-3.409905	1.221093	3.339914
H	-2.684247	1.236366	2.037200
O	-3.460597	-1.667616	2.463461
H	-3.409390	-1.221987	3.340475
H	-2.684950	-1.235921	2.037068

$[UO_2(OH)_5]^{3-}$

U	0.064087	0.151017	0.003649
O	0.078707	0.228146	1.884513
O	0.152156	0.146579	-1.878016
O	-2.014843	-0.923126	0.169805
O	2.375598	-0.474774	0.159556
O	1.257076	2.196216	-0.073255
O	0.316762	-2.264987	-0.199886
O	-1.592216	1.813203	-0.073309
H	2.257326	-1.371066	-0.226269

H	2.215638	1.995896	0.059426
H	-0.562015	-2.575515	0.124083
H	-1.139411	2.687894	-0.160862
H	-2.695567	-0.212294	0.125353
O	2.459012	-0.876452	2.815082
H	2.618394	-0.769005	1.812401
H	1.572822	-0.425483	2.811730
O	3.982727	1.339471	-1.085104
H	3.479485	0.574150	-0.662669
H	3.326963	1.639528	-1.774236
O	1.165772	-3.296261	2.199057
H	0.982390	-3.008301	1.249635
H	1.628150	-2.475136	2.542948
O	-0.084042	-2.411846	-2.885331
H	0.088177	-2.561433	-1.893265
H	0.031004	-1.424591	-2.844802
O	-0.146241	4.220842	1.080228
H	0.503580	3.546574	0.707895
H	-0.648691	3.657882	1.731645
O	1.799449	2.314964	-2.691844
H	1.545861	2.519771	-1.727428
H	1.285136	1.467071	-2.735805
O	-3.665643	0.885339	-1.712862
H	-2.885983	1.304177	-1.246426
H	-3.290686	0.030571	-2.055809
O	-1.749205	2.336337	2.561839
H	-1.942522	2.150833	1.581297
H	-1.055611	1.632889	2.656649
O	-1.740926	-3.008951	2.035020
H	-1.900246	-2.165333	1.524247
H	-0.768663	-2.981115	2.245950
O	-2.820946	-1.882795	-2.248959
H	-2.574739	-1.658520	-1.295222
H	-1.908243	-2.072344	-2.610631

$[UO_2(OH)_5]^{4-}$

U	0.005240	0.304227	-0.030724
O	-0.194458	0.438418	1.898003
O	0.147932	0.351101	-1.964229
O	-1.873277	-1.356874	0.306076
O	2.377448	-0.266277	0.320174
O	1.233303	2.423947	-0.040350
O	0.594628	-2.312170	-0.336080
O	-1.885655	1.794963	-0.286567
H	2.114026	-1.156093	-0.033678
H	2.038008	2.002664	0.340588
H	-0.329881	-2.320236	0.020305
H	-1.474826	2.312052	-1.012985

H	-2.201028	-0.793103	1.038774
O	2.055474	-0.861370	2.896773
H	2.358701	-0.659096	1.929622
H	1.156807	-0.427621	2.776325
O	4.239115	0.957847	-1.340659
H	3.634756	0.443426	-0.712590
H	3.537180	1.438399	-1.865690
O	1.293680	-3.433896	2.014489
H	1.106885	-3.104945	1.056116
H	1.531554	-2.549505	2.435023
O	-0.282661	-2.190562	-2.878609
H	0.077326	-2.416335	-1.938437
H	-0.148992	-1.198632	-2.766639
O	0.410078	4.534684	1.594879
H	0.805777	3.835194	0.983203
H	-0.379905	4.003074	1.901678
O	2.026194	2.331997	-2.575126
H	1.778641	2.552119	-1.599492
H	1.429408	1.525152	-2.604142
O	-3.917167	0.836486	-2.063052
H	-3.245756	1.174120	-1.397526
H	-3.577711	-0.097247	-2.184891
O	-1.742653	2.762563	2.216111
H	-1.902917	2.575387	1.224286
H	-1.119066	1.983161	2.337244
O	-1.564551	-3.559479	2.201930
H	-1.742567	-2.832809	1.535799
H	-0.562843	-3.521203	2.236375
O	-2.999538	-1.879488	-2.068794
H	-2.731894	-1.658142	-1.109782
H	-2.074982	-1.985874	-2.453713

