Supplementary materials

The strong interaction of actinyl ions and fullerenol driven by the hydrogen bonds

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Contents:

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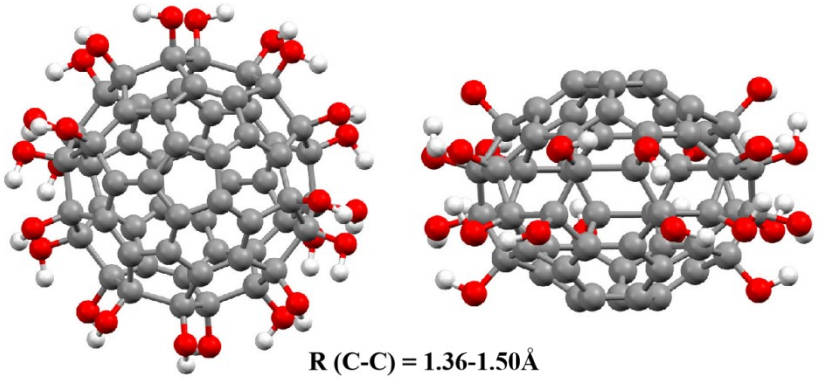

Figure S1. Relaxed structures of the most stable $C_{60}(OH)_{24}$ with 24 OH groups around the equator of C_{60} cage (Saturn-like shape), and key structural parameters including C-C, C-O, and O-H bond lenghts were also collected.

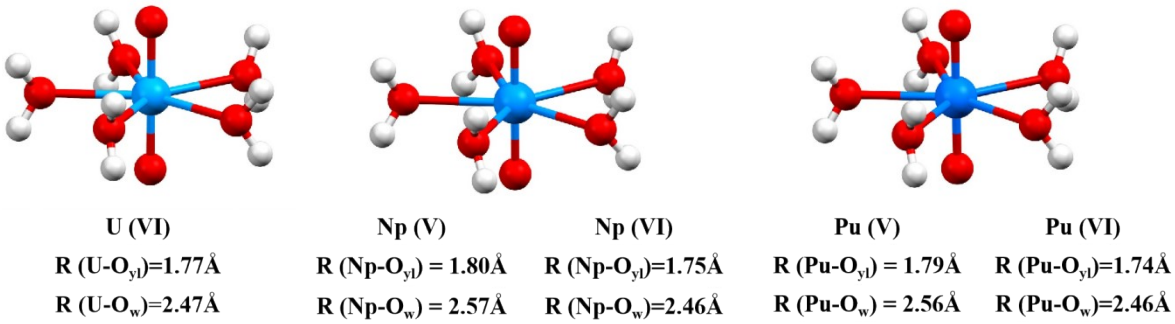

Figure S2. Relaxed structures of isolated actinyl complexes, U (V), U (VI), Np (V), Np (VI), Pu (V), and Pu (VI), and An-O_{yl} and An-O_w bond lengths in these complexes.

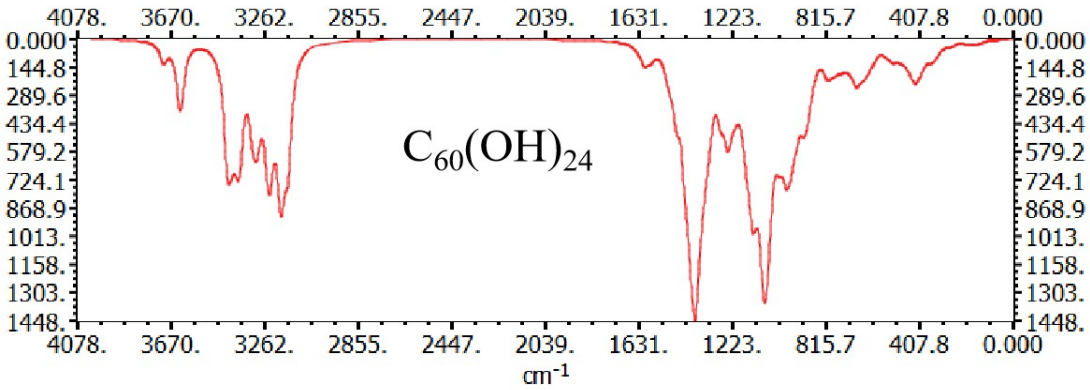

Figure S3. Simulated IR spectra for the most stable Saturn like isomer of $C_{60}(OH)_{24}$ fulerenol.

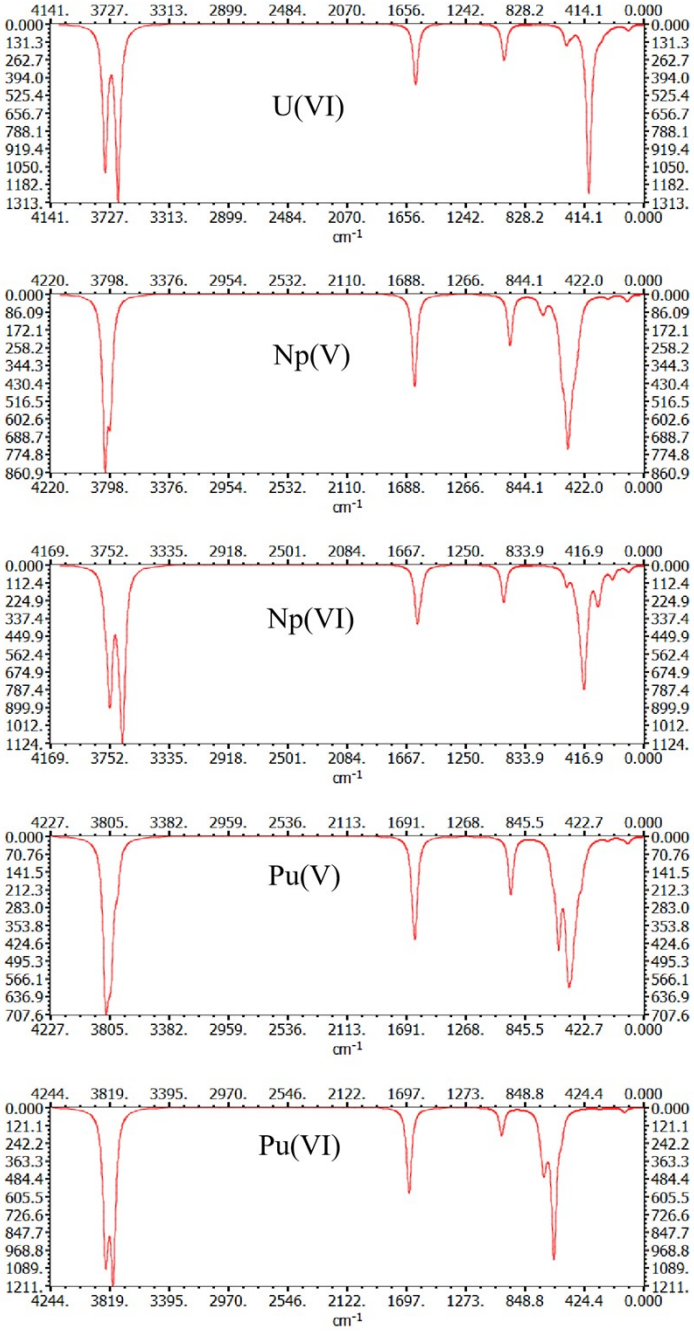

Figure S4. Simulated IR spectra of isolated actinyl complexes.

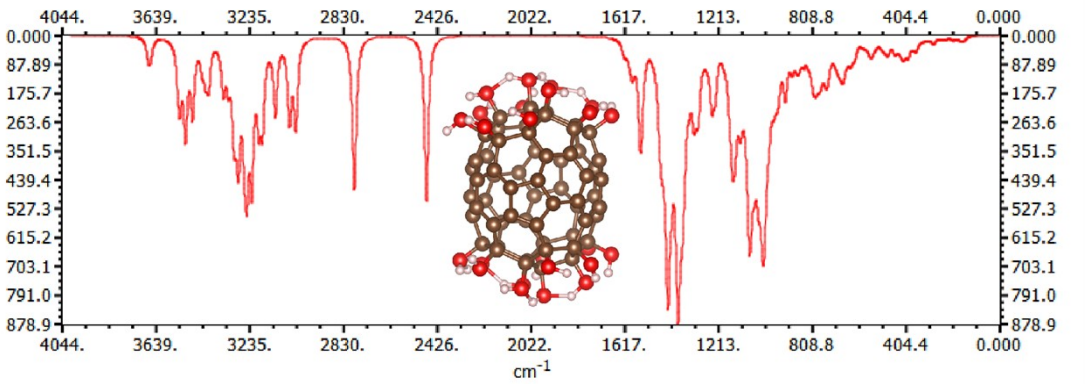

Figure S5. Simulated IR spectra and structure of a typical isomer (egg-like shape) of $C_{60}(OH)_{24}$ fulerenol (24 OH groups attached at opposite sides of C_{60} sphere).

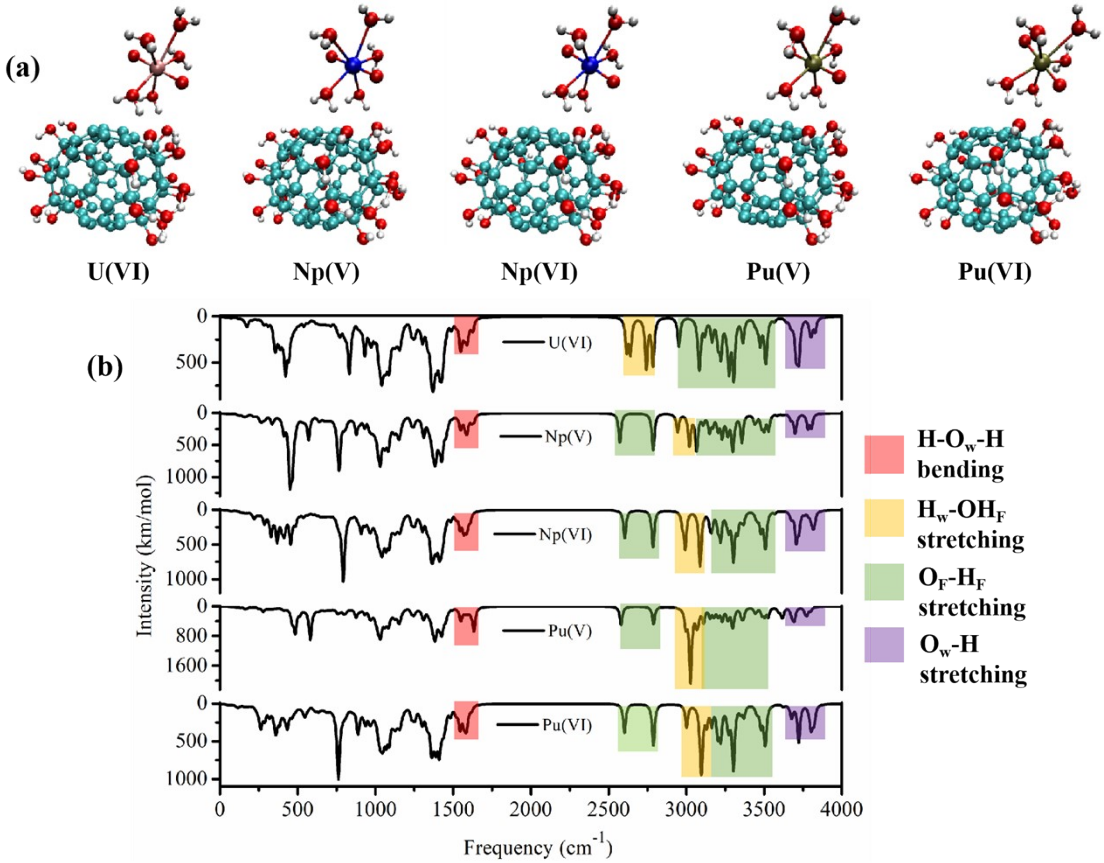

Figure S6. Structures (a) and IR spectra (b) of a typical isomer (egg-like shape) of $C_{60}(OH)_{24}$ fulerenol with actinyl ions adsorption.

Table S1. Cartesian coordinates of all relaxed complexes

$C_{60}(OH)_{24}/UO_2(H_2O)_5^{2+}$ ($C_{60}(OH)_{24}$/U(VI)-OS)

C	-1.93996340	3.53912904	-1.38439724
C	-0.85812950	3.39922445	-0.48539759
C	0.29349477	4.17440881	-0.63370892
C	0.40251692	5.09661916	-1.72980648
C	-0.66127622	5.18901715	-2.63780161
C	-1.86468447	4.45133614	-2.43556864
C	-2.94805256	2.43277331	-1.25293263
C	-2.17409754	1.29292226	-0.29027648
C	-0.85126255	2.05917049	0.24120187
C	0.47218205	1.39336424	-0.00962551
C	1.59207598	3.53915999	-0.49307906
C	1.74556666	5.05417001	-2.24089832
C	1.96821739	5.11138965	-3.61690080
C	0.88390334	5.24949752	-4.51298015
C	-0.42296778	5.32851894	-4.03811282
C	-1.69458102	5.12826748	-4.82433836
C	-2.73976465	4.49185753	-3.66281013
C	-3.39658025	3.08587553	-3.93396950
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C	-2.31927213	-0.42388193	-2.41890480
C	-2.75073796	0.80004575	-3.19896031
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C	3.21687472	4.52914723	-4.26849395
C	3.62432565	3.30669885	-3.49739176

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H	0.85427521	2.36199490	-9.28468428

$C_{60}(OH)_{24}/UO_2(H_2O)_4^{2+}$ ($C_{60}(OH)_{24}$/U(VI)-IS1)

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C	1.10057887	2.74908408	-0.15321760
C	-0.28812287	2.75612880	-0.34640433
C	-1.02633200	1.54001711	-0.43119521
C	-0.89938994	-0.99261517	-0.89636312
C	0.45861770	-1.86440989	-1.36742375
C	1.70190765	-0.97050070	-0.84462758
C	2.73813376	-0.57825663	-1.86040022
C	3.01597082	1.67003045	-0.87947997
C	1.90284395	3.70354009	-0.86823605
C	1.29082603	4.61327366	-1.73228651
C	-0.11299653	4.63149075	-1.88097630
C	-0.91272855	3.73752770	-1.17246020
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C	-2.06840241	-0.78792338	-1.93744570
C	0.59323165	-2.38088406	-2.89536842
C	-0.58392643	-1.87722326	-3.89897531
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C	-2.11248245	0.11832742	-4.13983168
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C	-2.76526129	3.71198225	-2.92659879
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C	3.08906407	3.00009998	-1.31763055
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C	3.50285691	4.16434943	-4.86028078
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C	3.90126653	1.60823664	-5.91697911
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O	2.77013894	6.41908310	-2.47389209
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O	2.46439881	-3.34991911	-4.23239979
O	4.03808256	-2.46485752	-2.51989220
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H	1.22143867	-2.91132006	0.04652575
H	3.20314816	-2.06236888	-0.17566305

