Supporting Information

Photophysical Tuning via Piperazine Nitrogen Torsion in a Ferrocene–Aminonaphthalimide Derivative

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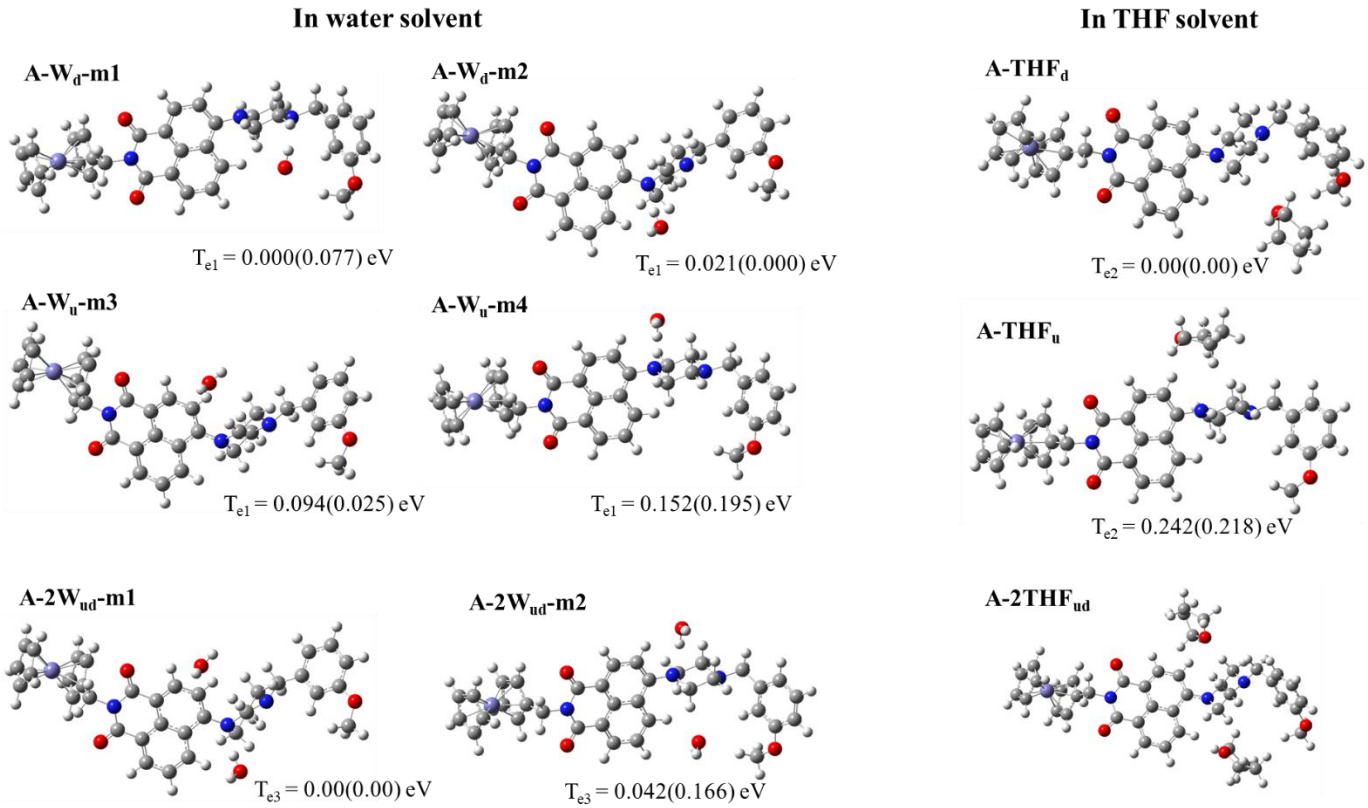

Figure S1. Calculated minimum structures of molecule **A** with explicit addition of one and two water or THF solvent molecules and relative energies T_e at the PBE0/6-31G(d,p) and in parenthesis at the PBE0/def2tzvp methods in water or THF solvent.

Table S1. Total energies (hartree) of the **A-W**, **A-2W**, **A-THF** and **A-2THF** molecular systems in water or THF solvent at the PBE0/6-31G(d,p) and PBE0/def2-tzvp levels of theory.

Molecule	PBE0/6-31G(d,p)	PBE0/def2-tzvp
A-W$_d$-m$_1$	-3081.371057	-3082.093155
A-W$_u$-m$_2$	-3081.370295	-3082.095990
A-W$_d$-m$_3$	-3081.367602	-3082.095070
A-W$_u$-m$_4$	-3081.365476	-3082.088812
A-2W$_{ud}$-m$_1$	-3157.719390	-3158.482490
A-2W$_{ud}$-m$_2$	-3157.717852	-3158.476399
A-THF$_u$	-3237.202079	-3237.966326
A-THF$_d$	-3237.210975	-3237.974336
A-2THF$_{ud}$	-3469.406774	-

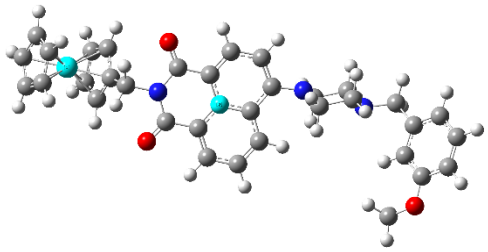

Figure S2. Charge transfer distance dCT (Fe…C_5), a diagnostic index for charge transfer

Table S2. Charge transfer distance dCT (Fe…C_5), a diagnostic index for charge transfer

Molecule	Methodology	Distance (Å)[Fe….C_5)]
A (H_2O)	PBE0/6-31G(d, p)	7.065
A-2W_{ud}-m_1	PBE0/6-31G(d, p)	7.058
A-2THF_{ud}	PBE0/6-31G(d, p)	7.070
A (THF)	PBE0/6-31G(d, p)	7.065
	TPSSh/6-31G(d, p)	7.091
	ωB97XD/6-31G(d, p)	7.044

Table S3. Total electronic energies (E, hartree), total free energies (G, Hartree), ΔE (eV) and ΔG(eV) of the **A** molecule in water or THF solvent at the PBE0/6-31G(d,p) level of theory.

	E	**G**	**ΔE**	**ΔG**
A (typeI in water)	-3005.009751	-3004.465463	0.230	0.191
A (typeII in water)	-3005.018195	-3004.472489	0.000	0.000
A (ts in water)	-3005.009179	-3004.458641	0.245	0.377
A (typeI in thf)	-3005.006217	-3004.459715	0.218	0.247
A (typeII in thf)	-3005.014214	-3004.468807	0.000	0.000
A (ts)	-3005.004004	-3004.454132	0.278	0.399

Table S4. Rate Constants for the **A** interconversion (**I → II & II → I)** at the PBE0/6-31G(d,p) level of theory. The solvent is implicitly included.

	Barrier (eV)	**$\Delta G^{\ddagger}$ (kJ/mol)**	**Rate Constant (s^{-1})**	**Lifetime (μs)**	**Interconversion**
I → II in THF	0.152	14.7	1.5×10^{8}	0.007	Fast
II → I in THF	0.399	38.5	3.2×10^{3}	310	Very slow
I → II in water	0.186	18.0	2.0×10^{7}	0.05	Moderately fast
II → I in water	0.377	36.4	1.3×10^{4}	77	Slow

Table S5. Main absorption and charge transfer peaks, λ (nm), energy differences ΔE (eV), f-values and the corresponding main excitations of the absorption spectrum of the **A**, **A-W**, **A-2W**, **A-THF** and **A-2THF** molecular systems in water or THF solvent at the PBE0/6-31G(d,p) level of theory.

Molecule	Method	solvent	λ (nm)	ΔE	f	
A	PBE0	THF	443.7	2.79	0.0009	0.969 |H → L>
	PBE0	THF	333.5	3.72	0.4260	0.989 |H-6 → L>
	PBE0	THF	225.0	5.51	0.4283	0.737 |H-6 → L+1>
	TPSSh	THF	353.5	3.51	0.2344	0.768 |H-6 → L>
	ωB97X-D	THF	308.9	4.01	0.5029	0.916 |H-5 → L>
	PBE0-D3	THF	333.5	3.72	0.4250	0.986 |H-6 → L>
	TPSSh-D3	THF	353.9	3.50	0.2740	0.833 |H-6 → L>
	PBE0	water	438.8	2.83	0.0002	0.806 |H → L>
	PBE0	water	333.5	3.72	0.4216	0.989 |H-6 → L>
	PBE0	water	224.4	5.52	0.4388	0.739 |H-6 → L+1>
A-W_d-m_1	PBE0	water	430.2	2.88	0.0007	0.989 |H → L>
	PBE0	water	334.2	3.71	0.4208	0.981 |H-5 → L>
A-W_d-m_2	PBE0	water	417.7	2.97	0.0031	0.965 |H → L>
	PBE0	water	399.9	3.10	0.3391	0.990 |H-2 → L>
A-W_u-m_3	PBE0	water	474.7	2.61	0.0001	0.989 |H → L>
	PBE0	water	417.2	2.97	0.3661	0.879 |H-2 → L>
A-W_u-m_4	PBE0	water	446.2	2.78	0.0009	0.982 |H → L>
	PBE0	water	332.8	3.73	0.4218	0.979 |H-5 → L>
A-2W_{ud}-m_1	PBE0	water	424.9	2.92	0.0023	0.984 |H → L>
	PBE0	water	401.8	3.09	0.3231	0.991 |H-2 → L>
A-2W_{ud}-m_2	PBE0	water	433.2	2.86	0.0005	0.958 |H → L>
	PBE0	water	333.7	3.72	0.2547	0.733 |H-5 → L>
A-THF_u	PBE0	THF	433.2	2.86	0.0005	0.997 |H → L>
	PBE0	THF	334.2	3.71	0.4152	0.981 |H-6 → L>
A-THF_d	PBE0	THF	418.9	2.96	0.3914	0.812 |H-2 → L>
A-2THF_{ud}	PBE0	THF	421.5	2.94	0.4067	0.988 |H → L>

Table S6. Main absorption and charge transfer peaks, λ (nm), cLR corrected values (eV) and λ (nm) of the absorption spectrum of the **A**, **A-W**, **A-2W**, **A-THF** and **A-2THF** molecular systems in water or THF solvent at the PBE0/6-31G(d, p) level of theory.

