

Supporting Information

The energy-based fragmentation approach for computing total energies, structures, and molecular properties of large systems at the *ab initio* levels

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Cartesian coordinates of all compounds	C	1.952466	-7.455546	0.479602
	O	2.201398	-8.557704	0.969677
1. Coordinates for ground state energies calculations.	N	2.765024	-6.406870	0.654759
(1) 1FGD (charge=-6)	C	3.905772	-6.347002	1.578950
a. conformer 1	C	3.480977	-6.547133	3.051754
	O	3.281830	-5.585210	3.785226
N -3.077051 0.773647 4.123127	C	4.669332	-5.030437	1.344936
C -2.634232 -0.627590 3.980241	C	5.964674	-4.910559	2.129417
C -1.876334 -0.811942 2.656793	C	6.017573	-4.119916	3.293714
O -2.248670 -0.189600 1.665617	C	7.114908	-5.608254	1.709571
C -3.826697 -1.594306 4.074144	C	7.207588	-4.043633	4.042448
S -4.730259 -1.553763 5.649064	C	8.300290	-5.534090	2.470136
N -0.800231 -1.623269 2.602407	C	8.340980	-4.765302	3.643955
C -0.077309 -1.921981 1.363316	O	9.472658	-4.742633	4.396034
C -0.816222 -2.960648 0.498332	N	3.269476	-7.812974	3.444629
O -1.722667 -3.653735 0.957543	C	2.853639	-8.357317	4.763348
C 1.283512 -2.450421 1.827199	C	1.707676	-7.650075	5.527182
C 0.921294 -3.206838 3.101104	O	1.402071	-8.026449	6.655970
C -0.212555 -2.370175 3.703629	C	4.067617	-8.689445	5.671935
N -0.386823 -3.101122 -0.754931	C	4.954238	-7.481885	6.060402
C -0.918540 -4.051334 -1.748811	C	4.866040	-9.865910	5.076114
C -0.739325 -5.545790 -1.408939	C	6.192078	-7.221517	5.189335
O -1.506826 -6.382429 -1.886168	N	1.020428	-6.697360	4.894742
C -0.281781 -3.742213 -3.122290	C	-0.010255	-5.794572	5.427490
C 1.205051 -4.131709 -3.282477	C	0.493207	-4.805110	6.491607
C 2.083806 -3.599368 -2.141743	O	0.074165	-3.651982	6.444617
O 2.585068 -4.431095 -1.350476	C	-1.300607	-6.533226	5.848349
O 2.123594 -2.362902 -1.970525	C	-2.247962	-6.982967	4.716113
N 0.287233 -5.892841 -0.628165	C	-2.826224	-5.805232	3.926780
C 0.661579 -7.278542 -0.331799	C	-1.613849	-7.962120	3.725344

N	1.420463	-5.175395	7.376185	S	-3.913199	-3.016062	6.817213
C	2.127841	-4.211463	8.226995	N	-3.930708	0.731572	8.026747
C	3.556773	-4.670885	8.582973	C	-5.093195	1.654294	8.049184
O	3.832294	-5.861578	8.718065	C	-5.099454	2.481220	6.751980
C	1.293882	-3.893397	9.486859	O	-4.039812	2.591498	6.127461
C	1.526251	-2.460250	9.976839	C	-4.980345	2.594790	9.271491
O	2.674990	-1.971968	9.909519	O	-4.662582	1.863023	10.437350
O	0.556721	-1.780659	10.376065	C	-6.257904	3.352555	9.618145
N	4.444615	-3.688637	8.737468	N	-6.229151	3.069428	6.334710
C	5.885044	-3.789818	9.030269	C	-6.308897	3.908228	5.116097
C	6.396255	-2.538093	9.799482	C	-7.215126	5.151863	5.235107
O	7.591608	-2.383709	10.043895	O	-6.846477	6.208816	4.719355
C	6.621740	-3.960261	7.685280	C	-6.776325	3.063122	3.914238
C	8.059712	-4.499494	7.768889	C	-5.667132	2.166312	3.363828
O	8.346099	-5.339095	8.652189	O	-5.760596	0.924120	3.479944
O	8.851819	-4.141717	6.859861	O	-4.650084	2.691918	2.856960
N	5.508993	-1.597550	10.173583	N	-8.373383	5.059960	5.901850
C	5.914297	-0.299486	10.739205	C	-9.313105	6.183651	6.127555
C	4.807157	0.711797	11.084204	C	-10.351590	5.845008	7.207068
O	5.131184	1.884713	11.258696	O	-10.546412	6.629001	8.129749
N	3.544726	0.276442	11.179024	C	-9.997796	6.639587	4.808765
C	2.310790	1.031441	11.465706	C	-10.888539	7.876402	5.068326
C	1.680123	1.648604	10.203488	C	-10.784302	5.524179	4.088596
O	1.653164	2.866799	10.027988	C	-11.381474	8.569637	3.791702
C	2.437735	2.006514	12.652657	N	-10.926771	4.644000	7.114185
C	2.914385	1.361580	13.942917	C	-11.636738	3.916242	8.174147
C	4.214049	1.606728	14.425267	C	-12.911951	4.584145	8.768727
C	2.059956	0.498414	14.654893	O	-13.426519	4.118767	9.787917
C	4.658054	0.991486	15.609930	C	-10.593022	3.399893	9.189313
C	2.501944	-0.116375	15.840409	C	-9.573964	2.433066	8.547637
C	3.801590	0.129560	16.318029	O	-8.761599	2.868333	7.688661
N	1.167800	0.783160	9.320987	O	-9.594777	1.239049	8.916431
C	0.542410	1.129459	8.026491	N	-13.487500	5.578347	8.072334
C	-0.794665	0.402821	7.751735	C	-14.875651	6.091259	8.205948
O	-1.399934	0.620889	6.698413	C	-15.509456	6.315147	6.815639
C	1.541619	0.919185	6.859317	O	-14.787548	6.792642	5.906672
C	2.009390	-0.549999	6.748139	C	-14.920407	7.364191	9.091932
C	2.737461	1.880522	6.989407	C	-16.356033	7.842418	9.406777
C	2.842522	-0.855152	5.497323	C	-16.432275	8.987224	10.443064
N	-1.258580	-0.460735	8.664283	O	-16.207128	10.164769	10.067971
C	-2.513383	-1.234907	8.637637	O	-16.803185	8.710329	11.612046
C	-3.838203	-0.432108	8.675324	O	-16.690674	5.929205	6.648276
O	-4.760766	-0.835181	9.381984	H	-3.522996	0.928212	5.017445
C	-2.408763	-2.289929	7.520643	H	-2.314101	1.422864	4.026580