H	-0.87523748	-2.48809516	0.28377789
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H	-0.34852701	7.36767407	-2.95839908
H	1.76179020	7.36295267	-3.37756482
H	-2.33240238	6.62111673	-3.55820198
H	-4.23486318	4.46417539	-2.01441424
H	-3.54032024	3.47528908	0.06333665
H	-4.08090096	1.21773730	-0.14179377
H	3.26673863	-3.53900961	-3.67910794
H	4.95461222	-2.21859765	-2.80332898
H	6.06816816	-0.27115580	-3.30207409
H	5.43758205	-1.00945899	-5.72453215
H	5.60359144	1.94104627	-6.73866912
H	-0.18125402	5.92965269	-7.04805949
H	3.75327449	5.42367588	-6.64951502
H	6.21837019	2.84107730	-4.31133481
H	5.32414357	4.74171056	-5.16015070
H	1.81461145	6.24094762	-6.81473843
U	-2.82134716	5.02828908	-8.34889761
O	-3.59632881	4.39330968	-10.65992109
O	-3.45023586	3.57756597	-7.51846030
O	-2.25449880	6.47985119	-9.23022191
O	-3.36940316	6.47160094	-6.51236306
O	-1.22240661	3.34056750	-9.34024599
O	-5.28120602	5.57502401	-8.54874178
H	-3.17430502	7.42120868	-6.59440752
H	-3.10492333	6.19015605	-5.54201725
H	-0.46682800	3.57767768	-9.90615415
H	-0.88112693	2.69778798	-8.67832468
H	-3.54111114	4.97302904	-11.43927643
H	-4.05974166	3.58117252	-10.92880602
H	-5.65910022	6.43518127	-8.80250381
H	-5.86935671	5.20032021	-7.86806573

$C_{60}(OH)_{24}/UO_2(H_2O)_3^{2+}$ ($C_{60}(OH)_{24}$/U(VI)-IS2)

C	-0.40316522	0.38248822	-0.47128377
C	0.99942255	0.34502265	-0.30112772
C	1.72712780	1.52482285	-0.13469902
C	1.05631712	2.79407868	-0.17497409
C	-0.32837005	2.81496630	-0.39242312
C	-1.07547746	1.60347992	-0.48367999
C	-0.96586412	-0.93421816	-0.92716519

C	0.39202413	-1.82295702	-1.36698137
C	1.63455086	-0.93727197	-0.82785554
C	2.69246918	-0.56311226	-1.82785590
C	2.97417271	1.69011054	-0.86057698
C	1.88158838	3.73452310	-0.88274591
C	1.29762568	4.65032652	-1.75820237
C	-0.10622396	4.69002232	-1.92500120
C	-0.92649519	3.80308530	-1.22996619
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C	-2.11486814	-0.72975641	-1.99023389
C	0.54957914	-2.35309683	-2.88797430
C	-0.60491404	-1.84824372	-3.91647955
C	-1.59845629	-0.83137054	-3.39343639
C	-2.11546693	0.15258411	-4.20651349
C	-2.69957034	1.21407848	-3.41466727
C	-2.61147255	2.50753291	-3.85668766
C	-2.71960754	3.76772671	-3.03511715
C	-1.70893045	4.81038195	-3.87361743
C	-0.52107376	5.50091308	-3.11723530
C	3.06935939	3.01403625	-1.30620314
C	2.42347048	4.35423763	-5.91674862
C	3.55552582	4.14302394	-4.85024589
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C	3.94785513	1.58214659	-5.88212603
C	2.53457426	1.82952471	-6.34927193
C	0.44863940	3.08441643	-6.54090887
C	-0.17881960	4.36217938	-6.00997030
C	1.06461363	5.24327150	-5.46048058
C	0.91146522	5.77337666	-3.94442083
C	2.06192222	5.26104959	-2.92704062
C	3.02521905	4.23666852	-3.45343546
C	4.13397636	2.20104884	-3.43317579
C	4.04569636	0.90816394	-2.99533748
C	4.15595223	-0.34646065	-3.81120738
C	3.83999067	-0.06133008	-5.32532588
C	2.38889082	-0.36965752	-5.60502391
C	1.79100449	0.61901919	-6.43760427
C	0.40388069	0.63732508	-6.65314761
C	-0.27617833	1.90174784	-6.69613796
C	-1.27211917	4.00100792	-5.04729048
C	-1.91178253	2.76951644	-5.08666048
C	-1.53193710	1.72855128	-5.98174967

C	-1.60542761	0.40767328	-5.52032919
C	-0.41631299	-0.30694871	-5.95024170
C	0.16702361	-1.21410806	-5.06941224
C	1.56786978	-1.25523518	-4.90816070
C	1.98911284	-2.08546769	-3.73308765
C	3.17538802	-1.40677558	-2.96738793
C	3.53993011	3.25857793	-2.63668489
C	3.36123364	0.63304574	-1.74623159
C	1.85509536	3.04504828	-6.37173925
O	2.28011662	-1.67118354	0.23912882
O	0.33246062	-2.95126035	-0.53867016
O	0.42205098	-3.73916323	-2.83159906
O	-1.56320233	-1.61129163	0.15698246
O	-3.08771911	-1.71954314	-1.76311445
O	-1.37937203	-2.94847434	-4.32804871
O	-4.27762870	0.46644414	-1.73724117
O	-3.38409272	1.87285608	0.08585574
O	5.48643895	-0.90252984	-3.73820157
O	2.81505213	6.42427095	-2.50264082
O	4.51610732	5.18228785	-5.07325054
O	1.02148789	7.17099650	-3.98260881
O	-1.01205588	6.77730983	-2.72936614
O	1.10778000	6.38084655	-6.28926185
O	-0.79233748	5.18052567	-7.06218566
O	-2.49161050	5.89711900	-4.39181828
O	-4.03367142	4.27921897	-3.04626277
O	-3.24737854	4.21231858	-0.72817917
O	2.43251261	-3.34967662	-4.18395420
O	3.98412351	-2.46594635	-2.44707083
O	4.62811070	-0.86049660	-6.14158271
O	4.78222437	1.63276950	-6.99069441
O	5.75349619	2.99104062	-5.05925035
O	2.99447922	5.05359821	-7.01172735
H	-1.00779770	-3.70405087	-3.80028755
H	1.15221617	-4.07907661	-3.42290139
H	1.11867771	-2.86833792	0.06771125
H	3.11342912	-2.03535606	-0.12104950
H	-0.97485451	-2.41916810	0.26473346
H	-2.86362084	-2.03397408	-0.83776123
H	-4.31195805	-0.53400090	-1.71517346
H	3.69826044	6.36744099	-2.91737546
H	-0.30157661	7.39999490	-3.07725736
H	1.82616381	7.37323146	-3.42342180
H	-2.19225731	6.68063922	-3.81378679

H	-4.19070702	4.51463248	-2.08427930
H	-3.59880128	3.54228201	-0.07013404
H	-4.13774097	1.30782909	-0.25290614
H	3.22294218	-3.54450429	-3.61625073
H	4.90795448	-2.23191895	-2.71823336
H	6.05368279	-0.30406136	-3.21977517
H	5.45242408	-1.04983921	-5.64942003
H	5.67223365	1.88321226	-6.67323631
H	-0.12782269	5.96376524	-7.08468110
H	3.85454951	5.39706654	-6.64110415
H	6.25051136	2.80342951	-4.24247103
H	5.38651563	4.70665352	-5.11362596
H	1.92868965	6.21662844	-6.85768701
U	-3.20362746	5.64508706	-6.73740418
O	-5.32935921	6.32186652	-7.86081489
O	-3.61331862	3.94707638	-7.11474193
O	-2.93713547	7.41387826	-6.69277314
O	-2.70435656	5.79539897	-9.19434806
O	-5.10960290	5.45655272	-5.15583574
H	-2.29657821	6.54450697	-9.66221664
H	-2.55259063	4.99680923	-9.73002749
H	-5.53351022	7.19728101	-8.23240867
H	-6.03291497	5.70650046	-8.13203887
H	-5.57759055	6.25425163	-4.85557228
H	-4.78797751	4.98370018	-4.32195976

$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{1+}$ ($C_{60}(OH)_{24}$/Np(V)-OS)

C	-1.95058119	3.51713263	-1.43397004
C	-0.88653222	3.36780576	-0.51628662
C	0.26972170	4.14561885	-0.63744943
C	0.39470387	5.07956312	-1.72249717
C	-0.65453573	5.18113831	-2.64626763
C	-1.86181025	4.44370379	-2.47152452
C	-2.95938227	2.40919758	-1.33481766
C	-2.20194291	1.25877562	-0.37385396
C	-0.89076855	2.02007974	0.18966557
C	0.43589579	1.36173035	-0.04456822
C	1.56680750	3.51766330	-0.47593136
C	1.74632584	5.04868030	-2.21177188
C	1.99027185	5.12455738	-3.58625773
C	0.91878643	5.26520127	-4.49614220
C	-0.39477285	5.33861310	-4.04048488
C	-1.65286076	5.15085509	-4.84825800
C	-2.71511548	4.49823491	-3.71293460

C	-3.36298980	3.09536462	-4.01331656
C	-3.48083012	1.97764744	-2.75764426
C	-1.92579948	-0.22464642	-0.95805356
C	-2.31392059	-0.43716421	-2.52484146
C	-2.73075643	0.79876318	-3.29551240
C	-2.39842078	0.96612209	-4.61776416
C	-2.53852275	2.35090910	-5.02398960
C	-1.67577031	2.87927133	-5.94360965
C	-1.35545651	4.33399537	-6.16291260
C	0.23360495	4.26502309	-6.73213016
C	1.33772649	5.04283908	-5.91835440
C	2.45536308	4.06154998	-1.42158022
C	3.91310840	1.72608360	-5.41184214
C	4.41561415	2.16042569	-3.99233510
C	4.30266473	1.05306413	-2.74468228
C	3.70090273	-0.36578732	-3.03942646
C	2.82092575	-0.29434875	-4.26172894
C	1.82829479	0.78640956	-6.20648980
C	1.84258910	2.11028413	-6.95489120
C	3.14868105	2.88477861	-6.38162693
C	2.86849259	4.36475332	-5.79002080
C	3.24700375	4.55402108	-4.22620429
C	3.64537243	3.32643567	-3.46288356
C	3.48109757	1.79371261	-1.73345166
C	2.61737895	1.26467237	-0.81242793
C	2.28640215	-0.18129193	-0.59375573
C	2.60579776	-1.03676678	-1.87044668
C	1.35277265	-1.19445726	-2.69592844
C	1.61737451	-1.03604872	-4.08680245
C	0.56672315	-0.93250282	-5.01009081
C	0.68462181	0.00202019	-6.09338500
C	0.50839694	2.78847810	-6.75655369
C	-0.62208472	2.05108073	-6.49354702
C	-0.61310036	0.63499111	-6.25747271
C	-1.49108250	0.09787922	-5.31189098
C	-0.78344015	-0.90061936	-4.52621864
C	-1.03077985	-0.96798106	-3.15766888
C	0.03595504	-1.13059141	-2.24601085
C	-0.38390559	-0.90706285	-0.82585184
C	0.71084164	-0.10764380	-0.04239993
C	3.33089621	3.17995924	-2.12962085
C	1.57508296	2.10481009	-0.25766120
C	2.90308448	0.62671178	-5.30298110
O	-1.05089603	2.18364174	1.62828183

O	-3.06693458	1.11841519	0.72512505
O	-2.75448539	-1.08641097	-0.23486205
O	-4.09728875	2.85273489	-0.61619879
O	-4.85624398	1.67273075	-2.62748563
O	-3.35962187	-1.37880558	-2.61826715
O	-4.68410725	3.33099087	-4.46034248
O	-3.75790673	5.43581022	-3.55349341
O	3.06807802	-0.72019007	0.50363572
O	4.34949016	5.50385878	-4.14978252
O	5.79916394	2.52663080	-4.14331240
O	3.69749612	5.25169183	-6.49823855
O	1.50396708	6.29727030	-6.55960452
O	4.01198656	3.04384765	-7.47580152
O	2.05898655	1.87704849	-8.36020907
O	0.26809428	4.80300446	-8.04032903
O	-2.17634650	4.87922533	-7.17798359
O	-2.20387673	6.39326052	-5.24006842
O	-0.55058411	-2.15684599	-0.17466195
O	0.68042382	-0.59017023	1.31221390
O	3.06191306	-2.29854844	-1.49881146
O	4.72468700	-1.27861870	-3.27914432
O	5.65597187	0.86280397	-2.25544594
O	5.04567811	1.28233024	-6.14607654
H	-3.58080909	-1.56702993	-1.67080344
H	-2.15907010	-1.85829482	-0.01597541
H	-2.54452900	1.47632378	1.49573924
H	-0.45878566	1.52605582	2.04489580
H	-4.06083516	2.28206485	0.21059031
H	-5.08105016	2.10046487	-1.74943763
H	-5.22041553	2.69822360	-3.89451506
H	5.14502304	4.98118518	-3.92692461
H	2.48541414	6.30274252	-6.76752105
H	4.28032027	5.65343633	-5.79412113
H	0.67740083	5.70388764	-7.90518638
H	-2.45396402	5.76269725	-6.80435650
H	-3.01552594	6.47362241	-4.65995021
H	-4.55091558	4.93231954	-3.89953363
H	-0.16004018	-2.00085537	0.72459667
H	1.62883837	-0.78810338	1.51819885
H	3.66047855	-0.01584785	0.82186660
H	3.52105614	-2.18703859	-0.64282514
H	5.47842134	-1.00466056	-2.72057102
H	2.95659041	2.30143956	-8.49977173
H	5.80963367	1.64482056	-5.62177950