Molecule	**λ (nm)**	**ΔE**	**ΔE_{cLR}**	**λ_{cLR}**	**Shift (λ)**
A-Wd-m1	334.2	3.71	3.71	334.0	**0.2**
A-Wd-m2	399.9	3.10	3.05	406.0	**-6.1**
A-Wu-m3	417.2	2.97	2.95	419.9	**-2.7**
A-Wu-m4	332.8	3.73	3.76	329.5	**3.3**
A-2Wud-m1	401.8	3.09	3.03	409.9	**-8.1**
A-2Wud-m2	333.7	3.72	3.72	333.7	**0**
A-THFd	418.9	2.96	2.95	420.5	**-1.6**
A-THFu	334.2	3.71	3.71	334.0	**0.2**
A-2THFud	421.5	2.94	2.94	421.6	**0.1**

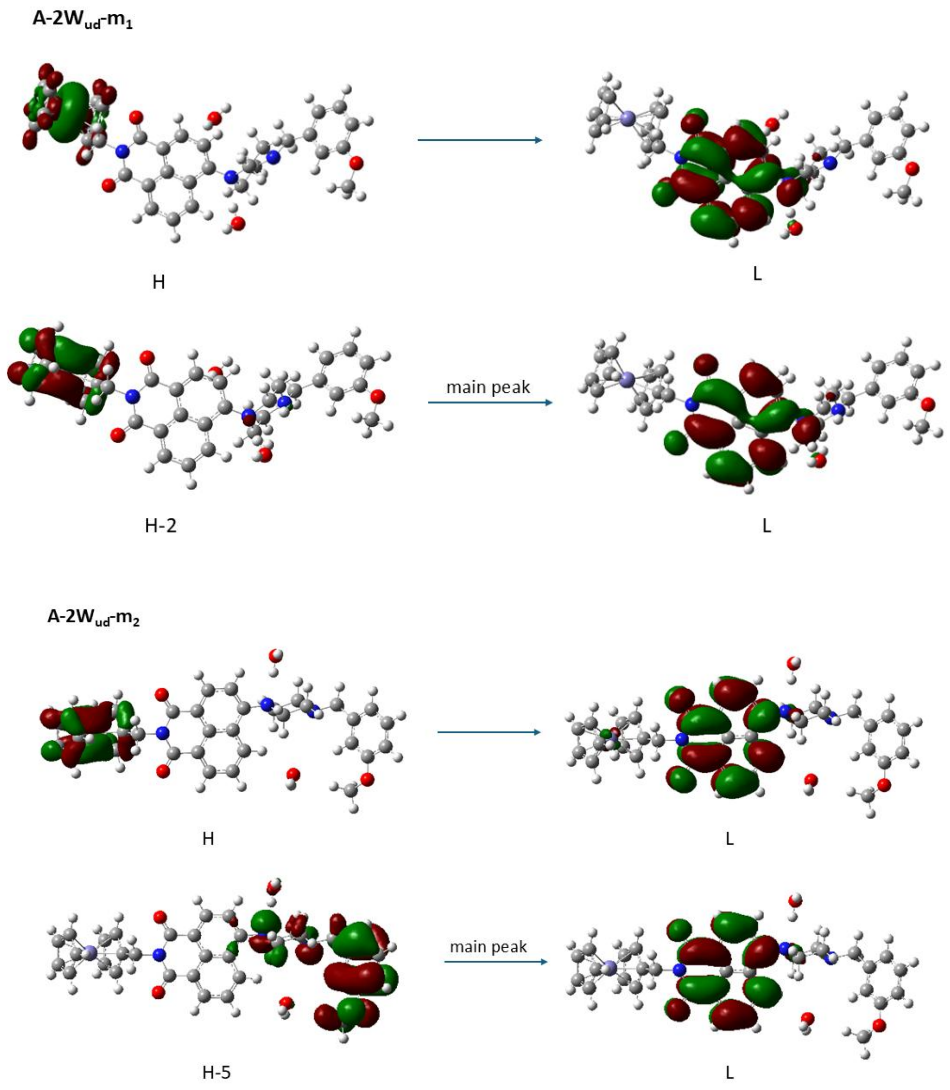

Figure S3. Natural Transition Orbitals involved in main UV-vis absorption peaks of A-2W_{ud}-m_1 and A-2W_{ud}-m_2 at PBE0/6-31G (d, p) in water solvent.

Table S7. Geometries

A (PBE0/6-31G(d,p) in THF solvent type I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.401699	-0.839683	0.260282
2	6	0	9.487981	-1.443283	-0.367797
3	6	0	8.301886	0.556152	0.286560
4	6	0	10.477155	-0.654053	-0.957704
5	1	0	9.562425	-2.527057	-0.397763
6	6	0	9.288843	1.338934	-0.311251
7	1	0	7.435881	0.998248	0.766249
8	6	0	10.385362	0.728640	-0.934287
9	1	0	11.324829	-1.124812	-1.447749
10	8	0	9.275238	2.695889	-0.340223
11	6	0	8.187119	3.355971	0.273982
12	1	0	7.234056	3.086951	-0.197388
13	1	0	8.131857	3.131336	1.345988
14	1	0	8.365031	4.423418	0.139745
15	6	0	7.354363	-1.675995	0.958403
16	1	0	7.564199	-1.673881	2.036610
17	1	0	7.448513	-2.727598	0.627091
18	6	0	5.542799	-1.326012	-0.591516
19	6	0	5.067069	-1.799737	1.697181
20	6	0	4.176715	-0.684132	-0.766256
21	1	0	5.479688	-2.395234	-0.871844
22	1	0	6.259671	-0.843216	-1.263219
23	6	0	3.693097	-1.162779	1.564634
24	1	0	4.979656	-2.886811	1.507381
25	1	0	5.429791	-1.666203	2.722578
26	1	0	3.809952	-0.870109	-1.780216
27	1	0	4.283786	0.407765	-0.643239
28	1	0	2.980936	-1.686209	2.209665
29	1	0	3.757961	-0.117720	1.914078
30	7	0	6.004234	-1.168714	0.780602
31	7	0	3.245933	-1.276703	0.183906
32	6	0	1.856873	-1.114726	-0.070967
33	6	0	1.166008	0.133930	0.049890
34	6	0	1.151524	-2.240122	-0.455827
35	6	0	1.799627	1.341648	0.434845
36	6	0	-0.231485	0.172997	-0.230767
37	6	0	-0.223681	-2.192428	-0.729932
38	1	0	1.695791	-3.174907	-0.540400
39	6	0	1.091046	2.518285	0.538950

40	1	0	2.861018	1.338793	0.650996
41	6	0	-0.938950	1.392645	-0.116971
42	6	0	-0.912684	-1.002666	-0.620487
43	1	0	-0.763309	-3.084933	-1.029615
44	6	0	-0.285660	2.547142	0.263676
45	1	0	1.598440	3.430317	0.836229
46	1	0	-0.855230	3.467120	0.343935
47	6	0	-2.358764	-0.972921	-0.911391
48	6	0	-2.387210	1.447678	-0.402064
49	8	0	-2.984684	-1.969367	-1.244372
50	8	0	-3.036949	2.479427	-0.307965
51	7	0	-2.998851	0.259851	-0.796659
52	6	0	-4.439853	0.302774	-1.078368
53	1	0	-4.634814	-0.450851	-1.841363
54	1	0	-4.654074	1.293309	-1.479935
55	6	0	-5.264092	0.040306	0.142645
56	6	0	-5.734472	1.019684	1.070008
57	6	0	-5.713017	-1.236648	0.599044
58	1	0	-5.565753	2.085352	0.989564
59	6	0	-6.478618	0.351869	2.082058
60	1	0	-5.525387	-2.177991	0.099833
61	6	0	-6.465290	-1.043122	1.790921
62	1	0	-6.990102	0.823103	2.911241
63	1	0	-6.964576	-1.816072	2.360551
64	6	0	-8.836759	-1.021063	-0.546092
65	6	0	-8.083572	-0.373115	-1.566867
66	1	0	-7.579098	-0.860413	-2.391069
67	6	0	-8.084564	1.025482	-1.293741
68	1	0	-7.580983	1.787663	-1.874064
69	6	0	-9.303141	-0.023781	0.357318
70	1	0	-9.885945	-0.198984	1.252164
71	6	0	-8.838276	1.240790	-0.104304
72	1	0	-9.005255	2.194775	0.378446
73	1	0	-9.002546	-2.086785	-0.457837
74	26	0	-7.277740	-0.002134	0.253842
75	1	0	11.142288	1.356521	-1.393847

A (PBE0/6-31G(d,p) in THF solvent type II)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.797293	-1.375999	0.617075
2	6	0	-8.230525	-1.924365	1.821301
3	6	0	-8.461726	-0.267935	0.078484
4	6	0	-9.331842	-1.373718	2.479708

5	1	0	-7.710076	-2.778768	2.245663
6	6	0	-9.556422	0.282003	0.744386
7	1	0	-8.091988	0.149750	-0.851181
8	6	0	-9.995359	-0.277720	1.951550
9	1	0	-9.670311	-1.801270	3.419324
10	8	0	-10.260115	1.355238	0.303217
11	6	0	-9.856148	1.953501	-0.911785
12	1	0	-8.831331	2.339317	-0.850452
13	1	0	-9.924025	1.249871	-1.750232
14	1	0	-10.542041	2.783596	-1.083682
15	6	0	-6.646184	-1.995567	-0.140700
16	1	0	-7.049749	-2.606580	-0.959358
17	1	0	-6.102421	-2.690703	0.526312
18	6	0	-5.001011	-0.282711	0.268849
19	6	0	-4.852669	-1.612725	-1.701195
20	6	0	-4.168792	0.823324	-0.369400
21	1	0	-4.331448	-0.959585	0.835677
22	1	0	-5.698477	0.166446	0.983312
23	6	0	-4.010739	-0.524903	-2.357336
24	1	0	-4.196871	-2.367952	-1.226323
25	1	0	-5.439887	-2.125387	-2.471381
26	1	0	-3.588222	1.322667	0.406112
27	1	0	-4.836965	1.561616	-0.831067
28	1	0	-3.318572	-0.945851	-3.089090
29	1	0	-4.688604	0.150758	-2.895386
30	7	0	-5.759351	-1.009901	-0.737092
31	7	0	-3.275512	0.285726	-1.397199
32	6	0	-1.950683	0.016477	-1.112663
33	6	0	-1.109313	1.059335	-0.573609
34	6	0	-1.367961	-1.223784	-1.383305
35	6	0	-1.519806	2.409256	-0.485891
36	6	0	0.223808	0.741894	-0.187627
37	6	0	-0.045171	-1.498116	-1.037087
38	1	0	-1.966461	-2.019706	-1.810396
39	6	0	-0.694578	3.379172	0.046122
40	1	0	-2.489629	2.693830	-0.878983
41	6	0	1.045892	1.745495	0.376994
42	6	0	0.747541	-0.551692	-0.411644
43	1	0	0.371656	-2.483615	-1.220134
44	6	0	0.585437	3.041795	0.506389
45	1	0	-1.031854	4.409491	0.093142
46	1	0	1.244498	3.788156	0.937680
47	6	0	2.115270	-0.890102	-0.015349
48	6	0	2.419818	1.425068	0.811596
49	8	0	2.612184	-1.996453	-0.193968
50	8	0	3.154560	2.253185	1.335470
51	7	0	2.857990	0.121510	0.602979
52	6	0	4.225901	-0.204978	1.021789

53	1	0	4.231416	-1.263792	1.280473
54	1	0	4.437386	0.390138	1.910515
55	6	0	5.232797	0.078116	-0.048917
56	6	0	5.956942	1.296147	-0.225954
57	6	0	5.637635	-0.818331	-1.084686
58	1	0	5.875146	2.166617	0.411249
59	6	0	6.811489	1.146087	-1.353510
60	1	0	5.271822	-1.828567	-1.211449
61	6	0	6.613545	-0.161436	-1.884900
62	1	0	7.509937	1.884350	-1.725529
63	1	0	7.135440	-0.589374	-2.730942
64	6	0	8.505177	-1.807073	0.301968
65	6	0	7.634620	-1.686716	1.423122
66	1	0	6.943382	-2.441420	1.775097
67	6	0	7.810342	-0.386336	1.978866
68	1	0	7.276173	0.020518	2.827636
69	6	0	9.218797	-0.582134	0.165052
70	1	0	9.941174	-0.349887	-0.606552
71	6	0	8.789581	0.295805	1.201036
72	1	0	9.128077	1.312150	1.354433
73	1	0	8.589498	-2.668397	-0.347701
74	26	0	7.219903	-0.261322	0.045713
75	1	0	-10.849273	0.166062	2.453748

