

Electronic Supplementary Information

Hydration of the Sulfuric Acid-Oxalic Acid Complex: Acid Dissociation and Its Atmospheric Implication

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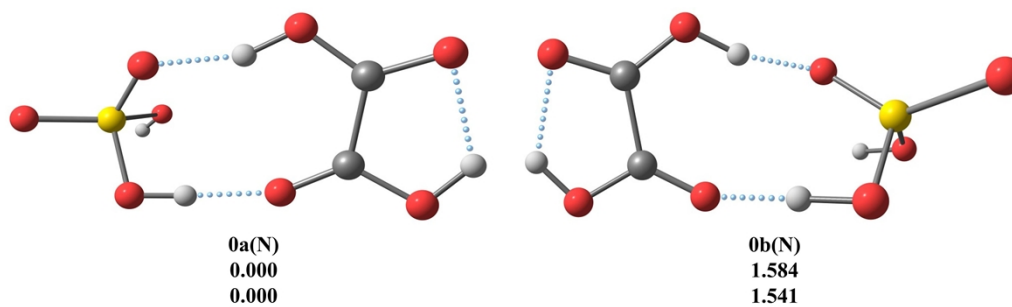


Figure S2.

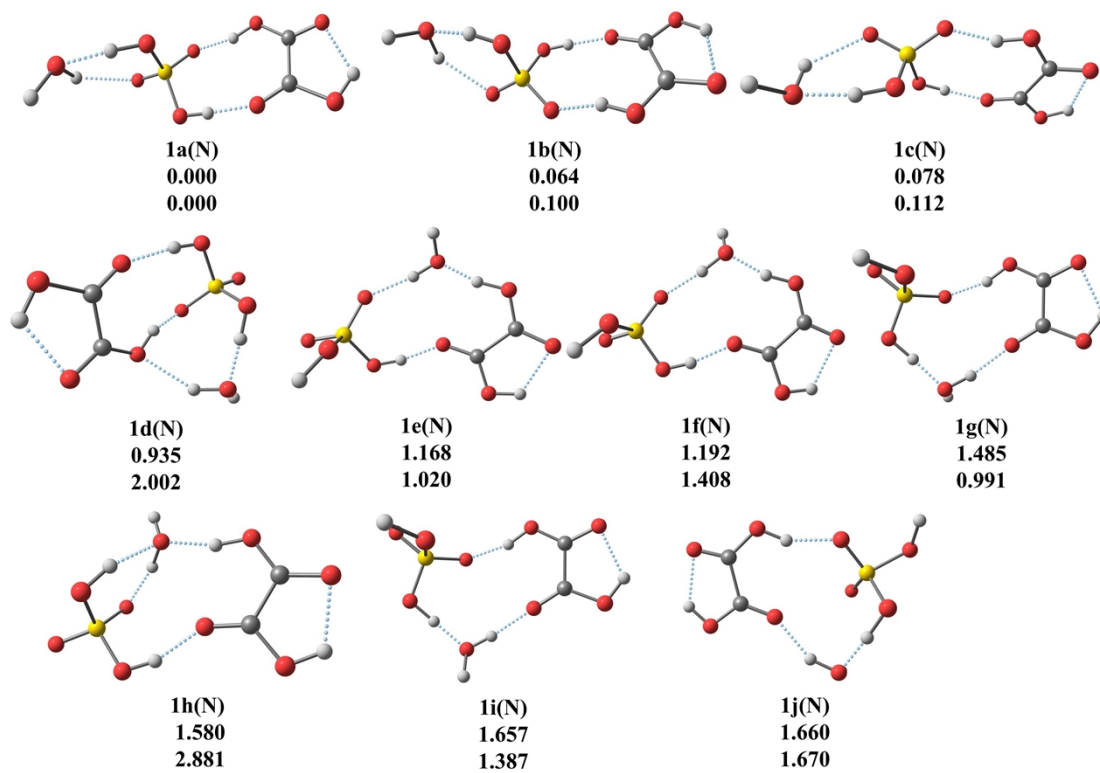


Figure S3.

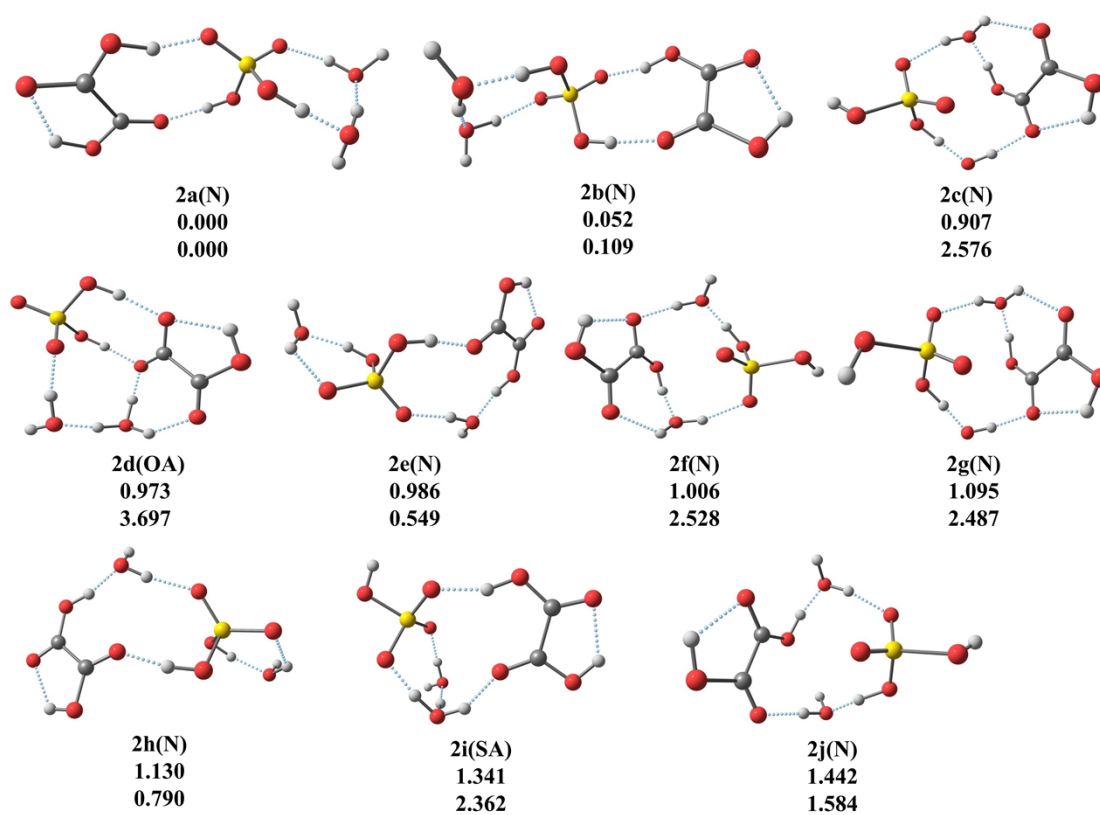


Figure S4.

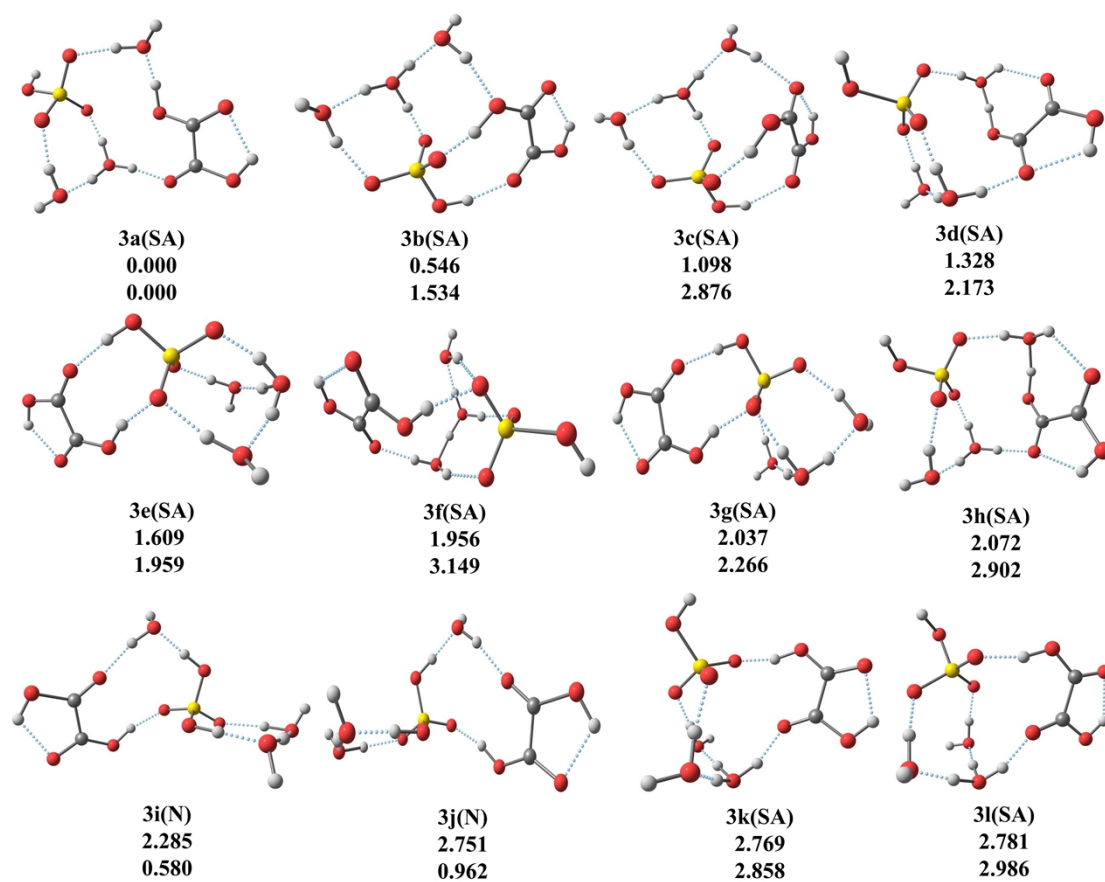


Figure S5.

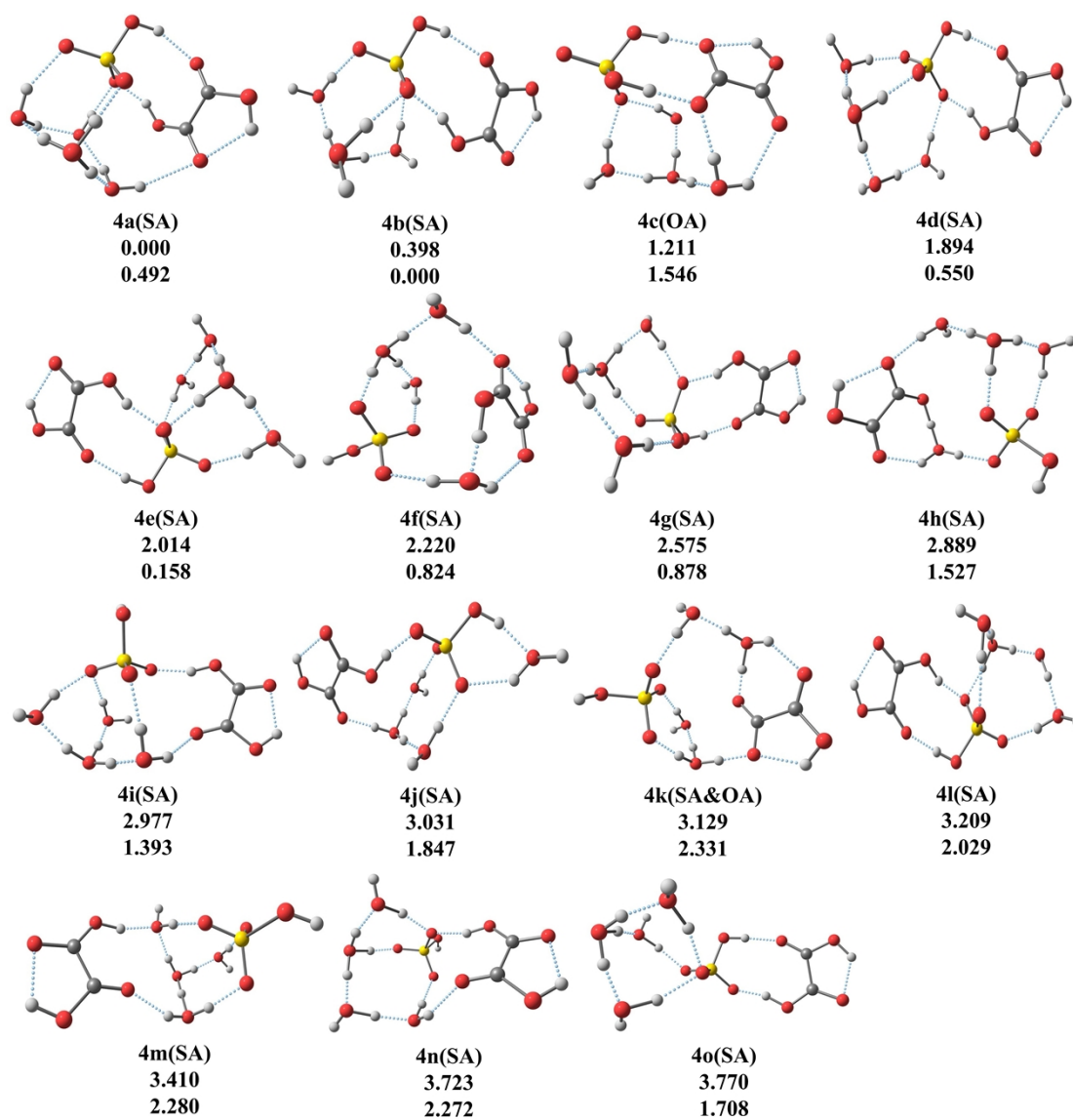


Figure S6.

