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Supplementary Information

For

Theoretical Study on the Mechanism of Water Oxidation Catalyzed by a Mononuclear Copper Complex: Important Roles of Redox Non-Innocent Ligand and the HPO_4^{2-} Anion

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S1. Optimized structure of 3pt, 4pt and TS'

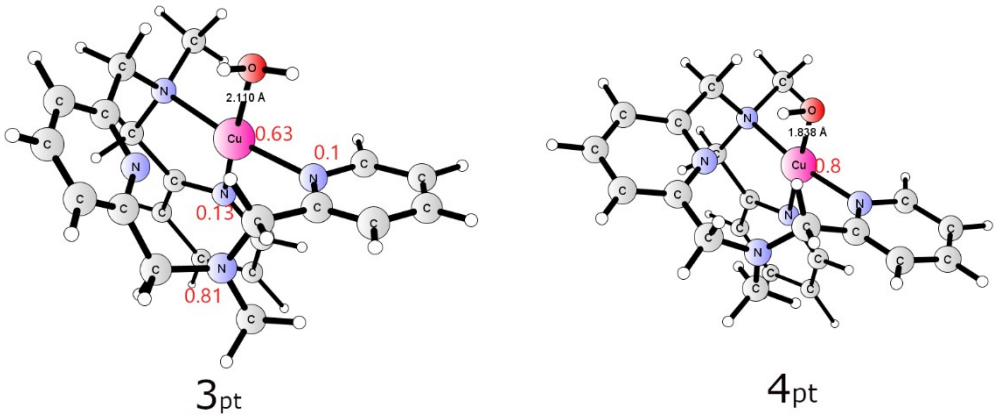

Figure S1. Optimized structure of 3_{pt} (Triplet), 4_{pt}(Doublet) and TS' (Doublet). Selected distances are shown in Angstrom in black. Spin densities on selected atoms are presented in red.

S2. Optimized structure of TS0Doublet and Int0Doublet

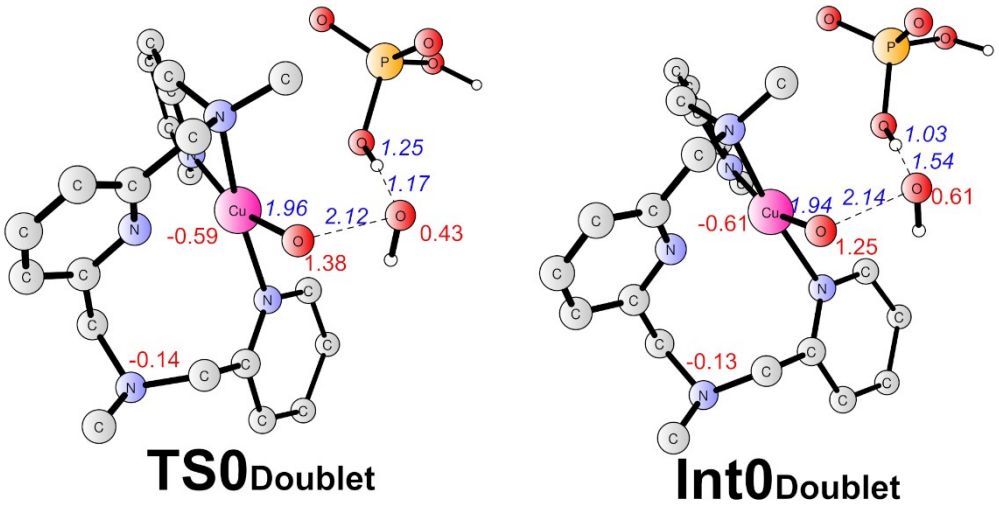

Figure S2. Optimized structure of $TS0_{Doublet}$ and $Int0_{Doublet}$. Selected distances are shown in Angstrom in black. Spin densities on selected atoms are presented in red.

S3. Gibbs free energy diagrams for water oxidation at B3LYP*-D3, PBE0-D3, and M06-D3 levels.

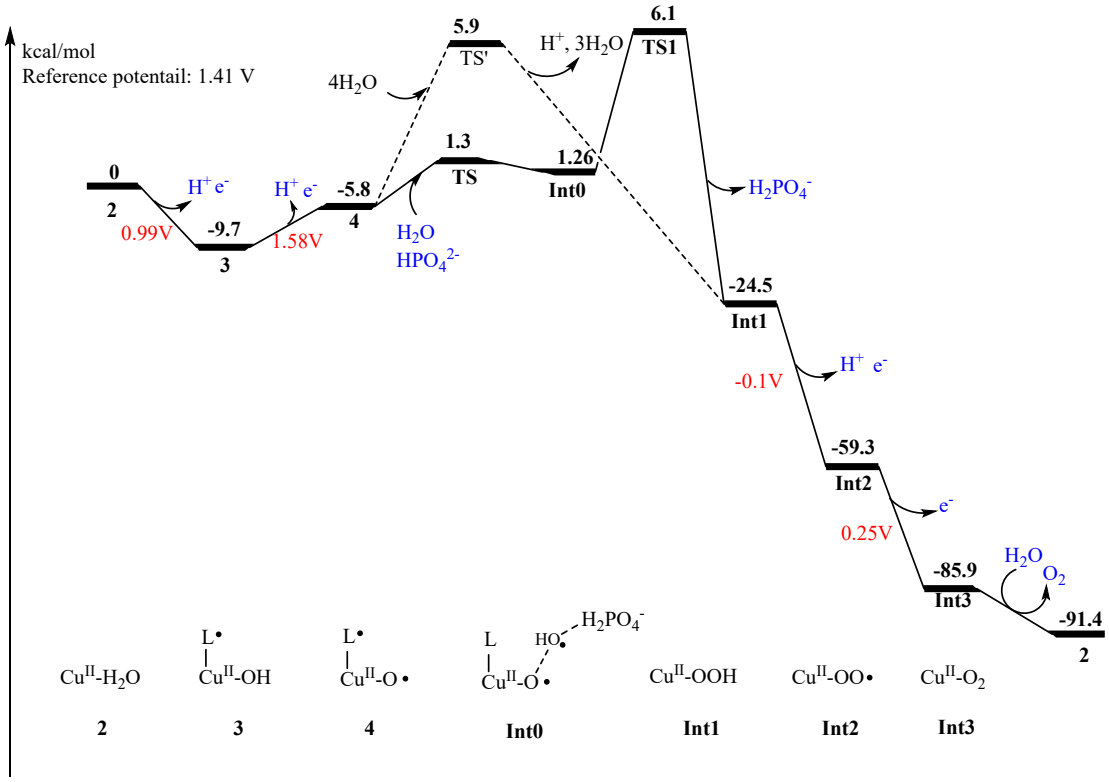

Figure S3. Energy diagram for water oxidation with B3LYP-15%-D3.