H	5.70558760	1.25128879	-1.36367551
H	6.25729543	2.02895138	-3.41862195
H	4.73176473	2.36631460	-7.29959943
Np	-2.01835615	2.47804643	-10.79504140
O	-4.59914038	2.46737951	-10.83599822
O	-2.09571422	4.21252603	-11.25398016
O	-1.93529261	0.73921551	-10.34563413
O	-0.02366487	2.10655441	-12.42176550
O	-3.17189187	2.95365122	-8.58963976
O	-2.87705874	1.86592067	-13.10767268
H	0.30710970	1.19364026	-12.35414034
H	0.55541910	2.62717739	-11.81932344
H	-3.17259827	2.24942976	-7.91582493
H	-2.89940134	3.78820908	-8.08153090
H	-4.71103793	2.77794057	-9.91332777
H	-4.95789567	3.17197205	-11.40232895
H	-3.10957159	0.93943171	-13.28836920
H	-2.31998568	2.16783676	-13.84606738
O	0.23723158	2.99487266	-9.89879529
H	0.25194205	3.83619037	-9.35118337
H	0.86405928	2.41311712	-9.36811677

$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{1+}$ ($C_{60}(OH)_{24}$/Np(V)-IS1)

C	-0.35075487	0.32289486	-0.46222307
C	1.05188822	0.27451437	-0.30683529
C	1.78938026	1.44930374	-0.12512561
C	1.12186937	2.72166220	-0.13405871
C	-0.26546287	2.75063411	-0.33673578
C	-1.02039020	1.54655560	-0.44085327
C	-0.92555508	-0.97973665	-0.93975439
C	0.42115769	-1.86539143	-1.41226114
C	1.67209136	-0.99651128	-0.86933337
C	2.72033213	-0.60681510	-1.86924485
C	3.03046823	1.62508389	-0.85329108
C	1.94214833	3.67519189	-0.83000734
C	1.34707952	4.60714923	-1.68576011
C	-0.05509477	4.64380536	-1.84446250
C	-0.87163640	3.75233907	-1.15203617
C	-2.31747238	3.42748167	-1.42990095
C	-2.42341769	1.82514632	-0.92063631
C	-2.88725760	0.73396821	-1.95924468
C	-2.07991997	-0.74840267	-1.98540850
C	0.55932669	-2.36733291	-2.94466078
C	-0.60553242	-1.84168406	-3.95367581

C	-1.58164622	-0.82713511	-3.39485931
C	-2.09434036	0.18369204	-4.16998685
C	-2.67879131	1.23618808	-3.36041196
C	-2.58875057	2.53577018	-3.76812802
C	-2.71048504	3.77719817	-2.92015035
C	-1.70262463	4.86187475	-3.76184259
C	-0.48648022	5.50107140	-2.99594878
C	3.12305618	2.96353494	-1.27636430
C	2.42736623	4.39941462	-5.85151568
C	3.56809900	4.16197487	-4.80280223
C	4.36488176	2.69145397	-4.82637189
C	3.94585356	1.61554144	-5.88842617
C	2.53081069	1.87653897	-6.33874106
C	0.45089887	3.13807011	-6.45096297
C	-0.17627865	4.41144958	-5.91431924
C	1.07071669	5.28729517	-5.37008898
C	0.93626033	5.78667520	-3.83860719
C	2.09631844	5.24404930	-2.84707492
C	3.05384278	4.23099838	-3.40108484
C	4.15155656	2.19005277	-3.43066966
C	4.06270685	0.88771156	-3.01825269
C	4.16011385	-0.34839450	-3.86104015
C	3.83838706	-0.03669742	-5.36597075
C	2.38598368	-0.33929086	-5.64099663
C	1.78256188	0.66904764	-6.44883588
C	0.39401470	0.69594231	-6.64728943
C	-0.28489544	1.96738516	-6.64982857
C	-1.24857149	4.04910153	-4.93223244
C	-1.90275103	2.84086967	-5.00307776
C	-1.52674958	1.79432804	-5.90924546
C	-1.60897103	0.46806134	-5.48944563
C	-0.42690039	-0.24879126	-5.94872465
C	0.16166944	-1.17418668	-5.09146726
C	1.56658541	-1.22919892	-4.95140942
C	1.99321305	-2.08408749	-3.79757448
C	3.18791164	-1.42407869	-3.03073766
C	3.57551184	3.23420974	-2.60610155
C	3.39584702	0.58780047	-1.76687766
C	1.85796612	3.09580084	-6.31874394
O	2.33300788	-1.76262969	0.17741795
O	0.37036553	-3.01377665	-0.60325102
O	0.44177563	-3.75912669	-2.90885969
O	-1.50876216	-1.67668681	0.14716665
O	-3.05998908	-1.74240823	-1.75681708

O	-1.34034134	-2.94882527	-4.42726658
O	-4.23914410	0.44312856	-1.67423869
O	-3.31956819	1.80174316	0.16736086
O	5.50182118	-0.89813426	-3.80465327
O	2.86915436	6.39493266	-2.39958837
O	4.53898897	5.20088621	-5.02025952
O	1.06160858	7.18637125	-3.85309795
O	-0.92609011	6.75923412	-2.50518270
O	1.11115384	6.44373046	-6.17137237
O	-0.75770704	5.18356465	-7.01293240
O	-2.49207824	5.95543347	-4.20291566
O	-4.01122329	4.26397525	-2.93670946
O	-3.15655782	4.17719441	-0.57923128
O	2.43532545	-3.34322323	-4.27842612
O	4.00962933	-2.50073499	-2.54822957
O	4.63094349	-0.82212691	-6.19823717
O	4.78173688	1.68912524	-7.00036950
O	5.76548150	3.00042561	-5.04712172
O	2.99415750	5.10700810	-6.94747083
H	-0.95934160	-3.70921265	-3.91936952
H	1.17144109	-4.07602452	-3.51174652
H	1.16555838	-2.93191716	-0.00803993
H	3.15232960	-2.11943500	-0.21967690
H	-0.92054452	-2.48674191	0.22190248
H	-2.82535454	-2.06002538	-0.83731376
H	-4.25776472	-0.55756208	-1.66697266
H	3.72996994	6.34456943	-2.85918107
H	-0.25498830	7.39095953	-2.89496293
H	1.86206244	7.36366684	-3.28347710
H	-2.26555489	6.67190395	-3.54733908
H	-4.16464792	4.54858295	-2.00255147
H	-3.51470381	3.49264345	0.05293893
H	-4.07562422	1.25266869	-0.19393061
H	3.23144964	-3.53657045	-3.71785422
H	4.92520851	-2.25033480	-2.83052692
H	6.04441748	-0.30762110	-3.25210987
H	5.46233155	-0.98990309	-5.71128006
H	5.66438339	1.94576721	-6.66791772
H	-0.16826042	6.00456427	-7.02209162
H	3.85354510	5.44480285	-6.57325526
H	6.24768464	2.79043801	-4.22719529
H	5.40134841	4.71411924	-5.06943322
H	1.91419485	6.29193166	-6.75521370
Np	-2.81631387	4.98801678	-8.36137149

O	-3.63242114	3.79920979	-10.49129460
O	-3.42995626	3.55197452	-7.47036587
O	-2.21988000	6.42743177	-9.26541286
O	-3.58402654	6.44885059	-6.50341429
O	-1.07225954	3.35797884	-9.42339203
O	-5.27304677	5.54500979	-8.78700117
H	-3.30131120	7.37238868	-6.61217853
H	-3.26457654	6.18156172	-5.57932594
H	-0.23430136	3.78059462	-9.68208342
H	-0.82518822	2.71165063	-8.72611925
H	-2.90480573	3.19330899	-10.72595553
H	-4.40396804	3.23448783	-10.31197572
H	-5.48254575	6.38277140	-9.23407269
H	-5.76867742	5.55047727	-7.94866442

$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{1+}$ ($C_{60}(OH)_{24}$/Np(V)-IS2)

C	-0.44360372	0.38959139	-0.50870676
C	0.95452357	0.34761188	-0.31119584
C	1.68222985	1.52932475	-0.13638892
C	1.01187343	2.79898174	-0.19106685
C	-0.36937684	2.82084285	-0.43119538
C	-1.11620656	1.61036153	-0.53127171
C	-1.00143790	-0.92624395	-0.97003897
C	0.35986833	-1.81791357	-1.38587567
C	1.59327398	-0.93358864	-0.82708090
C	2.66744821	-0.56291043	-1.80569249
C	2.94348974	1.69321926	-0.83255005
C	1.84927779	3.74047310	-0.88351086
C	1.27705052	4.65998654	-1.76752693
C	-0.12364627	4.69998936	-1.95452791
C	-0.95583894	3.81230972	-1.27304598
C	-2.38911674	3.46480060	-1.59411282
C	-2.50524974	1.87032122	-1.05445240
C	-2.94259077	0.75125090	-2.07696508
C	-2.12919542	-0.72606343	-2.05040161
C	0.54136819	-2.35300017	-2.90233522
C	-0.59852147	-1.85613853	-3.95396310
C	-1.59442297	-0.83375483	-3.44486114
C	-2.09083397	0.15420730	-4.25887309
C	-2.70179643	1.21973172	-3.48350673
C	-2.60294844	2.50888180	-3.91976947
C	-2.72004547	3.77677646	-3.10759913
C	-1.67974679	4.80430540	-3.93140164
C	-0.52252613	5.51090010	-3.15332493

C	3.04471696	3.02256770	-1.28169987
C	2.46683457	4.35058481	-5.91081520
C	3.57484292	4.13923278	-4.82222225
C	4.37708694	2.67551205	-4.79176915
C	3.99003197	1.57732563	-5.84264896
C	2.58803393	1.82389961	-6.34181963
C	0.50602544	3.08011338	-6.56976394
C	-0.13119615	4.35426039	-6.03078059
C	1.10169996	5.24169044	-5.48005777
C	0.92451147	5.77706597	-3.96289757
C	2.05493401	5.26366631	-2.92857282
C	3.02278708	4.23813021	-3.43623254
C	4.12926772	2.20385601	-3.39102944
C	4.03478112	0.91117355	-2.95190035
C	4.15707911	-0.34150269	-3.76612038
C	3.87264039	-0.06243002	-5.28541359
C	2.42902447	-0.37455941	-5.59140719
C	1.84603094	0.61201635	-6.43993637
C	0.46402202	0.63041056	-6.67694671
C	-0.21566690	1.89584320	-6.73204137
C	-1.17051194	3.95423720	-5.03647014
C	-1.85918252	2.77190048	-5.13091305
C	-1.47935811	1.72499120	-6.02898796
C	-1.56913663	0.40932293	-5.57295917
C	-0.37055569	-0.30788151	-5.98044817
C	0.19590653	-1.21058027	-5.08623845
C	1.59644801	-1.25409148	-4.90480632
C	1.99547235	-2.08229607	-3.72234644
C	3.16710395	-1.40245070	-2.93784930
C	3.52947707	3.26366254	-2.60502654
C	3.33632221	0.63655727	-1.71218848
C	1.90966552	3.03979518	-6.37801191
O	2.22494431	-1.67589393	0.25504389
O	0.28834991	-2.94780779	-0.55256568
O	0.42800885	-3.74405195	-2.83805456
O	-1.61062496	-1.59973150	0.11750058
O	-3.11200624	-1.71680909	-1.82183448
O	-1.32319247	-2.97566278	-4.41217322
O	-4.29970523	0.46201600	-1.81484064
O	-3.43590742	1.87677414	0.00594640
O	5.49858507	-0.88532992	-3.66292710
O	2.81927475	6.42641490	-2.49456504
O	4.54823918	5.18013800	-5.02685199
O	1.04214524	7.17682179	-4.00294045

O	-1.01723217	6.78568184	-2.77143463
O	1.15716091	6.37988209	-6.30451569
O	-0.78757699	5.15617615	-7.06276723
O	-2.44237654	5.86206121	-4.52157047
O	-4.02921557	4.30253829	-3.14581327
O	-3.28292070	4.21807367	-0.79925027
O	2.45396029	-3.35073900	-4.16285058
O	3.98006255	-2.46518959	-2.41127789
O	4.68672051	-0.86615826	-6.07906049
O	4.86029684	1.62744120	-6.92906193
O	5.78299142	2.98515433	-4.97888911
O	3.06623373	5.04227770	-6.99983469
H	-0.94888789	-3.72281081	-3.87996195
H	1.17481884	-4.07004463	-3.41543426
H	1.06984254	-2.85232889	0.05913363
H	3.05830527	-2.03466807	-0.10998910
H	-1.01978928	-2.40532232	0.22513867
H	-2.89552961	-2.01445249	-0.89062766
H	-4.31196763	-0.53967623	-1.78348895
H	3.68817251	6.36358595	-2.93796608
H	-0.30897331	7.40462615	-3.12060992
H	1.83174680	7.37085185	-3.42303661
H	-2.20681854	6.65817332	-3.95803094
H	-4.19973431	4.53223369	-2.18915903
H	-3.64740446	3.53467216	-0.16308483
H	-4.17462248	1.30513478	-0.35935979
H	3.23642164	-3.52789566	-3.57828960
H	4.90137577	-2.21662662	-2.67668348
H	6.02498798	-0.28039347	-3.11042078
H	5.50913654	-1.01476927	-5.57153274
H	5.73330758	1.88833299	-6.57590421
H	-0.16176614	5.94757402	-7.10327846
H	3.90745304	5.39725936	-6.60249927
H	6.24117254	2.79721639	-4.14014036
H	5.41281866	4.69494548	-5.04810081
H	1.96802298	6.21032370	-6.87389233
Np	-3.31064949	5.78070487	-6.88346744
O	-5.46505997	6.20476267	-8.11963422
O	-3.64547155	4.02532955	-7.06256586
O	-3.02601999	7.55536442	-6.83072706
O	-2.68189732	5.66173337	-9.36316517
O	-5.16787041	5.69610583	-5.19015164
H	-1.99932721	6.23537399	-9.74993057
H	-2.44815985	4.74982563	-9.61068561

H	-5.61423214	6.87726874	-8.80369012
H	-6.06665397	5.46300293	-8.29872557
H	-5.47124860	6.53460891	-4.80574811
H	-4.80604840	5.15714202	-4.42717300

$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{2+}$ ($C_{60}(OH)_{24}$/Np(VI)-OS)