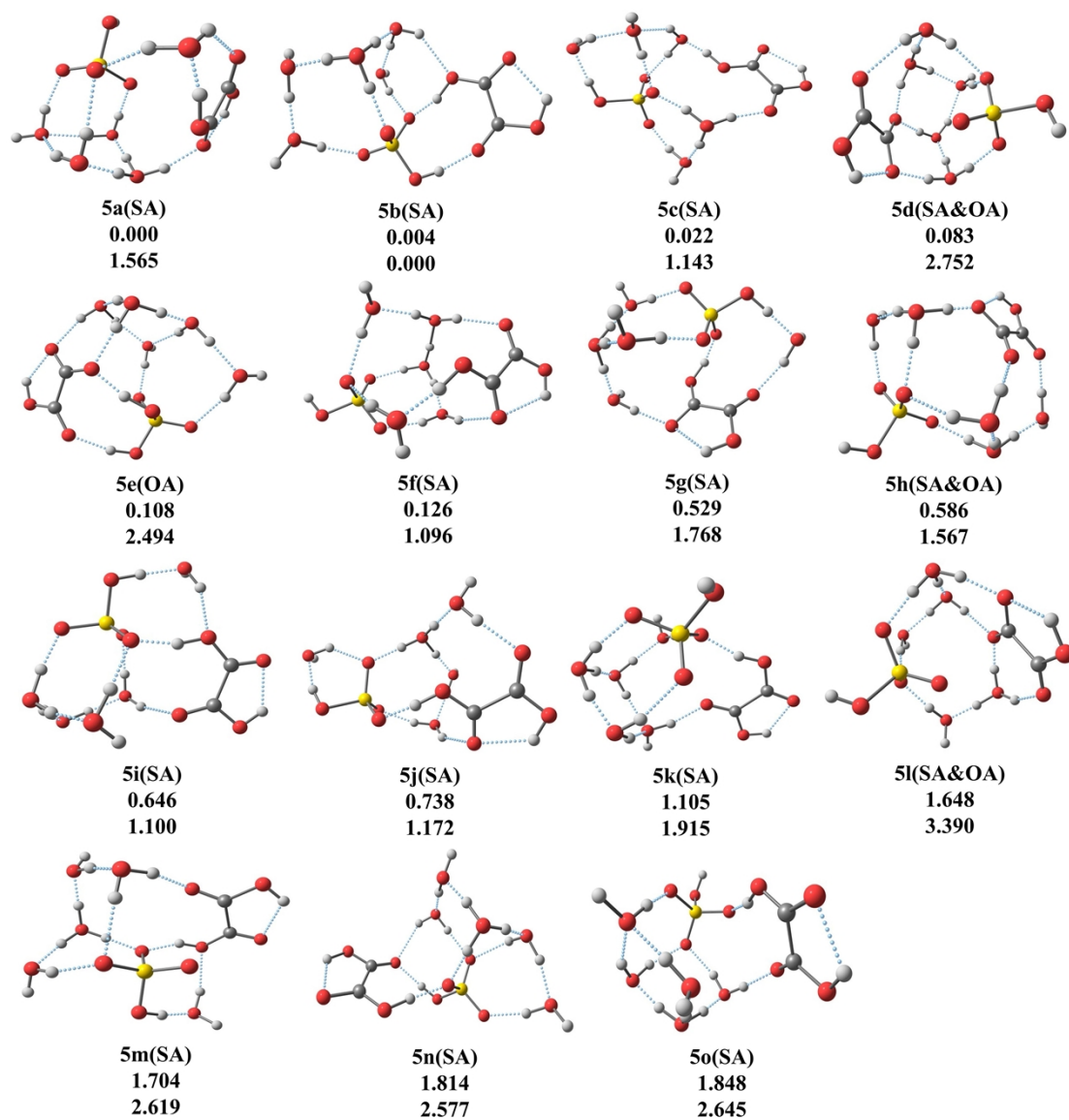


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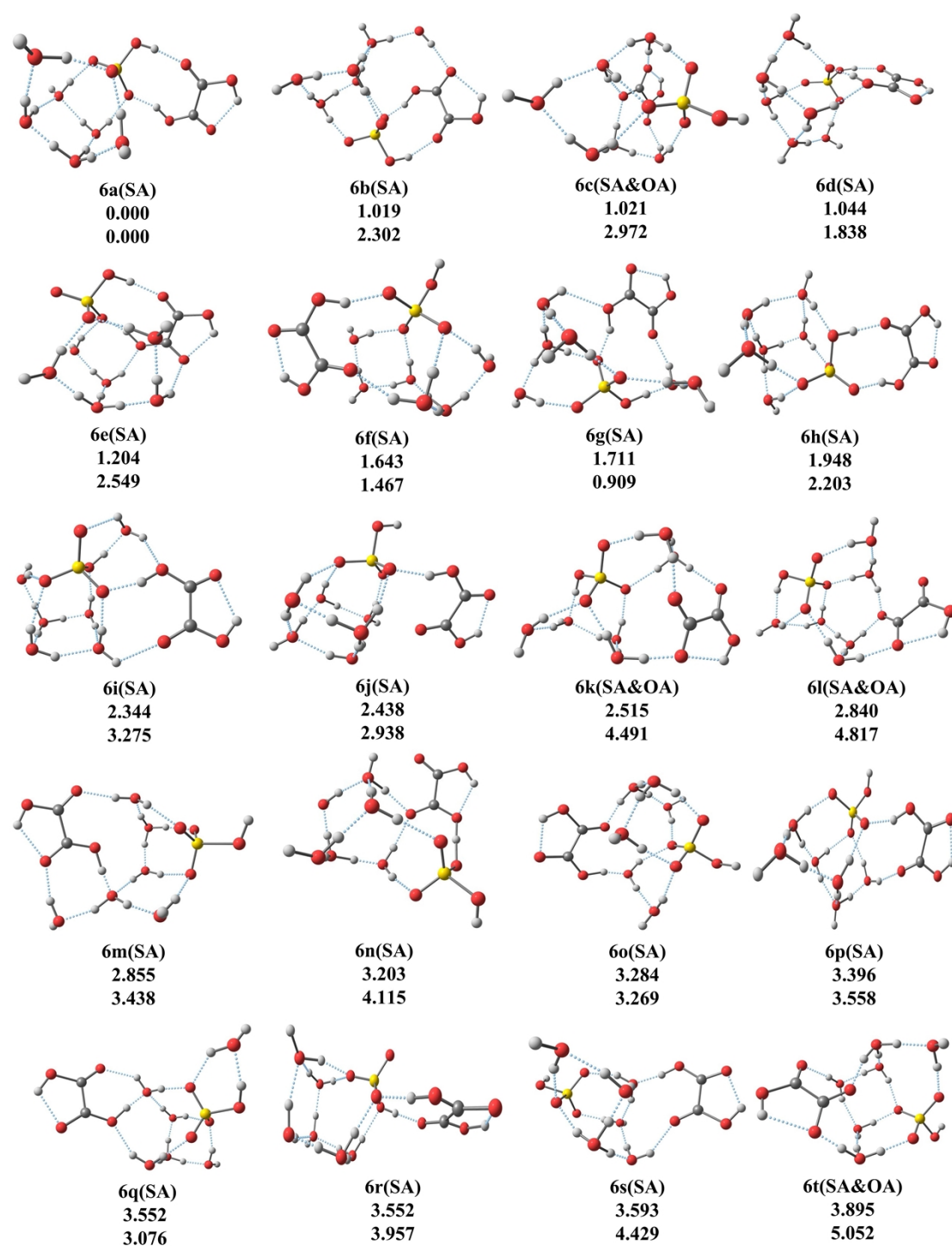


Table S1.

isomer	ΔE (0 K)	ΔH (298.15 K)	ΔG (298.15 K)
0a(N)	-15.11	-14.93	-5.49
0b(N)	-13.52	-13.35	-3.95
1a(N)	-11.01	-11.79	-2.28
1b(N)	-10.94	-11.74	-2.18
1c(N)	-10.93	-11.72	-2.17
1d(N)	-10.07	-10.96	-0.28
1e(N)	-9.84	-10.50	-1.26
1f(N)	-9.81	-10.52	-0.87
1g(N)	-9.52	-10.11	-1.29
1h(N)	-9.43	-10.52	0.60
1i(N)	-9.35	-9.94	-0.89
1j(N)	-9.35	-9.99	-0.61
2a(N)	-10.74	-11.66	-1.79
2b(N)	-10.69	-11.64	-1.68
2c(N)	-9.83	-10.83	0.78
2d(OA)	-9.77	-11.47	1.91
2e(N)	-9.76	-10.41	-1.24
2f(N)	-9.74	-10.70	0.74
2g(N)	-9.65	-10.65	0.69
2h(N)	-9.61	-10.28	-1.00
2i(SA)	-9.40	-10.60	0.57
2j(N)	-9.30	-10.10	-0.21

Table S2.

isomer	ΔE (0 K)	ΔH (298.15 K)	ΔG (298.15 K)
3a(SA)	-11.64	-12.72	-1.42
3b(SA)	-11.09	-12.42	0.11
3c(SA)	-10.54	-11.90	1.45
3d(SA)	-10.31	-11.61	0.75
3e(SA)	-10.03	-11.32	0.54
3f(SA)	-9.68	-10.79	1.73
3g(SA)	-9.60	-10.90	0.85
3h(SA)	-9.56	-10.89	1.48
3i(N)	-9.35	-9.88	-0.84
3j(N)	-8.88	-9.37	-0.46
3k(SA)	-8.87	-9.93	1.44
3l(SA)	-8.86	-9.95	1.57
4a(SA)	-11.55	-12.75	-0.60
4b(SA)	-11.15	-12.13	-1.09
4c(OA)	-10.34	-11.45	0.46
4d(SA)	-9.66	-10.50	-0.54
4e(SA)	-9.54	-10.34	-0.93
4f(SA)	-9.33	-10.17	-0.26
4g(SA)	-8.98	-9.81	-0.21
4h(SA)	-8.66	-9.59	0.44
4i(SA)	-8.57	-9.17	0.30
4j(SA)	-8.52	-9.34	0.76
4k(SA&OA)	-8.42	-9.48	1.24
4l(SA)	-8.34	-9.25	0.94
4m(SA)	-8.14	-9.04	1.19
4n(SA)	-7.83	-8.45	1.18

4o(SA)	-7.78	-8.63	0.62
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Table S3.

isomer	ΔE (0 K)	ΔH (298.15 K)	ΔG (298.15 K)
5a(SA)	-9.01	-9.75	0.29
5b(SA)	-9.01	-9.34	-1.27
5c(SA)	-8.99	-9.79	-0.13
5d(SA&OA)	-8.93	-10.03	1.48
5e(OA)	-8.90	-9.77	1.22
5f(SA)	-8.89	-9.24	-0.17
5g(SA)	-8.48	-9.13	0.50
5h(SA&OA)	-8.43	-9.09	0.30
5i(SA)	-8.37	-8.78	-0.17
5j(SA)	-8.27	-8.69	-0.10
5k(SA)	-7.91	-8.33	0.64
5l(SA&OA)	-7.36	-8.27	2.12
5m(SA)	-7.31	-7.71	1.35
5n(SA)	-7.20	-7.76	1.31
5o(SA)	-7.16	-7.57	1.37

Table S4.

isomer	ΔE (0 K)	ΔH (298.15 K)	ΔG (298.15 K)
6a(SA)	-10.42	-10.92	-1.41
6b(SA)	-9.40	-10.25	0.89
6c(SA&OA)	-9.40	-10.43	1.56
6d(SA)	-9.38	-10.02	0.43
6e(SA)	-9.22	-9.62	1.14
6f(SA)	-8.78	-8.77	0.06
6g(SA)	-8.71	-9.18	-0.50
6h(SA)	-8.47	-9.03	0.79
6i(SA)	-8.08	-8.64	1.86
6j(SA)	-7.98	-8.40	1.53
6k(SA&OA)	-7.91	-9.06	3.08
6l(SA&OA)	-7.58	-8.62	3.41
6m(SA)	-7.57	-8.18	2.03
6n(SA)	-7.22	-7.77	2.70
6o(SA)	-7.14	-7.33	1.86
6p(SA)	-7.03	-7.54	2.15
6q(SA)	-6.87	-7.51	1.66
6r(SA)	-6.87	-7.48	2.55
6s(SA)	-6.83	-7.39	3.02
6t(SA&OA)	-6.53	-7.30	3.64

Table S5.

OA-SA

15

0a(N)	E[DF-MP2-F12]	-1077.546603
S	-2.155144	-0.087265
O	-1.157259	-1.082729
O	-3.488063	-0.163645
O	-2.195704	-0.115577
O	-1.600052	1.345079
H	-2.997166	0.357858
H	-0.602890	1.343755
C	2.113063	0.763053
C	2.415545	-0.764837
O	3.229355	1.460227
O	1.012461	1.273117
O	3.585661	-1.090889
O	1.420382	-1.609144
H	3.943835	0.769542
H	0.512638	-1.195728

15

0b(N)	E[DF-MP2-F12]	-1077.543874
S	-2.134264	-0.119739
O	-1.110121	-0.921288
O	-3.112861	-0.706580
O	-1.419254	1.044451
O	-2.958282	0.630688
H	-0.474040	1.141999
H	-2.358588	0.825724
C	2.133332	0.760992
C	2.400851	-0.774573
O	3.269407	1.431309
O	1.041969	1.302873
O	3.567101	-1.122565
O	1.386771	-1.599259
H	3.970170	0.724357
H	0.487746	-1.171787

Table S6.

OA-SA-W

18

1a(N)	E[DF-MP2-F12]	-1153.925402
S	1.649241	-0.242045
O	2.919658	-0.430760
O	0.579099	-1.198193
O	1.861876	-0.154586
O	1.140898	1.191607
H	2.830200	0.129652
H	0.159999	1.252384
O	4.405091	0.388829
H	4.459775	0.156149
H	4.699653	1.310415
C	-2.866717	-0.693247
C	-2.536765	0.811473
O	-1.914964	-1.581806
O	-4.021045	-0.958274
O	-1.447222	1.270289
O	-3.619852	1.553366
H	-1.013288	-1.225038
H	-4.331634	0.896043

18

1b(N)	E[DF-MP2-F12]	-1153.925289
S	1.647526	-0.167220
O	0.589174	-1.124432
O	2.912831	-0.297043
O	1.881380	-0.180756
O	1.114017	1.279702
H	2.862926	0.052861
H	0.132656	1.311828
O	4.428945	0.345468
H	5.003732	-0.311937
H	4.465952	0.156208
C	-2.558654	0.791194
C	-2.864921	-0.730245
O	-3.653232	1.505198
O	-1.476041	1.282994
O	-4.014666	-1.032486
O	-1.898187	-1.593484
H	-4.354910	0.824259
H	-1.003074	-1.204696

18

1c(N)	E[DF-MP2-F12]	-1153.925265
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S	1.647301	-0.165743	-0.426035
O	0.588906	-1.122643	-0.695114
O	2.912149	-0.294086	-1.108337
O	1.113243	1.281564	-0.732757
O	1.882188	-0.182435	1.129289
H	0.131738	1.312838	-0.533120
H	2.864003	0.049982	1.305823
O	4.430326	0.341728	1.201760
H	5.004560	-0.317398	1.621012
H	4.466847	0.154991	0.241801
C	-2.864584	-0.730935	0.188404
C	-2.559007	0.790838	0.050374
O	-1.897456	-1.593575	0.011494
O	-4.014320	-1.033923	0.462617
O	-1.476554	1.283603	-0.199853
O	-3.654062	1.504019	0.248498
H	-1.002345	-1.204394	-0.226232
H	-4.355434	0.822448	0.433844

18

1d(N) E[DF-MP2-F12] -1153.923566

S	-2.008348	-0.399811	-0.121517
O	-1.117271	0.116526	-1.173157
O	-3.399644	-0.526560	-0.416713
O	-1.487341	-1.809305	0.339249
O	-1.767613	0.461367	1.175050
H	-0.490748	-1.799840	0.306302
H	-1.441854	1.403034	0.937585
O	-0.774127	2.808533	0.656676
H	0.017079	2.635415	0.110177
H	-1.322544	3.420690	0.142088
C	2.197030	-0.927325	0.108102
C	2.263054	0.575433	-0.293735
O	3.394475	-1.381307	0.442414
O	1.190977	-1.605584	0.133025
O	3.328572	1.148508	-0.161048
O	1.165496	1.150722	-0.736844
H	3.998776	-0.600302	0.355462
H	0.344141	0.546120	-0.862755