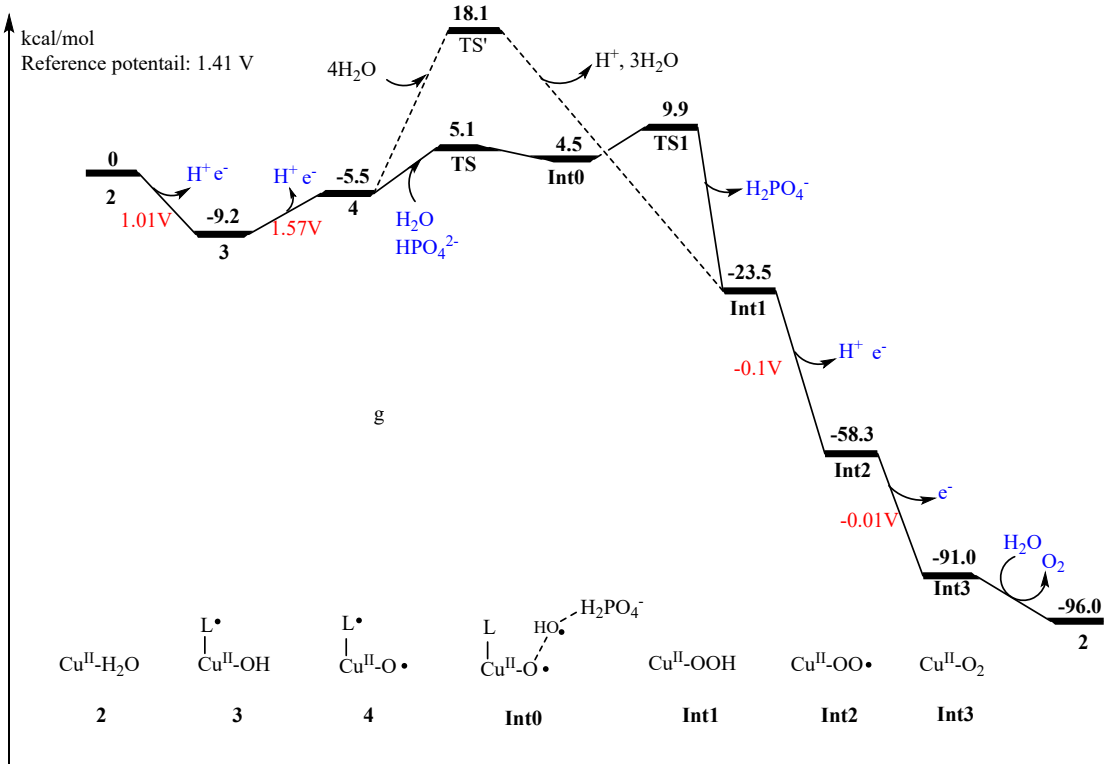

Figure S4. Energy diagram for water oxidation with PBE0-D3.

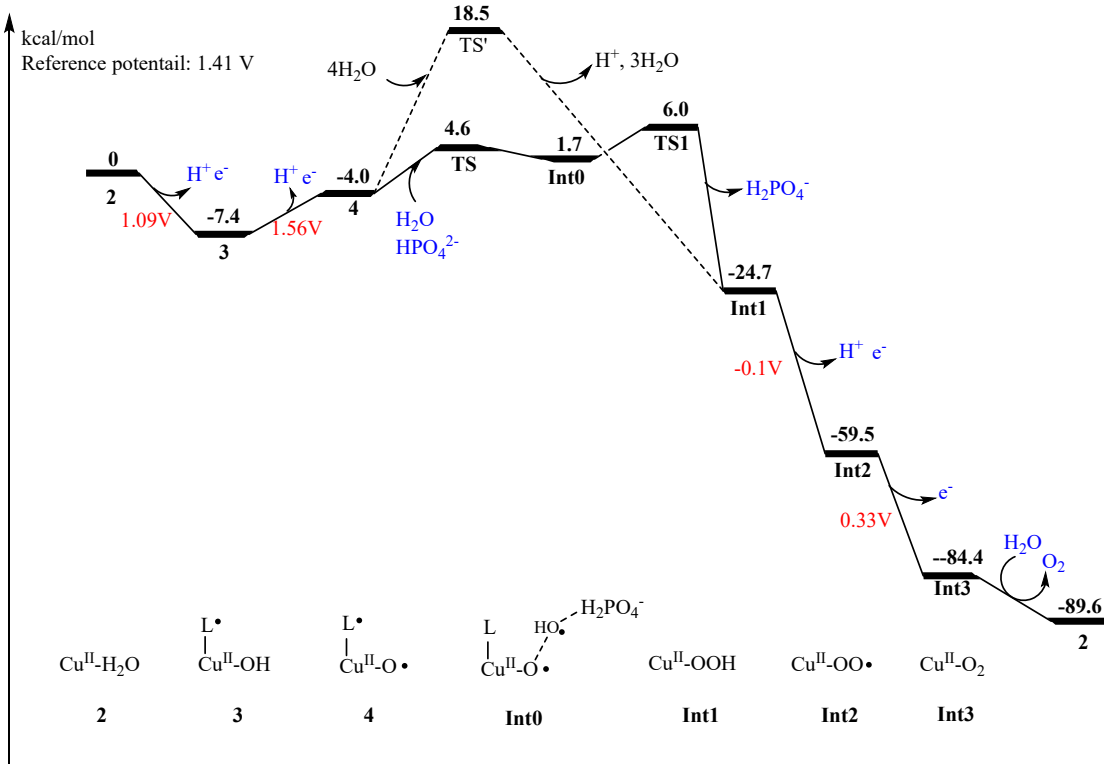

Figure S5. Energy diagram for water oxidation with M06-D3.

S4. Coordinates for all structures.