$[NpO_2(OH)_5]^{3-}$

Np	0.063220	0.215891	-0.004101
O	0.082462	0.281207	1.851875
O	0.106125	0.228907	-1.862273
O	-1.954559	-0.991013	0.172664
O	2.339033	-0.485833	0.143732
O	1.277013	2.221202	-0.093830
O	0.341286	-2.265827	-0.250910
O	-1.625931	1.807084	-0.045048
H	2.178896	-1.368688	-0.259430
H	2.229504	2.015031	0.077435
H	-0.582216	-2.472186	0.019101
H	-1.195271	2.693036	-0.153458
H	-2.644892	-0.289527	0.200847
O	2.429143	-0.947155	2.781184
H	2.574756	-0.820080	1.777052

H	1.548119	-0.492597	2.803212
O	3.996938	1.341571	-0.985344
H	3.479974	0.563289	-0.601082
H	3.378425	1.636092	-1.709933
O	1.137254	-3.367868	2.106752
H	0.933428	-3.044698	1.166560
H	1.601211	-2.558068	2.470548
O	-0.072453	-2.347308	-2.905664
H	0.118962	-2.494082	-1.908097
H	0.012101	-1.360004	-2.868871
O	-0.203763	4.231762	0.981616
H	0.472503	3.567388	0.639977
H	-0.673322	3.687948	1.673149
O	1.881807	2.305287	-2.691032
H	1.606442	2.518151	-1.733430
H	1.355772	1.467262	-2.745215
O	-3.681250	0.836837	-1.737760
H	-2.914249	1.247453	-1.249297
H	-3.306374	-0.027121	-2.058919
O	-1.730256	2.383810	2.575854
H	-1.948059	2.168297	1.606607
H	-1.028521	1.689986	2.671224
O	-1.728762	-2.919454	2.292701
H	-1.852481	-2.163220	1.656049
H	-0.737252	-3.012583	2.335667
O	-2.811267	-1.914080	-2.239417
H	-2.556248	-1.689084	-1.287104
H	-1.897415	-2.076994	-2.613572

$[NpO_2(OH)_5]^{4-}$

Np	0.037406	0.222655	-0.009772
O	-0.053125	0.332282	1.896889
O	0.155258	0.270870	-1.918250
O	-1.991052	-1.260264	0.243677
O	2.476287	-0.291328	0.233083
O	1.162662	2.427460	-0.045314
O	0.487177	-2.313144	-0.274017
O	-1.926645	1.733741	-0.153623
H	2.231583	-1.172222	-0.138948
H	1.955289	2.058748	0.404825
H	-0.449074	-2.381137	0.029476
H	-1.439768	2.379326	-0.711205
H	-2.510599	-0.516968	0.617536
O	2.284198	-0.869763	2.813017
H	2.524301	-0.684152	1.819081
H	1.375231	-0.454520	2.739935
O	4.268543	0.948553	-1.484753
H	3.690984	0.435969	-0.828395
H	3.541882	1.453668	-1.950046