18

1e(N) E[DF-MP2-F12] -1153.923062

S	-2.519068	-0.070151	-0.018421
O	-3.887862	-0.294585	-0.375900

O	-1.879954	1.207059	-0.239504
O	-2.336958	-0.319136	1.567217
O	-1.675652	-1.226801	-0.666019
H	-2.937472	-1.043284	1.826946
H	-0.686081	-1.027095	-0.587546
O	0.606744	2.458997	-0.309407
H	-0.227043	1.936018	-0.282410
H	0.439243	3.257318	0.212188
C	1.936834	-0.823266	-0.183755
C	3.116490	0.132597	0.141345
O	2.318688	-2.085749	-0.170601
O	0.801848	-0.443303	-0.414696
O	4.198594	-0.398610	0.348958
O	2.879700	1.411113	0.178735
H	3.290671	-2.032986	0.047469
H	1.904638	1.704573	-0.017725

18

1f(N)	E[DF-MP2-F12]	
S	-2.527143	-0.105672 -0.131939
O	-1.810254	1.049424 -0.625421
O	-3.819689	-0.456418 -0.639965
O	-1.626702	-1.389782 -0.230210
O	-2.631164	0.157763 1.456451
H	-0.653980	-1.150418 -0.080616
H	-3.283042	-0.468569 1.824251
O	0.516707	2.400452 0.077187
H	-0.275915	1.858709 -0.145850
H	0.431734	3.220291 -0.430955
C	1.981610	-0.835955 0.041870
C	3.158721	0.175543 -0.005982
O	2.412793	-2.082194 0.013005
O	0.808762	-0.508216 0.095207
O	4.282142	-0.306980 -0.042847
O	2.879318	1.445968 -0.010468
H	3.404798	-1.984964 -0.025136
H	1.873402	1.698037 0.010479

18

1g(N)	E[DF-MP2-F12]	
S	2.168663	-0.455395 -0.048396
O	3.285412	-1.330047 -0.253548
O	0.991760	-0.526299 -0.895293
O	1.569848	-0.699678 1.435306

O	2.696675	1.004714	-0.003146
H	2.313730	-0.918645	2.027342
H	1.916532	1.707545	-0.047742
O	0.854225	2.741314	-0.082717
H	0.894616	3.288382	-0.881581
H	-0.022315	2.290809	-0.108630
C	-2.438903	0.595019	0.033499
C	-2.509116	-0.949881	-0.119594
O	-3.622997	1.096641	0.352254
O	-1.433194	1.254274	-0.122879
O	-3.591492	-1.481020	0.065022
O	-1.411926	-1.590384	-0.438730
H	-4.218543	0.302328	0.399438
H	-0.600996	-1.011049	-0.548080

18

1h(N)	E[DF-MP2-F12]	-1153.923934
S	-2.443146	-0.177562
O	-1.879354	0.585429
O	-3.839996	-0.455773
O	-1.696006	-1.562969
O	-2.029835	0.578196
H	-0.710375	-1.411841
H	-1.272688	1.186241
O	-0.045777	2.113936
H	-0.187388	3.065267
H	-0.615622	1.649368
C	2.039612	-0.838997
C	3.044550	0.342199
O	2.653308	-2.007725
O	0.832490	-0.688189
O	4.231707	0.069781
O	2.549859	1.556678
H	3.620369	-1.781747
H	1.539895	1.599588

18

1i(N)	E[DF-MP2-F12]	-1153.922185
S	2.181365	-0.453466
O	3.276487	-1.356797
O	0.980406	-0.532142
O	1.625709	-0.631251
O	2.730626	0.998721
H	2.375606	-0.906052

H	1.952506	1.700098	-0.146987
O	0.863527	2.696782	-0.288025
H	-0.006250	2.235622	-0.245261
H	0.839880	3.375667	0.402580
C	-2.458300	0.595644	0.049456
C	-2.526592	-0.947646	-0.124876
O	-3.647370	1.090308	0.362227
O	-1.453234	1.261391	-0.080275
O	-3.612368	-1.479204	0.038213
O	-1.426366	-1.587861	-0.432830
H	-4.241872	0.294021	0.388259
H	-0.611701	-1.011465	-0.526390

18

lj(N)	E[DF-MP2-F12]	-1153.92204
S	1.948444	-0.413161
O	1.754948	0.118516
O	0.984010	-1.362080
O	2.214213	0.723143
O	3.361748	-1.168934
H	1.722482	1.612318
H	3.312958	-1.893560
O	0.951663	2.792678
H	0.054314	2.388022
H	1.214449	3.031678
C	-2.586770	-0.908942
C	-2.214734	0.597472
O	-1.622634	-1.779511
O	-3.766455	-1.194093
O	-1.084362	1.021000
O	-3.285103	1.352503
H	-0.700795	-1.385742
H	-4.033712	0.700927

Table S7.

OA-SA-W₂

21

2a(N)	E[DF-MP2-F12]	-1230.303153
S	-1.206803	-0.556929
O	-0.091695	-1.486221
O	-2.462433	-1.042613
O	-1.374997	0.028759
O	-0.809452	0.675338

H	-2.245233	0.640064	1.252573
H	0.160153	0.872312	-1.024996
O	-4.920594	0.135817	-0.341284
H	-5.584060	-0.501018	-0.037646
H	-4.152887	-0.401133	-0.647038
O	-3.454325	1.402253	1.435112
H	-3.361743	2.331125	1.174838
H	-4.131060	0.992751	0.807360
C	2.877952	0.817606	-0.310035
C	3.295037	-0.507784	0.397169
O	3.915018	1.630670	-0.417729
O	1.766036	1.097082	-0.713333
O	4.461652	-0.592271	0.746921
O	2.401528	-1.443118	0.582282
H	4.661516	1.124012	0.003922
H	1.478328	-1.251740	0.229271

21

2b(N) E[DF-MP2-F12] -1230.303078

S	-1.210226	-0.616147	0.275402
O	-2.478364	-1.084347	0.792271
O	-0.075599	-1.520830	0.337142
O	-1.332350	-0.149876	-1.197210
O	-0.876243	0.693034	1.096511
H	-2.232918	0.392334	-1.392622
H	0.087311	0.917816	0.945614
O	-3.442442	1.125762	-1.663422
H	-3.911767	0.780566	-2.437879
H	-4.044948	0.965007	-0.868388
O	-4.746242	0.468430	0.522287
H	-4.025162	-0.134670	0.819911
H	-4.843705	1.128519	1.224398
C	3.287528	-0.478223	-0.325875
C	2.816755	0.886736	0.262011
O	2.431475	-1.460654	-0.427442
O	4.457912	-0.548584	-0.665816
O	1.694334	1.154497	0.642937
O	3.820393	1.746920	0.295928
H	1.498809	-1.272541	-0.099280
H	4.587308	1.235438	-0.080502

21

2c(N) E[DF-MP2-F12] -1230.30102

S	-1.844186	-0.299061	-0.332243
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O	-1.913577	-1.596053	0.321956
O	-0.699411	0.046603	-1.134703
O	-3.105882	-0.209211	-1.324788
O	-2.134793	0.792519	0.727229
H	-3.843153	-0.709481	-0.927771
H	-1.500417	1.648102	0.641032
O	-0.659151	2.817063	0.640797
H	0.286933	2.536883	0.487861
H	-0.667787	3.238119	1.514217
O	0.572392	-2.285469	1.454571
H	-0.333210	-2.242517	1.066714
H	1.166448	-2.575801	0.733629
C	2.492707	-0.389563	-0.540477
C	1.759392	0.600897	0.409666
O	3.077562	0.247389	-1.551251
O	2.535532	-1.589593	-0.382737
O	1.796981	1.800803	0.107811
O	1.159917	0.143106	1.457803
H	2.854770	1.201413	-1.423793
H	0.994239	-0.917014	1.475350

21

2d(OA)	E[DF-MP2-F12]	-1230.301898	
S	-2.231403	-0.234478	-0.112375
O	-3.644683	-0.075710	-0.228124
O	-1.341463	0.486707	-1.027652
O	-1.816367	0.142010	1.369385
O	-1.897939	-1.768611	-0.225199
H	-0.809639	0.068920	1.438093
H	-0.904445	-1.912790	-0.089396
O	1.706256	2.303774	0.720789
H	2.500373	1.922770	0.248293
H	0.978742	2.609690	0.005171
O	-0.091222	2.826928	-0.941903
H	-0.689350	3.568327	-0.766109
H	-0.659151	2.003295	-0.992059
C	1.294571	-0.872363	0.448119
C	2.699431	-0.638382	-0.196727
O	0.829776	0.025556	1.221949
O	0.739965	-1.939628	0.113019
O	3.310042	0.416280	-0.180732
O	3.152449	-1.722044	-0.809739
H	1.325043	1.379671	1.077557
H	2.422350	-2.385859	-0.726244

21

2e(N) E[DF-MP2-F12] -1230.301527
S -2.065825 0.379209 -0.309304
O -1.293491 1.602334 -0.323589
O -3.430241 0.387274 -0.785104
O -1.324371 -0.734210 -1.142447
O -2.028376 -0.154004 1.176297
H -0.329667 -0.682664 -0.979585
H -2.853724 -0.737180 1.316815
O 1.280366 2.506672 0.127009
H 1.133068 3.183828 0.803214
H 0.399021 2.097943 -0.043071
O -4.334565 -1.386024 1.217979
H -4.528444 -0.911130 0.383164
H -4.383030 -2.329323 1.000017
C 3.473845 -0.149701 0.322222
C 2.259878 -0.875355 -0.319594
O 3.358517 1.115813 0.598039
O 4.464357 -0.837338 0.530717
O 1.209081 -0.324400 -0.596191
O 2.513516 -2.155559 -0.518839
H 2.446535 1.557692 0.369640
H 3.448762 -2.260638 -0.188060

21

2f(N) E[DF-MP2-F12] -1230.300833
S -1.859523 -0.286260 -0.329943
O -0.749867 0.112895 -1.157561
O -1.912662 -1.627505 0.227295
O -2.094509 0.723566 0.820178
O -3.162858 -0.113852 -1.258917
H -1.485751 1.598615 0.741678
H -3.895051 -0.615708 -0.854330
O -0.661263 2.776533 0.763365
H 0.292373 2.505831 0.646867
H -0.858694 3.362193 0.016355
O 0.572686 -2.366233 1.327077
H -0.332768 -2.312355 0.940978
H 1.170241 -2.618337 0.595042
C 2.529311 -0.358836 -0.532730
C 1.765493 0.578432 0.446426
O 3.159786 0.334387 -1.478098
O 2.554176 -1.566670 -0.451410

O	1.808704	1.793225	0.210293
O	1.132454	0.065823	1.446902
H	2.940531	1.280434	-1.296588
H	0.979480	-0.995447	1.413932

21

2g(N) E[DF-MP2-F12] -1230.300641

S	-1.869825	-0.315814	-0.314139
O	-0.722057	0.025946	-1.127876
O	-1.845122	-1.521931	0.483409
O	-2.293695	0.900051	0.552005
O	-3.155760	-0.524995	-1.250713
H	-1.556203	1.671629	0.587266
H	-3.206849	0.221048	-1.877534
O	0.642716	-2.259675	1.501960
H	1.216797	-2.565523	0.771766
H	-0.272307	-2.210258	1.135923
O	-0.655103	2.790478	0.712153
H	-0.645313	3.107777	1.628447
H	0.284549	2.512580	0.516550
C	2.502426	-0.376171	-0.560576
C	1.768942	0.616311	0.387119
O	3.066504	0.256506	-1.586472
O	2.560807	-1.573659	-0.390605
O	1.782573	1.812575	0.066159
O	1.192743	0.165796	1.449998
H	2.834572	1.209195	-1.465532
H	1.044888	-0.903003	1.489949

21

2h(N) E[DF-MP2-F12] -1230.301314

S	2.060582	0.349261	0.325406
O	1.296550	1.578425	0.327614
O	3.419174	0.351713	0.819205
O	1.301677	-0.756631	1.146772
O	2.044763	-0.182698	-1.161583
H	0.308875	-0.699833	0.973400
H	2.890973	-0.735068	-1.304019
O	4.355700	-1.411957	-1.164069
H	5.018951	-1.108471	-1.802432
H	4.539621	-0.920781	-0.336105
O	-1.273707	2.504072	-0.104299
H	-0.395390	2.086494	0.059794
H	-1.120751	3.192978	-0.767148

C	-2.278766	-0.873346	0.305319
C	-3.485794	-0.135822	-0.335651
O	-2.541977	-2.151768	0.501577
O	-1.224078	-0.330659	0.583644
O	-4.481170	-0.813832	-0.550961
O	-3.359555	1.130733	-0.604208
H	-3.476750	-2.251112	0.168933
H	-2.446489	1.563440	-0.366479

21

2i(SA) E[DF-MP2-F12] -1230.300859

S	-1.757868	-0.802813	-0.080223
O	-0.633437	-1.706965	-0.351087
O	-2.087066	0.123999	-1.190265
O	-3.071101	-1.741905	-0.069149
O	-1.673755	-0.135055	1.226459
H	-2.824810	-2.582688	0.358073
H	-1.768058	1.518761	1.495723
O	-0.936199	2.325746	-0.985293
H	0.015951	2.029052	-0.910535
H	-1.447815	1.402420	-1.154659
O	-1.675565	2.512994	1.415007
H	-2.544984	2.889887	1.616467
H	-1.245030	2.559435	-0.006193
C	2.766207	-0.837547	0.220576
C	2.331748	0.575890	-0.257404
O	1.871102	-1.782463	0.284609
O	3.945597	-0.969483	0.514464
O	1.199191	0.865608	-0.593676
O	3.350918	1.416732	-0.248382
H	0.922888	-1.533435	0.013605
H	4.112538	0.857849	0.070542

21

2j(N) E[DF-MP2-F12] -1230.29973

S	-1.941969	-0.141809	-0.403370
O	-2.286998	1.131069	0.228528
O	-2.043677	-1.285075	0.623658
O	-3.149361	-0.499845	-1.397442
O	-0.737231	-0.221608	-1.187074
H	-3.978200	-0.168494	-1.004648
H	-0.009038	3.369400	0.381950
O	-0.283362	2.772048	1.095989
H	0.715824	1.653596	1.160483

H	-1.083180	2.294214	0.754224
O	0.029679	-2.004193	1.744351
H	-1.086915	-1.579266	1.077161
H	0.858433	-1.882578	1.191922
C	2.524244	-0.687351	-0.312544
C	1.981400	0.718638	0.041346
O	3.361394	-0.636310	-1.338845
O	2.228446	-1.721371	0.255636
O	2.273251	1.653702	-0.692582
O	1.244239	0.749324	1.120765
H	3.367493	0.315207	-1.613770
H	0.162204	-1.422775	2.509918

Table S8.