A (PBE0/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.401527	-0.840209	0.262020
2	6	0	9.487885	-1.445114	-0.364650
3	6	0	8.302135	0.555708	0.286059
4	6	0	10.477559	-0.657104	-0.955352
5	1	0	9.562027	-2.528957	-0.392896
6	6	0	9.289572	1.337249	-0.312554
7	1	0	7.436061	0.998819	0.764681
8	6	0	10.386198	0.725652	-0.934148
9	1	0	11.325315	-1.128886	-1.444274
10	8	0	9.276431	2.694166	-0.343626
11	6	0	8.188296	3.355586	0.269127
12	1	0	7.235335	3.086202	-0.202239
13	1	0	8.132505	3.132603	1.341451
14	1	0	8.366666	4.422759	0.133337
15	6	0	7.353638	-1.675089	0.961019

16	1	0	7.563029	-1.671339	2.039306
17	1	0	7.447591	-2.727239	0.631396
18	6	0	5.542838	-1.327038	-0.590193
19	6	0	5.065964	-1.796811	1.699080
20	6	0	4.176927	-0.685251	-0.766579
21	1	0	5.479645	-2.396702	-0.868821
22	1	0	6.260079	-0.845474	-1.262388
23	6	0	3.692403	-1.159264	1.565056
24	1	0	4.978065	-2.884132	1.510946
25	1	0	5.428395	-1.661846	2.724393
26	1	0	3.810483	-0.873098	-1.780308
27	1	0	4.283959	0.406904	-0.645564
28	1	0	2.979750	-1.681034	2.210889
29	1	0	3.758021	-0.113668	1.912656
30	7	0	6.003752	-1.167646	0.781854
31	7	0	3.245599	-1.275641	0.184424
32	6	0	1.856806	-1.113403	-0.071735
33	6	0	1.165742	0.135047	0.050091
34	6	0	1.151952	-2.238283	-0.459003
35	6	0	1.799269	1.342660	0.435525
36	6	0	-0.231701	0.174174	-0.230803
37	6	0	-0.223108	-2.190433	-0.733803
38	1	0	1.696378	-3.172901	-0.544393
39	6	0	1.090504	2.519101	0.540580
40	1	0	2.860817	1.339957	0.650903
41	6	0	-0.939407	1.393567	-0.115789
42	6	0	-0.912509	-1.001077	-0.622438
43	1	0	-0.762409	-3.082607	-1.035058
44	6	0	-0.286305	2.547857	0.265807
45	1	0	1.597851	3.431074	0.838119
46	1	0	-0.856047	3.467652	0.346938
47	6	0	-2.358567	-0.971308	-0.913441
48	6	0	-2.387654	1.448617	-0.400920
49	8	0	-2.984197	-1.967461	-1.247843
50	8	0	-3.037690	2.480042	-0.305300
51	7	0	-2.999017	0.261113	-0.796931
52	6	0	-4.440063	0.304003	-1.078443
53	1	0	-4.634894	-0.448650	-1.842430
54	1	0	-4.654612	1.295020	-1.478638
55	6	0	-5.264049	0.039637	0.142332
56	6	0	-5.734345	1.017598	1.071237
57	6	0	-5.712697	-1.238040	0.596973
58	1	0	-5.565783	2.083406	0.992316
59	6	0	-6.478141	0.348202	2.082502
60	1	0	-5.525060	-2.178629	0.096345
61	6	0	-6.464700	-1.046360	1.789322
62	1	0	-6.989467	0.818156	2.912508
63	1	0	-6.963724	-1.820215	2.357952

64	6	0	-8.836747	-1.021212	-0.547049
65	6	0	-8.083934	-0.371644	-1.567072
66	1	0	-7.579636	-0.857643	-2.392147
67	6	0	-8.085065	1.026549	-1.291882
68	1	0	-7.581789	1.789666	-1.871239
69	6	0	-9.303041	-0.025334	0.357955
70	1	0	-9.885612	-0.201940	1.252677
71	6	0	-8.838491	1.239987	-0.101925
72	1	0	-9.005510	2.193237	0.382260
73	1	0	-9.002378	-2.087086	-0.460342
74	26	0	-7.277670	-0.003233	0.253973
75	1	0	11.143524	1.352568	-1.394353

A (PBE0/6-31G(d,p) in water solvent type I)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.406083	-0.839218	0.254021
2	6	0	9.497508	-1.439959	-0.368716
3	6	0	8.301890	0.556408	0.278856
4	6	0	10.486974	-0.647998	-0.954646
5	1	0	9.575600	-2.523494	-0.397606
6	6	0	9.289097	1.342141	-0.315285
7	1	0	7.432805	0.996602	0.754685
8	6	0	10.390614	0.734773	-0.932789
9	1	0	11.338444	-1.116365	-1.440412
10	8	0	9.270991	2.699011	-0.345271
11	6	0	8.176137	3.356789	0.262546
12	1	0	7.227079	3.083594	-0.213837
13	1	0	8.116209	3.133241	1.334269
14	1	0	8.351259	4.424530	0.127731
15	6	0	7.358992	-1.679322	0.948385
16	1	0	7.570296	-1.683175	2.026245
17	1	0	7.452947	-2.728925	0.611335
18	6	0	5.543349	-1.326344	-0.596181
19	6	0	5.073705	-1.803766	1.693247
20	6	0	4.176579	-0.684693	-0.766525
21	1	0	5.480567	-2.395164	-0.878040
22	1	0	6.257516	-0.841916	-1.269607
23	6	0	3.699452	-1.166609	1.565335
24	1	0	4.986330	-2.890472	1.501708
25	1	0	5.438885	-1.672092	2.717861
26	1	0	3.807853	-0.869020	-1.780026

27	1	0	4.282869	0.406845	-0.641303
28	1	0	2.989578	-1.690623	2.212315
29	1	0	3.765140	-0.121765	1.914673
30	7	0	6.008650	-1.171052	0.774985
31	7	0	3.248472	-1.280105	0.185206
32	6	0	1.859047	-1.116903	-0.066107
33	6	0	1.168617	0.131898	0.058027
34	6	0	1.152490	-2.241506	-0.451688
35	6	0	1.803631	1.338690	0.443741
36	6	0	-0.229301	0.172117	-0.220590
37	6	0	-0.222955	-2.192695	-0.723450
38	1	0	1.695183	-3.176866	-0.539338
39	6	0	1.096080	2.515845	0.550568
40	1	0	2.865269	1.335956	0.658246
41	6	0	-0.935895	1.392141	-0.104341
42	6	0	-0.911602	-1.002671	-0.611200
43	1	0	-0.761858	-3.085331	-1.023885
44	6	0	-0.280855	2.545835	0.277113
45	1	0	1.604679	3.426994	0.848080
46	1	0	-0.847844	3.467212	0.359344
47	6	0	-2.357154	-0.971179	-0.900896
48	6	0	-2.383624	1.447985	-0.388656
49	8	0	-2.985121	-1.967154	-1.233963
50	8	0	-3.034002	2.479854	-0.291926
51	7	0	-2.996657	0.261490	-0.784865
52	6	0	-4.436149	0.307340	-1.075329
53	1	0	-4.627114	-0.442122	-1.843267
54	1	0	-4.646325	1.299182	-1.475368
55	6	0	-5.271290	0.041725	0.138136
56	6	0	-5.743998	1.018415	1.068533
57	6	0	-5.720609	-1.237393	0.590843
58	1	0	-5.572286	2.084073	0.994969
59	6	0	-6.491117	0.347202	2.077158
60	1	0	-5.527633	-2.178128	0.092589
61	6	0	-6.476663	-1.047576	1.781782
62	1	0	-7.001017	0.815401	2.909007
63	1	0	-6.973737	-1.822726	2.350327
64	6	0	-9.171087	-0.696222	0.015034
65	6	0	-8.414754	-0.893094	-1.176611
66	1	0	-8.206393	-1.844663	-1.647905
67	6	0	-7.957370	0.380844	-1.623102
68	1	0	-7.341153	0.566360	-2.493416
69	6	0	-9.181645	0.699181	0.304724
70	1	0	-9.658327	1.168463	1.155376
71	6	0	-8.431903	1.365038	-0.707866
72	1	0	-8.238930	2.428499	-0.761069
73	1	0	-9.638257	-1.472279	0.607106
74	26	0	-7.282987	-0.002120	0.246790

75	1	0	11.148162	1.363960	-1.389773

A (PBE0/6-31G(d,p) in water solvent type II)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.821474	-1.353943	0.640812
2	6	0	-8.284671	-1.887029	1.841283
3	6	0	-8.460038	-0.240602	0.082252
4	6	0	-9.389666	-1.315656	2.475453
5	1	0	-7.784481	-2.745502	2.281474
6	6	0	-9.558182	0.330818	0.724599
7	1	0	-8.068068	0.164319	-0.843936
8	6	0	-10.027431	-0.213550	1.927494
9	1	0	-9.751414	-1.731222	3.411796
10	8	0	-10.236961	1.411498	0.262851
11	6	0	-9.798319	1.997754	-0.947470
12	1	0	-8.768733	2.366150	-0.866742
13	1	0	-9.861473	1.291246	-1.783542
14	1	0	-10.466552	2.838349	-1.136555
15	6	0	-6.666585	-1.997962	-0.091012
16	1	0	-7.067010	-2.629859	-0.895172
17	1	0	-6.131156	-2.676877	0.598788
18	6	0	-5.012177	-0.285885	0.282722
19	6	0	-4.864517	-1.665037	-1.653540
20	6	0	-4.169618	0.799204	-0.377815
21	1	0	-4.349825	-0.952909	0.869091
22	1	0	-5.708824	0.186748	0.982661
23	6	0	-4.015255	-0.598268	-2.333314
24	1	0	-4.213659	-2.410697	-1.157711
25	1	0	-5.451309	-2.193760	-2.412818
26	1	0	-3.588523	1.310670	0.389056
27	1	0	-4.829257	1.532375	-0.859055
28	1	0	-3.325153	-1.039991	-3.054301
29	1	0	-4.687135	0.070329	-2.887271
30	7	0	-5.771417	-1.032908	-0.707932
31	7	0	-3.277226	0.228423	-1.388495
32	6	0	-1.952227	-0.028667	-1.106251
33	6	0	-1.111343	1.024878	-0.584974
34	6	0	-1.365036	-1.271337	-1.362508
35	6	0	-1.523777	2.375331	-0.520021
36	6	0	0.223441	0.716439	-0.196750
37	6	0	-0.042062	-1.536353	-1.013998
38	1	0	-1.961505	-2.075498	-1.776613