C	-1.94752018	3.52274889	-1.38994675
C	-0.86893872	3.39042804	-0.48580907
C	0.27963858	4.17054795	-0.63102768
C	0.38930378	5.08967651	-1.72961900
C	-0.67053733	5.17375333	-2.64300050
C	-1.87150660	4.43157991	-2.44407266
C	-2.95090213	2.41210876	-1.25951101
C	-2.17562568	1.27898701	-0.28968857
C	-0.85898851	2.05324731	0.24586023
C	0.46880334	1.39246799	0.00382365
C	1.58060956	3.54216183	-0.48205476
C	1.73492699	5.05262974	-2.23402762
C	1.96367338	5.10624441	-3.60918898
C	0.88291348	5.23495049	-4.51089979
C	-0.42636862	5.30911958	-4.04267155
C	-1.69333332	5.10315033	-4.83452999
C	-2.74128165	4.46546530	-3.67545435
C	-3.39010044	3.05570653	-3.94582898
C	-3.48944243	1.95831170	-2.67274169
C	-1.89945816	-0.21129468	-0.85638643
C	-2.29918229	-0.44051495	-2.41481436
C	-2.73469457	0.77694576	-3.20039609
C	-2.42025084	0.92043839	-4.53616174
C	-2.57309307	2.29620040	-4.95350592
C	-1.72121370	2.81262130	-5.89494537
C	-1.40469164	4.26343461	-6.13730792
C	0.17294413	4.19281487	-6.71843078
C	1.28904272	4.98732828	-5.93245330
C	2.45352589	4.07202099	-1.44006968
C	3.87993055	1.68514452	-5.40822479
C	4.40008428	2.14072607	-4.00001322
C	4.30880454	1.05023328	-2.73354401
C	3.70157894	-0.37266758	-3.00319529
C	2.80341947	-0.31865355	-4.21415065
C	1.78925090	0.72577783	-6.16831372
C	1.78835900	2.04166867	-6.93168713
C	3.09987029	2.82773928	-6.38457424
C	2.82279105	4.31490982	-5.81077784

C	3.21872865	4.52922092	-4.25308676
C	3.62830205	3.31075839	-3.47633276
C	3.49410992	1.80162282	-1.72292005
C	2.64312705	1.28453209	-0.78457874
C	2.31794565	-0.15926331	-0.53650564
C	2.62158999	-1.03025276	-1.80913397
C	1.35864045	-1.19923580	-2.61833102
C	1.60512092	-1.05944999	-4.01347550
C	0.54211792	-0.97370486	-4.92755080
C	0.64775560	-0.05959693	-6.02906185
C	0.45403333	2.71766650	-6.72775290
C	-0.67445649	1.97655400	-6.43982324
C	-0.65195502	0.56660470	-6.18711030
C	-1.52008855	0.04084497	-5.21785969
C	-0.80168595	-0.94401893	-4.42790815
C	-1.03043236	-0.99248922	-3.05437399
C	0.04608774	-1.13527500	-2.15285341
C	-0.35700864	-0.89158493	-0.72990002
C	0.74603321	-0.07867174	0.02982798
C	3.32894186	3.18111398	-2.14159187
C	1.60092109	2.13137340	-0.23583036
C	2.87244332	0.58541407	-5.27315758
O	-1.00177182	2.24328182	1.67439364
O	-3.02603393	1.15120245	0.81669583
O	-2.72563240	-1.06499332	-0.12724977
O	-4.08275032	2.85654442	-0.54191587
O	-4.85404711	1.64132957	-2.52612087
O	-3.37412646	-1.34815121	-2.49295842
O	-4.71062805	3.27978337	-4.38612895
O	-3.77760344	5.40438434	-3.51826848
O	3.10145457	-0.68946799	0.55514213
O	4.31090221	5.48108452	-4.20523077
O	5.77235400	2.51387299	-4.17627941
O	3.63735904	5.19307301	-6.54092943
O	1.44278102	6.22268750	-6.60878297
O	3.94307456	2.96951956	-7.49398441
O	1.97954736	1.81059376	-8.34114911
O	0.19076466	4.72106230	-8.03381723
O	-2.23831429	4.78771901	-7.15242550
O	-2.25449792	6.32936080	-5.25085989
O	-0.51803471	-2.12868613	-0.06341040
O	0.72371562	-0.53166820	1.38767824
O	3.07908171	-2.28667351	-1.43618710
O	4.71387576	-1.28977529	-3.25227146

O	5.66610217	0.86695834	-2.27248714
O	4.99986144	1.23673325	-6.15159928
H	-3.59927662	-1.52028098	-1.53972166
H	-2.13578588	-1.83877175	0.10299511
H	-2.50598959	1.51993569	1.58307600
H	-0.40349300	1.60517338	2.11208213
H	-4.04181379	2.30487575	0.29779320
H	-5.08021484	2.07430882	-1.64971188
H	-5.24886014	2.65279204	-3.81742110
H	5.11762929	4.98288123	-3.96695000
H	2.42725054	6.23842145	-6.81246457
H	4.23621526	5.60617060	-5.85616556
H	0.63916746	5.61252784	-7.90903086
H	-2.52643384	5.67623228	-6.79035894
H	-3.05314079	6.43492848	-4.65608244
H	-4.58241742	4.90669523	-3.84060239
H	-0.12405964	-1.96984959	0.83381462
H	1.67109586	-0.72998110	1.59989017
H	3.71931209	-0.00213492	0.86255662
H	3.53319766	-2.18326198	-0.57581866
H	5.48667044	-1.01788042	-2.71847440
H	2.88605466	2.22250350	-8.48889489
H	5.77569073	1.60072086	-5.64511949
H	5.74656711	1.24868470	-1.37980259
H	6.25257310	2.03209534	-3.45424572
H	4.67553634	2.30322040	-7.31606257
Np	-1.86679797	2.58058036	-10.96484055
O	-4.40183651	2.59117387	-11.04789316
O	-1.90454338	4.31446861	-11.32283207
O	-1.80499971	0.84309740	-10.62180215
O	-0.04275319	2.39089921	-12.72858896
O	-2.90256775	2.93895411	-8.78945310
O	-2.85032855	2.04759895	-13.24666209
H	0.50352208	1.58531864	-12.76094782
H	0.57954995	3.14029005	-12.75039138
H	-2.94771536	2.18348222	-8.17466830
H	-2.72300673	3.75615048	-8.19707372
H	-4.76779959	2.92827128	-10.21025897
H	-4.85772240	3.05466401	-11.77173157
H	-3.09799077	1.13066712	-13.46168337
H	-2.45692205	2.42684788	-14.05230477
O	0.14864776	2.92189591	-9.82468320
H	0.19310856	3.75755608	-9.24654646
H	0.80243598	2.31450107	-9.34436180

$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{2+}$ ($C_{60}(OH)_{24}$/Np(VI)-IS1)

C	-0.32759015	0.32507909	-0.42158519
C	1.07718105	0.29068388	-0.27781872
C	1.80569473	1.47123858	-0.11298393
C	1.12988026	2.73839437	-0.13064299
C	-0.25855479	2.75557677	-0.32470316
C	-1.00496081	1.54464571	-0.41193740
C	-0.89504807	-0.98790214	-0.88080636
C	0.45722049	-1.86802668	-1.35305947
C	1.70660221	-0.98395053	-0.82766287
C	2.74638003	-0.59755981	-1.84217623
C	3.03861711	1.64751193	-0.85770135
C	1.93899825	3.68855822	-0.84340325
C	1.33408583	4.60436862	-1.70587139
C	-0.06975538	4.63306886	-1.85548381
C	-0.87572090	3.74333401	-1.14888421
C	-2.32147443	3.40633968	-1.41247984
C	-2.41449826	1.80772627	-0.88317373
C	-2.87874970	0.70108952	-1.90684679
C	-2.06298708	-0.77267848	-1.92227576
C	0.58886719	-2.38122622	-2.88205734
C	-0.58275022	-1.86515127	-3.88413373
C	-1.56778863	-0.85761032	-3.33313484
C	-2.09933583	0.14007706	-4.12478840
C	-2.67989813	1.18766317	-3.31705906
C	-2.60056108	2.48869052	-3.74358296
C	-2.72511527	3.73417928	-2.90598742
C	-1.73614754	4.82113723	-3.76297175
C	-0.51093830	5.47632659	-3.01410881
C	3.12062292	2.97758689	-1.29362656
C	2.38935720	4.36245468	-5.87451179
C	3.54480350	4.14552188	-4.83411200
C	4.35288353	2.67874824	-4.84804775
C	3.92617793	1.58917809	-5.89461407
C	2.50415944	1.83537893	-6.33252410
C	0.41553137	3.08198242	-6.45366031
C	-0.21416800	4.35231455	-5.91596064
C	1.03160122	5.24206335	-5.38904421
C	0.90541931	5.76139112	-3.86660218
C	2.07697301	5.23777644	-2.87528460
C	3.03980031	4.22515489	-3.42752032
C	4.15037046	2.18885369	-3.44575416
C	4.07219891	0.89101721	-3.01935437

C	4.17434292	-0.35604969	-3.84738944
C	3.83428617	-0.05984443	-5.35372893
C	2.38001145	-0.37226220	-5.61279925
C	1.76302530	0.62368878	-6.42437191
C	0.37150483	0.63850592	-6.61635103
C	-0.31488363	1.90479019	-6.63293129
C	-1.29120934	4.00369806	-4.93403561
C	-1.93466833	2.77876586	-4.98808912
C	-1.55329084	1.73203303	-5.88738070
C	-1.61843623	0.40660731	-5.44609227
C	-0.43619087	-0.30737850	-5.90603765
C	0.16689026	-1.22006082	-5.04416086
C	1.57176290	-1.26339211	-4.90994037
C	2.01365750	-2.10333653	-3.74901254
C	3.21218575	-1.42825264	-2.99772532
C	3.56801750	3.23771685	-2.62903893
C	3.41167077	0.60126032	-1.76067630
C	1.82312512	3.05104480	-6.32458515
O	2.37212503	-1.72707014	0.22152386
O	0.41748459	-3.00629905	-0.53731120
O	0.46236254	-3.76834094	-2.84085213
O	-1.47299386	-1.67939159	0.20500955
O	-3.02732425	-1.77142745	-1.69308843
O	-1.35694533	-2.96401653	-4.30480438
O	-4.22562015	0.41337741	-1.62199740
O	-3.29795409	1.79514405	0.20940242
O	5.50905199	-0.90590570	-3.80255807
O	2.82872743	6.39873521	-2.44188780
O	4.49880241	5.18594613	-5.07715499
O	1.01959466	7.15788620	-3.90184477
O	-0.96043277	6.73590400	-2.54540372
O	1.04830411	6.38478775	-6.21375412
O	-0.80536925	5.13685524	-7.00879372
O	-2.54371780	5.90692170	-4.18848825
O	-4.03048548	4.19782310	-2.92675373
O	-3.16432606	4.16185859	-0.57859839
O	2.45177562	-3.36194549	-4.21997039
O	4.03303709	-2.49260505	-2.50694478
O	4.61438806	-0.84600724	-6.19002967
O	4.73774592	1.65550197	-7.02021864
O	5.74072584	2.99611850	-5.09401940
O	2.93407690	5.06812568	-6.97970619
H	-0.98135327	-3.72333915	-3.78412387
H	1.18557597	-4.10158827	-3.44395547

H	1.21159998	-2.92301475	0.05897578
H	3.20011098	-2.08521763	-0.15596508
H	-0.88221110	-2.48665687	0.29514434
H	-2.79015597	-2.09175672	-0.77332593
H	-4.25955008	-0.58559402	-1.61250949
H	3.70808656	6.35276738	-2.86485266
H	-0.29041726	7.37246914	-2.93215259
H	1.82432851	7.35510251	-3.34237853
H	-2.28017134	6.63692199	-3.55228926
H	-4.19385176	4.48895094	-1.99368576
H	-3.50766235	3.49771750	0.08286005
H	-4.06308597	1.24473655	-0.12298413
H	3.25367677	-3.55778102	-3.66804644
H	4.95131599	-2.25298660	-2.79064136
H	6.07889614	-0.31287930	-3.28056948
H	5.44485351	-1.03821416	-5.70886957
H	5.62968065	1.91682697	-6.71591355
H	-0.17947654	5.95383479	-7.00385400
H	3.80361291	5.40728943	-6.62472988
H	6.25246891	2.80128120	-4.28797408
H	5.36983184	4.71349888	-5.12984369
H	1.86368045	6.24026689	-6.79119728
Np	-2.77821365	4.99519670	-8.36180310
O	-3.59720366	4.29229259	-10.64431751
O	-3.38589071	3.53040197	-7.57186107
O	-2.16398452	6.43738303	-9.19150821
O	-3.47156441	6.37937161	-6.51248087
O	-1.03463278	3.47939712	-9.40216547
O	-5.18789884	5.63155878	-8.69331077
H	-3.38112651	7.34245048	-6.61595949
H	-3.17323506	6.15846083	-5.55371486
H	-0.21293807	3.84539135	-9.77425794
H	-0.75476277	2.76575823	-8.79013656
H	-3.17908828	4.58523943	-11.47253958
H	-3.96112633	3.40494917	-10.81048929
H	-5.55854253	6.20376868	-9.38623440
H	-5.80509780	5.64238885	-7.94104021

$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{2+}$ ($C_{60}(OH)_{24}$/Np(VI)-IS2)

C	-0.44958078	0.39202384	-0.50192521
C	0.94924867	0.36096642	-0.30130573
C	1.66867419	1.54475010	-0.12978000
C	0.99416670	2.81112062	-0.19563602
C	-0.38557292	2.82553434	-0.44310806

C	-1.12568244	1.61037069	-0.54046973
C	-0.99730399	-0.93162466	-0.95544809
C	0.37317516	-1.81882384	-1.35866792
C	1.60078218	-0.92384908	-0.80084217
C	2.67909967	-0.55592898	-1.78135674
C	2.93069771	1.70797537	-0.82966331
C	1.83147091	3.74880556	-0.89234912
C	1.26343586	4.65759400	-1.78553638
C	-0.13740611	4.69413919	-1.97961251
C	-0.97019124	3.80716817	-1.29816680
C	-2.40172762	3.45309436	-1.62368091
C	-2.51480090	1.85976910	-1.07027002
C	-2.94309467	0.72975314	-2.08608782
C	-2.12630759	-0.74165776	-2.04376013
C	0.56479228	-2.35949914	-2.87167281
C	-0.56714825	-1.86369125	-3.92602853
C	-1.57697284	-0.85066961	-3.43351139
C	-2.07967889	0.12906036	-4.26856093
C	-2.69170133	1.18763595	-3.49614040
C	-2.59677299	2.47993117	-3.94505389
C	-2.72470350	3.75330525	-3.14330747
C	-1.68497453	4.77426288	-3.96680463
C	-0.52863509	5.49267306	-3.18884719
C	3.02972551	3.02816187	-1.28521480
C	2.47732999	4.32601824	-5.92200264
C	3.58514616	4.12745756	-4.82827111
C	4.39599419	2.66672998	-4.78516861
C	4.00948483	1.55954481	-5.82895658
C	2.60556283	1.79645697	-6.33069988
C	0.52160204	3.04551191	-6.58716810
C	-0.12095199	4.31876656	-6.05059305
C	1.10865034	5.21383687	-5.50059761
C	0.92193737	5.75997540	-3.99042535
C	2.05034759	5.25896775	-2.94511812
C	3.02502678	4.23074247	-3.44334405
C	4.14150693	2.20066200	-3.38241925
C	4.04974459	0.91144427	-2.93462834
C	4.18240647	-0.34963386	-3.73672468
C	3.89677660	-0.07914367	-5.25974328
C	2.45335962	-0.39537883	-5.56677130
C	1.86925325	0.58287210	-6.42139119
C	0.48581298	0.59394217	-6.66695911
C	-0.19569021	1.85623015	-6.74184788
C	-1.17446963	3.92308802	-5.06834281