OA-SA-W₃

24

3a(SA)	E[DF-MP2-F12]	-1306.682386
S	-2.422317	-0.276323
O	-2.291732	0.632780
O	-1.542865	0.058175
O	-3.938546	0.006752
O	-2.370125	-1.705293
H	-4.163285	-0.669911
H	-0.946757	-2.518614
O	0.138189	1.948165
H	-0.477973	1.112536
H	-0.253892	2.466351
O	-0.034135	-2.902741
H	0.185249	-3.437513
H	0.838093	-1.773030
O	-0.979683	2.922065
H	-1.564631	2.120663
H	-1.574252	3.676034
C	3.240621	0.558626
C	2.572110	-0.831079
O	4.510405	0.531656
O	2.683544	1.566691
O	3.241053	-1.738750
O	1.343561	-0.844117
H	4.662056	-0.405383
H	1.098756	1.681689

24

3b(SA)	E[DF-MP2-F12]	-1306.680952
S	-1.190395	-1.227893
O	-2.583944	-1.587061
O	-0.574492	-0.546108
O	-0.425929	-2.599319
O	-0.949710	-0.434622
H	0.543368	-2.395056
H	-1.621737	0.869581
O	-2.142817	1.778283
H	-2.944870	1.495394
H	-1.506118	2.395807
O	-0.447087	3.192928
H	-0.005183	3.927274
H	0.269203	2.566524
O	-4.011143	0.731516
H	-4.168449	1.011135
H	-3.619560	-0.183398
C	2.403783	0.839209
C	2.815598	-0.630366
O	1.231004	1.059383
O	3.214508	1.715802
O	2.112774	-1.609125
O	4.062810	-0.676791
H	0.536284	0.236995
H	4.359290	0.269891

24

3c(SA)	E[DF-MP2-F12]	-1306.680492
S	-1.284126	-1.181939
O	-2.732333	-1.130716
O	-0.813717	-0.991565
O	-0.871766	-2.656434
O	-0.551208	-0.275525
H	0.099104	-2.730535
H	-0.943003	1.120334
O	-1.277824	2.120551
H	-2.180215	2.038050
H	-0.560849	2.676206
O	0.650985	3.418134
H	1.429997	2.811651
H	0.968813	4.167055
O	-3.464525	1.499163
H	-3.347642	0.511425
H	-4.288997	1.691227

C	2.024420	0.453811	0.523024
C	2.364606	-0.914998	-0.138214
O	1.159666	0.503165	1.479830
O	2.624367	1.449927	0.096938
O	1.836320	-1.967439	0.142659
O	3.322485	-0.784297	-1.053152
H	0.433249	-0.266424	1.484190
H	3.541792	0.179458	-1.063313

24

3d(SA)	E[DF-MP2-F12]	-1306.678853
S	-2.016102	-0.692691
O	-1.404884	-1.999319
O	-2.469851	0.054723
O	-1.201136	0.108524
O	-3.399463	-1.022427
H	-0.742837	1.492674
H	-3.204189	-1.674735
O	-0.385147	2.431122
H	-0.914290	2.615822
H	0.604451	2.290843
O	0.725168	-2.044324
H	-0.098699	-2.144908
H	1.471769	-2.469933
O	-1.776070	2.567577
H	-2.113873	1.630751
H	-2.557920	3.139388
C	3.117732	-0.432278
C	2.047784	0.615168
O	4.005470	0.080857
O	3.133631	-1.583034
O	2.097316	1.719041
O	1.184111	0.302963
H	3.712157	1.011754
H	1.034811	-0.831578

24

3e(SA)	E[DF-MP2-F12]	-1306.680732
S	1.017958	0.957183
O	2.331812	1.299712
O	1.025026	0.790887
O	0.402671	-0.228311
O	0.114531	2.196158
H	1.502137	-1.529972

H	-0.837788	1.922490	0.430520
O	3.946722	-0.588573	0.195790
H	3.732657	-0.668954	-0.828241
H	3.421403	0.267822	0.460741
O	3.180542	-0.504563	-2.216427
H	2.329645	-0.016216	-2.020919
H	2.930171	-1.307679	-2.696767
O	2.275702	-2.154786	1.322964
H	3.389946	-1.319975	0.679568
H	2.378013	-2.366533	2.262771
C	-2.896493	-1.112226	-0.140920
C	-3.188935	0.414193	-0.020754
O	-1.683973	-1.548001	0.076117
O	-3.841609	-1.827347	-0.436881
O	-2.377943	1.278416	0.242711
O	-4.470443	0.659395	-0.245143
H	-0.988294	-0.853827	0.335157
H	-4.856951	-0.237767	-0.434048

24

3f(SA)	E[DF-MP2-F12]	-1306.679672
S	2.266343	-0.389205
O	1.720975	0.144990
O	2.853969	0.640879
O	1.330534	-1.292871
O	3.459083	-1.404718
H	-0.214954	-1.279212
H	4.116830	-0.909752
O	0.835903	2.228752
H	0.416478	1.515700
H	1.729775	1.799700
O	-0.219650	2.112086
H	0.282812	2.218860
H	0.346286	1.398468
O	-0.006625	0.101096
H	0.542276	-0.527564
H	0.217242	-0.060756
C	-2.159832	-1.011522
C	-3.165011	0.136074
O	-0.985448	-0.734404
O	-2.511186	-1.990545
O	-2.864290	1.220737
O	-4.398071	-0.192277
H	-1.145920	1.755419

H -4.324826 -1.100694 0.362709

24

3g(SA) E[DF-MP2-F12] -1306.67982

S	1.106670	-1.063135	0.214252
O	2.455823	-1.541084	-0.068439
O	0.590934	-0.138473	-0.873840
O	0.198560	-2.349897	0.135342
O	0.925841	-0.443121	1.536279
H	-0.751070	-2.055848	0.064845
H	1.421423	1.160121	1.713302
O	1.776401	2.090712	1.590949
H	1.057224	2.691609	1.838194
H	2.109703	2.075859	0.140803
O	2.293875	1.834674	-0.868262
H	3.195040	1.291693	-0.895123
H	1.584518	1.114583	-1.037303
O	4.253868	0.242869	-0.920796
H	4.991507	0.343907	-0.300858
H	3.717498	-0.535564	-0.596865
C	-2.728084	1.028772	-0.253091
C	-3.086800	-0.481298	-0.121783
O	-1.480240	1.365645	-0.458971
O	-3.646070	1.826220	-0.147525
O	-2.297064	-1.402899	-0.140574
O	-4.393505	-0.640695	0.021702
H	-0.815041	0.602788	-0.568540
H	-4.755605	0.284559	0.015842

24

3h(SA) E[DF-MP2-F12] -1306.678055

S	-1.998642	-0.578849	-0.159603
O	-1.833279	0.060313	1.159764
O	-1.566763	-1.981255	-0.225458
O	-3.613390	-0.621431	-0.303691
O	-1.481646	0.236479	-1.272999
H	-3.828799	-1.281433	-0.987803
H	-1.480159	1.910372	-1.236569
O	-0.460612	2.200071	1.299239
H	-0.966633	1.290086	1.326565
H	0.536295	2.006441	1.182467
O	0.862048	-2.675891	0.549805
H	-0.067863	-2.515092	0.199945
H	1.460699	-2.766114	-0.216960

O	-1.304538	2.865037	-0.983337
H	-0.800485	2.616202	0.396506
H	-2.150304	3.331931	-1.054798
C	2.944765	-0.250055	-0.519159
C	2.031967	0.349635	0.587985
O	3.660130	0.687345	-1.140065
O	2.987600	-1.427581	-0.797637
O	1.998507	1.596333	0.666516
O	1.354694	-0.432781	1.332924
H	3.384454	1.543102	-0.732498
H	1.208666	-1.524499	0.983339

24

3i(N)	E[DF-MP2-F12]	-1306.678448
S	-1.342999	0.069167 0.677604
O	-2.519886	-0.547135 1.259642
O	-0.101817	0.003487 1.432955
O	-1.024669	-0.533724 -0.723910
O	-1.726484	1.560404 0.413342
H	-1.893259	-0.698513 -1.307525
H	-0.903071	2.126101 0.114411
O	0.256931	2.984146 -0.333777
H	0.454252	3.690843 0.299142
H	1.057407	2.409326 -0.346450
O	-3.090473	-0.930263 -2.122639
H	-3.866658	-0.861933 -1.481400
H	-3.116195	-1.828859 -2.484309
O	-4.854688	-0.726682 -0.176094
H	-4.142059	-0.622195 0.499793
H	-5.389478	0.078682 -0.118767
C	3.070485	-1.136626 0.210849
C	3.131748	0.302583 -0.373649
O	2.014539	-1.483538 0.899879
O	4.025756	-1.865315 -0.007260
O	2.266687	1.139354 -0.228908
O	4.259020	0.494031 -1.044966
H	1.298295	-0.779233 0.978118
H	4.736030	-0.374746 -0.963967

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3j(N)	E[DF-MP2-F12]	-1306.677741
S	-1.344795	0.010419 -0.693514
O	-0.099757	-0.147052 -1.427247
O	-2.522192	-0.655655 -1.213747

O	-1.042409	-0.432212	0.770179
O	-1.716931	1.527798	-0.597546
H	-1.908847	-0.426221	1.377161
H	-0.889134	2.110532	-0.355869
O	-3.110525	-0.469417	2.221331
H	-3.292275	0.382609	2.644826
H	-3.877020	-0.647483	1.592397
O	0.277808	3.001473	0.029683
H	1.069545	2.420383	0.115766
H	0.498033	3.640609	-0.664489
O	-4.799274	-1.043301	0.275557
H	-5.532649	-0.476032	-0.002472
H	-4.096850	-0.927442	-0.408540
C	3.121388	0.308489	0.367042
C	3.075203	-1.171648	-0.105032
O	4.244310	0.562328	1.024330
O	2.248891	1.123295	0.155534
O	4.036853	-1.871822	0.170064
O	2.024713	-1.579281	-0.768789
H	4.729781	-0.305615	1.012520
H	1.304680	-0.888323	-0.901916

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3k(SA)	E[DF-MP2-F12]	-1306.677939
S	-1.555166	-1.139582
O	-2.639879	-0.280842
O	-0.536250	-1.458573
O	-2.347937	-2.518010
O	-0.958743	-0.705293
H	-1.695493	-3.179940
H	-1.232193	0.814511
O	-0.542665	2.834919
H	-1.242278	2.523136
H	0.290237	2.300808
O	-2.255951	1.972459
H	-2.432416	1.060153
H	-1.975250	1.830589
O	-1.299135	1.799991
H	-0.904819	2.463119
H	-2.215149	1.956865
C	2.380253	0.644226
C	2.822122	-0.845917
O	3.339451	1.426331
O	1.295951	1.039456

O	3.980933	-1.057693	-0.175474
O	1.963804	-1.760201	0.500996
H	4.083911	0.790406	-0.492705
H	0.995218	-1.456544	0.663456

24

3l(SA)	E[DF-MP2-F12]	-1306.678032	
S	1.533389	-1.143287	-0.094614
O	0.519967	-1.419284	0.941765
O	0.985133	-0.631437	-1.354957
O	2.673654	-0.372956	0.436013
O	2.134410	-2.576123	-0.548978
H	2.293663	2.041552	-2.297032
H	2.449848	-3.034429	0.251461
O	0.587354	2.817797	0.151928
H	1.273754	2.459517	0.880405
H	-0.256547	2.288266	0.295699
O	2.268401	1.860646	1.753152
H	2.449694	0.958960	1.339511
H	1.959535	1.686430	2.654793
O	1.375463	1.878235	-2.034785
H	1.302567	0.889404	-1.858562
H	0.960717	2.492662	-0.790963
C	-2.380608	0.658602	0.146594
C	-2.836722	-0.828084	0.152730
O	-3.332638	1.444880	-0.323330
O	-1.294782	1.048194	0.537549
O	-3.999912	-1.029116	-0.171037
O	-1.987730	-1.749598	0.500459
H	-4.082281	0.812973	-0.510313
H	-1.015764	-1.455748	0.650651

Table S9.

OA-SA-W₄

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4a(SA)	E[DF-MP2-F12]	-1383.063495	
S	-0.705915	-1.539170	-0.013333
O	-0.112740	-0.661100	-1.057621
O	-0.557764	-0.903404	1.341280
O	-2.059153	-1.988956	-0.282479
O	0.189106	-2.849140	0.021611
H	-3.303196	-0.544273	-0.571878
H	1.121000	-2.555666	0.186216

O	-1.545588	1.324999	-1.837277
H	-0.938657	0.519503	-1.642623
H	-1.179232	2.073401	-1.209118
O	-3.567086	0.403842	-0.632138
H	-2.465093	1.003519	-1.412254
H	-3.374002	0.749903	0.270490
O	-2.163514	1.298744	1.633494
H	-2.459127	1.464560	2.540906
H	-1.622647	0.464870	1.664133
O	-0.687977	3.005578	-0.109280
H	-1.045428	2.564759	0.696146
H	0.283811	2.987957	-0.011426
C	2.041517	1.041713	0.391600
C	2.737407	-0.271736	-0.060424
O	1.157720	0.970717	1.352108
O	2.367722	2.093442	-0.146735
O	2.508626	-1.364774	0.412615
O	3.635474	-0.044246	-1.010761
H	0.683230	0.063270	1.415480
H	3.601845	0.929415	-1.178339

27

4b(SA)	E[DF-MP2-F12]	-1383.06175
S	-0.766270	1.292821
O	-0.474825	0.692879
O	-2.133809	1.768354
O	-0.330360	0.364505
O	0.129495	2.591541
H	-1.498614	-0.559645
H	1.070441	2.283739
O	-3.057238	-1.947669
H	-2.187567	-2.011811
H	-3.571103	-1.085037
O	-0.962345	-1.943955
H	-0.191142	-2.349603
H	-0.740721	-0.968930
O	-4.110873	0.243274
H	-4.949638	0.513339
H	-3.426278	0.905089
O	-2.204558	-1.204845
H	-2.733499	-1.749413
H	-1.787667	-1.814208
C	3.221474	0.356737
C	2.706351	-1.114418

O	4.510584	0.395025	-0.247483
O	2.555006	1.342150	0.294941
O	3.504634	-1.988775	-0.214285
O	1.457824	-1.341038	0.410730
H	4.760554	-0.555229	-0.388472
H	0.880315	-0.518915	0.647561

27

4c(OA) E[DF-MP2-F12] -1383.059763

S	-2.304977	-0.818806	-0.104709
O	-1.911738	0.308053	0.777794
O	-3.704371	-1.029477	-0.295926
O	-1.630185	-0.575569	-1.499568
O	-1.649537	-2.118690	0.444941
H	0.561814	2.300159	1.273918
H	-0.607232	-2.103687	0.350234
O	0.595024	3.051329	0.576375
H	1.237247	2.710243	-0.231456
H	-0.374084	3.098038	0.225403
O	-1.881946	2.909775	-0.085127
H	-2.071938	1.963985	0.145667
H	-2.197289	3.034791	-0.992555
O	1.970174	2.180348	-1.298324
H	1.609816	1.248825	-1.374453
H	2.899581	2.003180	-1.062277
O	0.329755	1.003023	2.132428
H	0.199127	1.088115	3.088256
H	-0.503406	0.606452	1.767525
C	2.958503	-0.919298	-0.048795
C	1.436504	-1.090167	-0.336785
O	3.446930	-1.915632	0.693262
O	3.622179	0.016399	-0.434955
O	0.891180	-2.061678	0.251766
O	0.883703	-0.249509	-1.101648
H	2.674086	-2.499815	0.883609
H	-0.607467	-0.439587	-1.373198

27

4d(SA) E[DF-MP2-F12] -1383.059369

S	0.790455	-1.115497	-0.331611
O	0.048487	-0.099880	-1.136932
O	2.017657	-1.566502	-0.980610
O	0.972854	-0.655753	1.067613
O	-0.138029	-2.395035	-0.281344

