Supporting information

Unveiling a Photoinduced Hydrogen Evolution Reaction Mechanism via Concerted Formation of Uranyl Peroxide

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Figure S1. Alternative dimerization mechanism

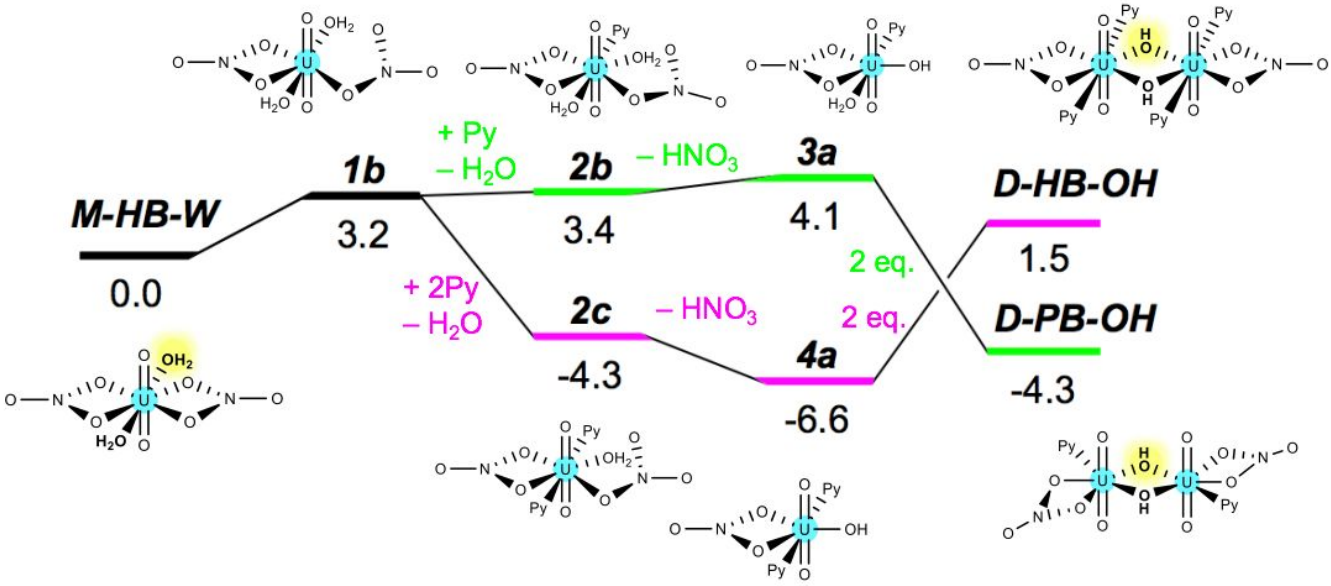


Figure S1: Formation of ***D-HB-OH*** and ***D-PB-OH*** promoted by nitrate ligand (Gibbs energies in kcal·mol^{-1}).

In first place, we considered that ***M-HB-W*** underwent a change of hapticity of the nitrate ligand (η^2 to η^1) motivated through an intramolecular hydrogen bond. Both ***2a*** and ***2b*** result from the respectively addition of one and two pyridine ligands. While the intramolecular acid-base reaction is mostly favored for the ***D-HB-OH*** compound, the energy barrier regarding the dimerization is considerably high. On the other hand, the condensation of ***D-PB-OH*** is energetically downhill.

Figure S2. Scalar ZORA UV-Vis spectra

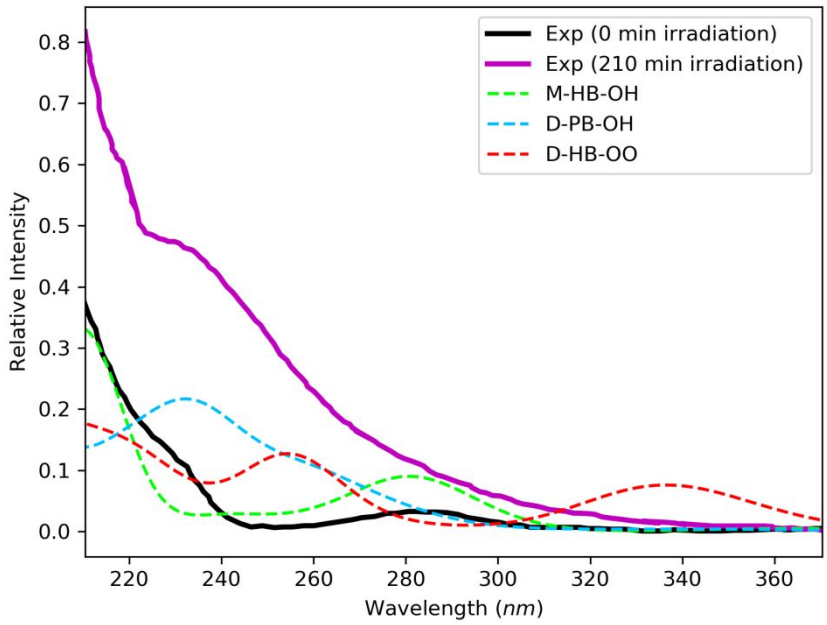


Figure S2: Comparison between the experimental and the computed UV-Vis spectra (scalar ZORA). All scalar TD-DFT computed spectra are shifted by –10 kcal.mol^{-1}.

Figure S3. Scalar and Spin-Orbit spectra comparison for ***M-HB-Py***.

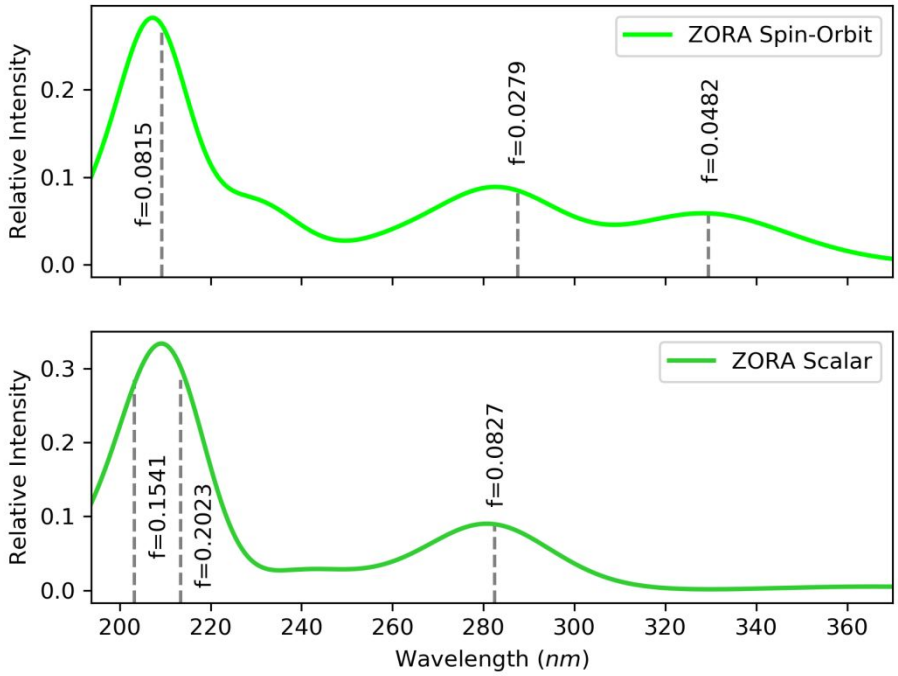


Figure S3: Comparison between the scalar and spin-orbit spectra of ***M-HB-Py***. Oscillator strength are marked in stick lines. Top and bottom spectra have been shifted –15 kcal.mol^{-1} and –10 kcal.mol^{-1} respectively.

Figure S3 presents a comparison between the scalar and spin-orbit ZORA bands for the monomer ***M-HB-Py***. Top and bottom spectra have been shifted taking as a reference the experimental peak at 213 nm. The first relevant difference concerns the oscillator strength values which are systematically lower for the spin-orbit bands. This can be understood because of the coupling of spin-forbidden singlet states (i.e., f =0) with triplet states. While the top spectra presents three peaks, the botom one only has two bands. Nonetheless, Table 1 and Table S2 show that the type of transitions involved in both spectra are very similar. They consist in π–transitions from the pyridine and nitrate ligands to the uranium f(ϕ). Therefore, we can

conclude that the effect of the spin-orbit coupling for the monomer ***M-HB-Py*** does not cause a sever change compared to employing ZORA Scalar.

Figure S4. Scalar and Spin-Orbit spectra comparison for ***D-PB-OH***.