C	-1.85674166	2.72543496	-5.15647114
C	-1.46080515	1.68455333	-6.04541442
C	-1.54704810	0.36523720	-5.57625204
C	-0.34582827	-0.34827070	-5.97342412
C	0.22372921	-1.24292075	-5.07134491
C	1.62142270	-1.27710901	-4.87907930
C	2.02025052	-2.09588502	-3.68808997
C	3.18865643	-1.40707222	-2.90376489
C	3.52733920	3.26272234	-2.60765132
C	3.34028479	0.64451546	-1.69753576
C	1.92235932	3.01095388	-6.38244194
O	2.22183083	-1.64592461	0.28848267
O	0.30016797	-2.94112816	-0.52397125
O	0.43543626	-3.74531069	-2.81042759
O	-1.61422545	-1.60249217	0.12105832
O	-3.09793407	-1.73467711	-1.82933019
O	-1.34044798	-2.96688609	-4.33711745
O	-4.29874742	0.44741299	-1.84191728
O	-3.44448304	1.87581949	-0.01591076
O	5.51329666	-0.89909783	-3.63225543
O	2.79574479	6.42450200	-2.51528257
O	4.54429785	5.17102088	-5.03530069
O	1.02892946	7.15646398	-4.03992565
O	-1.03969806	6.76649511	-2.83497312
O	1.15439223	6.33909722	-6.33858040
O	-0.79238849	5.13180239	-7.05918432
O	-2.43754998	5.83198530	-4.57051087
O	-4.03367305	4.27099753	-3.19672404
O	-3.30569369	4.20885047	-0.85151826
O	2.47469467	-3.36332020	-4.11773044
O	3.99060445	-2.46005915	-2.36168501
O	4.70281557	-0.88336116	-6.05272646
O	4.86706336	1.60226833	-6.91965300
O	5.79112584	2.98431395	-4.98242300
O	3.06995335	5.01188862	-7.01193768
H	-0.98283504	-3.71648021	-3.78834709
H	1.18138734	-4.08881794	-3.38065770
H	1.07291391	-2.84939264	0.09893553
H	3.06874410	-2.00438242	-0.04434280
H	-1.02512486	-2.40731186	0.24769184
H	-2.89175280	-2.03953621	-0.89634376
H	-4.33209548	-0.55239636	-1.81429368
H	3.68283402	6.37021511	-2.92229273
H	-0.32540998	7.39072060	-3.16946717

H	1.81809231	7.36842612	-3.46400652
H	-2.18177865	6.63277874	-4.00545123
H	-4.22057872	4.49500617	-2.23830170
H	-3.66524876	3.54459957	-0.19255910
H	-4.19052425	1.30570839	-0.36147728
H	3.25624439	-3.54891462	-3.53418516
H	4.91856295	-2.22577132	-2.61841291
H	6.06582089	-0.29668511	-3.10252231
H	5.52183529	-1.05856792	-5.54676336
H	5.74441740	1.87939691	-6.58865298
H	-0.14384036	5.91266701	-7.12497511
H	3.91435323	5.37414701	-6.62603756
H	6.27537184	2.79710733	-4.15797191
H	5.41853228	4.70189280	-5.05284713
H	1.97233623	6.17543528	-6.90516590
Np	-3.26198270	5.73858624	-6.91208369
O	-5.38782904	6.24561016	-8.13262796
O	-3.63597423	4.00994474	-7.09087589
O	-2.96297592	7.48910361	-6.84017666
O	-2.62861461	5.91227109	-9.32344285
O	-5.11329615	5.67612095	-5.24113237
H	-2.45214838	6.72665188	-9.82423355
H	-2.60844789	5.16994816	-9.95132346
H	-5.76048817	7.12951613	-8.29213312
H	-6.12373648	5.60932540	-8.16000018
H	-5.42887084	6.50509514	-4.84269812
H	-4.79076458	5.11223908	-4.47486351

$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{1+}$ ($C_{60}(OH)_{24}$/Pu(V)-OS)

C	-1.96065117	3.53395602	-1.51452159
C	-0.91545237	3.36388712	-0.57875559
C	0.24778893	4.13479151	-0.66471381
C	0.40196707	5.08367884	-1.73292065
C	-0.62737233	5.20484638	-2.67631833
C	-1.84341094	4.47392209	-2.53725589
C	-2.97898996	2.43165208	-1.45189806
C	-2.24883270	1.26203884	-0.49231021
C	-0.94316911	2.00514955	0.10722861
C	0.38368190	1.33979296	-0.11106251
C	1.53662338	3.49233519	-0.48891015
C	1.76264181	5.04840716	-2.19615625
C	2.03499941	5.13941354	-3.56391850
C	0.98430171	5.30013099	-4.49433657
C	-0.33710723	5.37540091	-4.06275680

C	-1.57943527	5.21093766	-4.89818410
C	-2.67036989	4.55142550	-3.79591583
C	-3.31828219	3.15640824	-4.12843155
C	-3.47325112	2.02358397	-2.89090735
C	-1.97211875	-0.21650890	-1.08996839
C	-2.32992471	-0.40483196	-2.66680162
C	-2.72025018	0.84558617	-3.42741778
C	-2.35697671	1.02819584	-4.73923807
C	-2.47641614	2.42000371	-5.12792615
C	-1.59459504	2.95573097	-6.02517415
C	-1.26370280	4.41188806	-6.22000193
C	0.33793676	4.33578821	-6.75903240
C	1.42967525	5.09470238	-5.91166634
C	2.44627554	4.04134833	-1.40756461
C	3.97177533	1.75044392	-5.39755717
C	4.44747455	2.16123805	-3.96239635
C	4.30321397	1.03740538	-2.73273053
C	3.69641163	-0.37279842	-3.05890544
C	2.84142774	-0.27708122	-4.29715343
C	1.89597314	0.83798528	-6.24588111
C	1.93542451	2.17201514	-6.97462092
C	3.23491250	2.92871412	-6.36623304
C	2.95293224	4.40303716	-5.76063803
C	3.30055417	4.56660755	-4.18639295
C	3.67198396	3.32402444	-3.43212675
C	3.46588081	1.76942727	-1.72775529
C	2.58013801	1.23462350	-0.83196705
C	2.23331859	-0.21158863	-0.63903495
C	2.57180165	-1.05159958	-1.92126177
C	1.33460387	-1.18683247	-2.77404411
C	1.62875871	-1.01141589	-4.15701223
C	0.59806022	-0.88747521	-5.09984696
C	0.74432133	0.06139225	-6.16732367
C	0.60199503	2.85745460	-6.79253805
C	-0.53961814	2.12505068	-6.56815417
C	-0.54509638	0.70623875	-6.34897224
C	-1.44560792	0.16197326	-5.42997570
C	-0.76148465	-0.85211893	-4.64324621
C	-1.03752761	-0.93592741	-3.28115838
C	0.00936597	-1.11918835	-2.35038328
C	-0.43759847	-0.91260361	-0.93610310
C	0.64699582	-0.13205967	-0.12062296
C	3.33115186	3.16202278	-2.10897797
C	1.53148281	2.07576020	-0.28933395

C	2.95152905	0.65739220	-5.32378855
O	-1.12627641	2.14786551	1.54356080
O	-3.13654005	1.11446549	0.58717312
O	-2.82131532	-1.08033563	-0.39432497
O	-4.12763923	2.87428077	-0.75077972
O	-4.85427692	1.73061752	-2.79538887
O	-3.37963765	-1.33783448	-2.79452481
O	-4.62673171	3.40345563	-4.60917312
O	-3.71003764	5.49295734	-3.64493412
O	2.98610675	-0.77161379	0.46696766
O	4.40929994	5.50185310	-4.07089902
O	5.83337070	2.52668338	-4.07838056
O	3.80227740	5.29335034	-6.43842645
O	1.61611683	6.35604687	-6.53067979
O	4.11972401	3.09755008	-7.44053177
O	2.17433290	1.95703445	-8.37717658
O	0.40646002	4.87851644	-8.06109132
O	-2.06086332	4.97960103	-7.24206817
O	-2.10381328	6.46762248	-5.27777016
O	-0.62638199	-2.16917215	-0.30499958
O	0.58326468	-0.62622781	1.22778834
O	3.00994855	-2.32194410	-1.55882547
O	4.71728370	-1.29037871	-3.29014490
O	5.64527565	0.83186957	-2.22136964
O	5.11535873	1.30845822	-6.11431995
H	-3.62244374	-1.53808637	-1.85509830
H	-2.23744508	-1.86059185	-0.17475928
H	-2.62888522	1.45672572	1.37387246
H	-0.55280901	1.47460206	1.96150506
H	-4.11395784	2.29259085	0.06873406
H	-5.09518243	2.14785680	-1.91673343
H	-5.18135460	2.77255629	-4.05817506
H	5.19761995	4.96823427	-3.84787483
H	2.60046688	6.35949759	-6.72124420
H	4.37484166	5.68171420	-5.71973750
H	0.80741745	5.77960051	-7.91469627
H	-2.30756248	5.87304462	-6.87228913
H	-2.92992276	6.54890948	-4.71991011
H	-4.49820346	5.00433281	-4.01997060
H	-0.25633230	-2.02882572	0.60498851
H	1.52501776	-0.83652799	1.45203529
H	3.57889235	-0.07837448	0.80801409
H	3.45684241	-2.22732532	-0.69447774
H	5.46380132	-1.02895776	-2.71611875

H	3.07227017	2.38365009	-8.50206125
H	5.87234294	1.66232208	-5.57548938
H	5.68141935	1.20235165	-1.32136757
H	6.27628833	2.01596570	-3.35323533
H	4.82871789	2.40932651	-7.26546357
Pu	-2.07269222	2.36884118	-10.37955938
O	-4.63153733	2.02273223	-10.54589448
O	-2.27155389	4.03614418	-10.98239653
O	-1.87523031	0.70463116	-9.75629768
O	-0.27100915	1.87771212	-12.22266501
O	-3.43697115	3.06799229	-8.34692629
O	-2.92991741	1.63642097	-12.66203813
H	0.07332757	0.97436627	-12.11028382
H	0.34435638	2.45327392	-11.71008371
H	-3.44420043	2.47814487	-7.56929545
H	-3.06490115	3.92767096	-7.97041440
H	-4.88276725	1.09823922	-10.37666455
H	-4.83945560	2.51116486	-9.72232150
H	-2.19769976	1.91073652	-13.24571703
H	-3.68547545	2.21024217	-12.87965498
O	0.29693320	3.01741870	-9.89726356
H	0.32744049	3.88759763	-9.40734128
H	0.96187197	2.47809960	-9.37057959

$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{1+}$ ($C_{60}(OH)_{24}$/Pu(V)-IS1)

C	-0.35647427	0.31394562	-0.46835899
C	1.04532960	0.27040136	-0.30559058
C	1.77841645	1.44661221	-0.11943680
C	1.10819206	2.71758658	-0.13147057
C	-0.27812680	2.74258842	-0.34221094
C	-1.02899167	1.53634718	-0.45173376
C	-0.92537907	-0.99059437	-0.94844480
C	0.42625140	-1.87252543	-1.41396131
C	1.67214354	-0.99939972	-0.86597841
C	2.72401002	-0.60640402	-1.86205256
C	3.02125079	1.62505491	-0.84509946
C	1.92928507	3.67237521	-0.82488743
C	1.33664089	4.60095252	-1.68522357
C	-0.06443163	4.63488377	-1.85174110
C	-0.88226601	3.74118223	-1.16301322
C	-2.32598921	3.41249521	-1.44898030
C	-2.43028738	1.81072874	-0.93932796
C	-2.88601540	0.71686670	-1.97914987
C	-2.07445847	-0.76354405	-2.00030661

C	0.57371292	-2.37609634	-2.94538125
C	-0.58732680	-1.85446092	-3.96066090
C	-1.56810461	-0.84157374	-3.40688474
C	-2.07914032	0.16747181	-4.18515270
C	-2.67161583	1.21860011	-3.37934014
C	-2.58206980	2.51812193	-3.78693859
C	-2.71118081	3.76071731	-2.94144505
C	-1.70098548	4.84632191	-3.77853818
C	-0.49184829	5.48999205	-3.00659591
C	3.11232685	2.96119599	-1.26799402
C	2.44038306	4.39264623	-5.84865562
C	3.57488459	4.15788964	-4.79318679
C	4.37724488	2.69117731	-4.81258928
C	3.96596741	1.61314642	-5.87610095
C	2.55244910	1.87018227	-6.33353184
C	0.46951448	3.12667739	-6.45977380
C	-0.16337444	4.39851639	-5.92322171
C	1.07828432	5.27801331	-5.37480190
C	0.93444875	5.77748814	-3.84306598
C	2.09036006	5.23741508	-2.84538535
C	3.05158929	4.22362201	-3.39403928
C	4.15786800	2.18887082	-3.41780768
C	4.07063819	0.88734345	-3.00492727
C	4.17531091	-0.34993908	-3.84550135
C	3.85967866	-0.03979981	-5.35241576
C	2.40918044	-0.34522895	-5.63369857
C	1.80754987	0.66087868	-6.44592057
C	0.42001665	0.68440169	-6.65164153
C	-0.26148235	1.95398334	-6.65857507
C	-1.23581344	4.03111648	-4.94230167
C	-1.88805012	2.82304057	-5.01728504
C	-1.50550285	1.77774756	-5.92214937
C	-1.58843196	0.45190122	-5.50287929
C	-0.40205977	-0.26201764	-5.95553969
C	0.18397909	-1.18526143	-5.09480785
C	1.58856130	-1.23657830	-4.94782093
C	2.01154405	-2.08968268	-3.79152637
C	3.20025931	-1.42558412	-3.01928395
C	3.57241820	3.23132068	-2.59655345
C	3.39570151	0.58789566	-1.75692914
C	1.87616610	3.08764192	-6.31866267
O	2.33415548	-1.76143328	0.18077413
O	0.37516105	-3.01975563	-0.60355991
O	0.46051574	-3.76795232	-2.90713174