H	2.245232	0.066484	1.453852
H	-1.070576	-2.095046	-0.106596
O	2.952413	2.768756	0.509071
H	2.204369	2.711489	-0.173118
H	3.727026	3.108781	0.037744
O	1.013872	2.507209	-1.234239
H	0.734979	1.559507	-1.276088
H	0.199498	2.989025	-1.021441
O	4.434594	-1.048094	0.026210
H	4.857717	-1.841957	0.385342
H	3.599582	-1.357259	-0.426611
O	3.173699	0.505220	1.600609
H	3.802080	-0.099458	1.036994
H	3.133215	1.458473	1.152609
C	-3.138965	0.981950	0.020096
C	-3.411986	-0.525048	0.302765
O	-1.967654	1.328799	-0.448778
O	-4.045517	1.764198	0.256166
O	-2.618745	-1.430193	0.147831
O	-4.648387	-0.701341	0.744159
H	-1.303645	0.572935	-0.618566
H	-5.032989	0.214497	0.766443

27

4e(SA)	E[DF-MP2-F12]	-1383.058982
S	-0.780898	-1.294836
O	-2.135644	-1.823816
O	-0.429403	-0.374828
O	-0.451881	-0.666234
O	0.158187	-2.556006
H	-1.164262	0.801296
H	1.091389	-2.220468
O	-1.592383	1.671216
H	-2.131707	2.426492
H	-2.252105	1.466390
O	-2.372782	1.127454
H	-3.176058	0.476228
H	-1.562066	0.549965
O	-2.455118	2.860742
H	-2.424894	1.894590
H	-1.877219	3.622461
O	-4.121555	-0.655530
H	-3.480821	-1.223075
H	-4.445690	-1.201732

C	3.273415	-0.367616	-0.135445
C	2.808887	1.087390	-0.444995
O	4.578397	-0.400048	0.092462
O	2.561486	-1.349558	-0.110761
O	3.667575	1.955479	-0.429503
O	1.546614	1.306343	-0.708735
H	4.864135	0.547267	-0.003539
H	0.931916	0.497589	-0.681252

27

4f(SA)	E[DF-MP2-F12]	-1383.05698
S	2.023326	-0.742225
O	1.787241	-2.026900
O	1.072736	-0.412095
O	3.419334	-0.906675
O	2.244829	0.359676
H	4.096112	-1.217724
H	1.727083	1.744419
O	-0.711132	-2.565974
H	-1.192834	-2.876725
H	0.248369	-2.454295
O	-0.886182	3.009216
H	-0.880211	2.722481
H	-1.548912	2.411358
O	0.842345	2.076469
H	1.477708	2.301552
H	0.948783	1.098684
O	1.340441	2.672831
H	0.428273	2.812483
H	1.145579	2.575035
C	-2.180164	0.147611
C	-2.652902	-0.863945
O	-1.559081	-0.277981
O	-2.455800	1.342133
O	-2.484858	-2.063217
O	-3.280613	-0.244335
H	-1.200745	-1.363736
H	-3.258118	0.714874

27

4g(SA)	E[DF-MP2-F12]	-1383.058189
S	-0.641797	-0.949984
O	-0.101560	0.423547
O	-0.596669	-1.269702

O	-1.949106	-1.168813	-1.152743
O	0.311132	-1.954226	-1.277625
H	-3.052966	-0.116261	-1.092646
H	1.247714	-1.708091	-1.045911
O	-3.678085	0.702411	-1.030608
H	-3.988245	0.769427	-0.015827
H	-3.034019	1.482513	-1.245144
O	-2.662054	-0.819069	2.584286
H	-2.997213	-1.688579	2.846934
H	-1.886063	-1.002940	1.987698
O	-4.369661	0.724461	1.378004
H	-3.723127	0.120664	1.884369
H	-4.368929	1.576525	1.838232
O	-1.816961	2.395928	-1.469151
H	-1.675255	2.708838	-2.374879
H	-1.084088	1.747548	-1.279900
C	3.499601	-0.301379	-0.008632
C	3.124987	1.098549	0.566889
O	4.781869	-0.558751	0.201021
O	2.747299	-1.063999	-0.579198
O	4.023814	1.721542	1.111985
O	1.900944	1.535967	0.438186
H	5.111507	0.248079	0.681514
H	1.244216	0.924633	-0.038022

27

4h(SA)	E[DF-MP2-F12]	-1383.055516
S	-1.960600	-1.111619
O	-1.342228	-2.266153
O	-0.945184	-0.246121
O	-2.869429	-1.728432
O	-2.942279	-0.383674
H	-2.318993	-2.357908
H	0.540491	3.234807
O	1.018732	-2.029007
H	1.677940	-2.413544
H	0.104671	-2.154823
O	0.671830	3.325095
H	1.490316	2.777962
H	-0.451247	2.723429
O	-1.224682	2.288434
H	-1.083306	1.262906
H	-2.135136	2.399293
O	-3.420907	2.229646

H	-3.386427	1.238435	0.569466
H	-4.246060	2.417711	-0.022344
C	2.429033	0.537640	0.299445
C	3.175460	-0.633909	-0.417999
O	1.641721	0.289932	1.268921
O	2.675667	1.674377	-0.156215
O	3.046452	-1.812723	-0.157145
O	3.984302	-0.180566	-1.370836
H	1.337253	-0.854062	1.467355
H	3.861184	0.802861	-1.352152

27

4i(SA)	E[DF-MP2-F12]	-1383.057816
S	1.184230	1.351474
O	1.055378	0.701604
O	0.031110	1.210676
O	2.443731	1.023132
O	1.289891	2.911827
H	3.617838	0.011033
H	1.348749	3.434973
O	0.494227	-1.970275
H	-0.370131	-1.989730
H	0.648683	-1.000239
O	4.121028	-0.791008
H	4.268606	-0.669782
H	3.129599	-1.927179
O	2.361603	-2.509138
H	2.093281	-2.040177
H	1.532355	-2.340552
O	1.752005	-1.075444
H	1.999659	-0.208651
H	0.796757	-0.994903
C	-3.408814	0.512719
C	-2.898995	-0.948059
O	-2.537687	1.454747
O	-4.609935	0.695320
O	-1.741720	-1.292609
O	-3.897203	-1.768131
H	-1.569242	1.164313
H	-4.696401	-1.176277

27

4j(SA)	E[DF-MP2-F12]	-1383.056587
S	1.939154	-0.660390

O	2.299168	0.461679	-0.721328
O	0.953771	-1.590107	-0.397658
O	3.244767	-1.532286	0.358941
O	1.545570	-0.187226	1.531771
H	4.048129	-0.954951	0.141399
H	0.492782	0.976162	1.897993
O	5.038351	0.246680	-0.421313
H	5.548473	-0.007086	-1.205212
H	4.227403	0.685364	-0.762530
O	0.431772	2.058785	-1.751341
H	1.135072	1.445272	-1.382694
H	0.119915	1.635080	-2.564781
O	-0.172327	1.702122	2.117081
H	-0.836364	2.180892	0.932025
H	0.311057	2.369816	2.625105
O	-1.321436	2.481207	0.034991
H	-0.647047	2.285986	-0.742143
H	-2.139752	1.896343	-0.080681
C	-3.624872	-0.148739	-0.125961
C	-2.427732	-1.130994	-0.224161
O	-4.772506	-0.795972	-0.009801
O	-3.544285	1.068270	-0.147695
O	-2.661057	-2.327744	-0.142172
O	-1.296129	-0.511805	-0.391196
H	-4.514187	-1.754846	-0.006931
H	-0.421588	-1.102223	-0.384622

27

4k(SA&OA)	E[DF-MP2-F12]	-1383.055643
S	2.204052	0.222047
O	2.164299	0.165418
O	1.550040	1.402796
O	3.792370	0.388424
O	1.808149	-1.028329
H	3.903362	0.485563
H	0.940549	-2.114911
O	-1.539536	2.187716
H	-2.332408	2.283596
H	-0.704441	2.683314
O	0.477591	3.293644
H	0.944032	2.600431
H	1.122330	3.561735
O	1.391391	-2.070451
H	1.733004	-1.203193

H	2.172875	-2.562746	2.474803
O	0.388805	-2.787022	-0.036822
H	0.732812	-2.603359	0.931770
H	-0.607397	-2.481381	-0.109890
C	-3.272462	0.079589	-0.450741
C	-2.069322	-0.740570	0.119157
O	-4.028383	-0.645810	-1.268374
O	-3.501430	1.247117	-0.197742
O	-1.980669	-1.911218	-0.349837
O	-1.290600	-0.218581	0.954739
H	-3.580913	-1.529104	-1.300966
H	-1.394149	1.103556	1.241578

27

4l(SA)	E[DF-MP2-F12]	-1383.056918
S	0.775116	-1.205863
O	0.265671	-0.212382
O	2.068425	-1.764921
O	0.702691	-0.625939
O	-0.223174	-2.428976
H	4.704162	-0.844699
H	-1.150184	-2.078186
O	1.739528	1.960340
H	1.249470	1.100052
H	1.429914	2.129899
O	4.200293	1.566393
H	2.795195	1.787229
H	4.662396	1.590133
O	0.892684	2.061649
H	-0.005281	2.429733
H	0.776525	1.073150
O	4.508667	-0.790775
H	3.621162	-1.223553
H	4.383791	0.651215
C	-2.968954	1.042026
C	-3.420569	-0.445109
O	-1.697879	1.324415
O	-3.834570	1.873856
O	-2.684422	-1.402583
O	-4.738911	-0.541910
H	-1.074546	0.550526
H	-5.049355	0.393475

27

4m(SA)	E[DF-MP2-F12]	-1383.056522
S	-2.328966	-1.052292
O	-1.009112	-1.188598
O	-3.264643	-0.177230
O	-2.908622	-2.555270
O	-2.273360	-0.759137
H	-3.785252	-2.574977
H	-1.100296	0.226384
O	-0.617510	2.478798
H	-1.621047	2.542608
H	-0.186949	1.984629
O	-0.416649	0.937437
H	0.463093	0.521275
H	-0.520879	1.778692
O	0.387752	0.797906
H	0.145201	0.946060
H	-0.170149	0.005044
O	-3.085050	2.448989
H	-3.753705	2.763360
H	-3.254771	1.469042
C	3.054092	-0.177079
C	3.707229	-0.187270
O	3.898296	-0.600321
O	1.915135	0.184727
O	4.873769	-0.533081
O	2.967759	0.185682
H	4.732551	-0.802551
H	2.005614	0.403987

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4n(SA)	E[DF-MP2-F12]	-1383.056096
S	1.232509	-1.377019
O	0.818811	-0.766360
O	0.337574	-1.094081
O	1.049515	-2.972612
O	2.652598	-1.160621
H	1.381477	-3.211506
H	3.105568	0.139430
O	2.545314	2.892089
H	3.221255	3.281808
H	1.769854	2.574707
O	1.295931	0.393349
H	0.863570	-0.212397
H	1.486422	-0.149663

O	0.610610	2.020719	-1.693353
H	-0.219574	2.057093	-1.174640
H	0.730051	1.053133	-1.845045
O	3.241045	0.974381	1.136825
H	2.973502	1.832447	0.524686
H	2.530594	0.845558	1.871714
C	-2.732019	0.964202	-0.043466
C	-3.212363	-0.455161	0.364924
O	-3.762332	1.753240	-0.327082
O	-1.569018	1.301917	-0.091840
O	-4.415777	-0.652103	0.412137
O	-2.302947	-1.359578	0.635027
H	-4.557817	1.178857	-0.176358
H	-1.349335	-1.054121	0.527890

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4o(SA)	E[DF-MP2-F12]	-1383.056288	
S	-0.609421	-0.528062	-0.665379
O	0.549082	-1.411872	-0.832206
O	-1.783060	-0.939160	-1.440330
O	-0.937579	-0.300697	0.777921
O	-0.217181	0.901944	-1.251715
H	-2.273876	-1.245888	1.359120
H	0.747410	1.055379	-1.049573
O	-2.175630	1.965747	1.545645
H	-1.967607	2.211550	2.458929
H	-1.546694	1.233032	1.294699
O	-3.184435	-1.505133	1.674569
H	-3.399010	-2.330078	1.213143
H	-3.970739	-0.276110	1.242707
O	-4.289554	0.668907	0.938079
H	-3.518025	1.286156	1.253049
H	-4.232771	0.651921	-0.117597
O	-4.018508	0.452940	-1.555685
H	-3.916482	1.252378	-2.093151
H	-3.145066	-0.041500	-1.614345
C	3.709085	-0.577729	0.454913
C	3.411154	0.834728	-0.140096
O	2.798417	-1.507221	0.400360
O	4.814298	-0.723199	0.959593
O	2.366518	1.204155	-0.637927
O	4.475184	1.614145	-0.020607
H	1.929937	-1.283695	-0.086570
H	5.141796	1.029385	0.435162

Table S10.0A-SA-W₅

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5a(SA) E[DF-MP2-F12] -1459.437949

S	1.203060	-1.426677	-0.359352
O	0.911639	-1.432766	1.088419
O	2.638549	-1.380011	-0.667651
O	0.669088	-2.893750	-0.798274
O	0.408335	-0.449336	-1.125818
H	0.705136	-2.947514	-1.771070
H	1.219295	1.082833	-1.608146
O	0.482380	2.897921	0.446082
H	0.891203	2.223447	1.149391
H	-0.501556	2.697329	0.328647
O	3.727425	0.961980	0.014415
H	3.478927	0.027827	-0.237086
H	4.693821	0.994121	0.058519
O	1.685701	1.239676	1.931747
H	2.554573	1.185233	1.467044
H	1.313040	0.335110	1.829026
O	1.646607	1.978013	-1.573826
H	2.548851	1.784827	-1.227392
H	0.959711	2.587155	-0.463890
O	-1.627903	-1.800405	1.937137
H	-2.186549	-2.158006	1.219295
H	-0.684705	-1.907476	1.639181
C	-2.998708	-0.004408	-0.555222
C	-2.164398	0.984180	0.309368
O	-3.406254	0.558633	-1.691226
O	-3.250323	-1.145827	-0.240298
O	-1.955370	2.109669	-0.175462
O	-1.734493	0.610887	1.459733
H	-3.037723	1.474579	-1.679454
H	-1.787399	-0.468735	1.680868

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5b(SA) E[DF-MP2-F12] -1459.437439

S	-0.648956	-1.389099	-0.203085
O	-1.921312	-1.888556	-0.700465
O	0.016152	-0.447260	-1.167347

O	-0.688937	-0.801250	1.154077
O	0.289204	-2.663460	-0.128500
H	-4.633910	-1.832938	0.891570
H	1.224199	-2.341158	-0.037268
O	-4.112411	1.279969	1.121080
H	-4.492062	1.859221	0.443889
H	-2.676148	1.491848	1.366500
O	-1.471763	1.601268	-2.269766
H	-1.323035	1.756781	-3.213219
H	-1.013471	0.753722	-2.053596
O	-0.547344	3.009033	-0.200740
H	0.409075	2.821106	-0.187398
H	-0.865236	2.612778	-1.064075
O	-1.642666	1.557317	1.558388
H	-1.188007	2.189023	0.846195
H	-1.255984	0.618800	1.415797
O	-4.363357	-1.170575	0.239419
H	-3.483138	-1.477883	-0.100614
H	-4.250914	0.331495	0.788340
C	3.442218	-0.551415	0.251832
C	3.008584	0.932018	0.055668
O	4.696439	-0.619575	0.675428
O	2.747298	-1.524531	0.050966
O	3.820163	1.794368	0.349840
O	1.808254	1.180701	-0.407425
H	4.985005	0.326681	0.754821
H	1.204355	0.372898	-0.646204