1(doulet) E_{opt} = -2728.4741576 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.084594	-0.016131	-0.024999
2	7	0	2.086351	-0.072486	-0.000078
3	7	0	0.508258	1.518305	-1.445289
4	7	0	-1.224075	1.543984	0.698693
5	6	0	-0.470336	1.551364	-2.546154
6	1	0	-0.220934	2.348233	-3.268272
7	1	0	-1.473002	1.741865	-2.142777
8	1	0	-0.474843	0.581185	-3.059598
9	6	0	-2.334485	1.447705	1.441368
10	1	0	-2.605788	0.448359	1.787976
11	6	0	-2.719677	3.808608	1.270765
12	1	0	-3.307617	4.701843	1.494116
13	6	0	2.754501	0.622036	-0.930185
14	6	0	-3.113425	2.559688	1.757452
15	1	0	-4.011055	2.441860	2.366751
16	6	0	-1.571692	3.901368	0.480379
17	1	0	-1.242811	4.856333	0.066913
18	6	0	-0.843744	2.740742	0.214049
19	6	0	0.421315	2.738880	-0.608773
20	1	0	0.485525	3.642949	-1.236423
21	1	0	1.285007	2.746283	0.075434
22	6	0	4.814712	-0.161987	0.012405
23	1	0	5.906441	-0.197238	0.017966
24	6	0	4.148635	0.612846	-0.943164
25	1	0	4.694534	1.189939	-1.691216
26	6	0	1.883021	1.300700	-1.955111
27	1	0	2.330847	2.245044	-2.306409
28	1	0	1.814192	0.630709	-2.826236
29	7	0	0.388116	-1.549868	1.436615
30	7	0	-1.351715	-1.456155	-0.692004
31	6	0	-0.588337	-1.491381	2.538203
32	1	0	-0.393395	-2.289539	3.275439
33	1	0	-1.602586	-1.620979	2.140317
34	1	0	-0.523986	-0.513619	3.032503
35	6	0	-2.453132	-1.275189	-1.432242
36	1	0	-2.643193	-0.258636	-1.783095

37	6	0	-3.021822	-3.597876	-1.247972
38	1	0	-3.678738	-4.443173	-1.465389
39	6	0	2.698182	-0.811115	0.933945
40	6	0	-3.317900	-2.324208	-1.739921
41	1	0	-4.205475	-2.139408	-2.347249
42	6	0	-1.882159	-3.777566	-0.460484
43	1	0	-1.628277	-4.753639	-0.043359
44	6	0	-1.064046	-2.677002	-0.202148
45	6	0	0.201437	-2.769741	0.615541
46	1	0	0.196083	-3.669828	1.252174
47	1	0	1.057891	-2.851320	-0.072813
48	6	0	4.090249	-0.892106	0.960335
49	1	0	4.590468	-1.503840	1.712746
50	6	0	1.775580	-1.434449	1.948555
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52	1	0	1.753950	-0.768970	2.825690

2(doulet) E_{opt} = -2728. 8533366 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.268956	0.129593	0.768744
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3	7	0	0.234977	-2.035647	-0.974034
4	7	0	2.190536	-0.551762	0.550708
5	6	0	0.339205	-1.369909	-2.267039
6	1	0	0.507650	-2.087622	-3.096806
7	1	0	1.172752	-0.654055	-2.258779
8	1	0	-0.583765	-0.808692	-2.477975
9	6	0	3.130399	0.264906	1.063143
10	1	0	2.766982	1.160521	1.573269
11	6	0	4.880767	-1.146646	0.251272
12	1	0	5.939087	-1.383977	0.121086
13	6	0	-2.183222	-2.157736	-0.665054
14	6	0	4.489421	0.001617	0.945213
15	1	0	5.217720	0.688677	1.378345
16	6	0	3.901913	-1.986178	-0.277017
17	1	0	4.173160	-2.890840	-0.824280
18	6	0	2.547862	-1.674551	-0.101759
19	6	0	1.480253	-2.652325	-0.551762
20	1	0	1.916982	-3.313413	-1.326951
21	1	0	1.267794	-3.293464	0.320808

22	6	0	-4.328518	-1.234102	-1.232374
23	1	0	-5.202694	-1.182387	-1.885550
24	6	0	-3.282826	-2.115462	-1.527102
25	1	0	-3.305072	-2.743492	-2.419664
26	6	0	-0.916678	-2.946365	-0.905883
27	1	0	-0.768814	-3.628785	-0.055165
28	1	0	-1.011368	-3.567899	-1.816457
29	7	0	-1.476650	1.255062	1.380263
30	7	0	0.475907	1.713631	-0.516224
31	6	0	-0.946623	1.985808	2.554004
32	1	0	-1.712195	2.660750	2.973535
33	1	0	-0.071981	2.579272	2.255337
34	1	0	-0.638679	1.260622	3.318343
35	6	0	1.558777	1.968337	-1.271374
36	1	0	2.350276	1.219298	-1.267933
37	6	0	0.632058	4.059169	-1.989706
38	1	0	0.694310	4.987371	-2.561975
39	6	0	-3.083212	-0.473444	0.671599
40	6	0	1.673578	3.127966	-2.029362
41	1	0	2.568177	3.294681	-2.631002
42	6	0	-0.490727	3.787864	-1.209365
43	1	0	-1.327846	4.485815	-1.155472
44	6	0	-0.544638	2.592404	-0.489025
45	6	0	-1.774854	2.179569	0.266628
46	1	0	-2.331783	3.060120	0.627461
47	1	0	-2.426642	1.658482	-0.452179
48	6	0	-4.220229	-0.372772	-0.135190
49	1	0	-4.980397	0.381783	0.073926
50	6	0	-2.708614	0.497235	1.763942
51	1	0	-3.524948	1.208214	1.969355
52	1	0	-2.483380	-0.047827	2.690718
53	8	0	-0.172565	-1.266386	2.191097
54	1	0	0.465761	-1.999082	2.175843
55	1	0	-0.955891	-1.574997	1.629491

3(triplet) E_{opt} = -2804.1802599 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	7	0	-1.997162	-0.643068	-0.668566
5	6	0	-1.485917	-1.129300	2.578475
6	1	0	-1.373913	-1.493226	3.613394
7	1	0	-2.502452	-1.301714	2.212313
8	1	0	-1.269033	-0.045487	2.592689
9	6	0	-3.044956	-0.092756	-1.296936
10	1	0	-2.894126	0.911453	-1.701186
11	6	0	-4.382187	-2.044169	-0.905196
12	1	0	-5.318118	-2.599270	-0.997091
13	6	0	1.954179	-1.786920	1.270420
14	6	0	-4.260982	-0.760767	-1.437543
15	1	0	-5.088677	-0.277759	-1.959026
16	6	0	-3.286857	-2.613971	-0.249506
17	1	0	-3.342671	-3.613395	0.184579
18	6	0	-2.102880	-1.884211	-0.152770
19	6	0	-0.866190	-2.442238	0.500581
20	1	0	-0.987388	-3.516169	0.737157
21	1	0	-0.025982	-2.348841	-0.205642
22	6	0	4.071983	-2.476248	0.384659
23	1	0	4.928672	-3.153705	0.369651
24	6	0	3.015981	-2.691580	1.276892
25	1	0	3.018004	-3.536546	1.967763
26	6	0	0.840196	-1.904641	2.281912
27	1	0	0.883279	-2.883222	2.796258
28	1	0	0.952443	-1.131484	3.057096
29	7	0	1.597207	1.434713	-1.248416
30	7	0	-0.533281	1.894136	0.388871
31	6	0	1.282316	2.211544	-2.461382
32	1	0	2.145990	2.821219	-2.780903
33	1	0	0.431539	2.876224	-2.257755
34	1	0	1.002027	1.520109	-3.266541
35	6	0	-1.703112	2.160889	0.993606
36	1	0	-2.508060	1.440720	0.842978
37	6	0	-0.823070	4.183751	1.931523
38	1	0	-0.936043	5.088283	2.533405
39	6	0	2.881427	-0.560690	-0.453294
40	6	0	-1.890399	3.293579	1.778959
41	1	0	-2.856118	3.471789	2.254452
42	6	0	0.388927	3.903736	1.301831
43	1	0	1.245817	4.573306	1.395227
44	6	0	0.504368	2.738355	0.539426
45	6	0	1.807649	2.320289	-0.087622
46	1	0	2.409261	3.201614	-0.366372
47	1	0	2.376315	1.771353	0.677257