39	6	0	-0.699974	3.356108	-0.004985
40	1	0	-2.494244	2.653034	-0.916170
41	6	0	1.043882	1.730908	0.350905
42	6	0	0.750447	-0.578948	-0.402612
43	1	0	0.375140	-2.524064	-1.183773
44	6	0	0.580484	3.028670	0.459848
45	1	0	-1.039667	4.386136	0.025341
46	1	0	1.236964	3.784327	0.878714
47	6	0	2.118236	-0.907189	-0.003740
48	6	0	2.418123	1.420181	0.788289
49	8	0	2.620229	-2.014731	-0.167072
50	8	0	3.152633	2.258415	1.298421
51	7	0	2.859940	0.115336	0.598408
52	6	0	4.227559	-0.203393	1.025539
53	1	0	4.232116	-1.255948	1.308128
54	1	0	4.438050	0.409713	1.901964
55	6	0	5.237508	0.054694	-0.049288
56	6	0	5.941345	1.278464	-0.271825
57	6	0	5.654948	-0.870602	-1.055433
58	1	0	5.844709	2.171193	0.331539
59	6	0	6.796574	1.102731	-1.396089
60	1	0	5.303036	-1.889299	-1.149085
61	6	0	6.619230	-0.226414	-1.880895
62	1	0	7.478898	1.840271	-1.798207
63	1	0	7.143751	-0.674006	-2.715028
64	6	0	8.985373	-1.253441	0.081444
65	6	0	8.020299	-1.902907	0.904625
66	1	0	7.656989	-2.914806	0.781735
67	6	0	7.596915	-0.976244	1.901421
68	1	0	6.856015	-1.161442	2.668463
69	6	0	9.158994	0.074220	0.569734
70	1	0	9.812426	0.826616	0.147820
71	6	0	8.301206	0.245593	1.694754
72	1	0	8.188329	1.150957	2.276656
73	1	0	9.483716	-1.685948	-0.776258
74	26	0	7.228525	-0.246902	0.049525
75	1	0	-10.883364	0.246051	2.411968

A (ωB97XD/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.389775	-0.799609	0.268995

2	6	0	9.533010	-1.327013	-0.322032
3	6	0	8.190546	0.584760	0.286743
4	6	0	10.481907	-0.470928	-0.884113
5	1	0	9.684480	-2.402170	-0.347141
6	6	0	9.135603	1.433340	-0.285820
7	1	0	7.279160	0.961218	0.735608
8	6	0	10.291469	0.901490	-0.870996
9	1	0	11.374871	-0.881484	-1.345121
10	8	0	9.022090	2.786655	-0.325402
11	6	0	7.862657	3.369107	0.238169
12	1	0	6.953118	3.021924	-0.266214
13	1	0	7.783651	3.151755	1.309718
14	1	0	7.964346	4.444685	0.096209
15	6	0	7.372472	-1.706243	0.930685
16	1	0	7.579217	-1.737730	2.007644
17	1	0	7.503611	-2.738645	0.556722
18	6	0	5.557770	-1.355209	-0.622332
19	6	0	5.076618	-1.917369	1.651831
20	6	0	4.184338	-0.720805	-0.782408
21	1	0	5.510226	-2.414898	-0.936181
22	1	0	6.271082	-0.841087	-1.272530
23	6	0	3.692432	-1.293457	1.535268
24	1	0	5.008096	-2.996845	1.420615
25	1	0	5.432114	-1.814686	2.682114
26	1	0	3.820715	-0.876642	-1.801710
27	1	0	4.283598	0.366012	-0.622384
28	1	0	2.981711	-1.852243	2.150221
29	1	0	3.741302	-0.263579	1.926985
30	7	0	6.006485	-1.236480	0.760570
31	7	0	3.254836	-1.353457	0.145870
32	6	0	1.863815	-1.178202	-0.103801
33	6	0	1.184841	0.075682	0.044088
34	6	0	1.152629	-2.287641	-0.507740
35	6	0	1.829487	1.268822	0.463194
36	6	0	-0.206549	0.134266	-0.239704
37	6	0	-0.224483	-2.221262	-0.780734
38	1	0	1.686847	-3.225051	-0.612127
39	6	0	1.134437	2.447184	0.590323
40	1	0	2.887883	1.251600	0.688910
41	6	0	-0.902257	1.360224	-0.103946
42	6	0	-0.898690	-1.029300	-0.652463
43	1	0	-0.768739	-3.104465	-1.095865
44	6	0	-0.242034	2.496630	0.304949
45	1	0	1.647619	3.346005	0.913135
46	1	0	-0.798707	3.421783	0.402701
47	6	0	-2.348176	-0.978740	-0.944990
48	6	0	-2.352138	1.435348	-0.397507
49	8	0	-2.985007	-1.964179	-1.283405

50	8	0	-2.991354	2.469328	-0.282173
51	7	0	-2.973877	0.262670	-0.825508
52	6	0	-4.418187	0.321908	-1.092900
53	1	0	-4.634628	-0.422180	-1.857756
54	1	0	-4.634153	1.315166	-1.483630
55	6	0	-5.224665	0.056678	0.141124
56	6	0	-5.677709	1.034724	1.076797
57	6	0	-5.663302	-1.221445	0.601966
58	1	0	-5.504284	2.098655	0.997349
59	6	0	-6.409561	0.365689	2.097017
60	1	0	-5.477106	-2.161005	0.100981
61	6	0	-6.400605	-1.029143	1.803404
62	1	0	-6.904035	0.834612	2.936304
63	1	0	-6.887204	-1.802620	2.381146
64	6	0	-9.139511	-0.665993	0.043560
65	6	0	-8.387942	-0.874205	-1.148723
66	1	0	-8.186401	-1.828630	-1.614702
67	6	0	-7.924046	0.393853	-1.603372
68	1	0	-7.308838	0.570408	-2.475014
69	6	0	-9.140867	0.730482	0.325235
70	1	0	-9.612860	1.207322	1.172909
71	6	0	-8.389480	1.385723	-0.692604
72	1	0	-8.189535	2.446477	-0.752013
73	1	0	-9.610716	-1.435023	0.639636
74	26	0	-7.237365	0.016278	0.270511
75	1	0	11.015492	1.578498	-1.311474

A (TPSSh/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.434958	-0.836272	0.269300
2	6	0	9.513208	-1.444573	-0.379711
3	6	0	8.339301	0.564815	0.299228
4	6	0	10.498363	-0.655186	-0.987674
5	1	0	9.584580	-2.528405	-0.411368
6	6	0	9.323094	1.346361	-0.316676
7	1	0	7.483353	1.011115	0.792691
8	6	0	10.411328	0.732969	-0.961181
9	1	0	11.336207	-1.127924	-1.492123
10	8	0	9.315135	2.714816	-0.344732
11	6	0	8.226164	3.380523	0.297024
12	1	0	7.268706	3.109788	-0.162883

13	1	0	8.194144	3.148479	1.367774
14	1	0	8.410335	4.445697	0.158706
15	6	0	7.390691	-1.673729	0.985475
16	1	0	7.593494	-1.652109	2.064414
17	1	0	7.487201	-2.728409	0.666957
18	6	0	5.566801	-1.350598	-0.584517
19	6	0	5.085415	-1.799251	1.725480
20	6	0	4.194380	-0.707639	-0.768868
21	1	0	5.503962	-2.423886	-0.846021
22	1	0	6.286541	-0.875498	-1.258192
23	6	0	3.705972	-1.158405	1.583824
24	1	0	4.999216	-2.886920	1.542859
25	1	0	5.451060	-1.653065	2.747830
26	1	0	3.825407	-0.904994	-1.779335
27	1	0	4.295369	0.384628	-0.649350
28	1	0	2.990596	-1.669716	2.234145
29	1	0	3.772379	-0.106129	1.908367
30	7	0	6.027797	-1.165100	0.797006
31	7	0	3.257693	-1.305421	0.192678
32	6	0	1.860362	-1.131217	-0.066273
33	6	0	1.170997	0.124050	0.049392
34	6	0	1.150926	-2.260851	-0.452297
35	6	0	1.809068	1.335862	0.429622
36	6	0	-0.233105	0.165507	-0.235617
37	6	0	-0.227050	-2.210987	-0.731003
38	1	0	1.692624	-3.197177	-0.532857
39	6	0	1.100585	2.519969	0.527624
40	1	0	2.870318	1.331227	0.645429
41	6	0	-0.939238	1.392514	-0.127685
42	6	0	-0.917983	-1.014302	-0.625122
43	1	0	-0.766845	-3.103226	-1.029871
44	6	0	-0.279366	2.551947	0.250357
45	1	0	1.610612	3.431760	0.820262
46	1	0	-0.845402	3.474103	0.325437
47	6	0	-2.365850	-0.983320	-0.920950
48	6	0	-2.389291	1.452324	-0.417446
49	8	0	-2.999595	-1.984815	-1.257707
50	8	0	-3.042634	2.493357	-0.331853
51	7	0	-3.007829	0.257625	-0.808115
52	6	0	-4.461217	0.305646	-1.103636
53	1	0	-4.645765	-0.455017	-1.861300
54	1	0	-4.660109	1.296647	-1.510235
55	6	0	-5.296673	0.053621	0.119980
56	6	0	-5.766304	1.045696	1.046556
57	6	0	-5.741338	-1.226933	0.595270
58	1	0	-5.593562	2.109835	0.961544
59	6	0	-6.506416	0.382433	2.074480
60	1	0	-5.546647	-2.174115	0.111149

61	6	0	-6.490917	-1.022424	1.795598
62	1	0	-7.006404	0.859508	2.906928
63	1	0	-6.977320	-1.791777	2.380456
64	6	0	-9.185276	-0.711142	0.055892
65	6	0	-8.437790	-0.909108	-1.148955
66	1	0	-8.230941	-1.860666	-1.620145
67	6	0	-7.994887	0.372134	-1.609638
68	1	0	-7.395497	0.558509	-2.490959
69	6	0	-9.204281	0.692132	0.339573
70	1	0	-9.678906	1.162434	1.190398
71	6	0	-8.468599	1.361872	-0.689881
72	1	0	-8.289213	2.426777	-0.753621
73	1	0	-9.642993	-1.487192	0.654714
74	26	0	-7.304707	0.004392	0.255718
75	1	0	11.162833	1.358313	-1.432384

A (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.401527	-0.840209	0.262020
2	6	0	9.487885	-1.445114	-0.364650
3	6	0	8.302135	0.555708	0.286059
4	6	0	10.477559	-0.657104	-0.955352
5	1	0	9.562027	-2.528957	-0.392896
6	6	0	9.289572	1.337249	-0.312554
7	1	0	7.436061	0.998819	0.764681
8	6	0	10.386198	0.725652	-0.934148
9	1	0	11.325315	-1.128886	-1.444274
10	8	0	9.276431	2.694166	-0.343626
11	6	0	8.188296	3.355586	0.269127
12	1	0	7.235335	3.086202	-0.202239
13	1	0	8.132505	3.132603	1.341451
14	1	0	8.366666	4.422759	0.133337
15	6	0	7.353638	-1.675089	0.961019
16	1	0	7.563029	-1.671339	2.039306
17	1	0	7.447591	-2.727239	0.631396
18	6	0	5.542838	-1.327038	-0.590193
19	6	0	5.065964	-1.796811	1.699080