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5c(SA)	E[DF-MP2-F12]	-1459.437539
S	1.958158	0.633754
O	1.184695	0.351233
O	1.592262	1.924139
O	3.464043	0.792455
O	1.873732	-0.510597
H	3.837382	-0.124093
H	0.791188	-1.792402
O	0.168129	-2.470291
H	0.622716	-2.719348
H	-0.916803	-1.694516
O	-0.105861	3.669066
H	0.610180	3.128620
H	0.341972	4.402544
O	1.765442	-2.139700

H	1.620217	-2.307602	2.515240
H	1.498278	-1.190729	1.404391
O	-0.876584	1.747384	1.299306
H	-0.646109	2.628173	0.764673
H	-1.789832	1.389015	1.026507
O	4.295372	-1.583452	0.617123
H	3.465477	-1.955401	1.009875
H	4.468495	-2.117153	-0.173604
C	-2.868801	-1.104522	-0.281317
C	-3.747481	0.084310	0.189599
O	-1.613145	-0.931278	-0.015039
O	-3.436343	-2.040475	-0.832412
O	-3.333715	1.093781	0.737214
O	-5.025797	-0.120917	-0.077218
H	-0.116695	1.093008	1.047287
H	-5.037142	-1.009696	-0.522796

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5d(SA&OA) E[DF-MP2-F12] -1459.437988

S	1.773121	-0.824838	-0.574389
O	0.509692	-1.410226	-0.996022
O	1.910936	-0.681572	0.898135
O	2.953334	-1.887430	-0.887899
O	2.143977	0.415064	-1.294165
H	2.868181	-2.157600	-1.820870
H	1.063549	1.362211	-1.852723
O	-0.863106	0.492194	2.729052
H	0.003472	0.999088	2.658212
H	-0.585278	-0.566310	2.633391
O	1.465535	1.642778	2.089159
H	2.167228	1.905818	2.703110
H	1.796561	0.829199	1.602340
O	-0.198275	-1.861461	2.336638
H	-0.922054	-2.116449	1.723077
H	0.596389	-1.714457	1.767266
O	0.078065	3.257659	0.148564
H	-0.720572	2.697350	0.332619
H	0.738586	2.908292	0.786881
O	0.358529	2.083078	-2.065100
H	0.331271	2.672884	-1.185186
H	-0.562055	1.608083	-2.057772
C	-2.477043	-0.968108	-0.322342
C	-1.969768	0.483060	-0.565106
O	-2.881740	-1.559115	-1.442025

O	-2.483757	-1.508243	0.765125
O	-1.847782	0.803971	-1.778107
O	-1.699134	1.198356	0.439464
H	-2.678429	-0.907949	-2.157689
H	-1.356108	0.707102	1.839709

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5e(OA) E[DF-MP2-F12] -1459.437917

S	-1.034325	-1.706143	0.253111
O	-0.413901	-0.828355	1.244212
O	-0.842731	-1.104454	-1.166950
O	-0.235990	-3.061182	0.230706
O	-2.428715	-2.044683	0.406776
H	0.715255	-2.834600	0.006317
H	-3.516839	-0.730787	-0.406814
O	-0.272327	2.722347	-1.359319
H	0.235985	1.855907	-1.479300
H	0.245970	3.134908	-0.537972
O	-2.443166	2.253646	-0.239164
H	-2.118953	2.098353	0.677744
H	-1.252359	2.479220	-0.968855
O	-3.935061	0.084922	-0.761360
H	-3.007325	1.458978	-0.471162
H	-4.842181	0.081394	-0.423707
O	-0.889495	1.725574	2.031650
H	-0.725426	0.769264	1.822483
H	-1.138260	1.755587	2.967223
O	1.040529	3.361765	0.708958
H	1.816290	2.779101	0.513671
H	0.508223	2.861338	1.368863
C	2.717282	-1.003542	-0.183396
C	2.149089	0.405411	-0.552285
O	3.898146	-0.908775	0.412677
O	2.163395	-2.065633	-0.396505
O	2.804928	1.364196	-0.094447
O	1.095297	0.457359	-1.262070
H	4.053193	0.070227	0.480413
H	0.050135	-0.545617	-1.225901

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5f(SA) E[DF-MP2-F12] -1459.436621

S	2.647158	-0.261208	0.159307
O	2.072411	-1.559217	0.505377
O	2.504989	0.800848	1.168981

O	4.225623	-0.580689	0.062549
O	2.232522	0.204244	-1.194969
H	4.701065	0.265122	-0.034900
H	1.158523	-0.897122	-1.902988
O	0.394234	-1.455698	-2.227024
H	0.523667	-2.320434	-1.805447
H	-0.791749	-0.810833	-1.739660
O	0.055492	1.096656	2.103045
H	-0.225599	0.111507	2.062079
H	1.024183	1.072834	1.820293
O	-1.046196	2.508799	0.431995
H	-0.494248	1.726026	1.338131
H	-0.415093	2.560930	-0.350179
O	0.831788	2.601927	-1.439824
H	1.391188	1.790111	-1.378634
H	0.600409	2.691819	-2.375419
O	-0.299866	-1.470397	1.932939
H	0.559823	-1.658234	1.483105
H	-0.980739	-1.863106	1.356039
C	-3.523595	0.092090	-0.017302
C	-2.397120	-0.808153	-0.586982
O	-4.487381	-0.623531	0.559897
O	-3.515914	1.303871	-0.048129
O	-2.335985	-1.977622	-0.198685
O	-1.605200	-0.197221	-1.408467
H	-4.187089	-1.562054	0.516452
H	-1.906735	2.153381	0.106462

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5g(SA)	E[DF-MP2-F12]	-1459.435387
S	-0.710202	-1.607683
O	-0.979346	-0.984068
O	-0.411188	-0.549293
O	-2.031886	-2.332808
O	0.294846	-2.674825
H	-2.818444	-1.670951
H	1.778804	-2.395758
O	-3.988492	-0.634028
H	-4.483198	-0.808297
H	-3.549542	0.234313
O	1.749801	-0.357849
H	1.807989	-1.049285
H	0.878812	-0.505642
O	2.722766	-2.173584

H	3.208183	-3.011176	-1.006993
H	3.223463	-1.118008	-0.090328
O	3.301043	1.895990	-0.648305
H	2.397909	2.297340	-0.501079
H	3.373292	1.795542	-1.609883
O	3.499379	-0.346880	0.562053
H	3.421436	0.562286	0.062312
H	2.808588	-0.359435	1.354495
C	-0.054982	2.038669	-0.578047
C	-1.467316	2.139782	0.060511
O	0.146344	1.200954	-1.534169
O	0.806504	2.816807	-0.139587
O	-2.452945	1.597107	-0.387553
O	-1.473153	2.930560	1.129955
H	-0.471686	0.310122	-1.510278
H	-0.547961	3.266510	1.211826

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5h(SA&OA) E[DF-MP2-F12] -1459.435734

S	-2.392891	-0.381595	-0.462083
O	-2.851491	0.811388	-1.174863
O	-1.423127	-1.199089	-1.190458
O	-1.992502	-0.084839	0.945085
O	-3.662785	-1.377079	-0.341486
H	-1.156324	1.305449	1.274894
H	-4.404328	-0.877674	0.047659
O	-0.704892	2.203627	1.355465
H	0.366747	2.094569	1.053002
H	-1.195302	2.774363	0.655070
O	-2.143275	3.321520	-0.465926
H	-2.474017	2.458475	-0.832516
H	-1.734201	3.787749	-1.209670
O	2.623980	-2.717565	-0.631194
H	3.027017	-1.807605	-0.580454
H	2.938450	-3.101623	-1.462190
O	-0.127528	-1.790340	2.159250
H	0.580810	-1.113410	2.011389
H	-0.947526	-1.288100	1.945886
O	0.166794	-2.940327	-0.035399
H	0.066217	-2.533391	0.961051
H	-0.421499	-2.326776	-0.581308
C	2.106489	0.829008	0.502241
C	3.330793	0.751501	-0.455886
O	1.737076	-0.206784	1.057789

O	1.611258	2.013785	0.577240
O	3.834730	-0.292558	-0.821615
O	3.770835	1.943629	-0.857178
H	1.159974	-2.822624	-0.329705
H	3.143964	2.590104	-0.451590

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5i(SA) E[DF-MP2-F12] -1459.435918

S	1.103077	1.488521	0.045818
O	0.721011	1.083282	1.403778
O	0.247928	0.779639	-0.980480
O	0.820862	3.026076	-0.111147
O	2.528663	1.353734	-0.279811
H	-0.156792	3.214472	0.112419
H	3.147577	-0.026416	-0.638700
O	-1.725125	3.432556	0.405675
H	-1.890642	3.526469	1.356401
H	-2.175840	2.602552	0.146230
O	0.843064	-1.611792	1.906956
H	0.790753	-0.627430	1.793839
H	0.199200	-1.956825	1.262192
O	3.215519	-2.373077	1.171307
H	3.861190	-2.261214	1.883923
H	2.303931	-2.102307	1.541753
O	3.414546	-0.981048	-0.904452
H	3.408660	-1.558941	-0.015360
H	2.600758	-1.294770	-1.476381
O	1.266799	-1.448548	-2.194051
H	0.705304	-2.159532	-1.842676
H	0.823847	-0.621640	-1.867142
C	-2.954906	-0.308139	-0.156025
C	-2.293074	-1.717758	-0.135959
O	-2.202954	0.724923	-0.438907
O	-4.145929	-0.245660	0.104230
O	-1.112939	-1.935712	-0.323888
O	-3.190945	-2.655308	0.133386
H	-1.180749	0.570486	-0.629633
H	-4.042538	-2.158371	0.251176

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5j(SA) E[DF-MP2-F12] -1459.43564

S	2.151916	-0.525180	-0.378755
O	2.092691	0.941127	-0.061462
O	2.247978	-1.348275	0.828346

O	1.067561	-0.952112	-1.289373
O	3.462558	-0.715705	-1.237191
H	-0.269977	-0.407808	-1.175929
H	4.157951	-0.061783	-0.900193
O	-0.209208	-2.204156	1.673995
H	-0.730866	-2.421829	0.877683
H	0.714263	-2.043333	1.351018
O	-1.577846	3.001851	-0.226074
H	-2.046269	3.764155	0.144498
H	-0.535122	2.365035	0.671244
O	0.166713	1.930804	1.299793
H	0.936656	1.526433	0.743799
H	-0.300095	1.153389	1.848288
O	-1.002818	0.087104	2.534107
H	-0.691898	-0.848129	2.230869
H	-0.929970	0.105680	3.499203
O	4.887064	1.275850	-0.241843
H	4.003232	1.590264	0.044249
H	5.375024	1.096721	0.576372
C	-3.528218	0.065347	-0.604046
C	-2.182895	-0.690941	-0.744869
O	-4.538500	-0.766931	-0.379381
O	-3.654431	1.271789	-0.667571
O	-2.168829	-1.895918	-0.499968
O	-1.202461	0.080456	-1.099609
H	-4.127425	-1.665379	-0.333876
H	-2.283270	2.355944	-0.493800

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5k(SA)	E[DF-MP2-F12]	-1459.436721
S	-1.048159	-1.704977
O	-0.685669	-1.127641
O	-0.106320	-1.379460
O	-2.451054	-1.490171
O	-0.844256	-3.303582
H	-3.152569	-0.050466
H	-1.303842	-3.600041
O	-3.417386	0.905306
H	-2.841704	1.127031
H	-2.956108	1.509712
O	-0.322968	3.080716
H	0.462071	2.513149
H	0.019649	3.965870
O	-0.883187	0.454871

H	-1.360399	-0.010362	3.494627
H	-0.620173	-0.245243	2.146739
O	-2.228210	2.282604	1.389093
H	-1.534283	2.728743	0.849857
H	-1.734094	1.638863	1.982407
O	-1.795378	1.345527	-2.213236
H	-1.205122	2.027003	-1.816455
H	-1.298858	0.495511	-2.131193
C	2.613540	0.893419	-0.105998
C	3.247220	-0.503523	0.139930
O	3.520996	1.755285	-0.541914
O	1.443100	1.163812	0.081520
O	4.451656	-0.593542	-0.049115
O	2.479255	-1.481856	0.531683
H	4.361174	1.219895	-0.565007
H	1.485605	-1.274358	0.597609

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5l(SA&OA) E[DF-MP2-F12] -1459.43418

S	-1.543612	0.561870	-1.108380
O	-1.958823	-0.823995	-1.401570
O	-0.138855	0.874325	-1.267788
O	-2.273200	1.476141	-2.231612
O	-2.111394	1.017926	0.200538
H	-3.207219	1.201459	-2.280888
H	-2.647947	-0.195890	1.373088
O	-0.693614	-2.500883	1.815214
H	0.082600	-1.891834	1.845816
H	-0.682195	-2.772128	0.487996
O	-2.804800	-0.915963	2.034731
H	-3.052333	-0.474253	2.859339
H	-1.497544	-1.922049	1.997864
O	-0.531793	-2.849374	-0.614603
H	0.436830	-2.553412	-0.721420
H	-1.089933	-2.090969	-1.002161
O	-0.664661	2.795350	1.536905
H	-0.580608	3.607267	1.014716
H	-1.224575	2.170983	0.981173
O	1.502918	1.629813	2.084139
H	0.619827	2.151461	1.830343
H	2.208936	1.795754	1.373609
C	1.957654	-0.846467	0.094303
C	2.917620	0.279790	-0.425106
O	1.384391	-0.710245	1.213965

O	1.862954	-1.819563	-0.694151
O	3.146572	1.341805	0.134726
O	3.483319	-0.051478	-1.571658
H	1.367767	0.610385	1.836314
H	3.088426	-0.937505	-1.787581

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5m(SA) E[DF-MP2-F12] -1459.435052

S	-0.550268	0.999238	-0.695825
O	0.688573	0.711313	-1.393726
O	-1.783444	0.529105	-1.350181
O	-0.486621	0.499100	0.740089
O	-0.742321	2.570177	-0.577492
H	-1.794018	-0.031177	1.386363
H	0.094478	2.934819	-0.129715
O	-2.709391	-0.381578	1.697836
H	-2.754399	-1.409710	1.390051
H	-3.377964	0.149895	1.114741
O	1.506739	3.303853	0.637112
H	2.178999	3.593171	0.000820
H	1.856742	2.465244	1.002448
O	-4.100488	0.913104	-0.018078
H	-3.340362	0.917733	-0.659640
H	-4.321722	1.842249	0.144079
O	-2.784972	-2.717659	0.839389
H	-2.453792	-3.419883	1.417959
H	-2.168615	-2.684823	0.021620
O	-1.233704	-2.421126	-1.220533
H	-0.312211	-2.380153	-0.886972
H	-1.423578	-1.509880	-1.524531
C	2.852949	-0.239961	0.620448
C	2.311171	-1.537291	-0.039306
O	2.013189	0.464234	1.354986
O	4.024195	0.050435	0.455995
O	1.215555	-2.008183	0.177041
O	3.217047	-2.081076	-0.844652
H	1.031031	0.248713	1.161986
H	4.010122	-1.494081	-0.775161

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5n(SA) E[DF-MP2-F12] -1459.435056