O	1.241587	-3.392622	2.081132
H	1.021628	-3.074451	1.130224
H	1.604853	-2.528871	2.448373
O	-0.174401	-2.277193	-2.883025
H	0.102763	-2.474368	-1.910329
H	-0.070319	-1.284580	-2.778409
O	0.238890	4.483904	1.597331
H	0.652274	3.809063	0.968122
H	-0.492953	3.900544	1.952376
O	1.981627	2.328420	-2.555617
H	1.730221	2.534729	-1.572651
H	1.417413	1.503618	-2.588336
O	-3.814095	0.841172	-2.078816
H	-3.158045	1.159507	-1.384092
H	-3.477236	-0.087883	-2.226982
O	-1.750368	2.579627	2.351830
H	-1.935914	2.379479	1.354054
H	-1.079714	1.844623	2.448259
O	-1.688224	-3.215967	2.299321
H	-1.853673	-2.490562	1.620628
H	-0.690581	-3.229340	2.322336
O	-2.937766	-1.918578	-2.158897
H	-2.676606	-1.674946	-1.192727
H	-2.012067	-2.035073	-2.527283

$[PuO_2(OH)_5]^{3-}$

Pu	0.080708	0.187696	0.020399
O	0.097185	0.285357	1.862471
O	0.128199	0.148246	-1.813099
O	-1.942764	-1.006370	0.272171
O	2.370176	-0.468020	0.128831
O	1.209732	2.248652	-0.129280
O	0.328293	-2.273739	-0.228724
O	-1.680175	1.754425	-0.077111
H	2.218808	-1.340124	-0.298652
H	2.152204	2.055221	0.096118
H	-0.585285	-2.445955	0.094635
H	-1.220085	2.627413	-0.139621
H	-2.488079	-0.273949	0.634492
O	2.477944	-0.988095	2.742649
H	2.599086	-0.833814	1.735020
H	1.598767	-0.539143	2.806206
O	4.000042	1.394166	-1.013331
H	3.492557	0.615907	-0.620482
H	3.364158	1.688661	-1.722496
O	1.205163	-3.413371	2.081470
H	0.972523	-3.082301	1.151325
H	1.675542	-2.603314	2.438219
O	-0.226899	-2.426251	-2.842062

H	0.015495	-2.534167	-1.849191
H	-0.112963	-1.444221	-2.861888
O	-0.228475	4.222692	1.113031
H	0.412301	3.561203	0.706944
H	-0.744549	3.642079	1.735914
O	1.849273	2.309730	-2.698180
H	1.554449	2.508652	-1.738132
H	1.354997	1.457701	-2.771689
O	-3.327531	1.073440	-2.334418
H	-2.728326	1.351972	-1.587378
H	-3.156634	0.093634	-2.373635
O	-1.862975	2.302438	2.534541
H	-2.014672	2.098663	1.543619
H	-1.134374	1.646795	2.665545
O	-1.635671	-2.937517	2.412725
H	-1.774821	-2.213184	1.742909
H	-0.645437	-3.057378	2.400943
O	-2.935827	-1.804227	-2.134541
H	-2.675410	-1.528100	-1.197233
H	-2.036819	-2.061481	-2.489015

$[PuO_2(OH)_5]^{4-}$

Pu	-0.021332	-0.064653	0.030263
O	-0.194136	-0.086774	1.943948
O	0.201198	-0.081382	-1.847298
O	-2.331700	-0.983915	-0.055975
O	2.490561	-0.177372	0.355379
O	0.994475	2.275001	0.001512
O	0.264786	-2.475532	0.007118
O	-1.789991	1.733635	-0.142520
H	2.554297	-1.126934	0.100602
H	1.819710	1.844799	0.322965
H	-0.442513	-2.681221	0.669158
H	-1.036544	2.342933	-0.317808
H	-2.683757	-0.067803	0.008022
O	2.428381	-0.818636	2.892468
H	2.628342	-0.484230	1.926090
H	1.447040	-0.664040	2.813518
O	4.175720	1.129214	-1.450870
H	3.657718	0.612369	-0.753201
H	3.397551	1.546817	-1.922767
O	2.475696	-3.310835	1.404361
H	1.664030	-3.078845	0.836934
H	2.475328	-2.521544	2.016200
O	-0.342691	-2.700452	-2.604964
H	-0.200346	-2.804600	-1.592466
H	-0.136246	-1.722475	-2.601029
O	0.174114	4.143373	1.891669