H	-3.775579	0.999515	3.417222	H	-3.084491	-7.497879	5.189626
H	-1.957056	-0.841539	4.800461	H	-3.603771	-6.162285	3.252303
H	-4.534776	-1.339550	3.281180	H	-2.056202	-5.314791	3.331248
H	-3.486057	-2.614750	3.894247	H	-3.266492	-5.082611	4.613210
H	0.069411	-1.015907	0.773985	H	-2.383161	-8.356569	3.062656
H	1.757660	-3.098690	1.089021	H	-1.151652	-8.783986	4.271011
H	1.938347	-1.612829	2.072163	H	-0.860999	-7.454983	3.122764
H	0.551905	-4.195968	2.829444	H	1.735641	-6.138974	7.390973
H	1.769096	-3.287756	3.781152	H	2.227856	-3.288939	7.654420
H	-0.954707	-3.019957	4.167901	H	0.231722	-4.002085	9.258540
H	0.194317	-1.678371	4.441380	H	1.538823	-4.600010	10.281415
H	0.413561	-2.536147	-1.041283	H	4.047599	-2.758592	8.712796
H	-1.992453	-3.880639	-1.828223	H	6.064228	-4.672141	9.646546
H	-0.849785	-4.269195	-3.890212	H	6.055950	-4.655999	7.064787
H	-0.388263	-2.674778	-3.322565	H	6.624558	-2.996886	7.171437
H	1.281607	-5.220602	-3.331481	H	4.520659	-1.778956	10.018889
H	1.567731	-3.739991	-4.235631	H	6.472065	-0.491993	11.655020
H	0.944081	-5.154990	-0.396069	H	6.591764	0.183264	10.034837
H	-0.152375	-7.747169	0.221242	H	3.385787	-0.696847	10.933860
H	0.786338	-7.810281	-1.274449	H	1.587429	0.280280	11.785654
H	2.607893	-5.579802	0.077224	H	3.097048	2.832169	12.385808
H	4.584518	-7.161313	1.327375	H	1.454775	2.441015	12.839063
H	4.908431	-4.948654	0.283499	H	4.876498	2.256509	13.870271
H	4.018883	-4.189840	1.591716	H	1.066048	0.297162	14.279689
H	5.133930	-3.596862	3.635259	H	5.661899	1.172173	15.964174
H	7.080975	-6.209387	0.813684	H	1.844412	-0.787873	16.372933
H	7.246635	-3.454473	4.945617	H	4.145224	-0.352951	17.220954
H	9.181892	-6.079493	2.177237	H	1.236737	-0.203567	9.569321
H	9.272495	-4.485768	5.331203	H	0.288636	2.189801	8.049874
H	3.325448	-8.489718	2.694766	H	1.026266	1.178615	5.933091
H	2.404050	-9.320557	4.527549	H	1.135798	-1.200623	6.732799
H	3.662339	-9.070224	6.610410	H	2.607974	-0.805771	7.620571
H	5.314016	-7.645527	7.077262	H	3.326080	1.877978	6.073344
H	4.343180	-6.579288	6.084634	H	3.373374	1.583369	7.824413
H	4.214872	-10.731410	4.958526	H	2.377494	2.894556	7.167102
H	5.677865	-10.129048	5.754911	H	3.798879	-0.334805	5.542006
H	5.282191	-9.594615	4.106069	H	3.035276	-1.927393	5.449006
H	6.894926	-8.050227	5.268440	H	2.301144	-0.548169	4.602435
H	5.910871	-7.082156	4.148388	H	-0.644732	-0.666680	9.450482
H	6.693928	-6.324472	5.546325	H	-2.528078	-1.802449	9.568972
H	1.432548	-6.404943	4.021346	H	-1.835007	-1.881040	6.693473
H	-0.295105	-5.151530	4.602958	H	-1.816228	-3.108875	7.927765
H	-1.046876	-7.398156	6.459630	H	-3.135500	1.025495	7.473333
H	-1.873066	-5.861186	6.489735	H	-6.026013	1.089910	8.111099

H	-4.181210	3.315702	9.094130	C	-2.526495	2.310715	1.706777
H	-5.043818	0.981507	10.312301	N	0.984184	-0.451547	1.625504
H	-6.097393	3.948562	10.515813	C	2.452974	-0.390433	1.707004
H	-6.539095	4.022698	8.807634	C	3.056989	0.865894	1.045179
H	-7.067511	2.645570	9.800589	O	2.538580	1.386588	0.056956
H	-7.090113	2.912913	6.867042	C	3.048314	-1.669017	1.071561
H	-5.315375	4.292701	4.879025	C	3.731833	-2.598550	2.085839
H	-7.641524	2.462267	4.201805	C	5.130546	-2.102372	2.482318
H	-7.089116	3.731676	3.110005	O	5.229463	-0.929450	2.911130
H	-8.558041	4.191135	6.405099	O	6.089370	-2.894562	2.338090
H	-8.734125	7.025019	6.508114	N	4.204894	1.318294	1.556464
H	-9.207603	6.958241	4.129059	C	5.054749	2.361767	0.965423
H	-10.315366	8.604799	5.643451	C	4.495735	3.792773	0.874467
H	-11.759205	7.589078	5.660954	O	5.251550	4.694542	0.518664
H	-11.041002	5.844767	3.080649	N	3.215662	4.037336	1.176532
H	-11.708519	5.304086	4.625999	C	2.587373	5.368042	1.061505
H	-10.180302	4.620581	4.011607	C	3.057663	6.393917	2.116621
H	-12.066293	7.919024	3.248129	O	2.854006	7.593587	1.927514
H	-11.914065	9.481326	4.063277	C	1.053636	5.223656	1.153419
H	-10.534047	8.826766	3.155848	C	0.288006	4.872907	-0.116605
H	-10.632820	4.085343	6.331066	C	-1.058464	5.281193	-0.225011
H	-12.032888	3.020868	7.696623	C	0.855959	4.097518	-1.150672
H	-10.061881	4.243415	9.633440	C	-1.833549	4.899708	-1.337992
H	-11.110623	2.874525	9.993503	C	0.078126	3.732091	-2.268457
H	-12.993319	5.926184	7.263656	C	-1.267610	4.117791	-2.353802
H	-15.483143	5.329979	8.690018	O	-2.027918	3.698333	-3.397661
H	-14.421829	7.142356	10.036824	N	3.630202	5.944913	3.239628
H	-14.373278	8.169146	8.598853	C	3.817829	6.733820	4.472423
H	-16.831782	8.175368	8.481550	C	5.099138	6.351717	5.231889
H	-16.930767	6.990205	9.779456	O	5.747620	5.358920	4.903906
				C	2.590894	6.598713	5.414213
b. conformer 2				C	2.412036	5.219563	6.101181
N	-4.875611	1.832813	4.375896	C	1.289325	7.055886	4.736105
C	-3.439904	2.084638	4.542807	C	2.235624	3.988336	5.198726
C	-2.630587	0.987371	3.840168	N	5.434164	7.109392	6.287941
O	-2.403903	-0.065623	4.441503	C	6.546123	6.792453	7.197515
C	-3.074884	2.203792	6.036093	C	7.144479	8.021398	7.904239
S	-1.351137	2.676551	6.335008	O	8.365934	8.140723	7.944940
N	-2.192483	1.191541	2.582684	C	6.047669	5.734429	8.203906
C	-1.348695	0.239938	1.861720	C	7.146523	5.171043	9.128124
C	0.153678	0.458241	2.141021	C	7.230611	5.916581	10.464281
O	0.563449	1.419995	2.791332	C	6.847159	3.704976	9.443423
C	-1.695885	0.480906	0.390505	N	6.315496	8.922295	8.444434
C	-1.887723	1.991296	0.355372	C	6.760020	10.163441	9.106075