20	6	0	4.176927	-0.685251	-0.766579
21	1	0	5.479645	-2.396702	-0.868821
22	1	0	6.260079	-0.845474	-1.262388
23	6	0	3.692403	-1.159264	1.565056
24	1	0	4.978065	-2.884132	1.510946
25	1	0	5.428395	-1.661846	2.724393
26	1	0	3.810483	-0.873098	-1.780308
27	1	0	4.283959	0.406904	-0.645564
28	1	0	2.979750	-1.681034	2.210889
29	1	0	3.758021	-0.113668	1.912656
30	7	0	6.003752	-1.167646	0.781854
31	7	0	3.245599	-1.275641	0.184424
32	6	0	1.856806	-1.113403	-0.071735
33	6	0	1.165742	0.135047	0.050091
34	6	0	1.151952	-2.238283	-0.459003
35	6	0	1.799269	1.342660	0.435525
36	6	0	-0.231701	0.174174	-0.230803
37	6	0	-0.223108	-2.190433	-0.733803
38	1	0	1.696378	-3.172901	-0.544393
39	6	0	1.090504	2.519101	0.540580
40	1	0	2.860817	1.339957	0.650903
41	6	0	-0.939407	1.393567	-0.115789
42	6	0	-0.912509	-1.001077	-0.622438
43	1	0	-0.762409	-3.082607	-1.035058
44	6	0	-0.286305	2.547857	0.265807
45	1	0	1.597851	3.431074	0.838119
46	1	0	-0.856047	3.467652	0.346938
47	6	0	-2.358567	-0.971308	-0.913441
48	6	0	-2.387654	1.448617	-0.400920
49	8	0	-2.984197	-1.967461	-1.247843
50	8	0	-3.037690	2.480042	-0.305300
51	7	0	-2.999017	0.261113	-0.796931
52	6	0	-4.440063	0.304003	-1.078443
53	1	0	-4.634894	-0.448650	-1.842430
54	1	0	-4.654612	1.295020	-1.478638
55	6	0	-5.264049	0.039637	0.142332
56	6	0	-5.734345	1.017598	1.071237
57	6	0	-5.712697	-1.238040	0.596973
58	1	0	-5.565783	2.083406	0.992316
59	6	0	-6.478141	0.348202	2.082502
60	1	0	-5.525060	-2.178629	0.096345
61	6	0	-6.464700	-1.046360	1.789322
62	1	0	-6.989467	0.818156	2.912508
63	1	0	-6.963724	-1.820215	2.357952
64	6	0	-8.836747	-1.021212	-0.547049
65	6	0	-8.083934	-0.371644	-1.567072
66	1	0	-7.579636	-0.857643	-2.392147
67	6	0	-8.085065	1.026549	-1.291882

68	1	0	-7.581789	1.789666	-1.871239
69	6	0	-9.303041	-0.025334	0.357955
70	1	0	-9.885612	-0.201940	1.252677
71	6	0	-8.838491	1.239987	-0.101925
72	1	0	-9.005510	2.193237	0.382260
73	1	0	-9.002378	-2.087086	-0.460342
74	26	0	-7.277670	-0.003233	0.253973
75	1	0	11.143524	1.352568	-1.394353

A-W_d-m_1 (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.183753	-0.815201	0.227428
2	6	0	9.078928	-1.512037	-0.580733
3	6	0	8.221057	0.584254	0.258978
4	6	0	10.008331	-0.812622	-1.354220
5	1	0	9.050441	-2.597792	-0.609100
6	6	0	9.140839	1.277335	-0.526633
7	1	0	7.506213	1.118275	0.874631
8	6	0	10.044243	0.572688	-1.334038
9	1	0	10.707261	-1.356262	-1.983529
10	8	0	9.232427	2.629649	-0.573891
11	6	0	8.363978	3.375687	0.260537
12	1	0	7.310574	3.149974	0.059452
13	1	0	8.569549	3.183043	1.320608
14	1	0	8.562226	4.425176	0.040956
15	6	0	7.187150	-1.553718	1.087305
16	1	0	7.395087	-1.349789	2.145012
17	1	0	7.312897	-2.640310	0.940737
18	6	0	5.369496	-1.507390	-0.514517
19	6	0	4.902502	-1.802845	1.800064
20	6	0	3.963914	-0.993582	-0.770717
21	1	0	5.399317	-2.602657	-0.655781
22	1	0	6.057838	-1.053669	-1.233316
23	6	0	3.480507	-1.301436	1.617086
24	1	0	4.929690	-2.900245	1.678694
25	1	0	5.240293	-1.566296	2.814494
26	1	0	3.627579	-1.343655	-1.751862
27	1	0	3.989655	0.106414	-0.802657
28	1	0	2.813686	-1.862829	2.279199
29	1	0	3.438415	-0.245029	1.922820
30	7	0	5.798288	-1.156404	0.840047

31	7	0	3.052779	-1.523752	0.239729
32	6	0	1.666055	-1.331700	-0.016310
33	6	0	1.020391	-0.052253	0.024660
34	6	0	0.922510	-2.457159	-0.319308
35	6	0	1.695827	1.160292	0.322581
36	6	0	-0.378279	0.010802	-0.251125
37	6	0	-0.451776	-2.383243	-0.588686
38	1	0	1.435278	-3.413016	-0.343537
39	6	0	1.018501	2.360464	0.347733
40	1	0	2.760881	1.160695	0.534836
41	6	0	-1.048918	1.256375	-0.218344
42	6	0	-1.100042	-1.166167	-0.556815
43	1	0	-1.021299	-3.276186	-0.824734
44	6	0	-0.358059	2.413810	0.078643
45	1	0	1.555372	3.275168	0.577987
46	1	0	-0.897105	3.355275	0.097802
47	6	0	-2.545254	-1.110214	-0.844833
48	6	0	-2.495326	1.337271	-0.501573
49	8	0	-3.204728	-2.107272	-1.106807
50	8	0	-3.113618	2.393021	-0.474835
51	7	0	-3.146596	0.146097	-0.813564
52	6	0	-4.584418	0.216345	-1.106361
53	1	0	-4.799993	-0.577485	-1.821430
54	1	0	-4.764479	1.184679	-1.573128
55	6	0	-5.425914	0.060004	0.121715
56	6	0	-5.861891	1.111395	0.986285
57	6	0	-5.920633	-1.169898	0.656056
58	1	0	-5.651983	2.163086	0.843818
59	6	0	-6.631650	0.534615	2.035469
60	1	0	-5.762891	-2.147473	0.220286
61	6	0	-6.668050	-0.876011	1.831264
62	1	0	-7.123256	1.074050	2.834539
63	1	0	-7.192044	-1.594151	2.448423
64	6	0	-9.351770	-0.538735	0.045615
65	6	0	-8.605530	-0.846575	-1.128723
66	1	0	-8.434707	-1.835779	-1.532854
67	6	0	-8.099843	0.374814	-1.661643
68	1	0	-7.478199	0.475626	-2.541982
69	6	0	-9.307978	0.872717	0.238145
70	1	0	-9.764889	1.417762	1.053754
71	6	0	-8.534553	1.437541	-0.817136
72	1	0	-8.300608	2.486503	-0.943483
73	1	0	-9.847804	-1.253280	0.689386
74	26	0	-7.437839	0.096129	0.230868
75	1	0	10.756245	1.130520	-1.934446
76	8	0	5.111504	1.621535	1.056333
77	1	0	5.405795	0.681000	1.016711
78	1	0	5.074204	1.818504	1.998152

A-W$_d$-m$_2$ (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.118437	-2.053069	0.686150
2	6	0	7.427951	-3.377759	0.388007
3	6	0	8.066368	-1.048833	0.457183
4	6	0	8.685708	-3.699114	-0.126313
5	1	0	6.689963	-4.157507	0.556078
6	6	0	9.317886	-1.374941	-0.064622
7	1	0	7.792604	-0.024158	0.682255
8	6	0	9.629764	-2.710038	-0.354357
9	1	0	8.927883	-4.732383	-0.358682
10	8	0	10.296926	-0.471745	-0.324151
11	6	0	10.026810	0.889713	-0.050954
12	1	0	9.182640	1.259850	-0.644777
13	1	0	9.815676	1.053025	1.012460
14	1	0	10.927735	1.438541	-0.326603
15	6	0	5.786009	-1.695354	1.302961
16	1	0	5.921270	-1.566847	2.385219
17	1	0	5.086405	-2.542701	1.176074
18	6	0	4.811098	-0.582832	-0.598760
19	6	0	4.123727	0.023751	1.594777
20	6	0	4.318984	0.761362	-1.120756
21	1	0	4.027121	-1.356840	-0.700927
22	1	0	5.664726	-0.901946	-1.205249
23	6	0	3.662306	1.391059	1.111840
24	1	0	3.269202	-0.680823	1.578441
25	1	0	4.452121	0.115520	2.636017
26	1	0	3.979999	0.683879	-2.156018
27	1	0	5.161794	1.463328	-1.104232
28	1	0	2.828820	1.732412	1.725482
29	1	0	4.481776	2.111323	1.215048
30	7	0	5.234386	-0.453161	0.787393
31	7	0	3.259461	1.368041	-0.308030
32	6	0	1.920676	1.077654	-0.599883
33	6	0	0.889058	1.951061	-0.098012
34	6	0	1.547476	0.005016	-1.403183
35	6	0	1.160406	3.182388	0.546493
36	6	0	-0.473764	1.597581	-0.312250
37	6	0	0.203268	-0.296606	-1.640298
38	1	0	2.301328	-0.651085	-1.819539

39	6	0	0.141255	3.975251	1.032407
40	1	0	2.183126	3.539217	0.613799
41	6	0	-1.501783	2.415874	0.212074
42	6	0	-0.808243	0.459072	-1.080730
43	1	0	-0.061329	-1.159446	-2.243067
44	6	0	-1.195954	3.579176	0.891178
45	1	0	0.376011	4.918845	1.514008
46	1	0	-2.006426	4.187106	1.279465
47	6	0	-2.208746	0.084806	-1.306121
48	6	0	-2.918558	2.046307	0.024461
49	8	0	-2.540242	-0.896267	-1.961263
50	8	0	-3.837215	2.701739	0.500245
51	7	0	-3.180126	0.909552	-0.734198
52	6	0	-4.586682	0.539820	-0.936929
53	1	0	-4.648625	0.056244	-1.911712
54	1	0	-5.158987	1.467296	-0.953603
55	6	0	-5.096049	-0.373034	0.134600
56	6	0	-5.695904	0.024580	1.369469
57	6	0	-5.047448	-1.801342	0.119980
58	1	0	-5.878522	1.046743	1.673299
59	6	0	-6.027644	-1.150083	2.101915
60	1	0	-4.652804	-2.403261	-0.687753
61	6	0	-5.626781	-2.279264	1.329115
62	1	0	-6.519397	-1.181616	3.065451
63	1	0	-5.761163	-3.317436	1.603595
64	6	0	-7.958049	-1.856134	-1.306206
65	6	0	-7.999469	-0.431715	-1.278013
66	1	0	-7.618436	0.230946	-2.044344
67	6	0	-8.606615	-0.032735	-0.051769
68	1	0	-8.767088	0.985808	0.276654
69	6	0	-8.538486	-2.337329	-0.096928
70	1	0	-8.639240	-3.375624	0.190943
71	6	0	-8.939303	-1.210537	0.678233
72	1	0	-9.397964	-1.243182	1.657845
73	1	0	-7.540260	-2.464643	-2.097541
74	26	0	-6.950904	-1.144411	0.300079
75	8	0	4.239817	4.085270	-0.616844
76	1	0	3.788434	4.654005	-1.248707
77	1	0	3.789128	3.227528	-0.709979
78	1	0	10.609396	-2.942963	-0.760099