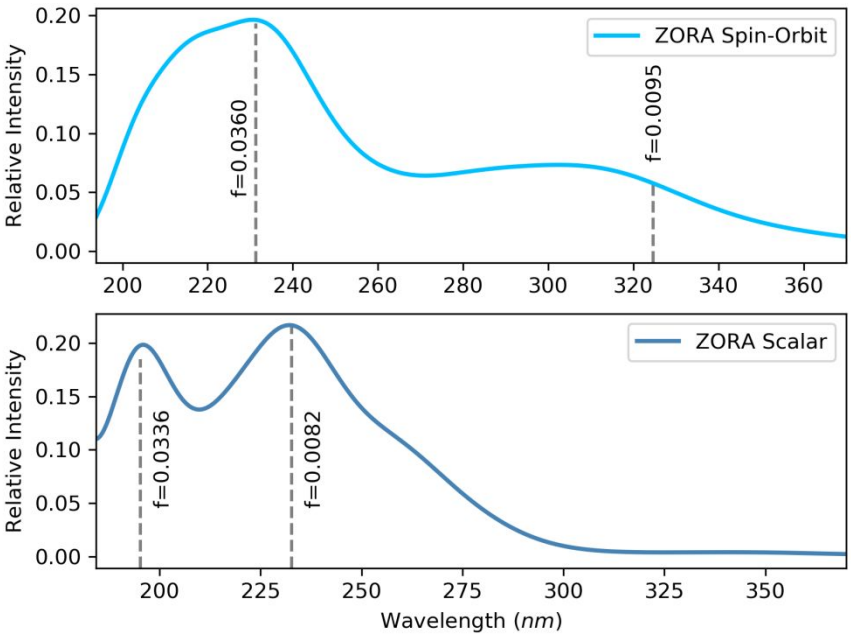


Figure S4: Comparison between the scalar and spin-orbit spectra of ***D-PB-OH***. Oscillator strength are marked in stick lines. Top and bottom spectra have been shifted –15 kcal.mol^{-1} and –10 kcal.mol^{-1} respectively.

Figure S4 presents a comparison between the scalar and spin-orbit ZORA bands for the dimer ***D-PB-OH***. Top and bottom spectra have been shifted taking as a reference the experimental peak at 213 nm. On the one hand, both spectra coincide in predicting the peak at ~215nm even though using ZORA scalar describes it as a double peak. On the other hand, top spectrum has an additional band at 322 nm but has a low oscillator strength value. In fact, TD-DFT spectra for ***D-PB-OH*** present very spread bands, that is why a summary of the main types of transitions could not be performed.

Figure S5. Scalar and Spin-Orbit spectra comparison for ***D-HB-OO***.

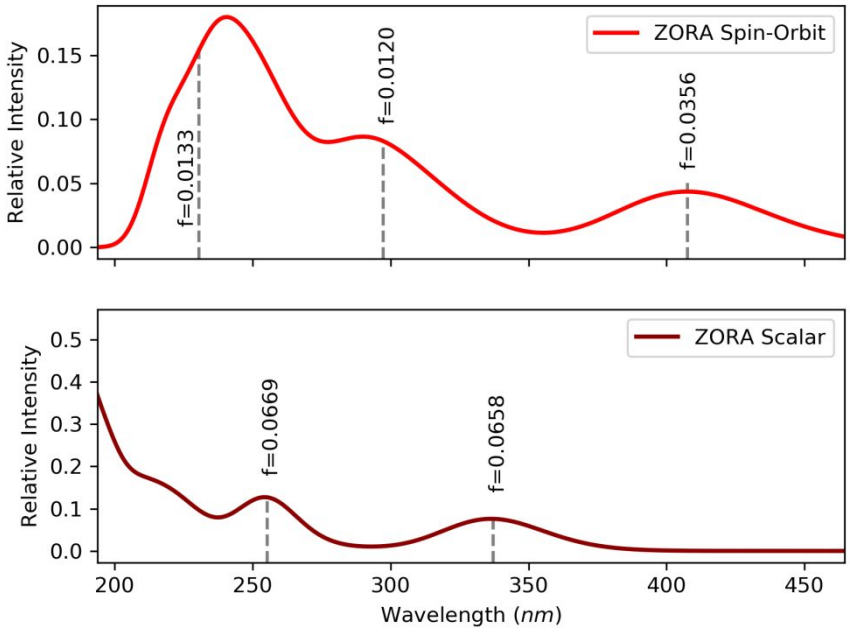


Figure S5: Comparison between the scalar and spin-orbit spectra of ***D-HB-OO***. Oscillator strength are marked in stick lines. Top and bottom spectra have been shifted –15 kcal.mol^{-1} and –10 kcal.mol^{-1} respectively.

Figure S5 presents a comparison between the scalar and spin-orbit ZORA bands for the product ***D-HB-OO.*** Top and bottom spectra have been shifted taking as a reference the experimental peak at 213 nm. If both curves are compared, it can be easily observed that the effect of ZORA has an important effect on the spectra. Hence, from the three compounds studied in the UV-vis section, spin-orbit coupling has its highest impact on the ***D-HB-OO*** compound. Indeed, scalar ZORA spectrum wrongly predicts the peroxide band at 334.8 nm, where no analogous peak appears in the experimental results (Figure S1). However, the spin-coupling spectrum correctly indicates that the $\pi(O_2^{2-})$ band is out of the range considered in the experiments (407.53 nm). In addition the oscillator strength values for the top spectrum are lower than for the ZORA scalar

curve. This can be understood as a consequence of coupling spin- forbidden singlet states (i.e., f =0) with triplet states. Overall, we assume that the spin-orbit coupling is needed when considering the spectra for the ***D-HB-OO***, which otherwise would lead to a wrong prediction of the peroxide band.

Table S1. Spin-Orbit ZORA bands for ***D-HB-OO***.

Table S1. Molecular spinors involved for the three main bands of the ***D-HB-OO***.

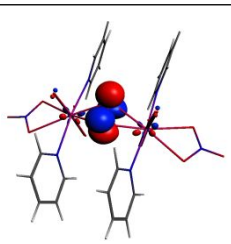
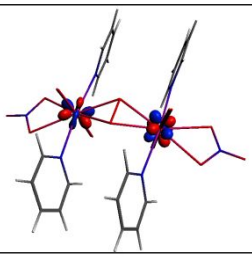
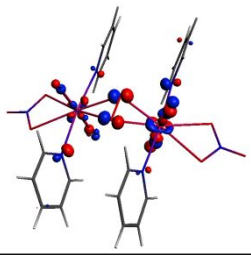
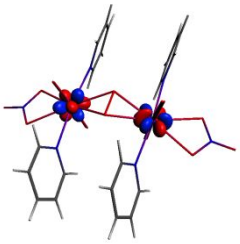
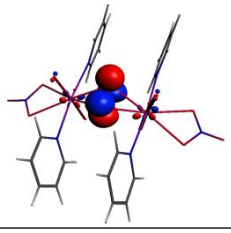
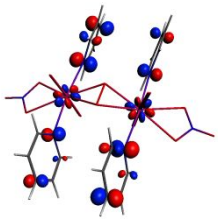
Intensity	**Excited State**	**From**	**From**
small	ν_{calc}=407.5 nm f=0.0356 $\pi(O_2^{2-}) \rightarrow$ f(δ),f(ϕ)		
medium	ν_{calc}=297.4 nm f = 0.0120 $\pi(O_2^{2-})$, n_N-*Py* → f(δ),f(ϕ)		
high	ν_{calc}= 230.6 nm f = 0.0133 $\pi(O_2^{2-}) \rightarrow$ f(δ),π(*Py*).		

Table S2. Scalar ZORA bands for ***M-HB-Py***.

Table S2. Molecular orbitals involved for the two main bands of the ***M-HB-Py***.

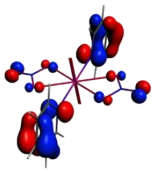
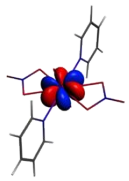
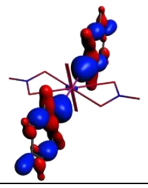
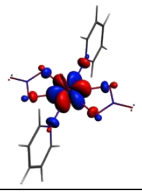
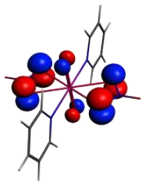
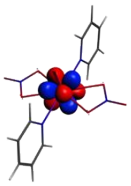
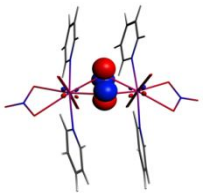
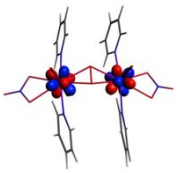
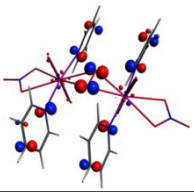
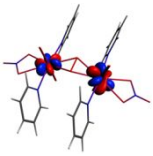
Intensity	Excited State	From	To
medium	ν_{calc}=282.5 nm f=0.083 $\pi(Py) \rightarrow f(\phi)$		
high	ν_{calc}=213.8 f = 0.200 n_N-$Py \rightarrow f(\phi)$		
weak	ν_{calc}=202.2 kcal·mol^{-1} f = 0.015 $\pi(O_{NO3}) \rightarrow f(\delta)$.		