C	5.843258	10.546453	10.296836	C	-5.357397	6.659560	6.378476
O	4.820281	9.893378	10.538761	C	-5.850744	5.375930	5.697530
C	6.842144	11.283505	8.040980	O	-5.076099	4.688529	5.029168
C	7.747575	12.472771	8.408135	C	-5.690778	7.909225	5.536117
O	8.380180	12.439126	9.490014	O	-5.431546	9.060749	6.308946
O	7.807560	13.417575	7.590311	C	-7.146977	8.054938	5.089657
N	6.218812	11.603878	11.025916	N	-7.137070	5.060831	5.853174
C	5.557220	12.183169	12.208949	C	-7.773184	3.818652	5.407672
C	4.984425	11.120729	13.181787	C	-9.123733	4.141313	4.752498
O	5.705062	10.215724	13.611808	O	-9.922693	4.893700	5.317317
C	4.570026	13.276127	11.745197	C	-7.945956	2.880934	6.615476
C	3.994438	14.087612	12.912274	C	-6.600824	2.485933	7.232323
O	4.750715	14.874336	13.522385	O	-6.044667	1.455667	6.789340
O	2.803432	13.857185	13.226049	O	-6.093214	3.242546	8.089170
N	3.706389	11.205189	13.565944	N	-9.350557	3.632273	3.536413
C	3.043432	10.311648	14.517154	C	-10.422818	4.118033	2.639519
C	2.710562	8.918067	13.974225	C	-10.987512	3.008760	1.721006
O	1.669848	8.377036	14.342400	O	-11.310964	3.244963	0.562086
N	3.554226	8.348293	13.102258	C	-9.898450	5.383545	1.904199
C	3.310313	7.083411	12.385401	C	-11.041862	6.212220	1.274841
C	2.029316	7.155574	11.520153	C	-8.767272	5.075443	0.902913
O	1.238333	6.215260	11.449779	C	-10.625492	7.638364	0.891085
C	3.347820	5.915481	13.398096	N	-11.044272	1.776246	2.239729
C	3.855816	4.584195	12.870201	C	-11.073593	0.503694	1.479975
C	5.206936	4.230414	13.053910	C	-9.802852	0.260792	0.617326
C	2.981636	3.673880	12.246128	O	-9.701563	-0.738933	-0.095082
C	5.679380	2.978685	12.619508	C	-12.416066	0.281545	0.741850
C	3.455828	2.427771	11.798551	C	-13.630207	0.115929	1.673807
C	4.803703	2.077517	11.988499	O	-13.463621	-0.442204	2.785019
N	1.773907	8.329405	10.931769	O	-14.750633	0.489861	1.250170
C	0.495114	8.671109	10.292937	N	-8.793014	1.123441	0.797276
C	0.161943	7.831955	9.044525	C	-7.365098	0.986560	0.454817
O	1.028095	7.496951	8.241876	C	-6.520071	1.378419	1.679135
C	0.404212	10.192786	10.009402	O	-6.959745	2.248432	2.474226
C	1.679808	10.905068	9.496279	C	-7.028591	1.837331	-0.792924
C	-0.025615	10.903954	11.304965	C	-5.591649	1.630287	-1.309836
C	2.311321	10.323780	8.226921	C	-5.284574	2.427087	-2.594157
N	-1.129946	7.537993	8.857149	O	-4.459018	3.373569	-2.528523
C	-1.692773	6.917587	7.652225	O	-5.815770	2.064423	-3.669286
C	-3.200857	7.223841	7.522401	O	-5.460112	0.756309	1.909091
O	-3.735170	8.068496	8.243975	H	-5.098828	1.544831	3.428634
C	-1.416150	5.403925	7.656040	H	-5.387311	2.681169	4.570006
S	-1.344532	4.677896	5.992853	H	-5.192648	1.129568	5.032004
N	-3.899319	6.573878	6.588843	H	-3.215071	3.039468	4.073280

H	-3.257831	1.242402	6.520576	H	6.265847	5.886368	10.968754
H	-3.726242	2.935659	6.518576	H	7.512172	6.955771	10.302426
H	-1.611689	-0.784049	2.127479	H	7.592182	3.308787	10.130955
H	-0.909790	0.156997	-0.292376	H	6.873722	3.122915	8.521717
H	-2.640427	-0.010973	0.150117	H	5.853821	3.622742	9.884295
H	-0.910656	2.465391	0.295600	H	5.328000	8.727619	8.481523
H	-2.522687	2.295089	-0.475963	H	7.762631	10.007331	9.508020
H	-2.122536	3.247480	2.092320	H	7.235518	10.858099	7.115534
H	-3.606850	2.388051	1.586955	H	5.834335	11.647434	7.832104
H	0.582000	-1.185563	1.070049	H	7.073661	12.065873	10.712164
H	2.731389	-0.354296	2.762076	H	6.328237	12.703672	12.777545
H	2.253716	-2.234555	0.580303	H	5.090768	13.961698	11.073958
H	3.770625	-1.406495	0.296624	H	3.757818	12.813104	11.181608
H	3.101448	-2.699494	2.972535	H	3.180717	12.022696	13.259144
H	3.815977	-3.588381	1.629779	H	3.691309	10.185774	15.383849
H	4.622441	0.745096	2.292936	H	2.116168	10.780206	14.845658
H	5.977956	2.410001	1.542297	H	4.390200	8.876756	12.865227
H	5.310355	2.052234	-0.047272	H	4.140534	6.950688	11.691986
H	2.619984	3.240551	1.369963	H	3.996331	6.197354	14.229201
H	2.833630	5.794940	0.088833	H	2.352280	5.774061	13.821359
H	0.808872	4.485128	1.919075	H	5.884720	4.925931	13.527484
H	0.649339	6.175891	1.499518	H	1.941588	3.931638	12.104562
H	-1.515857	5.852864	0.569385	H	6.719373	2.719377	12.750625
H	1.871157	3.737111	-1.076116	H	2.781642	1.745103	11.300438
H	-2.880407	5.163507	-1.401211	H	5.168233	1.124749	11.632148
H	0.492623	3.108956	-3.043953	H	2.491667	9.041552	10.977684
H	-2.976735	3.612381	-3.125457	H	-0.282704	8.427433	11.017195
H	3.851666	4.962021	3.291273	H	-0.387575	10.354833	9.275769
H	3.913277	7.784728	4.198048	H	2.433228	10.913814	10.283397
H	2.754181	7.312387	6.222595	H	1.424665	11.944647	9.286192
H	1.540386	5.279420	6.751375	H	-0.134856	11.974344	11.125811
H	3.266065	5.036154	6.752650	H	0.725707	10.756249	12.082921
H	0.510389	7.147508	5.487269	H	-0.980496	10.510012	11.652566
H	0.967219	6.340002	3.982740	H	1.555261	10.209358	7.449694
H	1.437131	8.029342	4.267875	H	3.089320	11.000282	7.872049
H	1.431077	4.145596	4.481384	H	2.772692	9.361244	8.443826
H	3.162777	3.766708	4.671709	H	-1.794917	7.855720	9.545607
H	1.984030	3.126671	5.817434	H	-1.199177	7.352981	6.785335
H	4.868146	7.917572	6.491566	H	-0.451808	5.216965	8.131626
H	7.352623	6.348480	6.610621	H	-2.181324	4.893858	8.243898
H	5.232671	6.143454	8.803372	H	-3.418586	5.872763	6.038452
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H	-7.283059	9.025934	4.613546	C	-0.373619	1.191999	2.782847
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H	-7.396842	7.284315	4.360290	O	-1.230081	-0.346917	1.117504
H	-7.722001	5.671720	6.400482	C	0.076444	0.371408	4.014149
H	-7.149728	3.323645	4.667156	C	1.452433	0.767152	4.570834
H	-8.561828	3.370619	7.372519	C	2.604744	0.360190	3.645960
H	-8.467815	1.979703	6.288576	O	2.804738	1.072798	2.636339
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H	-11.258143	4.425681	3.268016	N	0.846870	0.443538	0.779171
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H	-11.857507	6.285736	1.995038	C	0.798165	0.757530	-1.734779
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H	-8.312484	5.996130	0.543502	N	0.508542	2.041260	-1.494949
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H	-9.883742	7.615161	0.093120	O	1.907098	4.414256	-1.620148
H	-11.500006	8.184736	0.537594	C	-1.373710	3.396108	-2.318113
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H	-10.841749	1.692986	3.221854	C	-3.084922	2.357311	-3.880090
H	-11.023948	-0.287561	2.227758	C	-2.575088	1.217887	-1.792189
H	-12.597021	1.098266	0.042979	C	-4.005804	1.341508	-4.204186
H	-12.338537	-0.633416	0.153027	C	-3.482997	0.196338	-2.126189
H	-8.990605	1.908676	1.393787	C	-4.198240	0.262471	-3.330539
H	-7.142848	-0.055918	0.233669	O	-5.087009	-0.716748	-3.643417
H	-7.722818	1.568636	-1.590526	N	0.755450	5.239470	-3.361042
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H	-4.891072	1.929443	-0.528559	C	0.367477	7.631583	-3.774952
H	-5.435422	0.566257	-1.504733	O	-0.763411	7.302282	-4.124364
c. conformer 3				C	2.546409	6.558263	-4.530514
N	-6.474344	5.944190	0.081391	C	2.091612	6.512590	-6.011283
C	-5.606843	4.818980	-0.288352	C	3.608424	5.482357	-4.242121
C	-4.789014	4.370141	0.929821	C	1.277090	5.290322	-6.459292
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C	-4.689360	5.185823	-1.464923	C	-0.090855	10.074884	-3.925186
S	-5.531758	5.345627	-3.062456	C	0.565009	10.942386	-5.016516
N	-4.694543	3.056100	1.221233	O	1.792700	11.053618	-5.037996
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				O	-1.681349	13.769918	-6.636364