48	6	0	4.009521	-1.395181	-0.489091
49	1	0	4.809501	-1.199531	-1.206141
50	6	0	2.740491	0.543695	-1.477937
51	1	0	3.679550	1.123896	-1.538564
52	1	0	2.591135	0.061549	-2.453665
53	8	0	0.320504	-0.972059	-2.228898
54	1	0	-0.470495	-1.493054	-2.428528

3_{pt}(triplet) E_{opt} = -2804. 6538878 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.084652	0.310981	-0.864331
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3	7	0	-0.734559	-1.747859	1.802458
4	7	0	-1.982822	-0.467968	-0.676205
5	6	0	-1.734283	-1.165238	2.661349
6	1	0	-1.530630	-1.458118	3.703358
7	1	0	-2.742174	-1.466602	2.357616
8	1	0	-1.645475	-0.064217	2.605646
9	6	0	-2.945051	0.204716	-1.325771
10	1	0	-2.665829	1.179925	-1.732716
11	6	0	-4.515432	-1.564720	-0.945623
12	1	0	-5.511042	-2.001200	-1.049081
13	6	0	1.741907	-1.839628	1.313168
14	6	0	-4.231346	-0.308623	-1.480030
15	1	0	-4.985552	0.270627	-2.014637
16	6	0	-3.508465	-2.260935	-0.270733
17	1	0	-3.694295	-3.242601	0.167346
18	6	0	-2.245367	-1.682827	-0.154374
19	6	0	-1.104111	-2.380250	0.543618
20	1	0	-1.378583	-3.424276	0.785405
21	1	0	-0.225211	-2.408120	-0.114245
22	6	0	3.822115	-2.730506	0.512680
23	1	0	4.624421	-3.470315	0.556340
24	6	0	2.740106	-2.809314	1.396904
25	1	0	2.675785	-3.603194	2.142884
26	6	0	0.622601	-1.807905	2.322997
27	1	0	0.662140	-2.702136	2.974363
28	1	0	0.744227	-0.937722	2.988419
29	7	0	1.696341	1.286665	-1.285238
30	7	0	-0.333664	1.896822	0.415553

31	6	0	1.423471	2.077803	-2.502878
32	1	0	2.333391	2.603809	-2.837770
33	1	0	0.639854	2.815780	-2.285825
34	1	0	1.071852	1.407795	-3.297742
35	6	0	-1.464676	2.228685	1.060710
36	1	0	-2.324225	1.573510	0.917488
37	6	0	-0.409441	4.158790	2.014812
38	1	0	-0.437021	5.051411	2.643675
39	6	0	2.799300	-0.784602	-0.455374
40	6	0	-1.542576	3.351227	1.877577
41	1	0	-2.476984	3.584503	2.390081
42	6	0	0.758063	3.812966	1.336045
43	1	0	1.663067	4.417659	1.415391
44	6	0	0.766061	2.662597	0.544438
45	6	0	2.010571	2.167541	-0.135376
46	1	0	2.648523	3.006220	-0.456798
47	1	0	2.583724	1.593672	0.606735
48	6	0	3.861097	-1.700099	-0.420895
49	1	0	4.688844	-1.601387	-1.125934
50	6	0	2.762968	0.296948	-1.513896
51	1	0	3.744235	0.799291	-1.578166
52	1	0	2.581924	-0.177962	-2.489534
53	8	0	0.108350	-0.996436	-2.509102
54	1	0	-0.743812	-1.418262	-2.714237
55	1	0	0.699625	-1.741058	-2.300298

4(doublet) E_{opt} = -2803.5010593 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.123414	-0.468384	-0.907881
2	7	0	-0.923203	1.470302	0.072886
3	7	0	2.056450	2.193119	0.767294
4	7	0	1.936727	-0.827107	-0.700393
5	6	0	2.698195	3.408275	1.201641
6	1	0	3.281453	3.188949	2.116047
7	1	0	1.928544	4.147413	1.482205
8	1	0	3.355759	3.804031	0.421111
9	6	0	2.336546	-2.107915	-0.756717
10	1	0	1.563034	-2.846261	-0.979115
11	6	0	4.593280	-1.494247	-0.233746
12	1	0	5.637709	-1.750816	-0.043625

13	6	0	-0.372580	2.186751	1.052398
14	6	0	3.658813	-2.485605	-0.534956
15	1	0	3.939349	-3.538337	-0.593464
16	6	0	4.176423	-0.162390	-0.191123
17	1	0	4.880294	0.644888	0.018095
18	6	0	2.835649	0.139918	-0.442768
19	6	0	2.385587	1.591742	-0.510152
20	1	0	3.170647	2.195633	-0.976877
21	1	0	1.482676	1.622125	-1.157771
22	6	0	-2.186978	3.748140	0.977719
23	1	0	-2.690571	4.647155	1.339797
24	6	0	-0.970539	3.350291	1.542252
25	1	0	-0.501705	3.919753	2.346222
26	6	0	0.963604	1.670298	1.581454
27	1	0	1.123398	1.995157	2.616236
28	1	0	0.971241	0.573217	1.528006
29	7	0	-2.231658	-0.453588	-1.364159
30	7	0	-0.770027	-1.660600	0.654052
31	6	0	-2.379325	-1.285974	-2.567521
32	1	0	-3.423387	-1.291884	-2.928738
33	1	0	-2.075709	-2.314687	-2.327375
34	1	0	-1.717214	-0.899497	-3.352547
35	6	0	0.016979	-2.273629	1.556440
36	1	0	1.083778	-2.053876	1.507035
37	6	0	-1.863205	-3.387110	2.538865
38	1	0	-2.295331	-4.072994	3.271028
39	6	0	-2.083077	1.839640	-0.479861
40	6	0	-0.487210	-3.139298	2.520067
41	1	0	0.189361	-3.610544	3.234552
42	6	0	-2.678725	-2.737867	1.614700
43	1	0	-3.759573	-2.890370	1.606566
44	6	0	-2.100766	-1.861373	0.690668
45	6	0	-2.962459	-1.016990	-0.212582
46	1	0	-3.846761	-1.584291	-0.545115
47	1	0	-3.345145	-0.191897	0.409025
48	6	0	-2.756448	2.985924	-0.043981
49	1	0	-3.708158	3.267687	-0.498253
50	6	0	-2.585499	0.956351	-1.602949
51	1	0	-3.673263	1.083073	-1.740207
52	1	0	-2.091555	1.268656	-2.537025
53	8	0	0.274066	0.458298	-2.511765