H	0.565619	3.532549	1.184613
H	-0.566736	3.543040	2.193425
O	1.761526	2.230909	-2.516334
H	1.482946	2.418102	-1.529334
H	1.290395	1.354195	-2.555749
O	-3.410638	1.166004	-2.365453
H	-2.788312	1.420349	-1.610213
H	-3.195232	0.203293	-2.475967
O	-1.879561	2.220404	2.446338
H	-1.980202	2.119019	1.412918
H	-1.240039	1.462083	2.535110
O	-1.962446	-2.336954	2.165673
H	-2.285590	-1.858483	1.308521
H	-1.264171	-1.660191	2.371356
O	-3.105909	-1.871128	-2.419377
H	-2.917223	-1.543548	-1.458115
H	-2.174282	-2.176523	-2.618700

$[UO_2(CO_3)]^{5-}$

U	-0.001170	-0.000466	-2.816654
O	-0.140832	-1.914564	-2.790072
O	0.138850	1.913372	-2.780718
C	-0.010857	-0.008317	0.229246
O	-0.018907	-0.010775	1.489416
O	1.090645	-0.201031	-0.508354
O	-1.104415	0.187561	-0.520720
C	2.671670	0.120175	-4.353438
O	3.756702	0.258025	-4.975532
O	2.595247	-0.055955	-3.024134
O	1.466907	0.133131	-4.931131
C	-2.664535	-0.114230	-4.377723
O	-3.747119	-0.249274	-5.004857
O	-1.457402	-0.127606	-4.949020
O	-2.594762	0.058768	-3.047168
O	-3.447992	-1.205177	-0.775896
H	-3.362587	-0.868102	-1.721042
H	-2.597996	-0.778340	-0.440195
O	-3.068266	2.120540	-1.396937
H	-3.081310	1.438040	-2.144247
H	-2.298387	1.718418	-0.905306
O	0.292414	-1.784007	-6.479307
H	0.934043	-1.151074	-6.031222
H	-0.516950	-1.486139	-5.977614
O	-0.268321	1.794095	-6.477134
H	0.536204	1.495592	-5.968392
H	-0.913845	1.159044	-6.037127
O	3.058818	-2.124905	-1.378171
H	2.285959	-1.725066	-0.889055
H	3.076437	-1.438686	-2.121819

O	3.430752	1.199672	-0.741179
H	2.579741	0.768884	-0.413044
H	3.352113	0.866890	-1.688326
O	1.626461	-4.009025	-2.921772
H	0.854446	-3.360749	-2.967111
H	2.253258	-3.408829	-2.415720
O	-2.173315	-3.627337	-1.442766
H	-1.431589	-3.173600	-1.927226
H	-2.683541	-2.814334	-1.155835
O	1.564978	-4.297446	-5.785477
H	1.692804	-4.184850	-4.799435
H	1.074981	-3.452059	-6.004723
O	-1.624139	4.009841	-2.922828
H	-0.852839	3.360336	-2.963829
H	-2.255548	3.408968	-2.423444
O	-1.542630	4.306482	-5.784992
H	-1.677316	4.191323	-4.800169
H	-1.052806	3.460647	-6.003081
O	2.156753	3.622597	-1.404875
H	1.419594	3.171122	-1.898230
H	2.665676	2.808426	-1.118823