C	0.390935	11.424382	-8.257649	O	-8.394342	6.512296	-1.986592
C	1.374596	11.900662	-9.342090	C	-9.069862	6.664244	-4.794328
O	1.902988	13.031560	-9.226910	O	-9.158310	7.041783	-6.146117
O	1.602646	11.118464	-10.292282	C	-10.469800	6.147033	-4.450473
N	-0.324143	14.412669	-8.312025	N	-9.263594	8.561283	-1.683393
C	-0.945948	15.706062	-8.666565	C	-8.953591	8.667212	-0.252414
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C	-2.789448	16.779335	-10.075114	C	-6.641579	9.454476	-0.946913
O	-2.187446	17.461536	-10.934182	O	-5.887822	8.508347	-0.627290
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C	-1.202967	14.783043	-3.489747	C	-14.251806	8.089944	2.664671
C	-2.381146	13.900166	-3.035880	C	-13.430180	7.021154	0.500099
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C	-0.408314	15.464150	-2.363183	N	-11.449178	5.442359	2.384010
C	0.480442	14.510857	-1.583833	C	-10.997344	4.131433	2.877169
C	1.723654	14.119846	-2.117391	C	-11.956705	3.373687	3.836653
C	0.064031	13.994421	-0.342578	O	-11.570401	2.343931	4.392786
C	2.549213	13.226897	-1.410467	C	-9.525072	4.233779	3.338051
C	0.887624	13.099348	0.364317	C	-8.582303	4.715988	2.218191
C	2.131846	12.717378	-0.167991	O	-8.652602	5.895240	1.797691
N	-3.010526	13.232318	-4.007926	O	-7.739244	3.931675	1.725066
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C	-4.032854	11.029257	-4.592326	C	-14.406303	3.062465	4.420813
O	-3.126508	10.870799	-5.411225	C	-15.604340	3.277443	3.471355
C	-5.475977	13.100459	-4.265046	O	-15.744328	4.410919	2.949630
C	-5.390959	13.613724	-5.723541	C	-14.726030	3.450724	5.887509
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C	-4.927777	8.725999	-4.906479	O	-15.569054	1.973555	8.838216
C	-6.342290	8.140895	-5.101246	O	-16.313842	2.281196	3.198237
O	-6.597697	7.519097	-6.132459	H	-7.079380	6.183468	-0.692170
C	-4.077911	7.836158	-3.989579	H	-7.060602	5.688354	0.870971
S	-4.080628	6.049327	-4.306522	H	-5.926810	6.766499	0.306369
N	-7.251959	8.380349	-4.145803	H	-6.264217	4.011647	-0.600885
C	-8.637658	7.879578	-3.944327	H	-4.178333	6.125279	-1.239479
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H	-4.102712	3.164763	3.243849	H	-0.382276	9.169928	0.395269
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H	-4.038143	0.275926	0.769398	H	-1.235975	11.440115	-5.806855
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H	-0.642989	0.516229	4.822822	H	-1.802896	14.914132	-10.482923
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H	1.578716	0.282868	5.542479	H	-2.472328	18.392765	-5.746586
H	1.642404	0.902036	1.228808	H	-4.005106	17.513601	-5.786930
H	2.102474	-0.493642	-0.593910	H	-1.164652	15.608050	-5.440257
H	0.426201	-1.046304	-0.643188	H	-0.510903	14.095771	-3.977361
H	0.496169	2.342369	-0.531036	H	0.233221	16.230320	-2.801131
H	0.230964	2.608679	-3.500564	H	-1.098854	15.968181	-1.685452
H	-1.537431	3.703786	-1.286024	H	2.035570	14.491246	-3.083857
H	-1.615412	4.260144	-2.937172	H	-0.905435	14.265551	0.053147
H	-2.944014	3.190759	-4.554883	H	3.490900	12.914173	-1.838118
H	-2.036812	1.172143	-0.855211	H	0.549364	12.688005	1.304418
H	-4.572050	1.389010	-5.121186	H	2.755058	12.014809	0.365962
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H	-5.194892	-1.323168	-2.911202	H	-4.288261	12.102207	-2.777927
H	-0.049570	5.112195	-3.957809	H	-6.302831	12.390846	-4.204476
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H	3.193003	4.483139	-4.367631	H	-6.988410	15.080770	-5.721995
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H	1.125612	5.340622	-7.537759	H	-4.453567	8.756154	-5.888693
H	1.722250	9.099691	-3.469561	H	-3.051569	8.184095	-4.084708
H	-1.077180	9.764876	-4.273797	H	-4.386152	7.996903	-2.954120
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H	-0.844401	11.771417	-2.895404	H	-9.322447	8.689893	-4.187738
H	-1.117457	11.145359	-0.704848	H	-8.347581	5.854366	-4.684333
H	-2.646928	9.282497	-0.677082	H	-8.234102	7.240699	-6.393264
H	-1.972321	8.644572	-2.185424	H	-10.743081	5.356390	-5.148960
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H	-9.570333	9.413338	-2.124831	C	9.088233	1.615074	1.462098
H	-8.532278	7.727747	0.098493	C	9.005519	3.148539	1.480541
H	-8.269148	10.720703	-0.314698	C	9.510940	3.779038	0.179466
H	-7.555527	9.754173	0.984332	O	8.723484	3.786694	-0.793673
H	-9.994908	7.104220	1.378302	O	10.681973	4.217657	0.158793
H	-11.613232	8.675800	3.007485	N	8.851133	1.210231	-1.789925
H	-13.112632	9.036819	1.127099	C	9.498995	0.870561	-3.061654
H	-13.963153	8.780990	3.457726	C	8.583859	0.235484	-4.118370
H	-14.372444	7.099733	3.108171	O	9.002637	0.094995	-5.265838
H	-14.293014	7.342573	-0.080651	N	7.337616	-0.113158	-3.778056
H	-13.660951	6.050463	0.944238	C	6.345285	-0.786272	-4.643008
H	-12.583272	6.925905	-0.178104	C	5.738699	0.080045	-5.781455
H	-16.002455	7.806773	1.417136	O	4.607715	-0.147084	-6.204389
H	-16.315603	8.636423	2.947190	C	5.288241	-1.445617	-3.734496
H	-15.512866	9.509238	1.624203	C	5.652116	-2.863740	-3.332911
H	-11.417411	5.570878	1.387712	C	4.952202	-3.946649	-3.899766
H	-10.974814	3.486270	1.999860	C	6.703445	-3.111879	-2.427616
H	-9.454589	4.916261	4.186366	C	5.276169	-5.264746	-3.529771
H	-9.188141	3.251371	3.672445	C	7.031190	-4.435501	-2.073592
H	-13.454877	4.668916	3.452521	C	6.295358	-5.506821	-2.598541
H	-14.190756	1.996665	4.396473	O	6.534229	-6.774338	-2.174920
H	-13.819080	3.322883	6.480659	N	6.517395	1.037973	-6.298894
H	-15.014656	4.502107	5.929779	C	6.317559	2.001709	-7.408219
H	-16.784585	2.797037	6.015355	C	5.023417	2.837030	-7.506519
H	-15.602772	1.536941	6.357960	O	5.125916	3.975440	-7.954568
d. conformer 4				C	6.693614	1.410689	-8.790660
N	2.120854	-4.365478	1.105679	C	5.760639	0.290352	-9.316985
C	2.727923	-3.390137	0.184250	C	8.184579	1.025272	-8.832880
C	3.740784	-2.516255	0.936196	C	6.167452	-1.162712	-9.023724
O	3.395244	-1.408650	1.350612	N	3.860540	2.344484	-7.070311
C	1.644822	-2.593007	-0.570501	C	2.549087	3.003484	-7.160081
S	2.242032	-1.392974	-1.794963	C	2.236619	3.532227	-8.579481
N	4.985843	-2.996451	1.133816	O	2.056720	4.728749	-8.801997
C	6.119775	-2.194351	1.601355	C	2.370495	4.045204	-6.033579
C	6.442043	-0.938345	0.768517	C	2.337901	3.551625	-4.570548
O	5.941541	-0.730127	-0.335048	C	1.290437	2.461637	-4.334253
C	7.323143	-3.147170	1.588926	C	3.681163	3.044559	-4.038020
C	6.704976	-4.530360	1.753212	N	2.201451	2.609508	-9.543412
C	5.372676	-4.399341	1.025936	C	1.923802	2.866391	-10.968115
N	7.378188	-0.135332	1.281945	C	0.402997	2.970288	-11.271410
C	8.062418	0.928744	0.529136	O	-0.432962	2.804860	-10.376995
C	8.738345	0.381203	-0.750072	C	2.614268	1.747713	-11.784532
				C	2.986457	2.114494	-13.231823