4_{pt}(doublet) E_{opt} = -2803.9677673 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.327344	0.283263	-0.851558
2	7	0	2.004223	-1.030587	-0.131550
3	7	0	-0.034126	-2.258332	1.333577
4	7	0	-2.027433	-0.716160	-0.658649
5	6	0	-0.435217	-1.258374	2.281594
6	1	0	-0.111313	-1.560717	3.288617
7	1	0	-1.516548	-1.088375	2.243573
8	1	0	0.094121	-0.317973	2.034239
9	6	0	-3.114814	-0.073837	-1.107335
10	1	0	-2.955367	0.906796	-1.561426
11	6	0	-4.510117	-1.871703	-0.359250
12	1	0	-5.491437	-2.331973	-0.227453
13	6	0	2.367577	-1.886885	0.822915
14	6	0	-4.385357	-0.630133	-0.979301
15	1	0	-5.250509	-0.083441	-1.356422
16	6	0	-3.361173	-2.533793	0.081942
17	1	0	-3.419921	-3.517687	0.549653
18	6	0	-2.111102	-1.940274	-0.092695
19	6	0	-0.850103	-2.699466	0.218532
20	1	0	-1.091909	-3.761050	0.412645
21	1	0	-0.202269	-2.705274	-0.673353
22	6	0	4.657212	-1.194728	0.668085
23	1	0	5.700384	-1.258317	0.985064
24	6	0	3.690628	-2.003285	1.264436
25	1	0	3.948221	-2.708389	2.056585
26	6	0	1.306528	-2.811323	1.415820
27	1	0	1.317887	-3.769000	0.874999
28	1	0	1.536217	-3.000955	2.474008
29	7	0	1.224557	1.483386	-1.305769
30	7	0	-0.720459	1.642499	0.542963
31	6	0	0.696153	2.316211	-2.415958
32	1	0	1.483777	3.009019	-2.750899
33	1	0	-0.174216	2.885201	-2.066605
34	1	0	0.402794	1.655973	-3.240601
35	6	0	-1.851660	1.739135	1.264239
36	1	0	-2.595630	0.953093	1.147268
37	6	0	-1.079399	3.782453	2.258768
38	1	0	-1.224477	4.632203	2.929008
39	6	0	2.926415	-0.230323	-0.686798

40	6	0	-2.063142	2.797655	2.139030
41	1	0	-2.990943	2.840491	2.710641
42	6	0	0.093422	3.669339	1.512916
43	1	0	0.888776	4.412947	1.578364
44	6	0	0.251050	2.574209	0.666265
45	6	0	1.505589	2.295855	-0.088146
46	1	0	2.034853	3.216125	-0.378219
47	1	0	2.175026	1.722022	0.569967
48	6	0	4.272489	-0.284375	-0.319436
49	1	0	4.996687	0.384291	-0.787869
50	6	0	2.434051	0.737963	-1.736425
51	1	0	3.214357	1.478769	-1.971687
52	1	0	2.179501	0.208439	-2.664524
53	8	0	0.011023	-0.733840	-2.344949
54	1	0	0.695223	-1.357702	-2.039979

TS0(quartet) E_{opt} = -3522.812844 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.151726	-0.043839	-0.353681
2	7	0	-2.241066	-1.180323	-0.139915
3	7	0	-3.753687	1.610449	0.312615
4	7	0	-0.372831	2.066320	-0.058084
5	6	0	-5.084479	1.425347	-0.253955
6	1	0	-5.799453	1.180445	0.545985
7	1	0	-5.137396	0.617871	-1.012665
8	1	0	-5.416446	2.357640	-0.735922
9	6	0	0.714989	2.758851	0.333908
10	1	0	1.656662	2.205738	0.318929
11	6	0	-0.584876	4.745549	0.667669
12	1	0	-0.676911	5.794694	0.958286
13	6	0	-3.340896	-0.845037	0.552133
14	6	0	0.651883	4.097739	0.704822
15	1	0	1.560982	4.614816	1.016414
16	6	0	-1.697659	4.034080	0.227165
17	1	0	-2.676045	4.511495	0.151263
18	6	0	-1.565534	2.690479	-0.148885
19	6	0	-2.765806	1.955630	-0.703363
20	1	0	-3.252845	2.632845	-1.419948
21	1	0	-2.418756	1.082688	-1.292696
22	6	0	-4.416037	-2.895581	-0.120828
23	1	0	-5.271671	-3.574845	-0.106374

24	6	0	-4.456865	-1.692467	0.585310
25	1	0	-5.340094	-1.405307	1.158550
26	6	0	-3.345391	0.519029	1.210949
27	1	0	-4.032505	0.507046	2.070362
28	1	0	-2.334049	0.733304	1.587461
29	7	0	0.263850	-2.081991	-0.833884
30	7	0	0.632739	-0.596849	1.466312
31	6	0	1.486442	-2.147160	-1.657909
32	1	0	1.605574	-3.157541	-2.086939
33	1	0	2.353060	-1.933600	-1.025550
34	1	0	1.434469	-1.407887	-2.465674
35	6	0	1.010396	0.243708	2.442820
36	1	0	0.668079	1.275449	2.362573
37	6	0	2.205595	-1.502030	3.568435
38	1	0	2.835508	-1.857570	4.386904
39	6	0	-2.191844	-2.333733	-0.820607
40	6	0	1.791387	-0.168680	3.517000
41	1	0	2.073840	0.548682	4.288852
42	6	0	1.804126	-2.374248	2.558456
43	1	0	2.106080	-3.422737	2.559691
44	6	0	1.009158	-1.889608	1.518209
45	6	0	0.457224	-2.792473	0.450261
46	1	0	1.095480	-3.679389	0.312230
47	1	0	-0.518078	-3.156106	0.808279
48	6	0	-3.264650	-3.228205	-0.837641
49	1	0	-3.188286	-4.166246	-1.390693
50	6	0	-0.905852	-2.605293	-1.566270
51	1	0	-0.789241	-3.686100	-1.755426
52	1	0	-0.936624	-2.099860	-2.544542
53	8	0	-0.491929	0.312787	-2.238780
54	8	0	1.382237	1.243478	-2.681683
55	1	0	2.017439	1.000466	-1.771978
56	1	0	0.952765	2.082509	-2.441218
57	15	0	4.068675	-0.015933	-0.682510
58	8	0	2.714638	0.806913	-0.702241
59	8	0	5.214493	1.114293	-0.218283
60	1	0	5.354989	1.745107	-0.941331
61	8	0	4.081576	-1.027563	0.466695
62	8	0	4.433047	-0.516397	-2.080183