$[NpO_2(CO_3)]^{5-}$

Np	0.066651	0.055951	-2.874845
O	-0.009040	-1.823768	-2.929054
O	0.151416	1.953732	-2.790525
C	0.031415	-0.076781	0.190033
O	0.016213	-0.147005	1.449594
O	1.138025	-0.233052	-0.548763
O	-1.056525	0.159520	-0.554131
C	2.745454	0.208470	-4.401085
O	3.839805	0.350190	-5.009315
O	2.656612	0.005200	-3.075983
O	1.548511	0.245036	-4.992062
C	-2.608323	-0.108335	-4.430428
O	-3.687076	-0.280974	-5.057793
O	-1.404067	-0.066171	-5.004550
O	-2.545060	0.047638	-3.096960
O	-3.367365	-1.232806	-0.849551
H	-3.267771	-0.907608	-1.801833
H	-2.508082	-0.816268	-0.509217
O	-3.032242	2.076559	-1.418752
H	-3.041658	1.400141	-2.173265
H	-2.257207	1.675323	-0.933351
O	0.376761	-1.712059	-6.498119
H	1.015061	-1.068608	-6.058841
H	-0.436262	-1.404452	-6.006031
O	-0.221882	1.882864	-6.498647
H	0.589850	1.577200	-6.003694

H	-0.861927	1.235138	-6.067625
O	3.069378	-2.107401	-1.453311
H	2.309813	-1.685747	-0.954980
H	3.095184	-1.420724	-2.196206
O	3.459006	1.200851	-0.758506
H	2.610070	0.754184	-0.444352
H	3.393388	0.883332	-1.713231
O	1.592727	-4.022694	-2.874713
H	0.858818	-3.338777	-2.974195
H	2.242190	-3.412461	-2.403920
O	-2.926360	-3.900358	-0.951015
H	-2.084700	-3.817680	-1.447672
H	-3.146569	-2.904735	-0.875887
O	1.539597	-4.260987	-5.766467
H	1.664789	-4.161931	-4.779948
H	1.096558	-3.389137	-5.988356
O	-1.652969	4.029443	-2.901646
H	-0.866344	3.405330	-2.958203
H	-2.264852	3.397467	-2.412906
O	-1.523293	4.363595	-5.774510
H	-1.678672	4.227204	-4.796636
H	-1.021047	3.526043	-6.000102
O	2.191233	3.633285	-1.358315
H	1.456266	3.196242	-1.863816
H	2.700574	2.810581	-1.093523

$[PuO_2(CO_3)]^{5-}$

Pu	-0.000125	-0.000393	-2.989064
O	-0.003027	-1.894771	-2.990426
O	0.002495	1.893955	-2.988135
C	-0.001501	-0.002540	0.090625
O	-0.002181	-0.003756	1.351246
O	1.108813	0.021151	-0.655008
O	-1.111048	-0.024815	-0.656233
C	2.664595	0.000285	-4.529385
O	3.752854	0.001750	-5.165370
O	2.580641	-0.022046	-3.193919
O	1.459897	0.020161	-5.113010
C	-2.663832	0.000809	-4.531407
O	-3.751529	-0.000982	-5.168366
O	-1.458607	-0.017860	-5.114036
O	-2.581025	0.022057	-3.195901
O	-3.323550	-1.595568	-1.115945
H	-3.261640	-1.116449	-2.000687
H	-2.498771	-1.180862	-0.715713
O	-3.284869	1.594364	-1.053573
H	-3.221331	1.179545	-1.968130
H	-2.487916	1.113678	-0.666224
O	0.033461	-1.593937	-6.800172

H	0.770088	-1.116394	-6.304630
H	-0.723499	-1.178267	-6.283204
O	-0.031062	1.600474	-6.796298
H	0.725502	1.183867	-6.279566
H	-0.768057	1.121638	-6.302572
O	3.283871	-1.596304	-1.052967
H	2.486299	-1.117012	-0.665212
H	3.220920	-1.179766	-1.966805
O	3.320744	1.593692	-1.111588
H	2.495949	1.178546	-0.711968
H	3.259534	1.115112	-1.996663
O	1.860283	-3.926476	-1.526129
H	1.120916	-3.446931	-1.974365
H	2.450990	-3.134635	-1.338428
O	-2.215921	-3.926424	-2.124826
H	-1.454780	-3.449979	-2.538325
H	-2.667428	-3.133910	-1.701284
O	0.348455	-3.945238	-5.376838
H	0.330056	-3.484303	-4.503344
H	0.209766	-3.141076	-5.965786
O	-1.858222	3.924402	-1.517752
H	-1.118714	3.445561	-1.966452
H	-2.450198	3.132596	-1.333893
O	-0.351902	3.948565	-5.368765
H	-0.334371	3.485911	-4.496154
H	-0.210418	3.145864	-5.959014
O	2.215330	3.925135	-2.121632
H	1.454680	3.449275	-2.536679
H	2.665469	3.132302	-1.697239