Table S3. Scalar ZORA bands for ***D-HB-OO***.

Table S3. Transition orbitals involved for the 3 main bands of the ***D-HB-OO***.

Intensity	Excited State	From	To
weak	ν_{calc}= 334.8 nm f = 0.06 $\pi(O_2^{2-}) \rightarrow f(\delta)$.		
weak	ν_{calc}= 255.2 nm f = 0.07 $\pi(O_2^{2-})/\pi(Py) \rightarrow f(\phi)$		

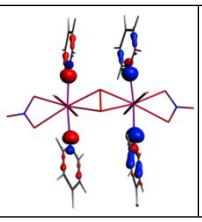
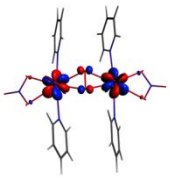
high	ν_{calc} = 181.1 nm f = 0.20 n_N-Py → f(ϕ)		

Table S4. Low-lying spin polarized excitation energies for ***M-HB-Py***.

Table S4. Low-lying spin polarized excitation energies for ***M-HB-Py***.

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.43506	5.47E-07	A
2	2.43509	3.92E-06	A
3	2.43579	1.14E-08	A
4	2.44071	1.85E-05	A
5	2.44072	1.97E-04	A
6	2.44138	1.19E-08	A
7	2.44655	1.58E-05	A
8	2.45219	5.94E-04	A
9	2.46386	2.09E-07	A
10	2.46407	4.46E-07	A
11	2.46431	1.86E-06	A
12	2.46515	4.50E-05	A
13	2.46951	6.51E-08	A
14	2.46975	2.56E-05	A
15	2.47002	4.39E-05	A

Table S5. Low-lying spin polarized excitation energies for ***D-PB-OH***.

Table S5. Low-lying spin polarized excitation energies for ***D-PB-OH***.

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.50036	1.33E-06	A
2	2.50051	5.01E-06	A
3	2.50108	3.83E-04	A
4	2.50316	4.68E-05	A
5	2.50328	5.59E-05	A
6	2.50399	4.99E-05	A
7	2.50522	2.87E-05	A
8	2.50774	1.31E-04	A

9	2.58458	1.86E-06	A
10	2.58475	2.60E-06	A
11	2.5852	8.31E-04	A
12	2.58683	9.89E-05	A
13	2.58742	9.14E-06	A
14	2.58801	5.76E-05	A
15	2.58881	3.06E-05	A

Table S6. Low-lying spin polarized excitation energies for ***D-HB-OO***.

Table S6. Low-lying spin polarized excitation energies for ***D-HB-OO.***

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.51762	4.60E-04	A
2	2.52219	2.77E-06	A
3	2.52618	2.91E-05	A
4	2.53499	2.18E-03	A
5	2.56263	1.40E-06	A
6	2.56433	1.07E-06	A
7	2.57772	8.21E-05	A
8	2.5809	4.84E-04	A
9	2.59072	7.46E-07	A
10	2.59866	1.08E-03	A
11	2.62728	1.86E-04	A
12	2.62964	3.56E-02	A
13	2.65213	2.10E-06	A
14	2.65782	8.09E-04	A
15	2.65815	2.35E-03	A

Table S7. Low-lying singlet-singlet excitation energies for ***M-HB-Py***.

Table S7. Low-lying singlet-singlet excitation energies for ***M-HB-Py.***

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.6032	2.92E-06	A
2	2.60896	1.17E-04	A
3	2.6349	4.19E-05	A
4	2.63609	9.69E-05	A
5	2.64047	2.07E-03	A
6	2.64112	2.76E-03	A
7	3.01465	4.11E-07	A
8	3.04524	7.05E-06	A
9	3.08087	1.18E-05	A
10	3.12256	4.79E-07	A
11	3.12804	3.51E-07	A
12	3.25119	1.54E-05	A
13	3.28323	2.74E-04	A

14	3.28918	8.27E-02	A
15	3.34476	1.50E-04	A

Table S8. Low-lying singlet-singlet excitation energies for ***D-PB-OH***.

Table S8. Low-lying singlet-singlet excitation energies for ***D-PB-OH.***

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.67921	1.52E-03	A
2	2.68183	1.27E-04	A
3	2.76818	1.17E-04	A
4	2.77062	1.60E-05	A
5	2.79959	2.15E-04	A
6	2.80209	1.12E-03	A
7	2.8074	2.72E-04	A
8	2.80969	5.37E-04	A
9	2.86199	6.05E-06	A
10	2.86444	2.13E-05	A
11	2.949	9.16E-05	A
12	2.95062	3.54E-04	A
13	3.03292	1.11E-03	A
14	3.03679	7.89E-04	A
15	3.24147	4.61E-03	A

Table S9. Low-lying singlet-singlet excitation energies for ***D-HB-OO***.

Table S9. Low-lying singlet-singlet excitation energies for ***D-HB-OO.***

Number	Energy (eV)	Oscillator Strength	Symmetry
1	2.74542	2.62E-06	A
2	2.78488	2.56E-06	A
3	2.80236	7.86E-04	A
4	2.82578	6.58E-02	A
5	2.84252	7.34E-03	A
6	2.86852	1.12E-03	A
7	3.03229	3.50E-05	A
8	3.04066	2.57E-03	A
9	3.0591	1.12E-04	A
10	3.06625	1.32E-04	A
11	3.07753	2.19E-05	A
12	3.08305	3.24E-04	A
13	3.08596	9.56E-05	A
14	3.09128	1.05E-03	A
15	3.09986	4.28E-04	A

Cartesian Coordinates

1_u2o4_2py
Energ (BONDING) = -6314.1179427 kcal.mol-1
y

	Atom	X	Y	Z
1	U	1.8566	0.2469	0.1761
2	H	0.3101	-1.4687	1.8312
3	O	2.8419	0.8296	-2.0419
4	O	0.1143	-0.3367	-1.3006
5	O	4.1156	1.2541	-0.3214
6	H	-2.8207	1.4925	-2.2899
7	H	-3.2911	-2.6394	-2.2602
8	O	4.8359	1.7276	-2.3553
9	N	3.9718	1.2900	-1.6058
10	O	2.5875	-1.4049	0.0949
11	O	1.1613	1.9055	0.3235
12	H	-3.9305	1.6896	-4.5143
13	H	4.9484	1.3748	5.7031
14	N	3.0824	0.6640	2.3738
15	C	2.5934	1.5578	3.2634
16	C	4.2345	0.0211	2.6708
17	C	3.2308	1.8356	4.4684
18	C	4.9312	0.2500	3.8532
19	C	4.4224	1.1731	4.7686
20	H	1.6658	2.0614	2.9873
21	H	4.5988	-0.6923	1.9303
22	H	5.8577	-0.2913	4.0457
23	H	2.7963	2.5651	5.1520
24	H	-4.4261	-2.6123	-4.4809
25	O	-1.5899	-2.4649	-0.1777
26	O	-2.0006	1.1045	0.1900
27	H	-4.7588	-0.4035	-5.6480
28	N	-3.0083	-0.5783	-2.1855
29	C	-3.1887	0.6079	-2.8112
30	C	-3.4542	-1.7018	-2.7933
31	C	-3.8094	0.7098	-4.0520
32	O	0.0926	-0.5790	1.4811
33	H	0.3365	-1.1393	-1.8176
34	U	-1.7760	-0.6802	0.0430
35	O	-2.9258	-1.0529	2.2218
36	C	-4.0862	-1.6787	-4.0326
37	O	-4.2384	-1.0290	0.4772
38	C	-4.2670	-0.4526	-4.6752
39	N	-4.1322	-1.1613	1.7584