S	-1.063513	-1.031911	0.629630
O	-0.367226	-0.618429	-0.646432
O	-1.571053	0.162954	1.335438

O	-2.046314	-2.083241	0.439422
O	0.081795	-1.687025	1.515455
H	-3.611446	-1.723567	-0.369231
H	0.876066	-1.086386	1.466455
O	-4.405016	-1.302125	-0.780344
H	-4.501676	-1.715622	-1.650205
H	-4.030405	0.319356	-0.648028
O	-3.616015	1.203309	-0.399155
H	-2.493045	1.411783	-1.189967
H	-3.188335	1.005477	0.461775
O	0.177993	2.283885	1.730710
H	-0.451217	1.521690	1.697775
H	1.049206	1.865390	1.837953
O	-1.534326	1.497236	-1.713339
H	-1.031134	0.676041	-1.403327
H	-1.010900	2.310440	-1.318375
O	-0.152340	3.340157	-0.645773
H	-0.509249	4.237235	-0.575339
H	0.013759	3.012189	0.299702
C	3.095962	-0.774626	-1.001457
C	3.077140	-0.020760	0.364269
O	1.990671	-1.284729	-1.470745
O	4.182033	-0.841927	-1.556552
O	2.140291	0.036445	1.145044
O	4.237451	0.566404	0.587012
H	1.127091	-1.031393	-0.992016
H	4.795336	0.296951	-0.194063

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5o(SA)	E[DF-MP2-F12]	-1459.435409
S	1.916511	-1.175376
O	2.371631	-0.045593
O	0.642811	-1.755347
O	3.053681	-2.284020
O	1.960097	-0.905111
H	2.790473	-3.109550
H	1.297723	0.398790
O	0.206766	2.867327
H	0.207190	2.058919
H	-0.455258	2.607577
O	-1.260443	1.970560
H	-1.882384	2.524617
H	-0.547534	1.699217
O	2.422315	2.466795

H	1.142009	2.795552	-0.428342
H	2.650522	1.589376	-0.101298
O	0.975780	1.284364	2.451200
H	1.075649	1.248993	3.413664
H	2.137396	2.241199	1.204844
O	0.318365	0.966295	-2.495772
H	-0.470345	0.396711	-2.350096
H	1.074819	0.455586	-2.113895
C	-2.618706	-1.040897	0.657521
C	-2.771115	-0.382874	-0.742527
O	-1.492694	-1.635674	0.951697
O	-3.576202	-0.966690	1.414291
O	-1.921757	-0.380345	-1.606578
O	-3.970721	0.174550	-0.870032
H	-0.767366	-1.596040	0.243336
H	-4.415180	-0.019181	-0.002300

Table S11.

0A-SA-W₆

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6a(SA)	E[DF-MP2-F12]	-1535.816637
S	0.400310	-1.227895
O	-0.218052	-0.024227
O	1.594162	-1.700359
O	0.607551	-1.013894
O	-0.638025	-2.411624
H	2.211740	-1.415863
H	-1.520241	-2.084329
O	2.357145	2.452915
H	1.575091	2.138204
H	2.050511	2.328605
O	3.628509	-0.078200
H	2.930890	-0.766128
H	4.199910	-0.441613
O	3.146620	-1.400973
H	3.877766	-0.034343
H	3.124556	-1.637102
O	4.179847	0.746843
H	3.157064	1.737648
H	4.207816	0.403930
O	0.321426	1.490703
H	0.279944	1.489168
H	0.328616	0.537987

O	1.693277	1.948344	-1.704847
H	2.428275	1.355271	-1.987079
H	0.926146	1.334799	-1.616166
C	-3.562407	1.018507	-0.290175
C	-3.752981	-0.416530	0.285597
O	-2.420132	1.335508	-0.838851
O	-4.516013	1.775877	-0.196321
O	-2.929202	-1.308565	0.264486
O	-4.958495	-0.547430	0.817168
H	-1.697833	0.627484	-0.817809
H	-5.381843	0.341391	0.670743

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6b(SA)	E[DF-MP2-F12]	-1535.81442
S	-0.662096	-1.803954
O	-0.309457	-1.044563
O	-2.064216	-2.210988
O	-0.185889	-1.097266
O	0.125736	-3.183555
H	-1.260947	0.394822
H	1.087652	-2.953032
O	-3.718885	-0.233409
H	-3.893427	0.219849
H	-3.162056	-1.067392
O	-1.950244	1.097376
H	-3.051257	0.396427
H	-1.558356	1.830147
O	-1.460003	1.311428
H	-1.175606	1.966264
H	-1.016275	0.469714
O	-3.977144	0.946073
H	-2.997285	1.096294
H	-4.408202	0.481636
O	-0.878404	3.031908
H	-1.370419	3.862527
H	0.086537	3.299852
O	1.675761	3.773002
H	1.927195	4.061838
H	2.280063	3.016002
C	3.059220	-0.878732
C	2.592816	0.506948
O	4.059786	-0.754427
O	2.594807	-1.941762
O	3.209860	1.497630

O	1.624865	0.568026	-1.061769
H	4.229237	0.217760	1.253762
H	0.991880	-0.274528	-1.160316

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6c(SA&OA) E[DF-MP2-F12] -1535.815023

S	-1.383651	-1.638167	-0.585581
O	-0.257471	-1.414613	-1.491412
O	-2.136669	-0.426061	-0.207276
O	-2.498124	-2.470665	-1.407270
O	-1.029619	-2.480087	0.578324
H	-2.059331	-3.243436	-1.808608
H	-0.468063	-1.922462	1.885305
O	-2.098964	2.253346	-1.079335
H	-2.392498	2.674076	-0.223909
H	-2.261070	1.290871	-0.957935
O	-1.290549	0.822777	2.093232
H	-0.407614	1.097180	1.719361
H	-1.720201	0.385417	1.310934
O	0.998813	0.550743	-2.988799
H	1.928425	0.444531	-2.707033
H	0.524308	-0.213056	-2.580193
O	-2.626778	3.186697	1.409036
H	-2.256191	2.423914	1.910534
H	-3.520642	3.328599	1.752375
O	0.380221	2.394958	-1.374747
H	-0.684440	2.378512	-1.243057
H	0.618858	1.684900	-2.118571
O	-0.115579	-1.414397	2.715920
H	0.862185	-1.078837	2.446857
H	-0.667673	-0.553172	2.698877
C	3.169974	0.206347	-0.067821
C	2.019368	0.270219	0.981044
O	4.146803	-0.628868	0.290669
O	3.162139	0.819693	-1.112310
O	2.105435	-0.614487	1.888556
O	1.119499	1.130846	0.835879
H	3.842765	-1.031244	1.139499
H	0.790301	2.006419	-0.538212

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6d(SA) E[DF-MP2-F12] -1535.814605

S	0.237798	-1.341497	-0.877400
O	-0.224903	-0.142242	-1.587008

O	1.569167	-1.822405	-1.212296
O	0.052816	-1.150307	0.608327
O	-0.741580	-2.537859	-1.270723
H	0.978113	-1.865733	1.876692
H	-1.640573	-2.260897	-0.969354
O	2.938757	0.199187	2.084536
H	2.245721	0.961980	1.973640
H	3.265173	0.001077	1.069168
O	2.568966	2.382483	-0.917519
H	1.986290	2.263541	-1.738218
H	3.168285	3.119260	-1.105941
O	3.582654	-0.133141	-0.299698
H	2.950708	-0.781552	-0.702609
H	3.334167	0.748216	-0.676106
O	1.342333	2.146741	1.568621
H	0.395572	1.919299	1.493737
H	1.649788	2.362054	0.653213
O	1.655811	-1.969041	2.595771
H	2.443701	-0.642480	2.402963
H	1.170847	-2.137817	3.416222
O	1.054689	1.778040	-2.958110
H	0.568988	1.008761	-2.557728
H	0.366788	2.378300	-3.279703
C	-3.347689	-0.061534	0.129650
C	-2.573966	1.073728	0.870590
O	-4.576499	0.339515	-0.177649
O	-2.911667	-1.162895	-0.123174
O	-3.168265	2.121702	1.067181
O	-1.343581	0.838453	1.256568
H	-4.628304	1.267626	0.169481
H	-0.919672	-0.056692	0.932893

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6e(SA)	E[DF-MP2-F12]	-1535.812952
S	1.342166	1.825606
O	0.967049	1.159988
O	2.662193	2.388429
O	1.060642	0.888000
O	0.315344	3.030209
H	2.091971	-0.443546
H	-0.570847	2.732940
O	2.551742	-1.324617
H	1.713722	-2.477196
H	2.976105	-1.354691

O	-1.315976	-0.140799	-2.073140
H	-0.450035	0.307750	-1.870718
H	-1.610830	0.210150	-2.925481
O	1.129877	-3.187093	-0.666433
H	0.145096	-3.041305	-0.977894
H	1.158356	-2.977793	0.378963
O	-1.274886	-2.750880	-1.412468
H	-1.303873	-1.816341	-1.762582
H	-1.890350	-2.732757	-0.656099
O	2.793780	-0.636884	2.173889
H	3.165351	-0.363271	3.024299
H	2.289243	0.138285	1.832274
O	1.091077	-2.635719	1.784838
H	0.256723	-2.136814	1.870297
H	1.793427	-1.951729	2.008160
C	-2.104213	-0.409109	0.840449
C	-2.677989	0.991519	0.486849
O	-0.863408	-0.504368	1.220256
O	-2.866241	-1.368373	0.751602
O	-2.047643	2.027492	0.485063
O	-3.971225	0.918698	0.202338
H	-0.209298	0.332676	1.117603
H	-4.194811	-0.043185	0.279477

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6f(SA)	E[DF-MP2-F12]	-1535.81334
S	1.169901	-1.619893
O	2.156782	-1.117889
O	0.012345	-2.253353
O	1.928502	-2.781151
O	0.851575	-0.646529
H	2.025594	-3.554653
H	1.325528	1.117477
O	1.470201	2.092425
H	2.124115	2.342984
H	0.548603	2.487688
O	1.261548	1.044412
H	1.519829	0.156310
H	0.309155	1.091502
O	-1.070284	2.843027
H	-1.549938	3.131373
H	-1.412810	1.930654
O	-1.683740	0.197340
H	-0.815867	-0.243674

H	-2.037823	-0.200722	2.807258
O	4.377802	0.443204	-0.416444
H	4.873311	0.345397	0.409714
H	3.685583	-0.264798	-0.411336
O	2.687454	2.411395	-0.737344
H	3.461522	1.763385	-0.605695
H	2.082964	1.940207	-1.449290
C	-2.407352	0.530962	-0.897534
C	-3.223293	-0.721262	-0.486445
O	-3.151977	1.631784	-0.818440
O	-1.252213	0.513178	-1.264007
O	-4.414636	-0.564272	-0.270482
O	-2.601994	-1.871848	-0.427077
H	-4.043476	1.294532	-0.535024
H	-1.601761	-1.811369	-0.511811

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6g(SA)	E[DF-MP2-F12]	-1535.811529
S	-1.140322	-1.245711
O	-0.589193	-1.164129
O	-2.599950	-1.347029
O	-0.656750	-0.050175
O	-0.595942	-2.512160
H	-1.692340	1.112367
H	0.482373	-2.686024
O	-1.605062	0.907254
H	-2.444720	0.623085
H	-1.256463	0.116455
O	1.801169	-2.992231
H	2.309466	-2.199357
H	1.845994	-3.005759
O	-2.353750	1.896073
H	-2.101200	2.399039
H	-3.278096	1.438992
O	1.488920	-2.709389
H	1.200037	-3.463852
H	0.673812	-2.180823
O	-1.652425	2.954529
H	-0.708901	3.157492
H	-1.663717	2.205967
O	-4.442184	0.478012
H	-4.985140	0.235911
H	-3.873185	-0.316408
C	3.083679	0.648310

C	2.258634	1.871366	-0.117349
O	4.387034	0.857753	-0.450032
O	2.591580	-0.364153	-1.040638
O	2.859489	2.848496	0.295118
O	0.949512	1.784572	-0.180576
H	4.457280	1.770189	-0.070928
H	0.566492	0.906655	-0.532015

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6h(SA)	E[DF-MP2-F12]	-1535.813654
S	-0.125093	-0.880598
O	1.080037	-1.575897
O	-0.286801	-0.853032
O	-1.349622	-1.295076
O	0.066632	0.666258
H	-2.660987	-2.054056
H	1.048340	0.858758
O	-4.229557	0.036769
H	-4.216430	0.661295
H	-3.386978	0.349421
O	-2.114689	0.835066
H	-1.413150	0.204923
H	-1.909275	1.661057
O	-4.049572	1.548562
H	-3.285721	2.119330
H	-3.722077	1.030770
O	-1.646274	2.640579
H	-0.977632	2.025595
H	-1.286433	3.534027
O	-3.529737	-2.282421
H	-3.341658	-2.992861
H	-4.018665	-0.918122
O	-2.891972	0.145586
H	-2.252738	-0.414758
H	-3.368247	-0.456653
C	3.789439	0.911828
C	4.325952	-0.507837
O	4.769928	1.797281
O	2.646524	1.204702
O	5.511682	-0.565942
O	3.521068	-1.531048
H	5.559593	1.252380
H	2.560029	-1.366574

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6i(SA)  E[DF-MP2-F12]  -1535.813332
S   0.901243   1.131792  -0.748864
O   2.201433   0.564970  -1.144911
O   0.564796   2.430724  -1.300140
O   -0.186793   0.116408  -0.916139
O   1.057293   1.333881   0.860756
H   0.011776  -1.534503  -0.420633
H   0.343886   2.021305   1.125748
O   1.546388  -1.204006   2.087111
H   1.312616  -0.282334   1.833155
H   2.913452  -1.432795   1.554558
O   -0.805115   3.147740   1.149044
H   -1.645322   2.678282   0.986461
H   -0.567872   3.496418   0.267407
O   3.814892  -1.594480   1.026392
H   3.466936  -1.945600   0.090439
H   4.190801  -0.658931   0.821402
O   4.524291   0.755100   0.238265
H   3.704444   0.926288  -0.293313
H   4.616182   1.503997   0.845302
O   2.784890  -2.248298  -1.197324
H   2.595362  -1.339924  -1.519767
H   1.890596  -2.575873  -0.931862
O   0.281230  -2.415730  -0.045644
H   0.973260  -1.759158   1.498266
H   -0.533754  -2.941849  -0.091467
C   -3.509991  -1.237173  -0.148994
C   -3.576600   0.289143   0.132943
O   -4.696574  -1.809942   0.040461
O   -2.506254  -1.827633  -0.476018
O   -4.627506   0.760092   0.530153
O   -2.478810   0.992333  -0.050180
H   -5.294472  -1.073022   0.321779
H   -1.671518   0.487944  -0.423958
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6j(SA)  E[DF-MP2-F12]  -1535.813156
S   0.422141  -1.738853  -0.192248
O   1.871956  -1.675708   0.008875
O   -0.062010  -1.186999  -1.462830
O   0.136234  -3.325450  -0.238467
O   -0.338852  -1.219696   0.980248
H   -0.796592  -3.464564  -0.488166
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H	0.152057	0.305628	1.639947
O	3.352695	0.043872	-1.779185
H	2.577261	0.499692	-2.175358
H	2.951581	-0.726096	-1.321653
O	2.964484	-0.124382	2.151139
H	2.740821	-0.886724	1.573464
H	3.507540	0.464181	1.567017
O	3.955107	1.595799	0.230690
H	3.835171	1.009306	-0.593044
H	4.823354	2.017997	0.161951
O	0.824441	1.275925	-2.174247
H	0.365235	0.423077	-1.950659
H	0.339484	1.658978	-2.919604
O	1.362104	2.612382	0.215817
H	2.338907	2.461988	0.179687
H	1.024148	2.262954	-0.646258
O	0.714341	1.030420	2.039088
H	0.901848	1.749167	1.256853
H	1.651909	0.563357	2.190916
C	-3.657555	-0.069843	0.225860
C	-2.875490	1.253863	0.001794
O	-2.973635	-1.112043	0.642962
O	-4.856604	-0.077625	0.005564
O	-1.691896	1.393600	0.207232
O	-3.684306	2.211960	-0.452109
H	-1.985504	-0.939851	0.735724
H	-4.575672	1.782009	-0.498998