Int0(quartet) E_{opt} = -3522.8175612 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	29	0	-0.190405	-0.007559	-0.408996
2	7	0	-2.198139	-1.248282	-0.147336
3	7	0	-3.839436	1.490600	0.422670
4	7	0	-0.533363	2.060673	-0.094088
5	6	0	-5.202052	1.276442	-0.052777
6	1	0	-5.852610	0.998483	0.790433
7	1	0	-5.289950	0.482109	-0.822333
8	1	0	-5.593073	2.207539	-0.491194
9	6	0	0.544468	2.798033	0.239904
10	1	0	1.497546	2.269197	0.275332
11	6	0	-0.782632	4.781763	0.444464
12	1	0	-0.888997	5.847895	0.658097
13	6	0	-3.303907	-0.958027	0.556016
14	6	0	0.465032	4.158136	0.516612
15	1	0	1.368664	4.709252	0.782171
16	6	0	-1.887822	4.021036	0.073346
17	1	0	-2.876011	4.475076	-0.019373
18	6	0	-1.738998	2.655684	-0.208787
19	6	0	-2.938446	1.859463	-0.671636
20	1	0	-3.504589	2.503880	-1.358831
21	1	0	-2.595686	0.993612	-1.267136
22	6	0	-4.325090	-3.020533	-0.162737
23	1	0	-5.162385	-3.722516	-0.162208
24	6	0	-4.396690	-1.835763	0.571605
25	1	0	-5.284828	-1.587401	1.155247
26	6	0	-3.337772	0.385797	1.256334
27	1	0	-3.976694	0.315380	2.149460
28	1	0	-2.317677	0.631488	1.587740
29	7	0	0.327112	-2.040015	-0.870846
30	7	0	0.613874	-0.522860	1.419801
31	6	0	1.552398	-2.057654	-1.689792
32	1	0	1.714165	-3.060448	-2.123580
33	1	0	2.407323	-1.819985	-1.050427
34	1	0	1.479572	-1.313313	-2.490814
35	6	0	0.920251	0.330925	2.410258
36	1	0	0.541077	1.348546	2.316281
37	6	0	2.137666	-1.366109	3.584795
38	1	0	2.748503	-1.696908	4.427762
39	6	0	-2.117105	-2.384984	-0.852184
40	6	0	1.674404	-0.049644	3.514775
41	1	0	1.897903	0.678469	4.295886
42	6	0	1.806992	-2.253488	2.562843
43	1	0	2.145854	-3.290530	2.579198

44	6	0	1.033076	-1.800745	1.491964
45	6	0	0.546004	-2.733557	0.417133
46	1	0	1.234927	-3.583955	0.291602
47	1	0	-0.410103	-3.151948	0.767109
48	6	0	-3.166049	-3.307119	-0.887327
49	1	0	-3.065838	-4.231464	-1.459404
50	6	0	-0.822054	-2.608002	-1.601017
51	1	0	-0.668109	-3.684546	-1.790102
52	1	0	-0.873907	-2.103264	-2.578647
53	8	0	-0.492171	0.337633	-2.278480
54	8	0	1.465593	1.186270	-2.630040
55	1	0	2.364505	0.954979	-1.360150
56	1	0	1.021103	2.017065	-2.385716
57	15	0	4.242747	-0.013001	-0.568640
58	8	0	2.908615	0.923080	-0.499230
59	8	0	5.421624	1.047233	-0.099510
60	1	0	5.599481	1.687072	-0.807357
61	8	0	4.179151	-1.042045	0.546719
62	8	0	4.474688	-0.450954	-2.003548

TS1(doublet) E_{opt} = -3522.808217 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.202899	-0.009847	-0.408195
2	7	0	-2.205022	-1.256061	-0.143500
3	7	0	-3.851610	1.483393	0.393701
4	7	0	-0.537080	2.065068	-0.088979
5	6	0	-5.205022	1.259288	-0.102959
6	1	0	-5.868219	0.982835	0.730887
7	1	0	-5.276031	0.460007	-0.869208
8	1	0	-5.593620	2.185663	-0.553433
9	6	0	0.532414	2.808324	0.259004
10	1	0	1.490697	2.289760	0.297029
11	6	0	-0.809979	4.781810	0.465018
12	1	0	-0.925278	5.845918	0.684040
13	6	0	-3.315283	-0.964851	0.551905
14	6	0	0.441156	4.166018	0.544262
15	1	0	1.338791	4.721665	0.820529
16	6	0	-1.906355	4.015991	0.078780
17	1	0	-2.896664	4.463966	-0.020565
18	6	0	-1.745400	2.653376	-0.210320
19	6	0	-2.935059	1.851290	-0.688483

20	1	0	-3.493199	2.491966	-1.385864
21	1	0	-2.578304	0.985770	-1.275834
22	6	0	-4.323730	-3.037945	-0.154003
23	1	0	-5.157714	-3.743881	-0.151243
24	6	0	-4.404495	-1.847046	0.569457
25	1	0	-5.296883	-1.597439	1.146126
26	6	0	-3.358581	0.384800	1.240836
27	1	0	-4.007844	0.320125	2.126996
28	1	0	-2.342780	0.634470	1.582399
29	7	0	0.328621	-2.043941	-0.864238
30	7	0	0.589971	-0.523423	1.429958
31	6	0	1.550454	-2.051402	-1.688959
32	1	0	1.707729	-3.046884	-2.141169
33	1	0	2.409516	-1.828670	-1.049399
34	1	0	1.475540	-1.293907	-2.477769
35	6	0	0.881096	0.332296	2.423140
36	1	0	0.475918	1.340680	2.336671
37	6	0	2.155387	-1.337172	3.576762
38	1	0	2.783851	-1.655440	4.411575
39	6	0	-2.115923	-2.397081	-0.840304
40	6	0	1.653499	-0.034314	3.520103
41	1	0	1.862704	0.694668	4.304400
42	6	0	1.839412	-2.227825	2.552518
43	1	0	2.206387	-3.255327	2.559957
44	6	0	1.040715	-1.791289	1.493426
45	6	0	0.556777	-2.732057	0.423838
46	1	0	1.248519	-3.580564	0.300362
47	1	0	-0.396787	-3.151929	0.779338
48	6	0	-3.160320	-3.324775	-0.871491
49	1	0	-3.053758	-4.253002	-1.436133
50	6	0	-0.820230	-2.617146	-1.589519
51	1	0	-0.663767	-3.693455	-1.778630
52	1	0	-0.876639	-2.111102	-2.566012
53	8	0	-0.463179	0.326348	-2.268930
54	8	0	1.534526	1.289131	-2.669553
55	1	0	2.386778	0.947591	-1.298049
56	1	0	1.024864	2.063667	-2.365556
57	15	0	4.261927	-0.025030	-0.576381
58	8	0	2.905994	0.883521	-0.440515
59	8	0	5.418376	1.025543	-0.041851
60	1	0	5.606981	1.693071	-0.720905
61	8	0	4.216275	-1.123426	0.470599
62	8	0	4.486386	-0.359388	-2.038976