40	O	-5.0955	-1.3731	2.4840

1ts_h2

Energy (BONDING) = -9509.4547149 kcal.mol-1

	Atom	X	Y	Z
1	U	-2.0203	-1.6361	2.4323
2	O	-4.5943	-1.7296	2.3825
3	O	-0.0408	-2.3910	1.8129
4	O	-3.7149	-1.3749	4.3503
5	H	-1.2055	0.8819	1.5422
6	O	-2.3640	0.2175	2.2546
7	O	-0.1697	-0.6499	1.4060
8	H	-3.4260	-2.3429	-3.8265
9	O	-2.2554	-3.4027	2.8136
10	H	-0.3923	0.7269	1.1750
11	N	-2.6841	-1.9856	-0.0294
12	C	-3.7773	-1.4131	-0.5773
13	C	-1.8510	-2.6816	-0.8348
14	C	-4.0785	-1.5200	-1.9325
15	C	-2.0829	-2.8312	-2.1991
16	C	-3.2174	-2.2425	-2.7601
17	H	-4.4254	-0.8548	0.0996
18	H	-0.9666	-3.1084	-0.3603
19	H	-1.3788	-3.4016	-2.8054
20	H	-4.9750	-1.0389	-2.3245
21	N	-4.7798	-1.5305	3.6425
22	O	-5.9081	-1.4914	4.1389
23	U	1.9989	-1.7397	1.0693
24	O	2.5420	-1.0167	2.6446
25	O	1.5905	-2.4538	-0.5521
26	O	4.2353	-0.9669	0.0821
27	O	4.2255	-2.9773	0.9256
28	N	4.8943	-2.0460	0.3341
29	O	6.0804	-2.1790	0.0315
30	H	1.5192	4.0986	-1.6537
31	H	1.6879	-7.4234	4.1656
32	N	1.9164	0.5780	-0.0632
33	C	2.4107	1.6731	0.5518
34	C	1.2871	0.7341	-1.2476
35	C	2.2875	2.9522	0.0151
36	C	1.1276	1.9780	-1.8515
37	C	1.6331	3.1092	-1.2078
38	H	2.9134	1.5068	1.5059
39	H	0.9017	-0.1760	-1.7101

40	H	0.6118	2.0524	-2.8092
41	H	2.6988	3.8058	0.5543
42	N	2.0369	-4.0367	2.2959
43	C	1.8857	-4.0738	3.6362
44	C	2.0646	-5.2032	1.6209
45	C	1.7623	-5.2659	4.3435
46	C	1.9426	-6.4385	2.2539
47	C	1.7873	-6.4720	3.6405
48	H	1.8631	-3.1080	4.1432
49	H	2.1879	-5.1354	0.5385
50	H	1.9678	-7.3535	1.6616
51	H	1.6444	-5.2427	5.4274
52	H	1.5107	-1.3147	7.7939
53	N	-0.7646	-1.3772	4.6479
54	C	0.2032	-0.4456	4.7816
55	C	-0.9285	-2.2836	5.6370
56	C	1.0374	-0.3893	5.8949
57	C	-0.1348	-2.2926	6.7800
58	C	0.8685	-1.3297	6.9118
59	H	0.3157	0.2578	3.9562
60	H	-1.7179	-3.0218	5.4904
61	H	-0.3036	-3.0478	7.5481
62	H	1.8083	0.3791	5.9526

3ts_u2o4_4py
Energ (BONDING) = -9541.5487086 kcal.mol-1
y

	Atom	X	Y	Z
1	U	1.7723	1.0980	0.0306
2	O	0.2940	-0.6996	-1.1593
3	O	3.6143	2.8336	0.0437
4	O	-0.6001	1.1669	-0.4993
5	O	4.2514	0.8103	0.5486
6	H	-1.6580	1.2931	2.2860
7	H	-4.5006	1.0452	-0.7260
8	O	5.7384	2.4449	0.5161
9	N	4.5839	2.0442	0.3751
10	O	2.1205	0.6881	-1.8734
11	O	1.3616	1.4449	1.7796
12	H	-0.3936	7.0268	-1.4874
13	H	3.3998	-4.8641	1.9490
14	N	2.4168	-1.2866	0.7955
15	C	2.1008	-1.7249	2.0316
16	C	3.0796	-2.1241	-0.0317
17	C	2.4370	-3.0001	2.4822
18	C	3.4507	-3.4112	0.3433
19	C	3.1250	-3.8587	1.6254
20	H	1.5612	-1.0224	2.6667
21	H	3.3152	-1.7382	-1.0248
22	H	3.9822	-4.0478	-0.3644
23	H	2.1575	-3.3062	3.4906
24	N	0.9769	3.5091	-0.5657
25	C	0.0850	4.1359	0.2313
26	C	1.3826	4.1369	-1.6887
27	C	-0.4281	5.3960	-0.0620
28	C	0.9148	5.3971	-2.0552
29	C	-0.0078	6.0395	-1.2279
30	H	-0.2199	3.5946	1.1277
31	H	2.1051	3.6030	-2.3088
32	H	1.2720	5.8592	-2.9759
33	H	-1.1451	5.8599	0.6161
34	U	-1.7767	-1.0066	-0.2018
35	O	-3.0615	-3.2083	0.0919
36	C	-4.7211	2.7916	0.5407
37	O	-4.0968	-1.4442	0.8432
38	C	-4.1966	3.4663	1.6441
39	N	-4.1124	-2.7178	0.6557

40	O	-5.0666	-3.4230	0.9919
41	H	-2.6429	3.4136	3.1647
42	H	-5.5867	3.1733	-0.0015
43	O	-2.6046	-0.7942	-1.8119
44	O	-1.0384	-1.1981	1.4517
45	H	-4.6461	4.3982	1.9913
46	H	1.3402	-6.4191	-2.0500
47	N	-0.5361	-3.1966	-0.9597
48	C	-0.2098	-4.1436	-0.0586
49	C	-0.1907	-3.3917	-2.2496
50	C	0.4622	-5.3124	-0.4087
51	C	0.4758	-4.5357	-2.6814
52	C	0.8118	-5.5145	-1.7444
53	H	-0.5016	-3.9491	0.9746
54	H	-0.4586	-2.5965	-2.9463
55	H	0.7281	-4.6470	-3.7364
56	H	0.7064	-6.0455	0.3606
57	N	-3.0401	1.0836	0.7499
58	C	-2.5368	1.7392	1.8168
59	C	-4.1179	1.6040	0.1299
60	C	-3.0870	2.9250	2.2967
61	H	1.2543	-0.0743	-1.8457
62	H	-0.7810	1.4928	-1.4060

3ts_u2o4_4py_wa
Energ (BONDING) = -9890.2748445 kcal.mol-1
y

	Atom	X	Y	Z
1	U	-2.0341	-1.5406	2.3387
2	O	-4.5840	-1.7779	2.1104
3	O	0.2633	-0.9991	2.6594
4	O	-3.8080	-2.0660	4.1265
5	H	-1.2943	1.0040	2.9890
6	O	-2.2743	0.3669	2.6849
7	O	-0.3710	-0.8785	0.6248
8	H	-4.1821	-1.1587	-3.7936
9	O	-1.8074	-3.3246	2.0058
10	H	-0.3774	0.0886	0.4663
11	N	-3.0103	-1.3631	-0.0923
12	C	-3.1970	-0.1713	-0.6957
13	C	-3.2501	-2.4825	-0.8052
14	C	-3.6152	-0.0536	-2.0191
15	C	-3.6740	-2.4521	-2.1322
16	C	-3.8566	-1.2160	-2.7535
17	H	-3.0018	0.7150	-0.0882
18	H	-3.0871	-3.4272	-0.2841
19	H	-3.8506	-3.3878	-2.6637
20	H	-3.7474	0.9354	-2.4588
21	N	-4.8352	-2.0316	3.3495
22	O	-5.9812	-2.2286	3.7621
23	U	1.9631	-1.5829	1.1226
24	O	2.4491	0.1789	1.0970
25	O	1.5117	-3.3466	1.1018
26	O	3.8675	-2.1120	-0.5413
27	O	4.4328	-2.1818	1.5624
28	N	4.7939	-2.3059	0.3318
29	O	5.9507	-2.5937	0.0117
30	H	0.1918	-1.1348	-5.1288
31	H	3.8637	-2.3927	7.3034
32	N	1.3516	-1.4620	-1.4334
33	C	1.8977	-0.5394	-2.2505
34	C	0.3941	-2.2708	-1.9330
35	C	1.5072	-0.3864	-3.5797
36	C	-0.0444	-2.1906	-3.2518
37	C	0.5183	-1.2277	-4.0916
38	H	2.6724	0.0942	-1.8151
39	H	-0.0322	-2.9977	-1.2398