O	-1.51118975	-1.68687124	0.13719821
O	-3.05327224	-1.75975121	-1.77583417
O	-1.31590656	-2.96402312	-4.43794923
O	-4.23795713	0.42333231	-1.69848276
O	-3.33013780	1.78532976	0.14496670
O	5.51687695	-0.89771547	-3.78060301
O	2.86356146	6.38519101	-2.39708309
O	4.54187314	5.20220995	-4.99654527
O	1.05728906	7.17707927	-3.85702196
O	-0.93649158	6.74603096	-2.51706019
O	1.11988245	6.43327427	-6.17513312
O	-0.75239416	5.16399934	-7.01607743
O	-2.48649964	5.93642548	-4.23185029
O	-4.01255956	4.24617770	-2.96625652
O	-3.16949179	4.16136646	-0.60249036
O	2.46011653	-3.34787883	-4.26832018
O	4.01999764	-2.49745641	-2.52505696
O	4.65777461	-0.82415458	-6.18000944
O	4.80791286	1.68736813	-6.98300458
O	5.77722097	3.00564896	-5.02580581
O	3.01309316	5.10051564	-6.94066501
H	-0.93929993	-3.72328115	-3.92587798
H	1.19122749	-4.08412325	-3.50872221
H	1.16668432	-2.93719195	-0.00460734
H	3.15224474	-2.12206754	-0.21571010
H	-0.92253604	-2.49584855	0.21603904
H	-2.82506842	-2.07576195	-0.85471570
H	-4.25558529	-0.57731484	-1.69271275
H	3.72115667	6.34167898	-2.86365133
H	-0.26925879	7.38101545	-2.90739749
H	1.85259669	7.35892007	-3.28335569
H	-2.27950849	6.65182727	-3.57024638
H	-4.17354445	4.53205249	-2.03403245
H	-3.52940314	3.47732928	0.02915421
H	-4.08263708	1.23235774	-0.21895350
H	3.25093286	-3.54196133	-3.70144562
H	4.93717385	-2.24731372	-2.80288132
H	6.05757412	-0.30518045	-3.22841524
H	5.48898435	-0.98756905	-5.69153852
H	5.68854985	1.94623757	-6.64725460
H	-0.16799729	5.98485181	-7.04083559
H	3.86588915	5.44684569	-6.56164656
H	6.25816081	2.79419650	-4.20558176
H	5.40713258	4.72020775	-5.04249933

H	1.92325845	6.28375217	-6.75755050
Pu	-2.85059818	4.95086700	-8.30031523
O	-3.80271894	3.92497846	-10.44238737
O	-3.40870206	3.48031677	-7.44891615
O	-2.30503996	6.42297822	-9.16279439
O	-3.77858464	6.38691463	-6.45464117
O	-1.18423316	3.36056911	-9.51217054
O	-5.30225095	5.57697352	-8.69648981
H	-3.46807900	7.30175104	-6.56686147
H	-3.42340572	6.11246457	-5.55043621
H	-0.36532572	3.78933588	-9.81620901
H	-0.89751453	2.70166940	-8.84610682
H	-3.15029296	3.25360305	-10.71359936
H	-4.61484564	3.43616306	-10.22183730
H	-5.40768373	6.35291442	-9.27367575
H	-5.57043027	5.87063694	-7.80447698

$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{1+}$ ($C_{60}(OH)_{24}$/Pu(V)-IS2)

C	-0.47942307	0.39476060	-0.53039823
C	0.91498086	0.36049385	-0.30708427
C	1.63497094	1.54465308	-0.12502447
C	0.96227835	2.81239272	-0.20013993
C	-0.41406853	2.82770812	-0.46758037
C	-1.15427429	1.61378420	-0.57544295
C	-1.02406666	-0.92646147	-0.99307841
C	0.34801042	-1.81581140	-1.37789192
C	1.56782890	-0.92267542	-0.80422615
C	2.65778696	-0.55397649	-1.76745854
C	2.90676480	1.70717008	-0.80407480
C	1.80901689	3.75050175	-0.88555574
C	1.25132206	4.66062233	-1.78725145
C	-0.14563862	4.69576459	-2.00208607
C	-0.98755947	3.80937099	-1.33018032
C	-2.41463770	3.45463523	-1.67482605
C	-2.53437753	1.86477951	-1.12625350
C	-2.94864256	0.73659238	-2.14815296
C	-2.13118439	-0.73860276	-2.09565426
C	0.55939526	-2.36266399	-2.88685345
C	-0.56192898	-1.87757124	-3.96284142
C	-1.56951952	-0.85448461	-3.47877850
C	-2.05319908	0.12678246	-4.30856481
C	-2.68229037	1.19552824	-3.55286080
C	-2.57779794	2.48179469	-3.99565295
C	-2.71832389	3.75323739	-3.19538232

C	-1.67013618	4.78618403	-4.00694662
C	-0.52394062	5.49778892	-3.21345048
C	3.01164873	3.03026958	-1.26013564
C	2.52235082	4.32593602	-5.90824650
C	3.60838393	4.12427824	-4.79707280
C	4.41706431	2.66525400	-4.74285285
C	4.05200863	1.55792129	-5.79254156
C	2.65807189	1.79668866	-6.31716729
C	0.57665254	3.04527631	-6.59019298
C	-0.07578801	4.32299182	-6.07529081
C	1.14531441	5.21772393	-5.51085784
C	0.93847123	5.76052393	-3.99983742
C	2.04961306	5.25612589	-2.94038610
C	3.02800044	4.22660470	-3.42240798
C	4.14445734	2.20063538	-3.34384280
C	4.04569753	0.91156369	-2.89732838
C	4.18666341	-0.34778771	-3.69878735
C	3.92897719	-0.08000069	-5.22516101
C	2.49171665	-0.39738191	-5.55423486
C	1.92160407	0.58195244	-6.41957150
C	0.54426847	0.59505538	-6.68152691
C	-0.13732532	1.85786481	-6.75770901
C	-1.13375552	3.92829548	-5.09534451
C	-1.81340565	2.74150526	-5.19423991
C	-1.41227531	1.68848348	-6.07584766
C	-1.50920545	0.37523255	-5.61484638
C	-0.30081097	-0.34085920	-5.99431288
C	0.25135487	-1.23604620	-5.08389505
C	1.64875204	-1.27431269	-4.87702444
C	2.02818437	-2.09333055	-3.68203763
C	3.18225928	-1.40330824	-2.88151328
C	3.52315375	3.26272994	-2.57659071
C	3.32165272	0.64518533	-1.66957096
C	1.97653426	3.01022915	-6.37400967
O	2.18762132	-1.65232527	0.29048691
O	0.26580512	-2.93879892	-0.53645252
O	0.45026430	-3.75331209	-2.81148576
O	-1.64919634	-1.59221692	0.08984829
O	-3.11581210	-1.73024650	-1.87730221
O	-1.27191189	-3.00332595	-4.42905496
O	-4.30912586	0.44563165	-1.90667505
O	-3.48145695	1.87384095	-0.08118509
O	5.52579071	-0.88899401	-3.56460212
O	2.81085763	6.41697968	-2.50330888

O	4.57852808	5.17132387	-4.97757744
O	1.05535779	7.16028891	-4.04497177
O	-1.02043382	6.77522675	-2.84529021
O	1.21368244	6.34882447	-6.34003399
O	-0.72015896	5.10646812	-7.11892292
O	-2.42898425	5.83764278	-4.60503369
O	-4.03224064	4.26493241	-3.26478645
O	-3.32241856	4.21152611	-0.90023074
O	2.49954462	-3.36335110	-4.10355610
O	3.98515589	-2.45623622	-2.32278020
O	4.75932686	-0.88677468	-5.99792228
O	4.94169867	1.60190348	-6.86266354
O	5.82377627	2.98128461	-4.90587780
O	3.14212732	5.00866446	-6.98973455
H	-0.91064725	-3.74550712	-3.88212923
H	1.20519847	-4.08210952	-3.37600073
H	1.03546899	-2.83880730	0.08798878
H	3.02437538	-2.01725493	-0.06084906
H	-1.05938131	-2.39562608	0.21456652
H	-2.91865741	-2.02016735	-0.94016246
H	-4.31999710	-0.55592859	-1.87053159
H	3.68105766	6.35792133	-2.94534449
H	-0.30554948	7.39060194	-3.18826314
H	1.83307212	7.36143045	-3.45322343
H	-2.17593049	6.63892378	-4.05901992
H	-4.22512553	4.50455709	-2.31587603
H	-3.69484449	3.53318973	-0.26364471
H	-4.21129192	1.29573156	-0.45557634
H	3.26773526	-3.53766557	-3.50068450
H	4.91160261	-2.20999003	-2.57277206
H	6.04344615	-0.27765255	-3.01095890
H	5.57505469	-1.02714462	-5.47775959
H	5.80748381	1.87042752	-6.49793950
H	-0.09859156	5.89388060	-7.18954601
H	3.96945386	5.37868914	-6.58072761
H	6.27081872	2.79460961	-4.06096616
H	5.44674341	4.69218425	-4.98157902
H	2.03048740	6.17923201	-6.89795127
Pu	-3.21457506	5.73308762	-7.01542073
O	-5.56815391	6.20293374	-7.90545844
O	-3.61395405	3.99594237	-7.09390247
O	-2.88259332	7.49301562	-6.99729674
O	-2.95908967	5.73004952	-9.51053239
O	-5.12263995	5.78727503	-5.24273481

H	-2.92106000	6.51008192	-10.08721683
H	-3.30143933	4.99149637	-10.04110867
H	-5.78953654	7.14750768	-7.96988375
H	-6.05512690	5.87477366	-7.12142278
H	-5.11318013	6.63540657	-4.76716183
H	-4.78196337	5.13586962	-4.56075558

$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{2+}$ ($C_{60}(OH)_{24}$/Pu(VI)-OS)

C	-1.93090464	3.54286769	-1.41506240
C	-0.86475251	3.39014251	-0.49926706
C	0.29596996	4.15508130	-0.62620212
C	0.43105002	5.07881971	-1.71811040
C	-0.61642773	5.18223332	-2.64347468
C	-1.82993611	4.45618455	-2.46320504
C	-2.95077303	2.44551599	-1.30281402
C	-2.20231252	1.29633276	-0.33070370
C	-0.88168604	2.04937538	0.22544608
C	0.43976688	1.37128010	-0.00446534
C	1.58647718	3.50841847	-0.46525932
C	1.78186988	5.02723012	-2.20657995
C	2.02788526	5.08589629	-3.57863740
C	0.95991838	5.23360786	-4.49268248
C	-0.35350207	5.32165341	-4.03924975
C	-1.61374772	5.14096926	-4.84710308
C	-2.68492715	4.51074203	-3.70437177
C	-3.34944516	3.11160533	-3.99165946
C	-3.47940907	2.00861019	-2.72687053
C	-1.93832618	-0.19318466	-0.90411306
C	-2.32020374	-0.40416268	-2.46836286
C	-2.73168763	0.82151369	-3.25148407
C	-2.39744701	0.96862413	-4.58594240
C	-2.52981916	2.34750285	-4.99391952
C	-1.65877670	2.85923026	-5.92336783
C	-1.32359538	4.30773860	-6.15565701
C	0.26194119	4.21703432	-6.71888323
C	1.38018549	4.99149469	-5.91128966
C	2.47720132	4.03183775	-1.41041601
C	3.91973843	1.65044365	-5.37539090
C	4.42925615	2.09030159	-3.95846945
C	4.30783216	0.99344597	-2.69984317
C	3.68401834	-0.41976418	-2.98479993
C	2.80118368	-0.34665805	-4.20633429
C	1.82607350	0.72356334	-6.16586550
C	1.85161054	2.04503412	-6.91920427

C	3.16765769	2.80999911	-6.35243209
C	2.90372060	4.29799385	-5.77454207
C	3.28352839	4.49684510	-4.21078608
C	3.66670032	3.26760654	-3.43678433
C	3.49089316	1.74954835	-1.69436285
C	2.62191151	1.23850361	-0.76914736
C	2.27436973	-0.20215291	-0.53353222
C	2.58063904	-1.06934793	-1.80808713
C	1.32542404	-1.21583308	-2.63353722
C	1.59031522	-1.07059191	-4.02405953
C	0.53862669	-0.96423877	-4.95090568
C	0.67194610	-0.04669517	-6.04623215
C	0.52312365	2.73860637	-6.72476770
C	-0.62172812	2.00959249	-6.45936709
C	-0.61527794	0.60033768	-6.21380608
C	-1.50543035	0.07780978	-5.25878143
C	-0.81069794	-0.92169561	-4.46719497
C	-1.05555171	-0.97604674	-3.09639946
C	0.00792789	-1.13730689	-2.18316091
C	-0.40832158	-0.89631041	-0.76327911
C	0.69692924	-0.10373256	0.01519642
C	3.34943543	3.13365690	-2.10660213
C	1.58457666	2.09610055	-0.22754846
C	2.89556816	0.56326403	-5.25929944
O	-1.04209912	2.23431087	1.65237459
O	-3.06764008	1.17196003	0.76362627
O	-2.78745643	-1.04139327	-0.19601521
O	-4.08632992	2.89839565	-0.59800614
O	-4.84778270	1.70588930	-2.59908867
O	-3.41897399	-1.28131853	-2.56818988
O	-4.65981512	3.35477059	-4.44993876
O	-3.70938250	5.46253175	-3.55199315
O	3.03726500	-0.75110806	0.56262288
O	4.38647562	5.43351938	-4.14268562
O	5.80728740	2.44638276	-4.11732286
O	3.73787074	5.16830519	-6.48980306
O	1.55592058	6.22714273	-6.57614158
O	4.02168124	2.94710671	-7.45182473
O	2.04025606	1.83084564	-8.32379222
O	0.31109720	4.73267185	-8.03101524
O	-2.13834863	4.84518667	-7.17474180
O	-2.14803519	6.37921556	-5.25844557
O	-0.59614969	-2.13485696	-0.10777333
O	0.65215648	-0.56757818	1.36816839