$[UO_2(CO_3)]^{4-}$

U	-0.001240	-0.000403	-2.982264
O	-0.031242	-1.822814	-2.985412
O	0.028833	1.822184	-2.982400
C	0.002237	-0.006896	0.018171
O	0.004195	-0.009808	1.267621
O	1.109103	-0.015061	-0.738577
O	-1.106655	0.004722	-0.735278
C	2.600403	-0.026725	-4.489430
O	3.679431	-0.038475	-5.119220
O	2.506688	-0.033403	-3.151603
O	1.390015	-0.005920	-5.066756
C	-2.606319	0.033264	-4.482773
O	-3.686815	0.047094	-5.110052
O	-1.397294	0.015593	-5.063034
O	-2.509593	0.034393	-3.145150
O	-2.828148	-2.087063	-1.381465
H	-2.907594	-1.492274	-2.180278
H	-2.151211	-1.527121	-0.907367

O	-2.792210	2.124880	-1.345982
H	-2.874960	1.556663	-2.163581
H	-2.139405	1.531125	-0.877440
O	-0.007104	-2.079121	-6.255384
H	0.732902	-1.495052	-5.922881
H	-0.749021	-1.511617	-5.902601
O	-0.000640	2.100809	-6.238565
H	0.741390	1.530711	-5.890260
H	-0.740414	1.516176	-5.907081
O	2.794267	-2.133282	-1.365785
H	2.141539	-1.543065	-0.892908
H	2.875738	-1.559781	-2.179870
O	2.832643	2.073961	-1.373249
H	2.157277	1.509537	-0.901704
H	2.909083	1.486459	-2.177758
O	1.361696	-4.485599	-2.114935
H	0.383958	-4.355213	-1.954901
H	1.765847	-3.587773	-1.917696
O	-1.499689	-4.463949	-2.286346
H	-1.143166	-4.334463	-3.211192
H	-1.849016	-3.559647	-2.027899
O	0.082988	-4.458850	-4.673268
H	0.710730	-4.340452	-3.904485
H	0.046124	-3.553650	-5.105698
O	-1.358892	4.481089	-2.073923
H	-0.381125	4.347684	-1.915673
H	-1.764733	3.582204	-1.884552
O	-0.083670	4.471054	-4.633904
H	-0.710041	4.348647	-3.864523
H	-0.049019	3.568542	-5.071630
O	1.500536	4.456058	-2.246530
H	1.144782	4.334541	-3.172668
H	1.852886	3.550093	-1.997067

$[NpO_2(CO_3)]^{4-}$

Np	0.000274	-0.000633	-2.979096
O	-0.012327	-1.804156	-2.985858
O	0.012596	1.802805	-2.973478
C	0.005293	-0.010520	0.010970
O	0.005580	-0.014332	1.261515
O	1.112113	-0.011747	-0.741969
O	-1.102599	-0.004436	-0.740948
C	2.608607	-0.010190	-4.477820
O	3.679339	-0.013166	-5.124459
O	2.531631	-0.020274	-3.143899
O	1.392941	0.003217	-5.045460
C	-2.612683	0.020474	-4.473493
O	-3.685719	0.028628	-5.116355