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6k(SA&OA)	E[DF-MP2-F12]	-1535.8122
S	1.408735	1.126744
O	1.007252	2.366256
O	0.476285	0.691070
O	1.696983	0.012816
O	2.794598	1.494478
H	0.818662	-1.368297
H	3.199992	0.659411
O	3.817281	-0.899477
H	4.604465	-0.926868
H	4.110309	-1.128392
O	-1.955639	2.311221
H	-2.694624	1.661307
H	-1.148920	1.778628
O	1.175866	-1.919659

H	2.151495	-1.802276	1.704639
H	0.849378	-0.986336	1.660869
O	-1.572663	2.459818	-1.085181
H	-1.786632	2.541461	-0.046894
H	-0.555112	2.494541	-1.097571
O	4.205341	-1.125901	-1.236132
H	3.350225	-0.657478	-1.396545
H	4.148695	-1.955465	-1.732507
O	0.484281	-2.281905	-0.748908
H	-0.589578	-2.276732	-0.804510
H	0.758310	-2.280730	0.264759
C	-2.358442	-0.953953	-0.702910
C	-3.584175	-0.645230	0.206975
O	-1.810225	-0.048704	-1.356160
O	-1.998863	-2.177477	-0.652452
O	-3.884514	0.464885	0.598173
O	-4.258004	-1.741829	0.556594
H	-1.797062	1.461826	-1.263147
H	-3.727473	-2.492117	0.194934

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6l(SA&OA) E[DF-MP2-F12] -1535.811973

S	1.863342	1.107807	-0.424100
O	1.196342	2.270415	-0.988636
O	1.459045	0.835970	0.994095
O	1.800147	-0.121343	-1.244430
O	3.407736	1.516468	-0.358749
H	0.592543	-1.538735	-1.633856
H	3.933371	0.681467	-0.251485
O	2.266505	-1.649658	1.883585
H	2.056539	-0.698902	1.707151
H	3.053371	-1.808638	1.324212
O	-0.956943	1.386447	1.765230
H	-1.231567	2.107009	1.062745
H	0.020593	1.200955	1.536189
O	0.141323	-2.713080	0.940044
H	1.020797	-2.329089	1.347993
H	-0.608648	-2.019742	1.066669
O	-1.272353	3.013077	-0.150696
H	-0.370117	2.903244	-0.548611
H	-1.417813	3.960866	-0.017937
O	4.119638	-1.190589	-0.314716
H	4.826331	-1.609974	-0.827588
H	3.337336	-1.112008	-0.911359

O	0.137604	-2.404985	-1.540428
H	-0.836297	-2.202065	-1.551938
H	0.240552	-2.683385	-0.125241
C	-2.518287	-0.957243	-0.038990
C	-3.684114	0.074312	-0.040281
O	-1.710870	-0.895534	0.949835
O	-2.465706	-1.738274	-1.011883
O	-3.793287	0.961047	0.772307
O	-4.531546	-0.130870	-1.056405
H	-1.449939	0.502645	1.523351
H	-4.147202	-0.893696	-1.552295

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6m(SA) E[DF-MP2-F12] -1535.810035

S	3.025745	-0.207185	-0.389748
O	2.827408	1.192798	0.040450
O	3.395576	-1.105744	0.722367
O	1.944097	-0.727920	-1.235631
O	4.341261	-0.078209	-1.322747
H	0.903036	2.417150	-2.157118
H	4.552421	-0.967544	-1.662147
O	-0.889293	2.227621	0.407468
H	-1.685402	2.837995	0.378476
H	-1.366723	1.030724	0.138540
O	0.996707	1.047918	2.233504
H	1.747145	1.245788	1.627144
H	0.240728	1.518396	1.823542
O	1.211745	-1.517621	2.087123
H	0.971802	-0.517646	2.192747
H	2.147903	-1.466873	1.690264
O	1.025455	2.744580	-1.253556
H	1.761621	2.189678	-0.876509
H	-0.199992	2.498926	-0.298925
O	0.213910	-2.509224	0.058643
H	-0.753115	-2.446176	-0.130672
H	0.648811	-1.952754	1.255523
O	-3.278669	3.305444	0.182471
H	-3.760897	3.722474	0.910929
H	-3.663508	2.401527	0.075617
C	-3.340525	-1.709625	-0.400096
C	-2.955780	-0.222236	-0.180969
O	-4.650863	-1.867767	-0.575008
O	-2.545728	-2.624385	-0.409346
O	-3.875840	0.610067	-0.172673

O	-1.694972	-0.035089	-0.029907
H	-5.033114	-0.959385	-0.512521
H	0.688844	-1.945892	-0.597811

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6n(SA)	E[DF-MP2-F12]	-1535.808882
S	0.885028	-2.376389 0.074031
O	-0.356322	-2.782695 -0.586608
O	0.775767	-1.495482 1.226964
O	1.540669	-3.722088 0.677785
O	1.885449	-1.873043 -0.933720
H	1.426458	-4.431212 0.018468
H	2.295222	-0.664590 -0.794727
O	-3.619103	-1.051092 1.122588
H	-4.375259	-0.891500 1.704914
H	-3.645975	-0.433898 -0.195652
O	-1.270700	-0.620318 -1.998614
H	-0.579716	0.000773 -1.677090
H	-0.999603	-1.489524 -1.603143
O	-3.543777	0.012926 -1.149033
H	-3.552816	1.024717 -1.004003
H	-2.579973	-0.256538 -1.522043
O	-3.487203	2.545742 -0.601201
H	-3.470058	3.197133 -1.316945
H	-2.640277	2.665202 -0.083920
O	-1.203535	2.474973 0.794128
H	-1.318471	0.827438 1.823059
H	-0.782332	3.250788 1.198802
O	-1.458554	-0.075648 2.179444
H	-2.789379	-0.694015 1.599265
H	-0.679619	-0.603674 1.888863
C	1.770181	1.287855 -0.487980
C	2.296419	2.611130 0.137159
O	0.570654	1.183186 -0.766180
O	2.692437	0.395931 -0.634255
O	1.560452	3.517318 0.447709
O	3.622705	2.642138 0.308765
H	-0.506674	2.144001 0.163109
H	3.966903	1.768425 0.019287

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6o(SA)	E[DF-MP2-F12]	-1535.809329
S	2.356707	-0.348699 0.278802
O	2.760838	0.899755 0.934400

O	1.542673	-1.227777	1.152482
O	1.776954	-0.178143	-1.063356
O	3.715586	-1.166531	-0.041377
H	1.890952	1.362329	-1.840060
H	4.222148	-1.246007	0.788065
O	1.730131	2.282662	-2.181092
H	0.580769	2.788680	-1.291680
H	2.576122	2.748028	-2.104872
O	0.605317	2.458136	1.613554
H	0.049817	1.703043	1.959173
H	1.482034	2.021406	1.459520
O	0.746916	-3.623678	-0.098044
H	0.171380	-4.156654	0.469999
H	1.084116	-2.895168	0.472000
O	-0.637653	0.134981	2.231855
H	0.103776	-0.442206	1.922700
H	-0.800757	-0.116717	3.152650
O	-0.548189	-1.872100	-1.703773
H	-0.102342	-2.618491	-1.212445
H	0.068436	-1.120455	-1.595913
O	-0.213593	2.986001	-0.660219
H	0.141389	2.787764	0.367698
H	-0.894423	2.259267	-0.844419
C	-2.710583	0.628508	-0.295307
C	-3.332774	-0.779500	-0.079138
O	-3.405851	1.552582	0.341898
O	-1.715929	0.862631	-0.966133
O	-4.361597	-0.792293	0.594116
O	-2.755749	-1.807648	-0.602710
H	-4.141386	1.018365	0.763221
H	-1.798015	-1.676664	-1.092601

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6p(SA)	E[DF-MP2-F12]	-1535.811178
S	0.702914	-1.440979
O	1.013540	-0.566714
O	-0.110683	-0.782738
O	-0.245466	-2.565130
O	1.861754	-2.158796
H	-0.400885	-3.267334
H	3.207141	-1.381211
O	1.120249	1.383600
H	1.320503	2.007072
H	0.605139	0.661994

O	-0.169309	1.995663	-1.852417
H	0.111247	1.057858	-1.949152
H	-1.004631	1.937161	-1.346180
O	3.476489	0.894429	-1.331361
H	2.777778	0.376623	-1.785801
H	2.982722	1.690473	-0.992457
O	3.976052	-0.741292	0.519282
H	3.782864	-0.295243	1.461002
H	3.843165	-0.002338	-0.232652
O	1.793671	2.829121	-0.384565
H	1.944401	3.781874	-0.466617
H	0.984629	2.604646	-0.971441
O	3.324367	0.282008	2.710049
H	2.456810	0.771273	2.475982
H	3.900541	0.903969	3.176044
C	-3.708964	-0.531742	0.663111
C	-3.462796	0.876216	0.056624
O	-2.664938	-1.300664	0.863556
O	-4.858772	-0.848900	0.917149
O	-2.368800	1.308743	-0.232840
O	-4.604023	1.536502	-0.101158
H	-1.782015	-0.895379	0.597487
H	-5.298515	0.910738	0.231210

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6q(SA)	E[DF-MP2-F12]	-1535.810492
S	-2.142113	0.816326
O	-1.574098	0.170541
O	-1.153187	1.660613
O	-3.280359	1.800385
O	-2.824096	-0.138625
H	-2.936325	2.753173
H	-3.468345	-1.647594
O	-0.986641	-1.510784
H	-1.690921	-0.921790
H	-0.179577	-0.952841
O	-3.563107	-2.613928
H	-2.133581	-3.138414
H	-4.323675	-2.938349
O	-1.129062	-3.239601
H	-0.625120	-2.787709
H	-0.981295	-2.595024
O	0.958949	0.369289
H	1.677234	0.945616

H	0.216592	0.945973	1.042531
O	-2.080085	4.120898	-0.401189
H	-2.496438	4.699011	0.255878
H	-1.453253	3.555515	0.101065
O	-0.070221	-2.065646	-1.565141
H	-0.599920	-1.222805	-1.610343
H	0.853078	-1.783142	-1.417321
C	3.541818	-0.441305	-0.616903
C	4.159615	0.613317	0.354039
O	2.277908	-0.760062	-0.453833
O	4.267391	-0.915345	-1.473783
O	3.574793	1.163300	1.263672
O	5.433737	0.834568	0.052322
H	1.775897	-0.252602	0.312003
H	5.615476	0.242882	-0.722361

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6r(SA)	E[DF-MP2-F12]	-1535.811667
S	0.026412	-0.978391
O	-0.818385	-2.028716
O	-0.400059	-0.497941
O	1.481708	-1.197088
O	-0.135552	0.326019
H	2.545366	-1.820309
H	-1.095633	0.582015
O	3.385116	-1.909844
H	3.329355	-2.749760
H	3.481585	-0.322238
O	4.158207	-0.793383
H	3.200293	-0.937357
H	4.335925	-1.368969
O	4.156337	1.629397
H	4.907506	2.164721
H	4.233735	0.731857
O	1.074751	1.440956
H	1.227533	1.956147
H	0.489883	0.651954
O	3.436148	0.649604
H	3.881301	1.069771
H	2.043223	1.069373
O	1.529139	2.461383
H	1.032201	1.831413
H	2.488437	2.243531
C	-3.966213	-0.175878

C	-3.768814	0.601753	-0.480625
O	-2.920146	-0.635426	1.490916
O	-5.116182	-0.298192	1.249852
O	-2.704189	0.858320	-1.005055
O	-4.938212	0.977974	-0.973803
H	-2.024799	-0.501863	1.039683
H	-5.597782	0.634225	-0.312092

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6s(SA) E[DF-MP2-F12] -1535.810622

S	3.014018	0.053254	-0.582600
O	2.226040	-0.799082	-1.481314
O	2.833122	1.496395	-0.813652
O	2.910356	-0.311573	0.849516
O	4.569155	-0.275689	-0.881230
H	0.305293	-0.301026	2.093206
H	4.703128	-0.224708	-1.845499
O	0.900050	0.595805	2.419282
H	0.361504	1.428585	2.075969
H	1.740005	0.497716	1.889132
O	0.334554	2.295386	-1.071502
H	1.314264	2.073902	-1.058680
H	0.191274	2.909288	-1.805900
O	-0.452413	-0.384190	-1.040314
H	0.413505	-0.705973	-1.396056
H	-0.359663	0.600419	-1.059377
O	-0.529074	2.495729	1.510685
H	-0.213102	2.623182	0.580163
H	-1.417536	2.103016	1.384159
O	-0.319581	-1.359870	1.567112
H	0.405488	-2.055418	1.538467
H	-0.453921	-1.079151	0.623993
O	1.882250	-2.844933	1.406505
H	2.451816	-2.068813	1.190310
H	2.281779	-3.261817	2.183467
C	-3.656247	0.343107	0.158835
C	-3.884611	-0.787052	-0.889358
O	-4.777970	0.610965	0.813529
O	-2.599785	0.911536	0.345656
O	-5.023517	-1.214510	-0.998134
O	-2.865241	-1.205932	-1.594337
H	-5.444410	-0.008172	0.411745
H	-1.962145	-0.799722	-1.354762

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6t(SA&OA) E[DF-MP2-F12] -1535.808752

S	-2.660698	-0.450059	-0.112475
O	-3.174967	0.804594	-0.661162
O	-1.999862	-1.337584	-1.071042
O	-1.879856	-0.237705	1.137704
O	-3.959925	-1.316504	0.319284
H	-0.679572	-1.252127	1.657620
H	-4.579840	-0.716404	0.773219
O	0.139742	-1.803651	1.843417
H	0.238038	-2.518772	0.337319
H	-0.085451	-2.383330	2.587045
O	-1.731017	2.744709	-1.870123
H	-2.305406	2.023830	-1.499817
H	-1.634427	2.546805	-2.813126
O	0.385663	2.673485	-0.397621
H	-0.013160	2.489911	0.618612
H	-0.419693	2.733535	-1.034656
O	0.188254	-2.684941	-0.657921
H	1.118531	-2.216893	-1.066689
H	-0.635646	-2.154416	-0.928326
O	1.661387	0.666025	2.564796
H	2.359038	0.869997	1.905527
H	1.359430	-0.240489	2.355038
O	-0.455252	2.115167	1.855147
H	-1.117736	1.408079	1.681861
H	0.339629	1.618843	2.231061
C	2.253209	-0.422168	-0.907960
C	3.588529	0.131465	-0.345377
O	1.239501	0.290543	-0.918482
O	2.320459	-1.652150	-1.266567
O	3.643295	1.049845	0.444245
O	4.670081	-0.533145	-0.769096
H	0.866263	1.807399	-0.623275
H	4.330729	-1.300308	-1.282414