O	3.01391036	-2.33500216	-1.43916591
O	4.68533980	-1.34987511	-3.22703381
O	5.65685560	0.78805049	-2.22593795
O	5.03953906	1.18800204	-6.10830757
H	-3.66177924	-1.45340223	-1.61789654
H	-2.21219284	-1.82566170	0.03774143
H	-2.55274166	1.53027994	1.53883781
H	-0.45450842	1.59089170	2.09649758
H	-4.06415243	2.34165514	0.23922212
H	-5.07976970	2.13588491	-1.72221831
H	-5.21650966	2.73215305	-3.89560929
H	5.18515792	4.92414041	-3.90099875
H	2.54108131	6.23193667	-6.77466484
H	4.33323521	5.57231150	-5.79723632
H	0.75256800	5.62466878	-7.90758977
H	-2.41039732	5.73836265	-6.81515331
H	-2.95157285	6.49637466	-4.67384529
H	-4.51785488	4.98364615	-3.89053893
H	-0.20888583	-1.98862449	0.79490307
H	1.59390989	-0.78092370	1.59085100
H	3.65970505	-0.07467322	0.88477678
H	3.46224656	-2.24506103	-0.57416537
H	5.46082739	-1.08399046	-2.69365191
H	2.94394263	2.24394096	-8.47450380
H	5.81615556	1.54106485	-5.59569416
H	5.73358534	1.15718293	-1.32763488
H	6.27448300	1.95561611	-3.39308666
H	4.73788697	2.26301300	-7.28032926
Pu	-1.97934797	2.60369050	-10.91066526
O	-4.51726405	2.62302615	-11.02177191
O	-1.98024935	4.33954700	-11.24531215
O	-1.95004323	0.86820749	-10.57347670
O	-0.24089189	2.39545530	-12.79343377
O	-3.07638993	2.99091768	-8.72631034
O	-2.97755063	2.05576760	-13.18168224
H	0.35783102	1.62808824	-12.76184464
H	0.33695653	3.17752054	-12.85627938
H	-3.16035720	2.24581442	-8.10589288
H	-2.81073434	3.78775863	-8.15848753
H	-4.82739753	2.96791979	-10.16418606
H	-4.90340979	3.19287154	-11.70987146
H	-3.38122627	1.17604464	-13.28666340
H	-2.34099236	2.15556959	-13.91220483
O	0.11845020	2.88592198	-9.82369997

H	0.21820913	3.73146178	-9.28938246
H	0.77356298	2.28052223	-9.37162393

$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{2+}$ ($C_{60}(OH)_{24}$/Pu(VI)-IS1)

C	-0.33892690	0.32006991	-0.43552348
C	1.06552083	0.28125948	-0.28615345
C	1.79573969	1.45893309	-0.11203121
C	1.12298219	2.72781053	-0.12590210
C	-0.26446921	2.74985763	-0.32592873
C	-1.01328344	1.54114141	-0.42283119
C	-0.90677635	-0.98947360	-0.90383187
C	0.44582915	-1.87015470	-1.37499544
C	1.69507249	-0.99220758	-0.83862333
C	2.74083693	-0.60390865	-1.84648078
C	3.03302922	1.63603530	-0.84979508
C	1.93768758	3.67982833	-0.82944354
C	1.33947173	4.60254909	-1.68902096
C	-0.06397606	4.63652994	-1.84429218
C	-0.87530051	3.74492292	-1.14618478
C	-2.32070830	3.41279049	-1.41902876
C	-2.42020820	1.81024171	-0.89816704
C	-2.88252994	0.70986318	-1.92979602
C	-2.07141294	-0.76486224	-1.94942790
C	0.58352858	-2.37285263	-2.90639174
C	-0.57972443	-1.84405999	-3.90828575
C	-1.56700404	-0.84128934	-3.35733536
C	-2.09372226	0.16491900	-4.15064368
C	-2.67470465	1.20299557	-3.33654841
C	-2.58764931	2.50982931	-3.75588682
C	-2.71293887	3.75151681	-2.91412538
C	-1.72044146	4.83692497	-3.76033203
C	-0.49685323	5.48707814	-3.00120076
C	3.11944506	2.96780220	-1.27845334
C	2.41437199	4.38006908	-5.85601725
C	3.56308890	4.15411552	-4.81044079
C	4.36825242	2.68619952	-4.82857201
C	3.94380180	1.60301142	-5.88316155
C	2.52442278	1.85500724	-6.32780833
C	0.43970853	3.10935201	-6.45602721
C	-0.18911438	4.37952809	-5.91223769
C	1.05807329	5.26278055	-5.37251399
C	0.92452712	5.77265995	-3.84572522
C	2.08955381	5.23999412	-2.85210392
C	3.05101220	4.22643572	-3.40568058

C	4.15773860	2.18844469	-3.42995570
C	4.07533521	0.88857976	-3.01049683
C	4.17822882	-0.35414094	-3.84497130
C	3.84495806	-0.04860201	-5.35105828
C	2.39106055	-0.35524045	-5.61812303
C	1.78056657	0.64615104	-6.42684951
C	0.38892162	0.66622445	-6.62533246
C	-0.29146198	1.93436761	-6.64011723
C	-1.26539267	4.02036776	-4.92741717
C	-1.91755254	2.79938811	-4.99620124
C	-1.53090235	1.76079238	-5.89985999
C	-1.60751679	0.43035012	-5.46824292
C	-0.42430085	-0.28350994	-5.92483685
C	0.17363532	-1.20190394	-5.06564297
C	1.57749037	-1.24835941	-4.92367182
C	2.01217129	-2.09596759	-3.76543422
C	3.20972288	-1.42918203	-3.00503453
C	3.57415315	3.23424351	-2.61028474
C	3.40776634	0.59354907	-1.75657705
C	1.84549357	3.07277589	-6.31698837
O	2.34990744	-1.74307450	0.21127540
O	0.39884549	-3.01343006	-0.56766114
O	0.44628064	-3.75906776	-2.87815803
O	-1.49292393	-1.68752646	0.17218820
O	-3.03728746	-1.76316845	-1.73357470
O	-1.37412791	-2.93220083	-4.32196000
O	-4.23188975	0.42649241	-1.65661296
O	-3.30864738	1.79498310	0.18973295
O	5.51063556	-0.90798277	-3.79850392
O	2.84451671	6.39392997	-2.40867967
O	4.51907587	5.19513820	-5.03887120
O	1.04061580	7.16840630	-3.87050644
O	-0.94948177	6.74223114	-2.53190847
O	1.08136677	6.40878897	-6.18530130
O	-0.79710652	5.16442335	-6.97818524
O	-2.51332133	5.91675680	-4.20759907
O	-4.01845559	4.21562555	-2.94346321
O	-3.16907275	4.16469810	-0.58917422
O	2.44593997	-3.35406084	-4.24054608
O	4.02547297	-2.49917306	-2.51950812
O	4.62409998	-0.83363887	-6.18883258
O	4.76144248	1.67176900	-7.00364369
O	5.75712260	3.00246159	-5.06685056
O	2.96671173	5.08504237	-6.95605794

H	-1.00719683	-3.69599933	-3.79860161
H	1.17173684	-4.09276947	-3.47955872
H	1.19035715	-2.93564438	0.03361966
H	3.18336165	-2.09621083	-0.15867367
H	-0.90457759	-2.49730283	0.26032615
H	-2.80500725	-2.09099450	-0.81457863
H	-4.27406123	-0.57169371	-1.65639511
H	3.72225257	6.35253035	-2.83575721
H	-0.27929452	7.38142032	-2.91508797
H	1.84157047	7.36287264	-3.30566324
H	-2.26926435	6.64858338	-3.56891198
H	-4.19182833	4.49721850	-2.00890985
H	-3.51516745	3.50051890	0.07051059
H	-4.07593763	1.25116454	-0.14628263
H	3.24659935	-3.55513452	-3.68811216
H	4.94546907	-2.26120394	-2.79948994
H	6.08016205	-0.32196982	-3.26823747
H	5.45526999	-1.02696894	-5.70939166
H	5.64955148	1.94198845	-6.69537161
H	-0.18776063	5.98294168	-6.98570630
H	3.83192985	5.42775034	-6.59617444
H	6.26772767	2.79690922	-4.26278426
H	5.39054825	4.72379557	-5.08948483
H	1.88839712	6.26453535	-6.77078315
Pu	-2.80045758	4.97703004	-8.36404348
O	-3.75439860	4.09572474	-10.53487496
O	-3.34487404	3.50789630	-7.53670650
O	-2.24230231	6.43919556	-9.19166248
O	-3.65472006	6.35637159	-6.51075511
O	-1.06310347	3.57455828	-9.60102369
O	-5.22138849	5.58141566	-8.76495594
H	-3.49707619	7.31153750	-6.60568213
H	-3.32207477	6.11955142	-5.58621064
H	-0.25178127	4.00434415	-9.92463661
H	-0.77077075	2.78133057	-9.11257301
H	-3.16306393	3.63746708	-11.15633090
H	-4.57338922	3.57278440	-10.48709688
H	-5.44915062	6.29236193	-9.38943248
H	-5.70661677	5.76788278	-7.94083987

$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{2+}$ ($C_{60}(OH)_{24}$/Pu(VI)-IS2)

C	-0.45287428	0.39034762	-0.50398218
C	0.94576347	0.35862503	-0.30183079
C	1.66540233	1.54194976	-0.12812123

C	0.99125540	2.80851744	-0.19402546
C	-0.38802410	2.82351935	-0.44354197
C	-1.12857461	1.60896059	-0.54250421
C	-1.00021822	-0.93244801	-0.96015733
C	0.37061813	-1.81957921	-1.36234536
C	1.59780058	-0.92583794	-0.80137920
C	2.67798759	-0.55759336	-1.77977804
C	2.92870003	1.70557975	-0.82553092
C	1.82951270	3.74668657	-0.88871226
C	1.26272780	4.65532575	-1.78294625
C	-0.13745875	4.69130776	-1.98075496
C	-0.97103457	3.80536968	-1.29939951
C	-2.40254877	3.45345785	-1.62538381
C	-2.51694426	1.85999868	-1.07383096
C	-2.94286979	0.73245499	-2.09284571
C	-2.12819518	-0.73944181	-2.05034957
C	0.56447488	-2.35731513	-2.87584152
C	-0.56457677	-1.85765703	-3.93024958
C	-1.57568867	-0.84699205	-3.43876163
C	-2.07662861	0.13613732	-4.27505877
C	-2.68750265	1.19211038	-3.50190555
C	-2.59054079	2.48661718	-3.94934588
C	-2.72562741	3.75549122	-3.14393114
C	-1.69454958	4.79044665	-3.96766911
C	-0.52732145	5.49507950	-3.18674829
C	3.02827720	3.02621659	-1.27994129
C	2.48471084	4.33074093	-5.91492916
C	3.59113257	4.13037840	-4.82022515
C	4.40140419	2.66869613	-4.77747201
C	4.01610303	1.56223349	-5.82286019
C	2.61297158	1.80055929	-6.32589492
C	0.53028831	3.05051717	-6.57903586
C	-0.11525068	4.32828320	-6.05764521
C	1.11494813	5.21988854	-5.49698516
C	0.92562464	5.76262604	-3.98651301
C	2.05206818	5.25916957	-2.93939187
C	3.02841621	4.23167204	-3.43634987
C	4.14402047	2.20091370	-3.37575685
C	4.05081940	0.91113086	-2.92958499
C	4.18432144	-0.34919720	-3.73278249
C	3.90118052	-0.07702296	-5.25583655
C	2.45798431	-0.39175935	-5.56570446
C	1.87584172	0.58807278	-6.41895654
C	0.49193768	0.60085748	-6.66599275

C	-0.18766228	1.86360935	-6.74048861
C	-1.19108713	3.94557322	-5.08476995
C	-1.85993828	2.73642194	-5.16402171
C	-1.45344309	1.69419208	-6.04630985
C	-1.54228668	0.37209933	-5.58041255
C	-0.34149566	-0.34217379	-5.97637067
C	0.22695053	-1.23891767	-5.07525190
C	1.62407959	-1.27412300	-4.88053209
C	2.02084956	-2.09438617	-3.68970742
C	3.18885860	-1.40744080	-2.90264064
C	3.52890537	3.26242512	-2.60093876
C	3.33905239	0.64296480	-1.69399397
C	1.92996063	3.01572905	-6.37479713
O	2.21496404	-1.64993474	0.28875041
O	0.29601489	-2.94328383	-0.53007948
O	0.43111853	-3.74284025	-2.81920277
O	-1.62041349	-1.60560309	0.11251641
O	-3.10011328	-1.73247724	-1.84054580
O	-1.34571471	-2.95712686	-4.33792876
O	-4.29975986	0.45159766	-1.85531578
O	-3.44764530	1.87359762	-0.02073074
O	5.51450348	-0.89957842	-3.62761001
O	2.79660394	6.42318389	-2.50494561
O	4.55065378	5.17359942	-5.02423985
O	1.03428541	7.15880419	-4.03395169
O	-1.02957310	6.76757515	-2.82247184
O	1.16457619	6.34562819	-6.33247929
O	-0.76502863	5.12257837	-7.08009954
O	-2.45391221	5.84287454	-4.54826124
O	-4.03781721	4.25780236	-3.20079995
O	-3.30484119	4.20999174	-0.85292241
O	2.47392373	-3.36181448	-4.12007788
O	3.98946317	-2.46216909	-2.36247677
O	4.70673417	-0.88147047	-6.04871797
O	4.87510850	1.60514887	-6.91215531
O	5.79653107	2.98603651	-4.97277635
O	3.07926670	5.01399576	-7.00475848
H	-0.99180688	-3.70761571	-3.78665687
H	1.17763599	-4.08693435	-3.38881603
H	1.06774945	-2.85235432	0.09456030
H	3.06426799	-2.00588880	-0.04050928
H	-1.03233218	-2.41134273	0.23892925
H	-2.89608694	-2.03918541	-0.90744867
H	-4.33668227	-0.54773928	-1.83092658