A-W_u-m_3 (PBE0/6-31G(d,p) in water solvent)

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	7.456882	-1.604522	0.673170
2	6	0	7.860524	-2.920364	0.460231
3	6	0	8.303363	-0.550213	0.310870
4	6	0	9.111445	-3.181751	-0.102307
5	1	0	7.200673	-3.739878	0.732071
6	6	0	9.548438	-0.817411	-0.258006
7	1	0	7.956238	0.464410	0.471527
8	6	0	9.955447	-2.142621	-0.462309
9	1	0	9.426850	-4.208016	-0.268358
10	8	0	10.433184	0.136542	-0.644096
11	6	0	10.065527	1.489917	-0.459789
12	1	0	9.162983	1.743245	-1.028536
13	1	0	9.898660	1.721567	0.598818
14	1	0	10.901522	2.084131	-0.829814
15	6	0	6.133547	-1.304612	1.338475
16	1	0	6.314900	-1.076908	2.397488
17	1	0	5.502419	-2.213079	1.320677
18	6	0	4.972453	-0.432949	-0.584545
19	6	0	4.347340	0.289608	1.597199
20	6	0	4.343168	0.824172	-1.169897
21	1	0	4.241127	-1.264467	-0.585879
22	1	0	5.817223	-0.736683	-1.210907
23	6	0	3.727243	1.565757	1.037670
24	1	0	3.558338	-0.481299	1.685086
25	1	0	4.726118	0.498797	2.604121
26	1	0	3.973899	0.650468	-2.182023
27	1	0	5.119084	1.598293	-1.231928
28	1	0	2.888666	1.856410	1.669654
29	1	0	4.469234	2.373934	1.050635
30	7	0	5.452379	-0.157396	0.761539
31	7	0	3.273302	1.362392	-0.340271
32	6	0	1.952742	1.103067	-0.627344
33	6	0	0.919510	1.989480	-0.140439
34	6	0	1.564789	0.025369	-1.434815
35	6	0	1.201019	3.234806	0.466440
36	6	0	-0.445565	1.647559	-0.357619
37	6	0	0.219204	-0.263371	-1.668779
38	1	0	2.315364	-0.637332	-1.849795
39	6	0	0.191606	4.053946	0.930394
40	1	0	2.229510	3.570711	0.536499
41	6	0	-1.465091	2.488484	0.147344
42	6	0	-0.790821	0.504145	-1.114311
43	1	0	-0.052679	-1.127979	-2.266282
44	6	0	-1.148094	3.665829	0.798231
45	1	0	0.436202	5.008057	1.385384
46	1	0	-1.953729	4.290800	1.169313

47	6	0	-2.190464	0.142756	-1.339828
48	6	0	-2.884809	2.131167	-0.038078
49	8	0	-2.534356	-0.842150	-1.984733
50	8	0	-3.798065	2.804589	0.424515
51	7	0	-3.155427	0.986386	-0.780013
52	6	0	-4.564871	0.630456	-0.984119
53	1	0	-4.628360	0.135036	-1.952848
54	1	0	-5.126497	1.564116	-1.014760
55	6	0	-5.089831	-0.262985	0.096251
56	6	0	-5.690803	0.156393	1.323304
57	6	0	-5.058115	-1.691749	0.098900
58	1	0	-5.862533	1.184231	1.614092
59	6	0	-6.040064	-1.005438	2.068038
60	1	0	-4.666360	-2.307584	-0.699706
61	6	0	-5.648936	-2.148417	1.310685
62	1	0	-6.536730	-1.019771	3.029467
63	1	0	-5.796838	-3.181595	1.596826
64	6	0	-7.952223	-1.695727	-1.361655
65	6	0	-7.998344	-0.272167	-1.307641
66	1	0	-7.615708	0.405550	-2.059884
67	6	0	-8.612416	0.102377	-0.077166
68	1	0	-8.777619	1.114267	0.269014
69	6	0	-8.536639	-2.200762	-0.164038
70	1	0	-8.635307	-3.244443	0.104430
71	6	0	-8.944664	-1.089565	0.629673
72	1	0	-9.407632	-1.141403	1.606430
73	1	0	-7.528883	-2.288385	-2.162019
74	26	0	-6.954674	-1.010485	0.261835
75	8	0	1.519566	-1.978395	1.303274
76	1	0	1.361294	-1.429325	0.525398
77	1	0	2.152498	-2.632247	0.989223
78	1	0	10.928176	-2.329354	-0.906712

A-W_u-m_4 (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.404836	-0.841520	0.253846
2	6	0	9.494786	-1.442453	-0.371247
3	6	0	8.302852	0.554214	0.282172
4	6	0	10.485027	-0.650609	-0.956060
5	1	0	9.571160	-2.526035	-0.402806
6	6	0	9.290868	1.339847	-0.310716

7	1	0	7.434811	0.994623	0.759701
8	6	0	10.390909	0.732245	-0.930644
9	1	0	11.335353	-1.119123	-1.443683
10	8	0	9.274992	2.696818	-0.337178
11	6	0	8.181949	3.354826	0.273640
12	1	0	7.231905	3.084690	-0.202518
13	1	0	8.122732	3.128334	1.344785
14	1	0	8.358837	4.422632	0.141681
15	6	0	7.356930	-1.681415	0.947183
16	1	0	7.567730	-1.686041	2.025132
17	1	0	7.450260	-2.730871	0.609525
18	6	0	5.542010	-1.326811	-0.597846
19	6	0	5.071398	-1.804207	1.691462
20	6	0	4.175691	-0.684197	-0.768522
21	1	0	5.478594	-2.395543	-0.879899
22	1	0	6.256767	-0.842770	-1.270936
23	6	0	3.697453	-1.166561	1.562947
24	1	0	4.983541	-2.890892	1.499977
25	1	0	5.436297	-1.672653	2.716193
26	1	0	3.807268	-0.867844	-1.782258
27	1	0	4.282937	0.407160	-0.642862
28	1	0	2.987135	-1.690460	2.209535
29	1	0	3.762954	-0.121645	1.912230
30	7	0	6.007006	-1.172040	0.773499
31	7	0	3.247011	-1.279619	0.182602
32	6	0	1.857472	-1.116401	-0.068026
33	6	0	1.168035	0.133394	0.051489
34	6	0	1.149507	-2.242365	-0.447048
35	6	0	1.804085	1.341173	0.432361
36	6	0	-0.230183	0.173351	-0.225692
37	6	0	-0.226358	-2.193971	-0.716699
38	1	0	1.691503	-3.178453	-0.531209
39	6	0	1.097462	2.519291	0.534743
40	1	0	2.865699	1.338383	0.647014
41	6	0	-0.935787	1.394383	-0.114160
42	6	0	-0.913934	-1.002868	-0.609396
43	1	0	-0.766404	-3.087733	-1.011672
44	6	0	-0.279562	2.549232	0.261741
45	1	0	1.606836	3.431187	0.828619
46	1	0	-0.845805	3.471367	0.340515
47	6	0	-2.360178	-0.972072	-0.895648
48	6	0	-2.383931	1.449840	-0.396490
49	8	0	-2.989529	-1.969610	-1.221438
50	8	0	-3.033383	2.482700	-0.304476
51	7	0	-2.998701	0.261546	-0.784508
52	6	0	-4.439399	0.306160	-1.068549
53	1	0	-4.634753	-0.450173	-1.828643
54	1	0	-4.651253	1.294556	-1.476326

55	6	0	-5.267755	0.051902	0.151668
56	6	0	-5.750505	1.038458	1.065389
57	6	0	-5.712945	-1.222704	0.619247
58	1	0	-5.589655	2.104537	0.974404
59	6	0	-6.498004	0.377472	2.079826
60	1	0	-5.518345	-2.168586	0.131352
61	6	0	-6.474507	-1.020643	1.804134
62	1	0	-7.018593	0.854821	2.899842
63	1	0	-6.973807	-1.790167	2.378456
64	6	0	-8.829607	-1.038152	-0.548507
65	6	0	-8.071664	-0.399223	-1.571802
66	1	0	-7.557527	-0.894024	-2.385551
67	6	0	-8.081478	1.002859	-1.316232
68	1	0	-7.576096	1.759788	-1.901920
69	6	0	-9.307676	-0.031783	0.338953
70	1	0	-9.895566	-0.198762	1.232107
71	6	0	-8.845358	1.229372	-0.135084
72	1	0	-9.020292	2.188407	0.334822
73	1	0	-8.990467	-2.103572	-0.447598
74	26	0	-7.281591	-0.001360	0.249908
75	1	0	11.149130	1.361364	-1.386606

A-2W$_{ud}$-m$_1$ (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.061520	-1.983654	-0.607378
2	6	0	-7.361734	-3.306093	-0.290022
3	6	0	-8.014940	-0.982396	-0.388672
4	6	0	-8.615643	-3.628297	0.232929
5	1	0	-6.619504	-4.083457	-0.450348
6	6	0	-9.262564	-1.309180	0.142143
7	1	0	-7.748490	0.040734	-0.629023
8	6	0	-9.565110	-2.642067	0.451013
9	1	0	-8.850564	-4.659834	0.479982
10	8	0	-10.246232	-0.408524	0.392998
11	6	0	-9.985022	0.950895	0.101778
12	1	0	-9.140672	1.333235	0.687566
13	1	0	-9.778971	1.102168	-0.964414
14	1	0	-10.887989	1.498017	0.374141
15	6	0	-5.733806	-1.626797	-1.234574
16	1	0	-5.872904	-1.521832	-2.318930
17	1	0	-5.026399	-2.465698	-1.093004
18	6	0	-4.764838	-0.469269	0.641036
19	6	0	-4.077589	0.088498	-1.566376