40	H	-0.8188	-2.8712	-3.6060
41	H	1.9766	0.3810	-4.1960
42	N	2.6765	-1.8934	3.6354
43	C	2.7141	-0.8579	4.4989
44	C	3.0583	-3.1078	4.0806
45	C	3.1343	-0.9937	5.8198
46	C	3.4909	-3.3283	5.3861
47	C	3.5315	-2.2523	6.2735
48	H	2.3976	0.1107	4.1097
49	H	3.0136	-3.9232	3.3571
50	H	3.7861	-4.3317	5.6942
51	H	3.1463	-0.1221	6.4748
52	H	0.1870	-2.6416	8.3447
53	N	-1.1498	-1.9589	4.7619
54	C	-1.3437	-1.0659	5.7535
55	C	-0.4761	-3.0929	5.0430
56	C	-0.8783	-1.2706	7.0500
57	C	0.0115	-3.3775	6.3158
58	C	-0.1898	-2.4499	7.3386
59	H	-1.8954	-0.1613	5.4910
60	H	-0.3298	-3.7830	4.2107
61	H	0.5458	-4.3110	6.4923
62	H	-1.0585	-0.5144	7.8147
63	H	0.2232	0.3617	3.0238
64	O	-0.1436	1.3539	3.3116
65	H	0.1990	1.9942	2.6568

1ts_h2_wa
Energy (BONDING) = -9848.1239487 kcal.mol-1

	Atom	X	Y	Z
1	U	2.3744	-1.8420	1.3898
2	O	4.5976	-2.6681	0.5347
3	O	0.2030	-1.5818	1.0041
4	O	4.6640	-0.7543	1.5768
5	H	2.6187	-3.4092	4.3456
6	O	2.9545	-2.6810	2.9425
7	O	0.2911	-2.3866	2.6352
8	H	1.0414	-7.7698	-0.9658
9	O	2.3857	-0.9531	-0.1957
10	H	0.3333	-2.9871	3.7552
11	N	1.9039	-4.2106	0.3479
12	C	2.8794	-5.0886	0.0327
13	C	0.6188	-4.5999	0.1949
14	C	2.6110	-6.3719	-0.4406
15	C	0.2715	-5.8664	-0.2727
16	C	1.2828	-6.7708	-0.5969
17	H	3.9043	-4.7385	0.1652
18	H	-0.1454	-3.8688	0.4608
19	H	-0.7831	-6.1242	-0.3767
20	H	3.4386	-7.0403	-0.6815
21	N	5.3201	-1.6784	0.9594
22	O	6.5295	-1.6299	0.7855
23	U	-1.8538	-1.4049	1.8859
24	O	-1.4460	0.1733	2.6906
25	O	-2.3494	-3.0000	1.1572
26	O	-4.1482	-1.2720	2.9703
27	O	-3.9747	-0.3727	0.9952
28	N	-4.7382	-0.6448	2.0056
29	O	-5.9195	-0.3331	2.0424
30	H	-2.4603	-4.0933	7.7607
31	H	-1.1901	0.7499	-4.2411
32	N	-2.1062	-2.4795	4.2461
33	C	-1.9198	-1.7486	5.3618
34	C	-2.4332	-3.7795	4.3767
35	C	-2.0331	-2.2897	6.6406
36	C	-2.5706	-4.3961	5.6188
37	C	-2.3621	-3.6395	6.7728
38	H	-1.6740	-0.6968	5.2029
39	H	-2.5844	-4.3256	3.4437

40	H	-2.8398	-5.4517	5.6728
41	H	-1.8688	-1.6574	7.5138
42	N	-1.6801	-0.4055	-0.5624
43	C	-0.6508	0.3941	-0.9047
44	C	-2.5372	-0.7907	-1.5273
45	C	-0.4437	0.8357	-2.2096
46	C	-2.3961	-0.4011	-2.8580
47	C	-1.3301	0.4290	-3.2070
48	H	0.0374	0.6608	-0.1028
49	H	-3.3615	-1.4297	-1.2079
50	H	-3.1149	-0.7478	-3.6015
51	H	0.4113	1.4747	-2.4321
52	H	1.7094	3.8682	4.3225
53	N	2.1695	0.4250	2.5921
54	C	1.4785	0.5293	3.7438
55	C	2.6987	1.5424	2.0524
56	C	1.2943	1.7454	4.3972
57	C	2.5546	2.7953	2.6418
58	C	1.8411	2.8993	3.8375
59	H	1.0532	-0.3987	4.1281
60	H	3.2553	1.4061	1.1239
61	H	2.9983	3.6706	2.1662
62	H	0.7215	1.7796	5.3242
63	H	0.8362	-3.3435	4.4210
64	O	2.1375	-3.8105	5.1476
65	H	2.1483	-4.7715	4.9715

3_u2o4_2py
Energ (BONDING) = -6254.4637479 kcal.mol-1
y

	Atom	X	Y	Z
1	U	1.8518	0.2520	0.1403
2	H	0.2601	-1.3801	1.9741
3	O	2.8918	0.8697	-2.0466
4	O	0.0946	-0.3169	-1.3082
5	O	4.1353	1.2606	-0.2943
6	H	-2.6269	1.4760	-2.4431
7	H	-3.4146	-2.5957	-2.1274
8	O	4.8950	1.7633	-2.3063
9	N	4.0142	1.3180	-1.5786
10	O	2.5736	-1.4063	0.0499
11	O	1.1764	1.9203	0.3030
12	H	-3.6789	1.5898	-4.7064
13	H	4.9153	1.3265	5.7046
14	N	3.0289	0.6185	2.3841
15	C	2.5948	1.5743	3.2372
16	C	4.1330	-0.0880	2.7169
17	C	3.2406	1.8533	4.4376
18	C	4.8357	0.1370	3.8967
19	C	4.3835	1.1253	4.7732
20	H	1.7067	2.1299	2.9323
21	H	4.4548	-0.8508	2.0063
22	H	5.7231	-0.4565	4.1171
23	H	2.8514	2.6350	5.0902
24	H	-4.5054	-2.6490	-4.3686
25	O	-1.5169	-2.4727	-0.1025
26	O	-2.1312	1.1479	0.1010
27	H	-4.6466	-0.5139	-5.7009
28	N	-2.9796	-0.5587	-2.1991
29	C	-3.0541	0.5880	-2.9101
30	C	-3.4969	-1.6884	-2.7295
31	C	-3.6427	0.6415	-4.1698
32	O	0.0345	-0.5633	1.4821
33	H	0.3058	-1.1023	-1.8547
34	U	-1.7805	-0.6576	0.0570
35	O	-2.8939	-1.3249	2.2608
36	C	-4.1040	-1.7122	-3.9821
37	O	-4.2717	-0.8612	0.6339
38	C	-4.1775	-0.5269	-4.7156
39	N	-4.1136	-1.2244	1.8581

40	O	-5.0652	-1.4600	2.5985

3_u2o4_4py
Energy (BONDING) = -9550.7615781 kcal.mol-1

	Atom	X	Y	Z
1	U	1.8081	0.9388	0.0479
2	H	0.9817	-1.8826	-0.0568
3	O	3.3713	2.9789	-0.1639
4	O	-0.5518	1.0590	0.2416
5	O	4.3795	1.0546	-0.1319
6	H	-3.1193	1.4748	2.1093
7	H	-3.4120	1.3143	-2.0266
8	O	5.5720	2.9033	-0.3060
9	N	4.4838	2.3345	-0.2047
10	O	1.7506	0.8873	-1.7667
11	O	2.0096	1.0623	1.8498
12	H	-0.9975	6.8392	-0.1766
13	H	5.0653	-4.7297	0.0174
14	N	3.2168	-1.3109	0.0304
15	C	3.4607	-1.9704	1.1835
16	C	3.6431	-1.8627	-1.1258
17	C	4.1232	-3.1951	1.2214
18	C	4.3052	-3.0880	-1.1727
19	C	4.5490	-3.7685	0.0216
20	H	3.0997	-1.4938	2.0960
21	H	3.4355	-1.2965	-2.0352
22	H	4.6219	-3.4935	-2.1338
23	H	4.2956	-3.6848	2.1800
24	N	0.7658	3.3782	-0.0429
25	C	0.3596	3.9926	1.0894
26	C	0.5574	4.0036	-1.2212
27	C	-0.2729	5.2337	1.0837
28	C	-0.0733	5.2430	-1.3114
29	C	-0.4990	5.8695	-0.1387
30	H	0.5442	3.4562	2.0214
31	H	0.9060	3.4795	-2.1125
32	H	-0.2244	5.7015	-2.2888
33	H	-0.5814	5.6861	2.0263
34	U	-1.8081	-0.9390	0.0484
35	O	-3.3743	-2.9779	-0.1703
36	C	-4.2883	3.0999	-1.1575
37	O	-4.3811	-1.0524	-0.1473
38	C	-4.5425	3.7706	0.0402
39	N	-4.4858	-2.3319	-0.2260