O	-1.399094	0.010032	-5.044897
O	-2.531643	0.021684	-3.139583
O	-2.816204	-2.100826	-1.391554
H	-2.902628	-1.499034	-2.185833
H	-2.139326	-1.541292	-0.917138
O	-2.779862	2.124505	-1.357225
H	-2.866986	1.550513	-2.171107
H	-2.126564	1.532134	-0.888383
O	-0.004155	-2.073494	-6.234232
H	0.736058	-1.492580	-5.896880
H	-0.746301	-1.504982	-5.881635
O	-0.005163	2.097664	-6.216772
H	0.738083	1.527322	-5.870147
H	-0.744137	1.513080	-5.882778
O	2.782640	-2.137756	-1.377839
H	2.131870	-1.546723	-0.903404
H	2.868320	-1.558905	-2.188272
O	2.819589	2.089773	-1.381511
H	2.145349	1.524651	-0.909608
H	2.903642	1.495539	-2.181643
O	1.351772	-4.488636	-2.124653
H	0.373746	-4.363456	-1.958450
H	1.754858	-3.589806	-1.927752
O	-1.501054	-4.470613	-2.285036
H	-1.152969	-4.344480	-3.214046
H	-1.856280	-3.567194	-2.027452
O	0.064214	-4.456837	-4.672394
H	0.698241	-4.347213	-3.906981
H	0.034822	-3.549867	-5.103534
O	-1.352242	4.481302	-2.087962
H	-0.374228	4.354505	-1.922617
H	-1.755663	3.580932	-1.898824
O	-0.066663	4.470142	-4.635837
H	-0.699790	4.355990	-3.870251
H	-0.039543	3.566488	-5.073791
O	1.499773	4.465093	-2.248793
H	1.151733	4.346661	-3.178738
H	1.856816	3.560020	-1.999304

$[PuO_2(CO_3)]^{4-}$

Pu	-0.005020	0.001863	-2.981601
O	-0.078149	-1.790028	-2.972180
O	0.068338	1.793376	-2.991859
C	-0.005048	-0.002867	0.014336
O	-0.002732	-0.005470	1.265834
O	1.100742	0.009726	-0.738560
O	-1.113706	-0.012067	-0.734637
C	2.600692	-0.027971	-4.480323
O	3.681035	-0.037816	-5.112959
O	2.512738	-0.030259	-3.146182

O	1.394455	-0.016337	-5.061408
C	-2.608440	0.035691	-4.479274
O	-3.688534	0.046544	-5.112657
O	-1.401996	0.034107	-5.059866
O	-2.520756	0.027102	-3.145598
O	-2.799728	-2.111689	-1.398754
H	-2.878153	-1.514748	-2.197161
H	-2.129906	-1.544875	-0.919712
O	-2.765823	2.119795	-1.354432
H	-2.859901	1.544985	-2.166979
H	-2.119779	1.518378	-0.884245
O	-0.021840	-2.075204	-6.222622
H	0.727002	-1.496832	-5.897493
H	-0.755977	-1.494138	-5.871928
O	0.020851	2.100442	-6.206168
H	0.755848	1.515561	-5.864682
H	-0.725870	1.520861	-5.879336
O	2.759810	-2.126658	-1.384073
H	2.106405	-1.540437	-0.906687
H	2.853860	-1.536661	-2.186509
O	2.810172	2.091535	-1.389640
H	2.136564	1.527233	-0.913524
H	2.884631	1.497045	-2.190440
O	1.373581	-4.483113	-2.151507
H	0.397257	-4.360692	-1.967084
H	1.778085	-3.585534	-1.945765
O	-1.470563	-4.470864	-2.258674
H	-1.145900	-4.354399	-3.197832
H	-1.837950	-3.568771	-2.008710
O	0.046041	-4.460878	-4.673773
H	0.696030	-4.359042	-3.920301
H	0.016045	-3.552566	-5.103466
O	-1.360089	4.476615	-2.097173
H	-0.382219	4.355988	-1.922746
H	-1.764461	3.579606	-1.891225
O	-0.058012	4.468543	-4.632800
H	-0.700851	4.352029	-3.875397
H	-0.021108	3.566195	-5.074060
O	1.486874	4.464871	-2.236189
H	1.148500	4.349461	-3.170030
H	1.853034	3.562371	-1.989157