O	2.557975	3.187146	-13.716665	O	-0.485979	-6.667559	-7.254610
O	3.718878	1.309780	-13.850474	C	-2.672198	-7.176221	-6.461426
N	0.043704	3.223304	-12.536447	N	-0.116252	-6.174924	-3.079706
C	-1.321110	3.395177	-13.075218	C	0.780726	-6.839150	-2.126754
C	-2.222129	4.283534	-12.184139	C	0.333931	-6.475681	-0.693312
O	-1.990381	5.489903	-12.081849	O	-0.183428	-5.375017	-0.485154
C	-1.904268	2.012319	-13.435079	C	2.196971	-6.339449	-2.453684
C	-3.301543	2.096912	-14.060922	C	3.272983	-6.873525	-1.515127
O	-3.401648	2.510609	-15.237396	O	4.070230	-7.732249	-1.951506
O	-4.268296	1.768065	-13.334533	O	3.328169	-6.346774	-0.386286
N	-3.227622	3.721588	-11.504135	N	0.508318	-7.360148	0.294277
C	-4.100565	4.419377	-10.553420	C	-0.115386	-7.262256	1.631400
C	-3.444974	4.811577	-9.219763	C	0.836117	-7.743087	2.741226
O	-4.167908	5.039098	-8.250880	O	1.808622	-8.440951	2.463392
N	-2.110642	4.874106	-9.161976	C	-1.466462	-8.023053	1.622296
C	-1.278379	5.017427	-7.962733	C	-2.359468	-7.635319	2.822755
C	-1.443880	3.841730	-6.980802	C	-1.271318	-9.549002	1.535084
O	-1.823068	4.020771	-5.821182	C	-3.821464	-8.073170	2.669909
C	-1.430307	6.422953	-7.352455	N	0.559297	-7.343822	3.984443
C	-0.307547	6.812575	-6.407149	C	1.544659	-7.278001	5.075350
C	0.939400	7.209534	-6.926137	C	1.133801	-8.066683	6.345912
C	-0.490640	6.748875	-5.012716	O	1.921494	-8.148759	7.289222
C	1.995689	7.539297	-6.058168	C	1.804302	-5.790269	5.404276
C	0.565164	7.078824	-4.143253	C	1.994304	-4.908255	4.160279
C	1.809359	7.473883	-4.666145	O	3.139508	-4.716499	3.692134
N	-1.209746	2.613609	-7.465907	O	0.979735	-4.432874	3.594424
C	-1.587838	1.368850	-6.769755	N	-0.068823	-8.661736	6.354538
C	-0.496698	0.282371	-6.729513	C	-0.637588	-9.579334	7.368942
O	0.482762	0.295712	-7.470141	C	-1.577009	-10.593169	6.683275
C	-2.925241	0.813415	-7.334391	O	-2.259926	-10.185403	5.711299
C	-3.055456	0.758905	-8.875582	C	-1.351816	-8.780473	8.489529
C	-4.102167	1.631607	-6.777722	C	-1.828645	-9.655522	9.668415
C	-2.043108	-0.153089	-9.575967	C	-2.338909	-8.843292	10.879505
N	-0.703505	-0.695782	-5.844987	O	-3.442939	-8.251650	10.792936
C	0.081466	-1.922514	-5.695767	O	-1.657137	-8.858952	11.935465
C	-0.849862	-3.098019	-5.330061	O	-1.540004	-11.781367	7.078117
O	-2.024765	-2.896865	-5.019734	H	1.346580	-4.839420	0.664526
C	1.183574	-1.711048	-4.640618	H	2.805933	-5.067079	1.361773
S	0.639487	-1.084811	-3.023233	H	1.803397	-3.933614	1.968639
N	-0.342718	-4.334940	-5.367407	H	3.282585	-3.938921	-0.574242
C	-1.143446	-5.563729	-5.189731	H	1.003995	-3.298437	-1.097746
C	-0.397367	-6.581502	-4.315324	H	1.028320	-2.056115	0.152883
O	-0.011350	-7.661135	-4.760117	H	5.915722	-1.891379	2.628620
C	-1.578134	-6.113468	-6.561934	H	7.829079	-3.095751	0.623003