40	O	-5.5725	-2.8995	-0.3471
41	H	-4.3116	3.6681	2.1997
42	H	-4.5943	3.5154	-2.1178
43	O	-1.7483	-0.8865	-1.7660
44	O	-2.0131	-1.0650	1.8499
45	H	-5.0566	4.7329	0.0398
46	H	1.0024	-6.8392	-0.1637
47	N	-0.7684	-3.3820	-0.0342
48	C	-0.3294	-3.9778	1.0957
49	C	-0.5909	-4.0250	-1.2080
50	C	0.3064	-5.2171	1.0916
51	C	0.0420	-5.2634	-1.2967
52	C	0.5019	-5.8705	-0.1269
53	H	-0.4901	-3.4277	2.0241
54	H	-0.9658	-3.5162	-2.0974
55	H	0.1677	-5.7363	-2.2709
56	H	0.6417	-5.6537	2.0325
57	N	-3.2153	1.3104	0.0410
58	C	-3.4698	1.9601	1.1975
59	C	-3.6289	1.8730	-1.1147
60	C	-4.1299	3.1859	1.2392
61	O	0.5522	-1.0616	0.2313
62	H	-0.9846	1.8901	-0.0097

h2o

Energy (BONDING) = -331.51109940000003 kcal.mol-1

	Atom	X	Y	Z
1	H	0.76280.0000	-0.0282	
2	O	0.0000	0.0000	0.5807
3	H	-0.7628	0.0000	-0.0282

3_u2o2oh2_4py
Energy (BONDING) = -9533.3436048 kcal.mol-1

	Atom	X	Y	Z
1	U	1.8566	0.9674	0.1130
2	O	0.3230	-0.6684	0.8663
3	O	3.2711	2.8964	-0.7930
4	O	-0.3649	0.6296	0.8772
5	O	4.2529	0.9478	-0.7803
6	H	-3.4884	1.1062	2.2537
7	H	-2.5351	1.8130	-1.7218
8	O	5.3503	2.7181	-1.5209
9	N	4.3312	2.2068	-1.0499
10	O	1.2363	0.6051	-1.8059
11	O	2.4843	1.3308	1.8088
12	H	-1.3318	6.6188	-0.0416
13	H	4.6915	-4.8647	0.3166
14	N	2.9776	-1.3783	0.1963
15	C	3.5545	-1.8273	1.3308
16	C	3.0085	-2.1736	-0.8937
17	C	4.1798	-3.0694	1.4145
18	C	3.6132	-3.4277	-0.8921
19	C	4.2112	-3.8854	0.2830
20	H	3.5074	-1.1570	2.1905
21	H	2.5295	-1.7780	-1.7913
22	H	3.6082	-4.0313	-1.8000
23	H	4.6315	-3.3843	2.3556
24	N	0.5492	3.2184	0.0466
25	C	0.0111	3.7418	1.1682
26	C	0.4087	3.9034	-1.1079
27	C	-0.6702	4.9564	1.1786
28	C	-0.2563	5.1246	-1.1818
29	C	-0.8042	5.6638	-0.0170
30	H	0.1387	3.1580	2.0812
31	H	0.8501	3.4482	-1.9961
32	H	-0.3409	5.6364	-2.1408
33	H	-1.0855	5.3349	2.1130
34	U	-1.8639	-0.9726	0.1192
35	O	-3.2495	-2.8567	-0.8895
36	C	-3.5932	3.4499	-0.7742
37	O	-4.2206	-0.9025	-0.8484
38	C	-4.1741	3.8872	0.4171
39	N	-4.3028	-2.1548	-1.1538

40	O	-5.3107	-2.6463	-1.6586
41	H	-4.5785	3.3440	2.4822
42	H	-3.5870	4.0752	-1.6671
43	O	-1.1728	-0.5379	-1.8568
44	O	-2.5192	-1.3626	1.7985
45	H	-4.6398	4.8722	0.4788
46	H	1.4014	-6.5735	0.0633
47	N	-0.5737	-3.2258	0.0738
48	C	-0.0038	-3.6978	1.2033
49	C	-0.4330	-3.9450	-1.0597
50	C	0.7103	-4.8924	1.2405
51	C	0.2646	-5.1487	-1.1056
52	C	0.8464	-5.6339	0.0662
53	H	-0.1296	-3.0871	2.0985
54	H	-0.9017	-3.5364	-1.9564
55	H	0.3492	-5.6878	-2.0495
56	H	1.1509	-5.2280	2.1796
57	N	-2.9756	1.3671	0.2593
58	C	-3.5351	1.7966	1.4102
59	C	-3.0051	2.1888	-0.8113
60	C	-4.1420	3.0449	1.5289
61	H	0.3316	0.1800	-1.9596
62	H	-1.6152	-0.7674	-2.6997

singlet

Energy (BONDING) = -9535.1123835 kcal.mol-1

	Atom	X	Y	Z
1	U	-2.0484	-1.5456	2.2211
2	O	-4.5817	-1.8704	2.1606
3	O	0.1810	-0.8889	2.4414
4	O	-3.6878	-2.3238	4.0969
5	H	-1.6266	1.0157	2.9959
6	O	-2.3956	0.4281	2.8463
7	O	-0.3390	-0.7278	0.5794
8	H	-4.7218	-0.0334	-3.5091
9	O	-1.8848	-3.2780	1.5965
10	H	-0.2903	0.2322	0.3786
11	N	-3.1292	-0.9311	-0.0779
12	C	-3.9770	0.1118	-0.1963
13	C	-2.8479	-1.6529	-1.1826
14	C	-4.5678	0.4659	-1.4074
15	C	-3.3959	-1.3649	-2.4292
16	C	-4.2740	-0.2845	-2.5466
17	H	-4.1839	0.6725	0.7175
18	H	-2.1592	-2.4871	-1.0448
19	H	-3.1390	-1.9828	-3.2901
20	H	-5.2481	1.3173	-1.4493
21	N	-4.7539	-2.2390	3.3909
22	O	-5.8754	-2.4903	3.8405
23	U	1.9619	-1.6137	1.2119
24	O	2.4238	0.0490	0.6116
25	O	1.6695	-3.3197	1.7748
26	O	3.8855	-2.4442	-0.2538
27	O	4.4243	-1.9394	1.7965
28	N	4.8121	-2.3386	0.6336
29	O	5.9903	-2.6001	0.3890
30	H	-0.2590	-3.7070	-4.4971
31	H	3.5110	0.0794	7.2945
32	N	1.1960	-2.5125	-1.0961
33	C	1.4633	-1.8428	-2.2379
34	C	0.4166	-3.6139	-1.1666
35	C	0.9599	-2.2359	-3.4754
36	C	-0.1198	-4.0759	-2.3672
37	C	0.1519	-3.3729	-3.5425
38	H	2.1035	-0.9643	-2.1434
39	H	0.2164	-4.1219	-0.2223

40	H	-0.7413	-4.9713	-2.3716
41	H	1.2028	-1.6557	-4.3651
42	N	2.5874	-0.9383	3.6584
43	C	2.4473	0.3378	4.0767
44	C	3.0475	-1.8523	4.5376
45	C	2.7726	0.7436	5.3688
46	C	3.3878	-1.5288	5.8489
47	C	3.2505	-0.2062	6.2734
48	H	2.0603	1.0452	3.3428
49	H	3.1425	-2.8733	4.1657
50	H	3.7532	-2.3067	6.5182
51	H	2.6517	1.7885	5.6532
52	H	0.7265	-3.5509	7.7462
53	N	-0.9264	-2.2890	4.4644
54	C	-0.9282	-1.5276	5.5760
55	C	-0.3236	-3.4977	4.5150
56	C	-0.3390	-1.9388	6.7709
57	C	0.2730	-3.9880	5.6739
58	C	0.2666	-3.1953	6.8228
59	H	-1.4271	-0.5607	5.4979
60	H	-0.3228	-4.0727	3.5880
61	H	0.7388	-4.9744	5.6683
62	H	-0.3690	-1.2824	7.6402