TS'(doubelt) E_{opt} = -3109.033305 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.325094	-0.290178	-0.068559
2	7	0	-1.978074	-0.382693	-0.264588
3	7	0	-2.057631	2.815379	0.497042
4	7	0	1.099477	1.503839	0.390133
5	6	0	-3.203722	3.438790	-0.158501
6	1	0	-4.048617	3.498930	0.544192
7	1	0	-3.552406	2.896568	-1.061351
8	1	0	-2.944031	4.463196	-0.466658
9	6	0	2.357821	1.468880	0.864924
10	1	0	2.837414	0.490210	0.900753
11	6	0	2.319926	3.832848	1.233612
12	1	0	2.792451	4.757575	1.572378
13	6	0	-2.901705	0.448840	0.242736
14	6	0	3.008375	2.618558	1.294095
15	1	0	4.029757	2.552029	1.671386
16	6	0	1.028808	3.852225	0.711714
17	1	0	0.473352	4.787143	0.620134
18	6	0	0.431056	2.667018	0.262398
19	6	0	-0.920239	2.709609	-0.420893
20	1	0	-0.917821	3.612325	-1.046972
21	1	0	-0.990677	1.850912	-1.108415
22	6	0	-4.613757	-0.705596	-1.002775
23	1	0	-5.659777	-0.835168	-1.290225
24	6	0	-4.249130	0.308533	-0.113625
25	1	0	-4.996406	0.981743	0.309733
26	6	0	-2.400191	1.547988	1.162134
27	1	0	-3.167390	1.760929	1.921214
28	1	0	-1.506135	1.174611	1.683306
29	7	0	-0.062259	-2.237889	-0.621701
30	7	0	0.382637	-1.040832	1.797421
31	6	0	1.196142	-2.793422	-1.163119
32	1	0	1.011008	-3.791217	-1.593829
33	1	0	1.917102	-2.877856	-0.342161
34	1	0	1.595588	-2.121757	-1.926018
35	6	0	0.732930	-0.381562	2.915384
36	1	0	0.928682	0.686052	2.823592
37	6	0	0.571237	-2.394312	4.209695
38	1	0	0.656198	-2.931562	5.156715
39	6	0	-2.312892	-1.361839	-1.111455

40	6	0	0.833579	-1.023290	4.144341
41	1	0	1.116958	-0.451325	5.028894
42	6	0	0.189552	-3.068429	3.050778
43	1	0	-0.041609	-4.134705	3.060603
44	6	0	0.086345	-2.355699	1.855174
45	6	0	-0.475540	-2.966679	0.610385
46	1	0	-0.207997	-4.030155	0.519740
47	1	0	-1.571021	-2.920117	0.698798
48	6	0	-3.635536	-1.564514	-1.509881
49	1	0	-3.887953	-2.379163	-2.191185
50	6	0	-1.168451	-2.226106	-1.603524
51	1	0	-1.510783	-3.258435	-1.785920
52	1	0	-0.780949	-1.834456	-2.553019
53	8	0	0.446045	0.147958	-1.851055
54	8	0	1.626991	1.572009	-2.518426
55	1	0	1.195561	1.611514	-3.390193
56	8	0	3.502919	-0.154073	-2.923453
57	1	0	2.890769	-0.729668	-3.433565
58	1	0	3.599569	-0.591451	-2.043423
59	8	0	1.273796	-1.157756	-4.199952
60	1	0	1.029335	-2.092164	-4.117719
61	1	0	0.885020	-0.742694	-3.401364
62	8	0	3.818223	-1.161412	-0.384213
63	1	0	4.626300	-0.715812	-0.082140
64	1	0	4.074283	-2.095810	-0.443964
65	1	0	2.416024	0.935453	-2.658057

Int1(doublet) E_{opt} = -2879.4547845 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.111927	-0.440674	0.741386
2	7	0	0.960599	1.485549	-0.128209
3	7	0	-2.081462	2.200542	-1.225153
4	7	0	-1.924435	-0.752339	0.411809
5	6	0	-2.215823	3.653552	-1.244423
6	1	0	-1.994385	4.036655	-2.252308
7	1	0	-1.545394	4.175629	-0.530669
8	1	0	-3.250119	3.935753	-0.993707
9	6	0	-2.336454	-2.028839	0.515173
10	1	0	-1.571352	-2.762686	0.779932
11	6	0	-4.578078	-1.425141	-0.063331

12	1	0	-5.621571	-1.683396	-0.258293
13	6	0	0.452599	2.246150	-1.111210
14	6	0	-3.653500	-2.412269	0.289075
15	1	0	-3.941022	-3.460547	0.384437
16	6	0	-4.151416	-0.101303	-0.143417
17	1	0	-4.850444	0.699376	-0.391913
18	6	0	-2.811611	0.219561	0.117638
19	6	0	-2.360937	1.665068	0.112512
20	1	0	-3.187845	2.255873	0.530388
21	6	0	2.212118	3.860422	-0.777428
22	1	0	2.708056	4.798851	-1.036928
23	6	0	1.062851	3.457978	-1.461134
24	1	0	0.645243	4.065367	-2.265886
25	6	0	-0.806155	1.740303	-1.796734
26	1	0	-0.780293	2.049661	-2.852749
27	1	0	-0.787357	0.640494	-1.769971
28	7	0	2.207383	-0.493572	1.272823
29	7	0	0.813958	-1.700445	-0.791306
30	6	0	2.326532	-1.397225	2.423831
31	1	0	3.362844	-1.431729	2.807376
32	1	0	2.027979	-2.409703	2.116003
33	1	0	1.650939	-1.058641	3.218817
34	6	0	0.062307	-2.354397	-1.692890
35	1	0	-1.009895	-2.156026	-1.674016
36	6	0	1.985746	-3.457113	-2.602349
37	1	0	2.448382	-4.153812	-3.305170
38	6	0	2.072648	1.850439	0.525575
39	6	0	0.605360	-3.237658	-2.620402
40	1	0	-0.045305	-3.742671	-3.336081
41	6	0	2.766219	-2.765992	-1.677487
42	1	0	3.849349	-2.896803	-1.639214
43	6	0	2.148398	-1.876767	-0.792314
44	6	0	2.964683	-0.988281	0.111253
45	1	0	3.890310	-1.499011	0.425219
46	1	0	3.278891	-0.128942	-0.502207
47	6	0	2.736305	3.042897	0.226542
48	1	0	3.647099	3.314662	0.763778
49	6	0	2.550351	0.898303	1.605122
50	1	0	3.634887	1.019447	1.775064
51	1	0	2.031732	1.143613	2.543548
52	8	0	-0.297590	0.372433	2.475589
53	8	0	-1.005564	-0.617291	3.245358
54	1	0	-1.923987	-0.504415	2.945217
55	1	0	-1.512569	1.775129	0.810205