H	8.023563	-2.922849	2.393765	H	3.921755	2.074465	-4.467684
H	7.327638	-5.311649	1.316361	H	2.291072	1.647356	-9.260640
H	6.521819	-4.727294	2.810809	H	2.381349	3.818495	-11.242269
H	5.485136	-4.673498	-0.020704	H	3.543702	1.475347	-11.280060
H	4.648993	-5.059085	1.503541	H	1.975116	0.862858	-11.788782
H	7.760961	-0.382484	2.176852	H	0.816088	3.335844	-13.194153
H	7.314550	1.662022	0.220399	H	-1.228375	3.936087	-14.017141
H	10.100714	1.308707	1.194491	H	-1.233780	1.519465	-14.141574
H	8.918166	1.281367	2.487947	H	-1.947290	1.395516	-12.535214
H	7.972276	3.450203	1.668830	H	-3.451392	2.756561	-11.730710
H	9.607217	3.512671	2.317188	H	-4.463396	5.331855	-11.024948
H	8.598944	2.189260	-1.636584	H	-4.955386	3.780923	-10.334552
H	9.917579	1.782954	-3.485515	H	-1.618179	4.664005	-10.023791
H	10.319157	0.178495	-2.870965	H	-0.253986	4.952421	-8.316253
H	7.076977	0.021024	-2.809248	H	-1.448981	7.152931	-8.162936
H	6.865944	-1.592856	-5.160912	H	-2.386171	6.490130	-6.831663
H	5.136203	-0.839951	-2.840829	H	1.100440	7.216637	-7.996014
H	4.324280	-1.489085	-4.237801	H	-1.435935	6.410244	-4.612526
H	4.161813	-3.766944	-4.613294	H	2.960623	7.802919	-6.467037
H	7.250256	-2.287606	-1.989239	H	0.427168	6.999250	-3.075134
H	4.736265	-6.101960	-3.944907	H	2.630225	7.698944	-4.000747
H	7.817002	-4.634640	-1.362919	H	-0.886004	2.540620	-8.428905
H	5.679499	-7.252142	-2.072727	H	-1.763513	1.613036	-5.722005
H	7.453022	1.039879	-5.913747	H	-3.061414	-0.202334	-6.960407
H	7.070454	2.767838	-7.223772	H	-2.970339	1.761838	-9.293942
H	6.585105	2.234164	-9.499551	H	-4.050621	0.386751	-9.122114
H	5.707553	0.388325	-10.402266	H	-5.047219	1.188923	-7.090878
H	4.750921	0.452572	-8.940819	H	-4.054716	2.657072	-7.143649
H	8.445787	0.690420	-9.836659	H	-4.064527	1.649050	-5.688506
H	8.398199	0.228938	-8.118857	H	-2.035660	-1.136998	-9.106416
H	8.795077	1.892981	-8.583317	H	-2.323002	-0.260165	-10.624165
H	7.075486	-1.415331	-9.571119	H	-1.047704	0.284755	-9.533606
H	6.337757	-1.315277	-7.961013	H	-1.536487	-0.643764	-5.277882
H	5.369594	-1.829486	-9.351471	H	0.559242	-2.159361	-6.647989
H	3.873387	1.395865	-6.717280	H	1.710629	-2.651771	-4.483717
H	1.800717	2.236731	-6.989200	H	1.907036	-0.999202	-5.044188
H	3.145836	4.805512	-6.131021	H	0.618192	-4.450155	-5.652980
H	1.416535	4.539547	-6.207942	H	-2.053597	-5.306233	-4.648005
H	2.060406	4.408419	-3.956180	H	-1.975871	-5.287385	-7.152968
H	1.228674	2.238159	-3.269709	H	-0.084180	-7.301081	-6.639106
H	1.561187	1.552864	-4.870113	H	-3.541222	-6.757535	-5.954477
H	0.318277	2.813775	-4.677006	H	-2.316248	-8.046198	-5.910277
H	3.624443	2.936179	-2.955182	H	-2.963388	-7.484471	-7.465383
H	4.466366	3.759146	-4.282942	H	-0.496075	-5.291956	-2.767351