20	6	0	-4.273660	0.886459	1.132646
21	1	0	-3.978910	-1.239144	0.759212
22	1	0	-5.616304	-0.777078	1.256351
23	6	0	-3.614471	1.465359	-1.112918
24	1	0	-3.226924	-0.618740	-1.537755
25	1	0	-4.411326	0.163681	-2.607579
26	1	0	-3.940157	0.835779	2.171225
27	1	0	-5.114890	1.589323	1.093745
28	1	0	-2.780672	1.791137	-1.734246
29	1	0	-4.431040	2.186894	-1.228424
30	7	0	-5.190348	-0.369908	-0.746745
31	7	0	-3.210118	1.468805	0.307650
32	6	0	-1.874965	1.191377	0.611105
33	6	0	-0.839485	2.041176	0.076853
34	6	0	-1.502362	0.150441	1.460533
35	6	0	-1.107093	3.252164	-0.606857
36	6	0	0.522262	1.689316	0.300547
37	6	0	-0.157009	-0.144845	1.709167
38	1	0	-2.258025	-0.478362	1.915031
39	6	0	-0.085683	4.022371	-1.122771
40	1	0	-2.127910	3.613190	-0.680049
41	6	0	1.552509	2.482220	-0.257324
42	6	0	0.855530	0.580796	1.112185
43	1	0	0.105823	-0.979309	2.351610
44	6	0	1.249916	3.622774	-0.974935
45	1	0	-0.317006	4.951307	-1.633518
46	1	0	2.061904	4.212277	-1.387644
47	6	0	2.255493	0.208072	1.346663
48	6	0	2.968384	2.111225	-0.063464
49	8	0	2.582943	-0.747537	2.039853
50	8	0	3.887554	2.742598	-0.569081
51	7	0	3.227968	1.002346	0.736149
52	6	0	4.633654	0.629892	0.941628
53	1	0	4.699205	0.179492	1.931905
54	1	0	5.212559	1.553206	0.922666
55	6	0	5.128043	-0.322500	-0.102096
56	6	0	5.726746	0.028624	-1.351515
57	6	0	5.063071	-1.749026	-0.041727
58	1	0	5.919669	1.038362	-1.688644
59	6	0	6.041768	-1.172478	-2.047460
60	1	0	4.665452	-2.320575	0.786372
61	6	0	5.631349	-2.271749	-1.237484
62	1	0	6.528860	-1.240354	-3.011479
63	1	0	5.752505	-3.319614	-1.479313
64	6	0	7.974574	-1.775964	1.382979
65	6	0	8.042482	-0.355386	1.288818
66	1	0	7.677715	0.349030	2.025245
67	6	0	8.650969	-0.024980	0.043013

68	1	0	8.828814	0.974148	-0.332699
69	6	0	8.539956	-2.323285	0.194876
70	1	0	8.619839	-3.375463	-0.045167
71	6	0	8.957998	-1.241243	-0.633130
72	1	0	9.410943	-1.327634	-1.612132
73	1	0	7.549437	-2.339410	2.203238
74	26	0	6.972977	-1.120245	-0.250370
75	8	0	-1.329359	-2.236216	-1.031022
76	1	0	-1.143036	-1.585598	-0.343890
77	1	0	-1.944210	-2.842130	-0.604564
78	1	0	-10.541821	-2.875660	0.863356
79	8	0	-4.180143	4.208402	0.539934
80	1	0	-3.734747	3.353314	0.668031
81	1	0	-3.731531	4.797785	1.154678

A-2W$_{ud}$-m$_2$ (PBE0/6-31G(d,p) in water solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	8.111839	-0.621391	0.276689
2	6	0	9.142616	-1.209607	-0.451871
3	6	0	8.001064	0.773960	0.323785
4	6	0	10.064036	-0.406383	-1.127656
5	1	0	9.225661	-2.292266	-0.493992
6	6	0	8.924428	1.571071	-0.352198
7	1	0	7.173415	1.211456	0.870946
8	6	0	9.962284	0.974947	-1.082379
9	1	0	10.867244	-0.864902	-1.697709
10	8	0	8.901580	2.927422	-0.363024
11	6	0	7.942663	3.578082	0.452256
12	1	0	6.915835	3.322361	0.166778
13	1	0	8.088148	3.327491	1.510371
14	1	0	8.105345	4.647367	0.311670
15	6	0	7.129869	-1.470168	1.049837
16	1	0	7.325221	-1.350527	2.123671
17	1	0	7.307440	-2.536922	0.816725
18	6	0	5.319217	-1.405774	-0.537366
19	6	0	4.848589	-1.715705	1.777202
20	6	0	3.909678	-0.894360	-0.785727

21	1	0	5.359395	-2.495878	-0.722120
22	1	0	5.999826	-0.923241	-1.245910
23	6	0	3.429949	-1.206377	1.582151
24	1	0	4.859679	-2.817911	1.686589
25	1	0	5.177696	-1.462114	2.790932
26	1	0	3.575361	-1.199547	-1.781856
27	1	0	3.927004	0.203315	-0.751066
28	1	0	2.752413	-1.726099	2.265985
29	1	0	3.402904	-0.134192	1.825332
30	7	0	5.745392	-1.087748	0.818367
31	7	0	2.994438	-1.477774	0.205772
32	6	0	1.593329	-1.283428	-0.040648
33	6	0	0.947276	-0.002849	-0.028149
34	6	0	0.843371	-2.417610	-0.292916
35	6	0	1.615362	1.221808	0.227764
36	6	0	-0.456331	0.050797	-0.287681
37	6	0	-0.534613	-2.349854	-0.544388
38	1	0	1.346069	-3.379679	-0.290310
39	6	0	0.936543	2.420707	0.226183
40	1	0	2.680405	1.246908	0.423962
41	6	0	-1.130426	1.295346	-0.283379
42	6	0	-1.182922	-1.133940	-0.546197
43	1	0	-1.105608	-3.251142	-0.741941
44	6	0	-0.442101	2.464154	-0.028613
45	1	0	1.480490	3.339011	0.422729
46	1	0	-0.984850	3.403600	-0.031174
47	6	0	-2.632080	-1.089224	-0.818755
48	6	0	-2.580711	1.365729	-0.551232
49	8	0	-3.291717	-2.095349	-1.041865
50	8	0	-3.199292	2.421541	-0.548614
51	7	0	-3.234944	0.165872	-0.819425
52	6	0	-4.676091	0.226298	-1.098041
53	1	0	-4.898721	-0.587582	-1.788026
54	1	0	-4.862011	1.180924	-1.589984
55	6	0	-5.503955	0.104012	0.143011
56	6	0	-5.922828	1.177953	0.988182
57	6	0	-6.001050	-1.109811	0.710769
58	1	0	-5.707511	2.224652	0.819429
59	6	0	-6.684469	0.630598	2.058842
60	1	0	-5.855048	-2.098169	0.295700
61	6	0	-6.733096	-0.783982	1.887191
62	1	0	-7.163152	1.191596	2.850876
63	1	0	-7.255137	-1.484178	2.526228
64	6	0	-9.433911	-0.468910	0.122653
65	6	0	-8.703007	-0.804472	-1.053734
66	1	0	-8.543032	-1.802456	-1.440343
67	6	0	-8.195937	0.402986	-1.616250
68	1	0	-7.583836	0.482498	-2.505413

69	6	0	-9.379260	0.945736	0.286836
70	1	0	-9.823297	1.509552	1.096774
71	6	0	-8.614448	1.484811	-0.788006
72	1	0	-8.375392	2.529574	-0.937441
73	1	0	-9.926965	-1.167556	0.785868
74	26	0	-7.514159	0.157366	0.273854
75	1	0	10.670172	1.613401	-1.601984
76	8	0	3.482087	-4.356792	-0.092382
77	1	0	3.355510	-3.389933	0.006145
78	1	0	3.601757	-4.473254	-1.040727
79	8	0	4.538435	2.649634	0.415856
80	1	0	4.344835	3.165328	-0.374267
81	1	0	4.438682	3.282014	1.135591

A-THF$_u$ (PBE0/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.999005	-0.391049	0.567592
2	6	0	-9.145124	0.256368	0.113654
3	6	0	-7.796010	-1.741519	0.260977
4	6	0	-10.091067	-0.446920	-0.634633
5	1	0	-9.300061	1.307319	0.342849
6	6	0	-8.740480	-2.436499	-0.493534
7	1	0	-6.886009	-2.214896	0.612212
8	6	0	-9.897175	-1.784598	-0.940850
9	1	0	-10.985578	0.057841	-0.988701
10	8	0	-8.628433	-3.742953	-0.843621
11	6	0	-7.477578	-4.442570	-0.415643
12	1	0	-6.560916	-3.997961	-0.821799
13	1	0	-7.406717	-4.471732	0.678332
14	1	0	-7.582007	-5.459290	-0.795716
15	6	0	-6.995559	0.336598	1.431988
16	1	0	-7.172990	0.065332	2.481438
17	1	0	-7.175240	1.426354	1.359494
18	6	0	-5.209444	0.503934	-0.175613
19	6	0	-4.702881	0.458370	2.154102
20	6	0	-3.805410	0.032142	-0.514160
21	1	0	-5.236610	1.611485	-0.194386
22	1	0	-5.907895	0.138738	-0.935218
23	6	0	-3.290021	-0.018299	1.858939
24	1	0	-4.704263	1.563138	2.230841
25	1	0	-5.023948	0.056358	3.121653

26	1	0	-3.483477	0.483814	-1.457613
27	1	0	-3.830519	-1.061796	-0.659312
28	1	0	-2.600225	0.394629	2.601106
29	1	0	-3.268217	-1.117356	1.955812
30	7	0	-5.617822	-0.007288	1.124089
31	7	0	-2.889503	0.448738	0.538819
32	6	0	-1.497902	0.426746	0.236965
33	6	0	-0.744793	-0.780471	0.065093
34	6	0	-0.858986	1.646922	0.110188
35	6	0	-1.309253	-2.076587	0.167647
36	6	0	0.647822	-0.683240	-0.227263
37	6	0	0.512433	1.728744	-0.179149
38	1	0	-1.436019	2.559679	0.239252
39	6	0	-0.541803	-3.207656	-0.004236
40	1	0	-2.365139	-2.181005	0.384648
41	6	0	1.417194	-1.858177	-0.397417
42	6	0	1.262724	0.583857	-0.346207
43	1	0	1.001134	2.693349	-0.272120
44	6	0	0.829458	-3.101876	-0.286359
45	1	0	-0.998861	-4.188359	0.079604
46	1	0	1.445488	-3.984835	-0.421266
47	6	0	2.702453	0.696793	-0.645732
48	6	0	2.861614	-1.771353	-0.694008
49	8	0	3.271632	1.774132	-0.752336
50	8	0	3.563903	-2.762226	-0.838376
51	7	0	3.406566	-0.494915	-0.812198
52	6	0	4.843610	-0.396749	-1.099926
53	1	0	4.988319	0.519790	-1.671764
54	1	0	5.102811	-1.257297	-1.716731
55	6	0	5.670970	-0.375251	0.147115
56	6	0	6.215435	-1.512739	0.819054
57	6	0	6.034459	0.784561	0.898779
58	1	0	6.114142	-2.538258	0.489719
59	6	0	6.922268	-1.055270	1.966346
60	1	0	5.772119	1.801856	0.640634
61	6	0	6.809968	0.365092	2.015850
62	1	0	7.468494	-1.674462	2.665862
63	1	0	7.255940	1.012366	2.759650
64	6	0	9.509717	0.636205	0.243807
65	6	0	8.733773	1.062051	-0.872771
66	1	0	8.457020	2.082445	-1.103166
67	6	0	8.362903	-0.094907	-1.617562
68	1	0	7.756400	-0.106681	-2.513956
69	6	0	9.618887	-0.783521	0.188794
70	1	0	10.133270	-1.410060	0.905592
71	6	0	8.910310	-1.235594	-0.961726
72	1	0	8.791497	-2.265463	-1.271802
73	1	0	9.926573	1.276910	1.009757