Int2(triplet) E_{opt} = -2878.8350736 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.189265	-0.385530	0.684123
2	7	0	0.604333	1.650424	-0.175242
3	7	0	-2.547994	1.716566	-1.201614
4	7	0	-1.753749	-1.106355	0.484947
5	6	0	-2.976991	3.110711	-1.239357
6	1	0	-2.864026	3.509260	-2.259189
7	1	0	-2.409864	3.773839	-0.553725
8	1	0	-4.040480	3.180926	-0.963181
9	6	0	-1.892653	-2.437790	0.617232
10	1	0	-0.989960	-2.993217	0.883415
11	6	0	-4.218795	-2.320768	0.069072
12	1	0	-5.189498	-2.792461	-0.101145
13	6	0	-0.074407	2.273142	-1.154456
14	6	0	-3.106061	-3.088710	0.422656
15	1	0	-3.170629	-4.171290	0.543886
16	6	0	-4.075014	-0.939244	-0.043313
17	1	0	-4.927856	-0.305366	-0.293360
18	6	0	-2.826054	-0.345603	0.186852
19	6	0	-2.678177	1.160700	0.149635
20	1	0	-3.593612	1.582168	0.587835
21	6	0	1.316702	4.224521	-0.887079
22	1	0	1.598710	5.241225	-1.171024
23	6	0	0.262007	3.578609	-1.535206
24	1	0	-0.292121	4.071154	-2.336010
25	6	0	-1.220483	1.512294	-1.801709
26	1	0	-1.282033	1.804111	-2.861167
27	1	0	-0.981022	0.438914	-1.764968
28	7	0	2.271598	0.002862	1.226634
29	7	0	1.142388	-1.577945	-0.772232
30	6	0	2.619257	-0.825496	2.386571
31	1	0	3.655959	-0.638272	2.723271
32	1	0	2.522886	-1.885953	2.112195
33	1	0	1.928092	-0.615882	3.212175
34	6	0	0.552484	-2.455189	-1.599769
35	1	0	-0.538273	-2.486575	-1.584279
36	6	0	2.672189	-3.204481	-2.429350
37	1	0	3.277016	-3.848447	-3.071991

38	6	0	1.631782	2.251604	0.442423
39	6	0	1.277103	-3.285570	-2.450049
40	1	0	0.754070	-3.981573	-3.107935
41	6	0	3.282842	-2.283311	-1.579061
42	1	0	4.368958	-2.179395	-1.542245
43	6	0	2.483874	-1.469751	-0.769712
44	6	0	3.081473	-0.352712	0.049104
45	1	0	4.119137	-0.593247	0.335940
46	1	0	3.138513	0.521970	-0.617927
47	6	0	2.022978	3.551555	0.111930
48	1	0	2.869637	4.016231	0.621032
49	6	0	2.333443	1.442920	1.516796
50	1	0	3.375812	1.789697	1.634945
51	1	0	1.820488	1.610632	2.476215
52	8	0	-0.375685	0.409397	2.481677
53	8	0	-0.575875	-0.497719	3.359021
54	1	0	-1.847141	1.455056	0.815390

Int3(doublet) E_{opt} = -2878.6717152 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.377153	-0.177262	0.408158
2	7	0	-0.451500	1.697494	-0.139966
3	7	0	-3.057004	0.204894	-1.419712
4	7	0	-0.895635	-1.771355	0.195717
5	6	0	-4.161701	1.159057	-1.472235
6	1	0	-4.238587	1.583906	-2.484410
7	1	0	-4.060278	2.001219	-0.757470
8	1	0	-5.107531	0.643667	-1.245939
9	6	0	-0.289367	-2.966515	0.336384
10	1	0	0.772796	-2.948157	0.587861
11	6	0	-2.326103	-4.130193	-0.131681
12	1	0	-2.893009	-5.053168	-0.273022
13	6	0	-1.257338	1.944917	-1.189639
14	6	0	-0.965967	-4.170413	0.183888
15	1	0	-0.431753	-5.113215	0.309957
16	6	0	-2.955013	-2.891746	-0.241005
17	1	0	-4.022994	-2.821526	-0.454679
18	6	0	-2.221644	-1.713405	-0.054174
19	6	0	-2.921263	-0.373696	-0.079780
20	1	0	-3.934903	-0.535824	0.310448

21	6	0	-1.099226	4.312236	-0.746137
22	1	0	-1.354913	5.345780	-0.990041
23	6	0	-1.604037	3.262126	-1.513156
24	1	0	-2.256178	3.450654	-2.367171
25	6	0	-1.804586	0.755714	-1.954529
26	1	0	-1.980710	1.056185	-2.997215
27	1	0	-1.040530	-0.035947	-1.964034
28	7	0	1.719699	1.057554	1.319749
29	7	0	2.121366	-0.752110	-0.679881
30	6	0	2.249394	0.323485	2.486950
31	1	0	2.928944	0.969551	3.067871
32	1	0	2.800259	-0.561117	2.142056
33	1	0	1.416159	0.000238	3.123206
34	6	0	2.312669	-1.804018	-1.491284
35	1	0	1.468065	-2.482451	-1.625707
36	6	0	4.569445	-1.124264	-1.932540
37	1	0	5.536632	-1.273892	-2.417625
38	6	0	0.060685	2.701836	0.596354
39	6	0	3.522611	-2.025918	-2.142603
40	1	0	3.636657	-2.891993	-2.796271
41	6	0	4.364380	-0.027030	-1.095551
42	1	0	5.154247	0.703040	-0.911163
43	6	0	3.116622	0.136504	-0.491554
44	6	0	2.778365	1.352556	0.330064
45	1	0	3.669799	1.761551	0.831513
46	1	0	2.403484	2.128318	-0.356208
47	6	0	-0.244677	4.033056	0.322906
48	1	0	0.192276	4.828266	0.928851
49	6	0	0.968464	2.269614	1.717697
50	1	0	1.657014	3.075982	2.016344
51	1	0	0.356473	2.005152	2.593284
52	8	0	-1.193471	-0.088989	2.877753
53	8	0	-1.031360	-1.185772	3.334260
54	1	0	-2.418942	0.303712	0.635272