H	0.741700	-7.922568	-2.251583	C	6.570274	-1.167733	-0.372725
H	2.441879	-6.630740	-3.476807	C	5.857343	-1.198023	0.989198
H	2.209401	-5.248030	-2.411473	O	4.748268	-1.779043	1.053010
H	1.118609	-8.153562	0.144789	O	6.420879	-0.635526	1.954921
H	-0.325886	-6.212397	1.839044	N	4.967599	-3.152370	-3.288949
H	-1.997575	-7.708799	0.721771	C	5.609856	-4.216712	-4.083508
H	-2.347100	-6.550539	2.936526	C	4.843819	-5.536840	-4.240338
H	-1.968730	-8.080840	3.737992	O	5.472501	-6.571500	-4.442272
H	-2.225142	-10.041705	1.354984	N	3.516417	-5.508676	-4.117856
H	-0.859231	-9.927599	2.473693	C	2.582322	-6.628908	-4.328479
H	-0.590784	-9.801269	0.723066	C	1.185380	-6.027826	-4.580740
H	-3.893430	-9.160585	2.670400	O	0.948516	-4.893821	-4.161261
H	-4.398818	-7.689724	3.511606	C	2.618231	-7.533535	-3.078355
H	-4.236174	-7.676454	1.743011	C	1.603985	-8.665641	-2.984886
H	-0.263086	-6.775599	4.112201	C	0.935384	-8.891218	-1.764286
H	2.485103	-7.709248	4.730368	C	1.335176	-9.508230	-4.084059
H	0.955069	-5.404533	5.971725	C	-0.023005	-9.917469	-1.660347
H	2.689788	-5.714771	6.037550	C	0.360173	-10.522520	-3.978393
H	-0.628558	-8.603678	5.515451	C	-0.323202	-10.720247	-2.769519
H	0.165546	-10.158376	7.819121	O	-1.280509	-11.675247	-2.650121
H	-0.651987	-8.040517	8.881175	N	0.286619	-6.740144	-5.263660
H	-2.205971	-8.248510	8.067605	C	-1.007316	-6.254809	-5.778249
H	-2.628534	-10.314894	9.324144	C	-0.922749	-4.816075	-6.337674
H	-0.996570	-10.288188	9.989107	O	-1.369735	-3.837826	-5.734839
e. conformer 5				C	-2.206774	-6.602925	-4.860975
N	-0.792618	-0.860709	-4.291993	C	-2.292469	-5.932907	-3.469595
C	-1.587053	-0.898070	-3.049294	C	-2.333870	-8.131834	-4.738866
C	-0.641616	-0.833004	-1.837975	C	-1.531615	-6.572267	-2.300941
O	-0.497623	0.248327	-1.274057	N	-0.236335	-4.695942	-7.478766
C	-2.607072	-2.052515	-3.043344	C	0.405406	-3.471814	-7.989032
S	-4.232381	-1.660240	-3.725193	C	-0.518424	-2.326616	-8.454428
N	0.057533	-1.911137	-1.416550	O	-0.020468	-1.226726	-8.695555
C	1.376246	-1.779348	-0.794659	C	1.384953	-3.873092	-9.119319
C	2.438731	-1.470245	-1.871745	C	2.845205	-4.127110	-8.695679
O	2.126493	-1.366877	-3.060283	C	3.545822	-2.838044	-8.253468
C	1.615162	-3.123370	-0.101485	C	2.990073	-5.150553	-7.573527
C	0.975016	-4.105405	-1.074400	N	-1.830452	-2.535709	-8.583184
C	-0.214874	-3.323785	-1.644259	C	-2.788756	-1.428347	-8.750656
N	3.699139	-1.335888	-1.464848	C	-2.809301	-0.503663	-7.513728
C	4.818466	-0.863207	-2.293583	O	-2.593413	-0.948142	-6.389385
C	5.451778	-1.903167	-3.248115	C	-4.187387	-1.985916	-9.072717
O	6.405103	-1.570371	-3.953189	C	-5.295011	-0.953461	-8.828470
C	5.889993	-0.222079	-1.383065	O	-5.303618	0.062940	-9.558167
				O	-6.057463	-1.098886	-7.844656

N	-3.126605	0.777492	-7.714091	N	-2.673441	-9.272782	-8.401913
C	-3.267231	1.788240	-6.650703	C	-1.579028	-9.476362	-9.377467
C	-4.581957	2.593421	-6.773732	C	-1.825868	-10.707425	-10.271702
O	-4.793546	3.590277	-6.086898	O	-1.689039	-10.613886	-11.492753
C	-2.001586	2.668281	-6.593227	C	-0.220309	-9.638516	-8.661261
C	-1.509795	2.868656	-5.154460	C	0.433445	-8.340825	-8.166822
O	-1.153168	1.841604	-4.525446	O	1.263702	-8.430314	-7.233453
O	-1.449824	4.032098	-4.700508	O	0.144787	-7.245691	-8.702282
N	-5.516696	2.127439	-7.613100	N	-2.210553	-11.844917	-9.676523
C	-6.939730	2.471841	-7.543640	C	-2.646199	-13.087793	-10.353342
C	-7.694402	1.710334	-6.442365	C	-3.223714	-14.079098	-9.332765
O	-8.884620	1.951958	-6.243593	O	-4.341694	-14.551142	-9.505487
N	-7.003530	0.821384	-5.717616	C	-1.514700	-13.737036	-11.200137
C	-7.520868	-0.035041	-4.644284	C	-2.042531	-15.003986	-11.912500
C	-8.645188	-0.980675	-5.101680	C	-0.220911	-14.035875	-10.413198
O	-9.613702	-1.247460	-4.389168	C	-1.097931	-15.555000	-12.988337
C	-7.749361	0.767019	-3.348238	N	-2.480195	-14.294312	-8.244757
C	-6.439936	1.184976	-2.692137	C	-2.908325	-14.886959	-6.970357
C	-5.694696	2.259712	-3.213689	C	-3.494957	-16.328914	-7.005229
C	-5.913010	0.437443	-1.619378	O	-4.089953	-16.770761	-6.019931
C	-4.417987	2.555466	-2.704264	C	-3.723122	-13.826696	-6.200345
C	-4.644475	0.747799	-1.091980	C	-2.890886	-12.550927	-5.967722
C	-3.890778	1.798700	-1.644711	O	-2.885638	-11.653119	-6.847210
N	-8.432185	-1.559380	-6.286096	O	-2.208020	-12.478918	-4.919842
C	-9.156525	-2.703480	-6.866509	N	-3.218467	-17.094884	-8.073843
C	-8.167934	-3.856861	-7.152205	C	-3.291046	-18.576130	-8.168978
O	-8.314742	-4.614734	-8.108083	C	-2.050611	-19.134286	-8.900392
C	-9.958985	-2.256952	-8.113228	O	-1.609043	-18.495691	-9.886650
C	-9.063329	-1.605197	-9.195283	C	-4.621707	-19.034469	-8.822490
C	-11.095737	-1.310176	-7.681493	C	-4.821317	-20.567130	-8.794427
C	-9.782361	-1.352210	-10.525878	C	-6.216917	-21.037774	-9.264751
N	-7.111984	-3.922354	-6.338779	O	-6.452154	-21.111298	-10.496563
C	-5.825576	-4.526826	-6.658078	O	-7.042943	-21.417169	-8.396100
C	-5.732344	-6.052560	-6.454216	O	-1.501895	-20.152907	-8.417190
O	-6.233128	-6.620425	-5.484818	H	-1.389164	-1.079495	-5.080633
C	-4.766668	-3.744628	-5.857557	H	-0.455762	0.088616	-4.425650
S	-5.102336	-3.470922	-4.091216	H	-0.019613	-1.509933	-4.258053
N	-5.049744	-6.713926	-7.393188	H	-2.166125	0.026080	-3.025806
C	-4.709954	-8.152773	-7.471319	H	-2.203320	-2.875280	-3.624220
C	-3.564746	-8.277535	-8.497177	H	-2.770195	-2.390559	-2.020784
O	-3.509087	-7.438276	-9.398765	H	1.387638	-0.981530	-0.050868
C	-5.932640	-8.964044	-7.948263	H	2.672015	-3.339709	0.058275
O	-7.025074	-8.768701	-7.073970	H	1.077813	-3.144079	0.847772
C	-5.712060	-10.474607	-7.989101	H	1.692406	-4.331748	-1.861110