74	26	0	7.675890	-0.221453	0.282331
75	1	0	-10.619466	-2.344160	-1.526960
76	6	0	-3.482694	4.617787	0.765396
77	8	0	-2.200958	4.707324	0.136086
78	6	0	-2.368112	4.910691	-1.265602
79	6	0	-3.794378	4.485882	-1.580227
80	6	0	-4.520148	4.926091	-0.310655
81	1	0	-3.607945	3.599156	1.157846
82	1	0	-3.518288	5.318128	1.607592
83	1	0	-2.211895	5.972465	-1.509125
84	1	0	-1.608812	4.323178	-1.792164
85	1	0	-4.184435	4.947761	-2.490709
86	1	0	-3.849104	3.397176	-1.694624
87	1	0	-4.730024	6.000568	-0.348167
88	1	0	-5.464563	4.401627	-0.142289

A-THF$_d$ (PBE0/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.843145	-2.381402	0.666365
2	6	0	-7.290649	-2.856085	1.896409
3	6	0	-7.558520	-1.375072	0.007106
4	6	0	-8.454968	-2.331371	2.461362
5	1	0	-6.732472	-3.631772	2.413888
6	6	0	-8.718903	-0.852267	0.577657
7	1	0	-7.173522	-1.006757	-0.936932
8	6	0	-9.169460	-1.335881	1.813446
9	1	0	-8.804336	-2.700306	3.421664
10	8	0	-9.475313	0.122323	0.012006
11	6	0	-9.083880	0.600655	-1.263856
12	1	0	-8.095752	1.074686	-1.228328
13	1	0	-9.079077	-0.206652	-2.006232
14	1	0	-9.832685	1.341655	-1.547287
15	6	0	-5.617148	-2.970866	0.007070
16	1	0	-5.939164	-3.672783	-0.773869
17	1	0	-5.053100	-3.568130	0.747944
18	6	0	-4.099194	-1.128122	0.337088
19	6	0	-3.823715	-2.545854	-1.554818
20	6	0	-3.356294	0.010853	-0.352331
21	1	0	-3.383512	-1.719098	0.942863

22	1	0	-4.838361	-0.702182	1.023348
23	6	0	-3.075875	-1.425634	-2.268355
24	1	0	-3.107892	-3.212512	-1.035695
25	1	0	-4.358145	-3.149984	-2.296578
26	1	0	-2.815548	0.583775	0.401196
27	1	0	-4.081091	0.676338	-0.837380
28	1	0	-2.347304	-1.822037	-2.978192
29	1	0	-3.808926	-0.840544	-2.838849
30	7	0	-4.785473	-1.965966	-0.632694
31	7	0	-2.417438	-0.505757	-1.352062
32	6	0	-1.074633	-0.638332	-1.063514
33	6	0	-0.329376	0.501650	-0.580883
34	6	0	-0.381283	-1.832763	-1.277624
35	6	0	-0.860194	1.811568	-0.556520
36	6	0	1.028340	0.325500	-0.189751
37	6	0	0.960649	-1.969199	-0.925638
38	1	0	-0.906286	-2.699660	-1.660966
39	6	0	-0.124589	2.877492	-0.078987
40	1	0	-1.853488	1.987396	-0.954701
41	6	0	1.757949	1.426374	0.317974
42	6	0	1.666441	-0.925157	-0.352659
43	1	0	1.464058	-2.921384	-1.061481
44	6	0	1.182217	2.680669	0.386999
45	1	0	-0.553947	3.874097	-0.079865
46	1	0	1.772370	3.504082	0.775954
47	6	0	3.058919	-1.119134	0.052115
48	6	0	3.156865	1.254085	0.756212
49	8	0	3.653164	-2.184522	-0.070907
50	8	0	3.816225	2.171536	1.229595
51	7	0	3.709630	-0.014040	0.612048
52	6	0	5.101836	-0.195697	1.038564
53	1	0	5.200375	-1.233494	1.356904
54	1	0	5.262135	0.465401	1.890502
55	6	0	6.078571	0.111860	-0.053566
56	6	0	6.675560	1.382287	-0.319519
57	6	0	6.563862	-0.806200	-1.035105
58	1	0	6.506167	2.282006	0.256652
59	6	0	7.533772	1.243798	-1.446383
60	1	0	6.295493	-1.852463	-1.095191
61	6	0	7.464362	-0.109649	-1.889101
62	1	0	8.148531	2.022914	-1.877908
63	1	0	8.017190	-0.537347	-2.715306
64	6	0	8.987571	-1.570943	0.975357
65	6	0	8.532996	-0.605887	1.920340
66	1	0	7.819149	-0.780980	2.714858
67	6	0	9.164216	0.636089	1.620339
68	1	0	9.013230	1.569526	2.146477
69	6	0	9.898876	-0.924958	0.090737

70	1	0	10.404525	-1.384767	-0.748213
71	6	0	10.008074	0.438794	0.489394
72	1	0	10.611202	1.196338	0.006351
73	1	0	8.678838	-2.606862	0.925698
74	26	0	8.088677	-0.019787	0.034666
75	1	0	-10.074192	-0.915734	2.241699
76	6	0	-6.252988	3.628704	-0.923920
77	8	0	-6.090657	2.277698	-0.517380
78	6	0	-6.348215	2.280095	0.879605
79	6	0	-7.558189	3.200386	1.065966
80	6	0	-7.466507	4.155664	-0.144466
81	1	0	-5.349317	4.205628	-0.671213
82	1	0	-6.379200	3.641677	-2.009266
83	1	0	-6.523648	1.247419	1.190679
84	1	0	-5.471473	2.670112	1.421345
85	1	0	-8.483027	2.618318	1.033408
86	1	0	-7.525973	3.725147	2.024128
87	1	0	-8.374028	4.102670	-0.751689
88	1	0	-7.327909	5.198515	0.152031

A-2THF$_{ud}$ (PBE0/6-31G(d,p) in THF solvent)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.032104	1.334235	-1.853669
2	6	0	-7.488657	1.671536	-3.125316
3	6	0	-7.671496	0.319423	-1.132594
4	6	0	-8.588189	1.005012	-3.668918
5	1	0	-6.987259	2.451946	-3.691522
6	6	0	-8.762833	-0.349829	-1.685396
7	1	0	-7.282866	0.066825	-0.152375
8	6	0	-9.226492	-0.000934	-2.960362
9	1	0	-8.944875	1.268415	-4.660739
10	8	0	-9.439439	-1.350589	-1.065797
11	6	0	-9.000462	-1.745905	0.217588
12	1	0	-7.969418	-2.120813	0.193147
13	1	0	-9.064126	-0.921792	0.938308
14	1	0	-9.666866	-2.549827	0.531887
15	6	0	-5.882936	2.088643	-1.224846
16	1	0	-6.291173	2.866410	-0.565198
17	1	0	-5.319399	2.619232	-2.015759
18	6	0	-4.247858	0.318570	-1.224081
19	6	0	-4.127679	2.024245	0.426798
20	6	0	-3.450531	-0.643602	-0.351147

21	1	0	-3.554120	0.860570	-1.897318
22	1	0	-4.930970	-0.262469	-1.852456
23	6	0	-3.335319	1.087747	1.327464
24	1	0	-3.432373	2.641724	-0.173134
25	1	0	-4.718114	2.705878	1.048645
26	1	0	-2.841312	-1.275798	-0.996819
27	1	0	-4.124884	-1.293568	0.219020
28	1	0	-2.663068	1.655964	1.970458
29	1	0	-4.045903	0.549755	1.970149
30	7	0	-5.022426	1.245221	-0.414261
31	7	0	-2.589918	0.085176	0.581284
32	6	0	-1.235759	0.207470	0.374101
33	6	0	-0.440651	-0.965654	0.084592
34	6	0	-0.580323	1.440202	0.485613
35	6	0	-0.937581	-2.283430	0.217549
36	6	0	0.931307	-0.799847	-0.261651
37	6	0	0.774088	1.563849	0.185986
38	1	0	-1.138752	2.333462	0.750679
39	6	0	-0.149575	-3.378071	-0.081745
40	1	0	-1.941042	-2.448799	0.599883
41	6	0	1.710797	-1.934352	-0.590720
42	6	0	1.532364	0.478772	-0.225824
43	1	0	1.252173	2.537993	0.232603
44	6	0	1.169943	-3.204487	-0.518001
45	1	0	-0.552552	-4.378700	0.038251
46	1	0	1.797757	-4.052886	-0.770829
47	6	0	2.937111	0.661078	-0.582205
48	6	0	3.122396	-1.776978	-0.987607
49	8	0	3.504351	1.749110	-0.559613
50	8	0	3.825130	-2.724952	-1.319191
51	7	0	3.639086	-0.485676	-0.973867
52	6	0	5.045845	-0.319708	-1.354754
53	1	0	5.140617	0.679217	-1.780319
54	1	0	5.259387	-1.066175	-2.120233
55	6	0	5.975017	-0.483356	-0.192190
56	6	0	6.591925	-1.699994	0.231971
57	6	0	6.384172	0.544867	0.711602
58	1	0	6.476200	-2.658552	-0.255782
59	6	0	7.387347	-1.420098	1.378479
60	1	0	6.084530	1.582441	0.649299
61	6	0	7.258245	-0.031628	1.675606
62	1	0	8.000072	-2.131112	1.917172
63	1	0	7.756059	0.495447	2.479087
64	6	0	9.762467	0.667982	-0.259123
65	6	0	8.879664	1.178952	-1.254115
66	1	0	8.534274	2.201335	-1.333723
67	6	0	8.509780	0.100801	-2.109579
68	1	0	7.834799	0.161473	-2.953508

69	6	0	9.938567	-0.725468	-0.499929
70	1	0	10.539182	-1.402624	0.093112
71	6	0	9.164714	-1.076074	-1.643742
72	1	0	9.073692	-2.065917	-2.071353
73	1	0	10.205995	1.234723	0.548989
74	26	0	7.983173	-0.295651	-0.195833
75	1	0	-10.077491	-0.534341	-3.372216
76	6	0	-1.838634	5.298396	0.929244
77	8	0	-1.932385	4.200662	1.835907
78	6	0	-0.981170	4.368529	2.893319
79	6	0	-0.304998	5.718377	2.663322
80	6	0	-0.460602	5.899543	1.154751
81	1	0	-1.995447	4.919155	-0.085455
82	1	0	-2.627702	6.033467	1.148938
83	1	0	-1.500281	4.311765	3.856875
84	1	0	-0.259198	3.542281	2.845166
85	1	0	-0.840875	6.511995	3.195108
86	1	0	0.734492	5.727054	3.000030
87	1	0	-0.393304	6.941105	0.830781
88	1	0	0.299162	5.321534	0.616638
89	6	0	-4.011628	-2.901003	3.037233
90	8	0	-3.894613	-3.277990	1.664009
91	6	0	-4.936892	-4.191441	1.319585
92	6	0	-5.944280	-4.130370	2.459884
93	6	0	-5.032716	-3.849454	3.652424
94	1	0	-3.023582	-2.962948	3.505393
95	1	0	-4.354267	-1.857806	3.098522
96	1	0	-5.356240	-3.896221	0.351600
97	1	0	-4.517753	-5.202944	1.217609
98	1	0	-6.641808	-3.298338	2.310141
99	1	0	-6.525316	-5.050586	2.558668
100	1	0	-5.552254	-3.410992	4.508037
101	1	0	-4.546151	-4.773271	3.984001