H	3.68383322	6.37151090	-2.91196053
H	-0.31853817	7.39167060	-3.16330677
H	1.82045178	7.37006220	-3.45411113
H	-2.19163135	6.64314405	-3.99298439
H	-4.22781787	4.49243343	-2.24695530
H	-3.66520206	3.54799214	-0.19320274
H	-4.19576508	1.30854738	-0.36853412
H	3.25534265	-3.54846828	-3.53636814
H	4.91796271	-2.22797635	-2.61743634
H	6.06626911	-0.29977004	-3.09410398
H	5.52624622	-1.05629053	-5.54336060
H	5.75028005	1.88916079	-6.58082779
H	-0.12655390	5.90914545	-7.14390116
H	3.92354845	5.37614131	-6.61895077
H	6.28114264	2.79461039	-4.14951492
H	5.42525240	4.70530427	-5.03872251
H	1.98275599	6.18296045	-6.89775282
Pu	-3.24115387	5.72563645	-6.94950249
O	-5.40256001	6.24033808	-8.10922010
O	-3.61501809	4.00364112	-7.11488376
O	-2.92802253	7.46602415	-6.86842856
O	-2.64847857	5.84392520	-9.37243988
O	-5.10505887	5.68071026	-5.26798151
H	-2.54154583	6.65152294	-9.90299193
H	-2.71629181	5.09811864	-9.99288178
H	-5.78697511	7.13019208	-8.18749222
H	-6.14494656	5.62028650	-7.99936290
H	-5.36382517	6.52798383	-4.86741608
H	-4.77987871	5.12283824	-4.50326644

Table S2. Calculated formation energies (ΔE) in the gas phase and solvent of studied complexes at PBE-D3BJ level of theory

complexes	ΔE_{gas} (Kcal/mol)	ΔE_{sol} (Kcal/mol)
$C_{60}(OH)_{24}/UO_2(H_2O)_5^{2+}$	-101.80	-34.98
$C_{60}(OH)_{24}/UO_2(H_2O)_4^{2+}$	-79.50	-19.25
$C_{60}(OH)_{24}/UO_2(H_2O)_3^{2+}$	-70.36	-2.12
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{1+}$	-47.98	-29.37
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{1+}$	-28.40	-10.49
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{1+}$	-16.88	0.85
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{2+}$	-106.53	-34.68
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{2+}$	-84.03	-15.64
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{2+}$	-77.29	-3.92
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{1+}$	-48.29	-29.78
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{1+}$	-29.19	-11.04
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{1+}$	-17.12	-0.08
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{2+}$	-113.08	-39.60
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{2+}$	-91.89	-19.25
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{2+}$	-80.03	-9.06

Table S3. Calculated formation energies (ΔE) in the gas phase and solvent of studied complexes at wB97X-D3BJ level of theory.

complexes	ΔE_{gas} (Kcal/mol)	ΔE_{sol} (Kcal/mol)
$C_{60}(OH)_{24}/UO_2(H_2O)_5^{2+}$	-111.63	-46.28
$C_{60}(OH)_{24}/UO_2(H_2O)_4^{2+}$	-91.73	-29.92
$C_{60}(OH)_{24}/UO_2(H_2O)_3^{2+}$	-85.47	-19.00
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{1+}$	-61.24	-43.89
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{1+}$	-49.54	-31.83
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{1+}$	-39.84	-22.45
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{2+}$	-112.96	-46.93
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{2+}$	-93.72	-31.27
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{2+}$	-69.53	2.69
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{1+}$	-66.46	-47.40
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{1+}$	-54.93	-36.29
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{1+}$	-31.89	-13.91
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{2+}$	-105.65	-34.03
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{2+}$	-99.92	-28.22
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{2+}$	-102.03	-33.92

Table S4. Topological parameters relevant to the typical chemical bonds in actinyl/ $C_{60}(OH)_{24}$ complexes.

Species	BCP	ρ (r)	$\nabla^2\rho$	*H*(r)
$C_{60}(OH)_{24}/UO_2(H_2O)_5^{2+}$	An=O	0.303	0.216	-0.288
		0.301	0.220	-0.284
	An-OH_2	0.043	0.172	0.15E-2
		0.064	0.259	-0.15E-2
		0.045	0.176	0.12E-2
		0.078	0.308	-0.61E-2
		0.043	0.165	0.12E-2
	H---OH	0.067	0.169	-0.13E-1
		0.072	0.183	-0.17E-1
		0.071	0.173	-0.17E-2
$C_{60}(OH)_{24}/UO_2(H_2O)_4^{2+}$	An=O	0.302	0.208	-0.288
		0.299	0.214	-0.281
	An-OH_2	0.047	0.185	0.99E-3
		0.065	0.250	-0.21E-2
		0.046	0.195	0.20E-2
		0.046	0.187	0.16E-2
	An-OH	0.067	0.277	-0.21E-2
	H---OH	0.079	0.155	-0.26E-1
$C_{60}(OH)_{24}/UO_2(H_2O)_3^{2+}$	An=O	0.301	0.212	-0.286
		0.299	0.223	-0.281
	An-OH_2	0.054	0.199	-0.53E-3
		0.048	0.204	0.20E-2
		0.047	0.197	0.20E-2
	An-OH	0.055	0.216	-0.21E-3
		0.055	0.204	-0.86E-3
	H---OH	0.049	0.167	-0.96E-3
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{1+}$	An=O	0.285	0.208	-0.254
		0.286	0.203	-0.257
	An-OH_2	0.043	0.192	0.20E-2
		0.040	0.165	0.14E-2
		0.042	0.187	0.25E-3
		0.038	0.156	0.13E-2
		0.049	0.218	0.16E-2
	H---OH	0.050	0.171	-0.76E-3
		0.056	0.187	-0.41E-2
		0.051	0.185	-0.86E-3
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{1+}$	An=O	0.284	0.206	-0.254
		0.283	0.204	-0.251
	An-OH_2	0.037	0.155	0.18E-2

		0.041	0.169	0.16E-2
		0.041	0.179	0.22E-2
		0.049	0.214	0.13E-2
	An-OH	0.049	0.230	0.25E-2
	H---OH	0.055	0.185	-0.34E-2
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{1+}$	An=O	0.286	0.208	-0.256
		0.285	0.208	-0.254
	$An-OH_2$	0.046	0.196	0.14E-2
		0.043	0.200	0.30E-2
		0.040	0.179	0.25E-2
	An-OH	0.045	0.202	0.24E-2
		0.037	0.156	0.17E-2
	H---OH	0.039	0.148	0.29E-2
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{2+}$	An=O	0.310	0.189	-0.300
		0.310	0.189	-0.298
	$An-OH_2$	0.057	0.227	-0.14E-3
		0.046	0.174	0.11E-2
		0.044	0.179	0.17E-2
		0.072	0.288	-0.34E-2
		0.044	0.177	0.15E-3
	H---OH	0.054	0.163	-0.38E-2
		0.063	0.175	-0.11E-1
		0.064	0.185	-0.98E-2
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{2+}$	An=O	0.311	0.178	-0.300
		0.308	0.187	-0.296
	$An-OH_2$	0.045	0.180	0.12E-2
		0.045	0.187	0.20E-2
		0.046	0.189	0.21E-2
		0.061	0.239	-0.10E-2
	An-OH	0.061	0.259	-0.44E-3
	H---OH	0.067	0.171	-0.14E-1
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{2+}$	An=O	0.304	0.184	-0.289
		0.304	0.182	-0.289
	$An-OH_2$	0.051	0.195	0.55E-3
		0.046	0.201	0.24E-2
		0.046	0.207	0.26E-2
	An-OH	0.049	0.210	0.13E-2
		0.044	0.174	0.89E-3
	H---OH	0.041	0.149	0.19E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{1+}$	An=O	0.290	0.189	-0.261
		0.293	0.182	-0.267
	$An-OH_2$	0.041	0.181	0.18E-2
		0.038	0.160	0.16E-2
		0.041	0.177	0.16E-2

		0.035	0.145	0.13E-2
		0.045	0.203	0.17E-2
	H---OH	0.050	0.171	-0.74E-3
		0.052	0.178	-0.20E-2
		0.046	0.171	0.11E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{1+}$	An=O	0.290	0.189	-0.261
		0.288	0.189	-0.257
	An-OH_2	0.036	0.157	0.19E-2
		0.040	0.173	0.17E-2
		0.040	0.172	0.19E-2
		0.045	0.195	0.15E-2
	An-OH	0.048	0.229	0.28E-2
	H---OH	0.051	0.177	-0.11E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{1+}$	An=O	0.293	0.186	-0.266
		0.288	0.197	-0.257
	An-OH_2	0.043	0.207	0.33E-2
		0.040	0.172	0.18E-2
		0.036	0.153	0.13E-2
	An-OH	0.039	0.167	0.19E-2
		0.040	0.188	0.25E-2
	H---OH	0.039	0.144	0.25E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{2+}$	An=O	0.309	0.180	-0.294
		0.309	0.181	-0.295
	An-OH_2	0.062	0.275	-0.17E-4
		0.039	0.166	0.19E-2
		0.043	0.178	0.17E-2
		0.043	0.177	0.14E-2
		0.050	0.213	0.14E-2
	H---OH	0.044	0.150	0.70E-3
		0.056	0.178	-0.46E-2
		0.054	0.183	-0.26E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{2+}$	An=O	0.300	0.178	-0.280
		0.303	0.159	-0.285
	An-OH_2	0.040	0.181	0.26E-2
		0.041	0.191	0.26E-2
		0.042	0.191	0.25E-2
		0.050	0.228	0.18E-2
	An-OH	0.051	0.249	0.31E-2
	H---OH	0.052	0.186	-0.15E-2
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{2+}$	An=O	0.302	0.176	-0.284
		0.303	0.168	-0.285
	An-OH_2	0.045	0.214	0.34E-2
		0.044	0.204	0.30E-2
		0.045	0.198	0.18E-2

An-OH	0.041	0.182	0.23E-2
	0.041	0.196	0.28E-2
H---OH	0.039	0.148	0.31E-2

Table S5. The intrinsic bond strength indexes of typical chemical bonds in studied complexes.

Species	An-O_F		H_w---OH_F			An-O_{yl}	An-O_w
$C_{60}(OH)_{24}$/U(VI)-OS	-		0.08	0.09	0.08	0.38	0.03-0.09
$C_{60}(OH)_{24}$/U(VI)-IS1	0.06		0.09	-	-	0.36	0.04-0.05
$C_{60}(OH)_{24}$/U(VI)-IS2	0.05	0.05	0.06			0.36	0.04-0.05
$C_{60}(OH)_{24}$/Np(V)-OS	-		0.06	0.06	0.07	0.33	0.03-0.04
$C_{60}(OH)_{24}$/Np(V)-IS1	0.04		0.06	-	-	0.34	0.04-0.05
$C_{60}(OH)_{24}$/Np(V)-IS2	0.04	0.04	0.05	-	-	0.34	0.04-0.05
$C_{60}(OH)_{24}$/Np(VI)-OS			0.06	0.08	0.08	0.36	0.03-0.08
$C_{60}(OH)_{24}$/Np(VI)-IS1	0.05		0.08			0.37	0.03-0.06
$C_{60}(OH)_{24}$/Np(VI)-IS2	0.04	0.05	0.05			0.37	0.04-0.05
$C_{60}(OH)_{24}$/Pu(V)-OS	-		0.06	0.05	0.07	0.35	0.04-0.04
$C_{60}(OH)_{24}$/Pu(V)-IS1	0.04		0.06	-	-	0.35	0.03-0.04
$C_{60}(OH)_{24}$/Pu(V)-IS2	0.04	0.04	0.05	-	-	0.34	0.04-0.04
$C_{60}(OH)_{24}$/Pu(VI)-OS	-		0.05	0.07	0.07	0.36	0.04-0.05
$C_{60}(OH)_{24}$/Pu(VI)-IS1	0.04		0.06	-	-	0.37	0.04-0.05
$C_{60}(OH)_{24}$/Pu(VI)-IS2	0.04	0.04	0.05	-	-	0.37	0.04-0.05

Table S6. Symmetrical (w_{sym}) and asymmetrical ($w_{an\text{-}sym}$) harmonic vibrational frequencies as well as intensities (km/mol) of O=An=O for studied complexes, the frequency changes (Δw) after the adsorption on $C_{60}(OH)_{24}$ fulerenol relative to free one.

Species	w_{sym} (cm^{-1})	Δw_{sym} (cm^{-1})	$w_{an\text{-}sym}$ (cm^{-1})	$\Delta w_{an\text{-}sym}$ (cm^{-1})
$UO_2(H_2O)_5^{2+}$	882 (0.29)	-	977 (267.79)	-
$C_{60}(OH)_{24}/UO_2(H_2O)_5^{2+}$	845 (236.10)	-37	945 (174.54)	-32
$C_{60}(OH)_{24}/UO_2(H_2O)_4^{2+}$	839 (238.74)	-43	941 (126.15)	-36
$C_{60}(OH)_{24}/UO_2(H_2O)_3^{2+}$	836 (188.38)	-46	932 (104.99)	-45
$NpO_2(H_2O)_5^{1+}$	862 (0.15)	-	954 (245.13)	-
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{1+}$	827 (120.43)	-35	949 (63.12)	-5
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{1+}$	834 (189.88)	-28	934 (56.68)	-20
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{1+}$	779 (372.62)	-83	889 (185.51)	-65
$NpO_2(H_2O)_5^{2+}$	882 (0.48)	-	987 (234.93)	-
$C_{60}(OH)_{24}/NpO_2(H_2O)_5^{2+}$	824 (479.90)	-58	942 (192.03)	-45
$C_{60}(OH)_{24}/NpO_2(H_2O)_4^{2+}$	819 (122.13)	-63	940 (94.59)	-47
$C_{60}(OH)_{24}/NpO_2(H_2O)_3^{2+}$	803 (242.47)	-79	925 (83.06)	-62
$PuO_2(H_2O)_5^{1+}$	853 (0.42)	-	950 (228.06)	-
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{1+}$	789 (223.90)	-64	927 (138.12)	-23
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{1+}$	811 (153.78)	-42	914 (189.58)	-36
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{1+}$	766 (523.52)	-87	877 (55.87)	-73
$PuO_2(H_2O)_5^{2+}$	873 (0.00)	-	1019 (189.71)	-
$C_{60}(OH)_{24}/PuO_2(H_2O)_5^{2+}$	804 (177.39)	-69	946 (201.52)	-73
$C_{60}(OH)_{24}/PuO_2(H_2O)_4^{2+}$	816 (188.62)	-57	942 (150.97)	-77
$C_{60}(OH)_{24}/PuO_2(H_2O)_3^{2+}$	786 (352.77)	-87	916 (96.68)	-103