triplet

Energy (BONDING) = -9535.0616493 kcal.mol-1

	Atom	X	Y	Z
1	U	-2.0484	-1.5456	2.2211
2	O	-4.5817	-1.8704	2.1606
3	O	0.1810	-0.8889	2.4414
4	O	-3.6878	-2.3238	4.0969
5	H	-1.6266	1.0157	2.9959
6	O	-2.3956	0.4281	2.8463
7	O	-0.3390	-0.7278	0.5794
8	H	-4.7218	-0.0334	-3.5091
9	O	-1.8848	-3.2780	1.5965
10	H	-0.2903	0.2322	0.3786
11	N	-3.1292	-0.9311	-0.0779
12	C	-3.9770	0.1118	-0.1963
13	C	-2.8479	-1.6529	-1.1826
14	C	-4.5678	0.4659	-1.4074
15	C	-3.3959	-1.3649	-2.4292
16	C	-4.2740	-0.2845	-2.5466
17	H	-4.1839	0.6725	0.7175
18	H	-2.1592	-2.4871	-1.0448
19	H	-3.1390	-1.9828	-3.2901
20	H	-5.2481	1.3173	-1.4493
21	N	-4.7539	-2.2390	3.3909
22	O	-5.8754	-2.4903	3.8405
23	U	1.9619	-1.6137	1.2119
24	O	2.4238	0.0490	0.6116
25	O	1.6695	-3.3197	1.7748
26	O	3.8855	-2.4442	-0.2538
27	O	4.4243	-1.9394	1.7965
28	N	4.8121	-2.3386	0.6336
29	O	5.9903	-2.6001	0.3890
30	H	-0.2590	-3.7070	-4.4971
31	H	3.5110	0.0794	7.2945
32	N	1.1960	-2.5125	-1.0961
33	C	1.4633	-1.8428	-2.2379
34	C	0.4166	-3.6139	-1.1666
35	C	0.9599	-2.2359	-3.4754
36	C	-0.1198	-4.0759	-2.3672
37	C	0.1519	-3.3729	-3.5425
38	H	2.1035	-0.9643	-2.1434
39	H	0.2164	-4.1219	-0.2223

40	H	-0.7413	-4.9713	-2.3716
41	H	1.2028	-1.6557	-4.3651
42	N	2.5874	-0.9383	3.6584
43	C	2.4473	0.3378	4.0767
44	C	3.0475	-1.8523	4.5376
45	C	2.7726	0.7436	5.3688
46	C	3.3878	-1.5288	5.8489
47	C	3.2505	-0.2062	6.2734
48	H	2.0603	1.0452	3.3428
49	H	3.1425	-2.8733	4.1657
50	H	3.7532	-2.3067	6.5182
51	H	2.6517	1.7885	5.6532
52	H	0.7265	-3.5509	7.7462
53	N	-0.9264	-2.2890	4.4644
54	C	-0.9282	-1.5276	5.5760
55	C	-0.3236	-3.4977	4.5150
56	C	-0.3390	-1.9388	6.7709
57	C	0.2730	-3.9880	5.6739
58	C	0.2666	-3.1953	6.8228
59	H	-1.4271	-0.5607	5.4979
60	H	-0.3228	-4.0727	3.5880
61	H	0.7388	-4.9744	5.6683
62	H	-0.3690	-1.2824	7.6402

singlet

Energy (BONDING) = -9481.2326631 kcal.mol-1

	Atom	X	Y	Z
1	U	1.9080	0.9856	0.1465
2	O	0.3302	-0.6524	0.6903
3	O	3.3892	2.9649	-0.4450
4	O	-0.3436	0.6445	0.6929
5	O	4.3649	1.0184	-0.5155
6	H	-3.9675	1.0656	1.8548
7	H	-2.0699	1.8267	-1.7583
8	O	5.5197	2.8349	-1.0079
9	N	4.4680	2.2944	-0.6692
10	O	1.5096	0.8278	-1.7471
11	O	2.4307	1.2045	1.8903
12	H	-1.2820	6.6104	0.3498
13	H	4.5688	-4.9040	0.0185
14	N	2.9693	-1.3644	0.1000
15	C	3.6378	-1.8465	1.1701
16	C	2.8672	-2.1455	-0.9973
17	C	4.2261	-3.1089	1.1793
18	C	3.4279	-3.4174	-1.0658
19	C	4.1210	-3.9095	0.0413
20	H	3.6940	-1.1889	2.0382
21	H	2.3169	-1.7249	-1.8399
22	H	3.3151	-4.0079	-1.9749
23	H	4.7536	-3.4525	2.0694
24	N	0.6247	3.2289	0.2119
25	C	-0.0067	3.6208	1.3395
26	C	0.5712	4.0378	-0.8679
27	C	-0.6993	4.8254	1.4292
28	C	-0.1024	5.2566	-0.8587
29	C	-0.7473	5.6603	0.3116
30	H	0.0508	2.9372	2.1877
31	H	1.0911	3.6867	-1.7602
32	H	-0.1166	5.8731	-1.7571
33	H	-1.1893	5.0968	2.3642
34	U	-1.9136	-0.9918	0.1132
35	O	-3.3886	-2.9724	-0.4813
36	C	-3.3170	3.4583	-1.0659
37	O	-4.3718	-1.0294	-0.5426
38	C	-4.1695	3.8806	-0.0442
39	N	-4.4744	-2.3064	-0.6855

40	O	-5.5318	-2.8529	-0.9951
41	H	-5.0698	3.3052	1.8496
42	H	-3.0930	4.0956	-1.9213
43	O	-1.4999	-0.8219	-1.7782
44	O	-2.4451	-1.2262	1.8521
45	H	-4.6358	4.8661	-0.0818
46	H	1.3368	-6.5822	0.2546
47	N	-0.6237	-3.2309	0.1519
48	C	-0.0042	-3.6352	1.2815
49	C	-0.5420	-4.0179	-0.9423
50	C	0.7067	-4.8297	1.3581
51	C	0.1499	-5.2264	-0.9464
52	C	0.7849	-5.6416	0.2253
53	H	-0.0868	-2.9700	2.1422
54	H	-1.0513	-3.6566	-1.8366
55	H	0.1875	-5.8231	-1.8579
56	H	1.1887	-5.1104	2.2945
57	N	-2.9786	1.3552	0.0506
58	C	-3.8015	1.7692	1.0383
59	C	-2.7416	2.1940	-0.9812
60	C	-4.4135	3.0202	1.0274
61	H	-0.4496	-0.2585	-2.2750
62	H	0.4678	0.2556	-2.2698

triplet

Energy (BONDING) = -9481.184235 kcal.mol-1

	Atom	X	Y	Z
1	U	1.9080	0.9856	0.1465
2	O	0.3302	-0.6524	0.6903
3	O	3.3892	2.9649	-0.4450
4	O	-0.3436	0.6445	0.6929
5	O	4.3649	1.0184	-0.5155
6	H	-3.9675	1.0656	1.8548
7	H	-2.0699	1.8267	-1.7583
8	O	5.5197	2.8349	-1.0079
9	N	4.4680	2.2944	-0.6692
10	O	1.5096	0.8278	-1.7471
11	O	2.4307	1.2045	1.8903
12	H	-1.2820	6.6104	0.3498
13	H	4.5688	-4.9040	0.0185
14	N	2.9693	-1.3644	0.1000
15	C	3.6378	-1.8465	1.1701
16	C	2.8672	-2.1455	-0.9973
17	C	4.2261	-3.1089	1.1793
18	C	3.4279	-3.4174	-1.0658
19	C	4.1210	-3.9095	0.0413
20	H	3.6940	-1.1889	2.0382
21	H	2.3169	-1.7249	-1.8399
22	H	3.3151	-4.0079	-1.9749
23	H	4.7536	-3.4525	2.0694
24	N	0.6247	3.2289	0.2119
25	C	-0.0067	3.6208	1.3395
26	C	0.5712	4.0378	-0.8679
27	C	-0.6993	4.8254	1.4292
28	C	-0.1024	5.2566	-0.8587
29	C	-0.7473	5.6603	0.3116
30	H	0.0508	2.9372	2.1877
31	H	1.0911	3.6867	-1.7602
32	H	-0.1166	5.8731	-1.7571
33	H	-1.1893	5.0968	2.3642
34	U	-1.9136	-0.9918	0.1132
35	O	-3.3886	-2.9724	-0.4813
36	C	-3.3170	3.4583	-1.0659
37	O	-4.3718	-1.0294	-0.5426
38	C	-4.1695	3.8806	-0.0442
39	N	-4.4744	-2.3064	-0.6855

40	O	-5.5318	-2.8529	-0.9951
41	H	-5.0698	3.3052	1.8496
42	H	-3.0930	4.0956	-1.9213
43	O	-1.4999	-0.8219	-1.7782
44	O	-2.4451	-1.2262	1.8521
45	H	-4.6358	4.8661	-0.0818
46	H	1.3368	-6.5822	0.2546
47	N	-0.6237	-3.2309	0.1519
48	C	-0.0042	-3.6352	1.2815
49	C	-0.5420	-4.0179	-0.9423
50	C	0.7067	-4.8297	1.3581
51	C	0.1499	-5.2264	-0.9464
52	C	0.7849	-5.6416	0.2253
53	H	-0.0868	-2.9700	2.1422
54	H	-1.0513	-3.6566	-1.8366
55	H	0.1875	-5.8231	-1.8579
56	H	1.1887	-5.1104	2.2945
57	N	-2.9786	1.3552	0.0506
58	C	-3.8015	1.7692	1.0383
59	C	-2.7416	2.1940	-0.9812
60	C	-4.4135	3.0202	1.0274
61	H	-0.4496	-0.2585	-2.2750
62	H	0.4678	0.2556	-2.2698

monodentate

Energy (BONDING) = -2518.6394004 kcal.mol-1

	Atom	X	Y	Z
1	U	-0.1750	0.7186	0.1054
2	O	-2.1029	-0.7917	0.7887
3	O	0.5663	-1.5532	0.9955
4	O	-2.6351	1.1533	-0.0409
5	N	3.1230	-0.1804	-0.3793
6	N	-3.0386	0.0281	0.4510
7	O	-4.2298	-0.2370	0.5881
8	O	-0.1977	-0.0180	-1.5598
9	O	-0.1354	1.3840	1.7990
10	O	2.8959	-1.4232	-0.2958
11	H	1.4555	-1.6661	0.5344
12	O	4.1545	0.2734	-0.8890
13	O	2.2446	0.6529	0.1173
14	H	-0.1455	3.4677	-0.0938
15	H	0.0180	-2.3038	0.6951
16	O	-0.1448	2.7149	-0.7167

bidentate

Energy (BONDING) = -2519.1974766 kcal.mol-1

	Atom	X	Y	Z
1	U	-0.0831	0.5339	0.0872
2	O	-2.1995	-0.4849	1.1504
3	H	0.0480	3.2689	-0.2155
4	O	-2.4768	1.4615	0.2274
5	N	2.8565	0.0586	-0.4282
6	N	-3.0064	0.4774	0.8618
7	O	-4.1977	0.4523	1.1756
8	O	-0.4840	-0.2437	-1.5129
9	O	0.3191	1.2398	1.7179
10	O	4.0540	-0.1343	-0.6446
11	H	0.6204	-2.4985	0.7169
12	O	2.2490	1.1288	-0.7991
13	O	2.1225	-0.7997	0.1913
14	O	-0.0257	-1.9071	1.1495
15	H	-0.8816	-2.3726	1.0784
16	O	-0.1357	2.5100	-0.8017

u2o4_2oh_2py
Energ (BONDING) = -6302.891847899999 kcal.mol-1
y

	Atom	X	Y	Z
1	U	1.8422	0.3524	-0.0960
2	H	0.3476	-1.7777	-1.2589
3	O	2.3951	2.7802	0.0414
4	O	-0.2748	1.3750	-0.3452
5	O	4.0920	1.4295	0.2510
6	H	-2.7379	2.1680	1.9117
7	H	-4.6129	0.8943	-1.5748
8	O	4.4182	3.6110	0.3452
9	N	3.6709	2.6505	0.2181
10	O	2.1278	0.3714	-1.8834
11	O	1.6007	0.2750	1.6931
12	H	-4.4106	3.9886	2.2491
13	H	6.2701	-4.2614	0.4782
14	N	3.5972	-1.4700	0.1179
15	C	3.5940	-2.2962	1.1899
16	C	4.5517	-1.6392	-0.8264
17	C	4.5321	-3.3108	1.3503
18	C	5.5264	-2.6268	-0.7303
19	C	5.5175	-3.4784	0.3759
20	H	2.8139	-2.1239	1.9322
21	H	4.5203	-0.9547	-1.6750
22	H	6.2763	-2.7209	-1.5157
23	H	4.4878	-3.9503	2.2318
24	H	-6.3737	2.6514	-1.3721
25	O	-2.1359	-0.3303	-1.8852
26	O	-1.5905	-0.3046	1.6898
27	H	-6.2812	4.2417	0.5802
28	N	-3.6064	1.4621	0.1562
29	C	-3.5564	2.3145	1.2057
30	C	-4.6079	1.5994	-0.7427
31	C	-4.4940	3.3260	1.3878
32	O	0.2742	-1.3643	-0.3743
33	H	-0.3524	1.8034	-1.2226
34	U	-1.8427	-0.3469	-0.0987
35	O	-2.3805	-2.7796	-0.0250
36	C	-5.5852	2.5820	-0.6230
37	O	-4.0824	-1.4457	0.2421
38	C	-5.5285	3.4612	0.4602
39	N	-3.6546	-2.6625	0.1691

40	O	-4.3952	-3.6308	0.2755

u2o4_2oh_4py

Energy (BONDING) = -9598.359482099999 kcal.mol-1

	Atom	X	Y	Z
1	U	1.8083	0.9384	0.0529
2	H	0.9797	-1.8828	-0.0550
3	O	3.3721	2.9785	-0.1573
4	O	-0.5517	1.0588	0.2501
5	O	4.3798	1.0534	-0.1321
6	H	-3.1327	1.4850	2.1015
7	H	-3.3985	1.3078	-2.0368
8	O	5.5724	2.9021	-0.3037
9	N	4.4842	2.3334	-0.2014
10	O	1.7477	0.8892	-1.7615
11	O	2.0141	1.0581	1.8550
12	H	-1.0012	6.8366	-0.1879
13	H	5.0558	-4.7350	-0.0115
14	N	3.2141	-1.3126	0.0218
15	C	3.4598	-1.9781	1.1713
16	C	3.6368	-1.8596	-1.1380
17	C	4.1199	-3.2042	1.2012
18	C	4.2963	-3.0860	-1.1927
19	C	4.5415	-3.7729	-0.0024
20	H	3.1024	-1.5056	2.0873
21	H	3.4278	-1.2886	-2.0441
22	H	4.6100	-3.4870	-2.1567
23	H	4.2945	-3.7000	2.1560
24	N	0.7649	3.3775	-0.0452
25	C	0.3544	3.9925	1.0853
26	C	0.5609	4.0020	-1.2247
27	C	-0.2800	5.2325	1.0762
28	C	-0.0704	5.2409	-1.3180
29	C	-0.5019	5.8674	-0.1475
30	H	0.5372	3.4580	2.0186
31	H	0.9133	3.4776	-2.1142
32	H	-0.2168	5.6994	-2.2962
33	H	-0.5924	5.6851	2.0173
34	U	-1.8086	-0.9388	0.0539
35	O	-3.3752	-2.9772	-0.1663
36	C	-4.2809	3.0952	-1.1805
37	O	-4.3816	-1.0517	-0.1426
38	C	-4.5422	3.7715	0.0126
39	N	-4.4862	-2.3315	-0.2200

40	O	-5.5735	-2.8990	-0.3376
41	H	-4.3226	3.6786	2.1743
42	H	-4.5812	3.5043	-2.1452
43	O	-1.7485	-0.8866	-1.7604
44	O	-2.0135	-1.0643	1.8556
45	H	-5.0566	4.7336	0.0043
46	H	1.0220	-6.8274	-0.1776
47	N	-0.7683	-3.3806	-0.0364
48	C	-0.3282	-3.9792	1.0919
49	C	-0.5856	-4.0176	-1.2129
50	C	0.3147	-5.2148	1.0835
51	C	0.0542	-5.2522	-1.3054
52	C	0.5158	-5.8617	-0.1375
53	H	-0.4933	-3.4343	2.0226
54	H	-0.9616	-3.5080	-2.1010
55	H	0.1841	-5.7188	-2.2817
56	H	0.6501	-5.6548	2.0229
57	N	-3.2147	1.3110	0.0323
58	C	-3.4765	1.9658	1.1842
59	C	-3.6212	1.8690	-1.1281
60	C	-4.1365	3.1922	1.2166
61	O	0.5520	-1.0621	0.2366
62	H	-0.9845	1.8895	-0.0024

Energy (BONDING) = -2528.7700977 kcal.mol-1

	Atom	X	Y	Z
1	U	-0.0788	0.4365	0.1323
2	O	-2.2315	-0.3891	1.0682
3	H	0.7080	3.2454	-0.9165
4	O	-2.2879	1.5814	0.1583
5	N	2.7881	0.2292	-0.4943
6	N	-2.9445	0.6453	0.7617
7	O	-4.1319	0.7315	1.0228
8	O	-0.4809	-0.2892	-1.4649
9	O	0.3234	1.1619	1.7296
10	O	3.9771	0.1464	-0.7491
11	H	0.6476	-2.4989	0.8201
12	O	2.0745	1.2633	-0.8009
13	O	2.1312	-0.7079	0.1072
14	O	-0.0221	-1.8765	1.1667
15	H	-0.8615	-2.3777	1.1691
16	O	-0.1349	2.7503	-0.9012
17	H	-0.7949	3.3784	-0.5466