H	0.657168	-5.020900	-0.575078	H	-2.473791	-0.819316	-9.598674
H	-0.327372	-3.530226	-2.704578	H	-4.211122	-2.302402	-10.116646
H	-1.118996	-3.609309	-1.106446	H	-4.365753	-2.864455	-8.463422
H	3.896208	-1.483952	-0.472295	H	-3.381343	1.043659	-8.655378
H	4.435697	-0.073455	-2.941022	H	-3.344590	1.260713	-5.698660
H	6.665859	0.199769	-2.023287	H	-1.193821	2.188767	-7.150269
H	5.444953	0.615445	-0.843260	H	-2.196859	3.631306	-7.068828
H	6.632500	-2.176797	-0.786166	H	-5.289009	1.317767	-8.190162
H	7.595767	-0.819064	-0.226151	H	-7.049538	3.540468	-7.362154
H	4.190971	-3.375070	-2.685983	H	-7.400862	2.222004	-8.498479
H	5.785069	-3.832524	-5.088739	H	-6.063696	0.629317	-6.037121
H	6.579469	-4.443850	-3.640827	H	-6.710649	-0.722092	-4.412623
H	3.071961	-4.609052	-3.997949	H	-8.355179	1.648907	-3.558935
H	2.876232	-7.205621	-5.208167	H	-8.302616	0.148640	-2.641048
H	3.610080	-7.981046	-3.009152	H	-6.081734	2.836381	-4.040645
H	2.492762	-6.893765	-2.203648	H	-6.466068	-0.402518	-1.225948
H	1.141534	-8.263896	-0.910683	H	-3.825866	3.345866	-3.152460
H	1.851202	-9.368367	-5.024990	H	-4.232312	0.158910	-0.286129
H	-0.558592	-10.085423	-0.740544	H	-2.896459	2.016414	-1.275934
H	0.112638	-11.137147	-4.834348	H	-7.606398	-1.251511	-6.806063
H	-1.601734	-11.988030	-3.534318	H	-9.860326	-3.085236	-6.127292
H	0.616657	-7.612462	-5.676697	H	-10.424363	-3.145529	-8.543039
H	-1.193695	-6.851917	-6.669030	H	-8.215135	-2.258789	-9.399862
H	-3.087750	-6.270535	-5.405311	H	-8.670855	-0.655501	-8.828712
H	-3.344723	-5.903037	-3.184680	H	-11.775302	-1.132027	-8.512473
H	-1.954453	-4.910872	-3.558062	H	-10.681589	-0.358477	-7.343004
H	-2.305165	-8.602005	-5.720288	H	-11.656881	-1.758636	-6.861639
H	-3.269292	-8.396574	-4.245616	H	-10.562920	-0.602569	-10.400652
H	-1.502999	-8.539234	-4.168134	H	-9.061178	-0.984859	-11.256492
H	-1.910555	-7.573883	-2.099669	H	-10.218796	-2.281124	-10.894019
H	-0.469238	-6.616982	-2.521843	H	-7.106996	-3.284517	-5.561467
H	-1.678781	-5.969024	-1.405953	H	-5.644696	-4.350424	-7.717054
H	0.032129	-5.575483	-7.929254	H	-3.795519	-4.218627	-5.972270
H	0.976005	-3.045615	-7.165716	H	-4.688665	-2.753758	-6.305161
H	1.008643	-4.767919	-9.618965	H	-4.693216	-6.176309	-8.173225
H	1.402908	-3.088385	-9.876165	H	-4.386905	-8.532297	-6.504483
H	3.378944	-4.506907	-9.567531	H	-6.219446	-8.622178	-8.943586
H	4.599708	-3.040449	-8.067269	H	-6.773799	-8.076394	-6.441325
H	3.093915	-2.450454	-7.340912	H	-6.637903	-10.971770	-8.276898
H	3.458504	-2.087141	-9.037823	H	-4.945594	-10.731912	-8.718681
H	4.041395	-5.373175	-7.399204	H	-5.408201	-10.832837	-7.005349
H	2.479891	-6.073809	-7.855840	H	-2.784745	-9.982284	-7.673064
H	2.542730	-4.764767	-6.661341	H	-1.501738	-8.616976	-10.045304
H	-2.179590	-3.445530	-8.330610	H	-0.339630	-10.327240	-7.822322

H 0.481145 -10.097681 -9.360229
H -2.359912 -11.797776 -8.667253
H -3.459301 -12.826855 -11.030401
H -1.250795 -13.027479 -11.983529
H -2.991928 -14.764171 -12.393199
H -2.225760 -15.793016 -11.180643
H 0.587320 -14.262327 -11.106114
H -0.363876 -14.896440 -9.757898
H 0.075621 -13.168739 -9.823571
H -0.181009 -15.927517 -12.532060
H -1.587417 -16.381761 -13.503616
H -0.859653 -14.774300 -13.711016
H -1.592667 -13.820794 -8.229433
H -1.994400 -15.014133 -6.390698
H -4.629327 -13.580809 -6.756836
H -4.020188 -14.231556 -5.231656
H -2.755510 -16.653863 -8.854993
H -3.255628 -18.991768 -7.164526
H -5.448044 -18.574168 -8.278562
H -4.657562 -18.686058 -9.855807
H -4.063416 -21.036760 -9.425480
H -4.656370 -20.918726 -7.772342

(2) (H₂O)₁₆

a. isomer 1

O 5.605716 7.786617 13.739292
H 6.481749 7.422075 13.865420
H 5.739724 8.539704 13.163849
O 7.935593 6.554295 14.294011
H 7.805768 5.629995 14.081767
H 7.995460 6.575099 15.249111
O 7.570304 6.532830 17.051538
H 6.733979 6.983479 16.934452
H 8.004933 7.012834 17.756468
O 5.165318 7.602280 16.479715
H 4.536574 6.881619 16.519222
H 5.217533 7.824524 15.550138
O 6.293655 4.094919 16.757240
H 6.847690 4.828631 17.023591
H 5.423095 4.478136 16.649990
O 3.860245 5.152803 16.135242
H 4.006349 5.214820 15.191293
H 3.270473 4.405949 16.238246
O 4.577885 5.227260 13.508824

H 5.426209 4.795825 13.611010
H 4.790498 6.156026 13.417050
O 6.913620 3.957567 14.108580
H 6.790329 3.945020 15.057724
H 6.743651 3.056922 13.832571
O 3.296957 2.755331 13.324550
H 3.019582 2.756772 14.240680
H 3.563072 3.658642 13.152955
O 2.774914 2.586322 15.992420
H 3.613663 2.202223 16.247767
H 2.162167 1.850982 15.999396
O 5.251685 1.529639 16.412553
H 5.745311 2.273828 16.757153
H 5.506248 1.478730 15.491229
O 5.676053 1.486840 13.722442
H 4.859540 1.919157 13.472159
H 5.522151 0.559702 13.540888
O 1.495985 0.148347 15.708738
H 2.307722 -0.302983 15.940291
H 0.811391 -0.338585 16.167498
O 3.926263 -0.920401 16.162814
H 4.481562 -0.201776 16.465227
H 4.260924 -1.131920 15.291324
O 4.650503 -1.072453 13.481358
H 4.766459 -1.818611 12.893110
H 3.799057 -0.707230 13.240763
O 2.295333 0.159167 13.044385
H 2.498604 1.085503 12.914711
H 1.848591 0.127639 13.890353

b. isomer 2

O 1.817420 -3.234399 -1.178169
H 2.137024 -3.877476 -0.545288
H 2.525123 -2.593623 -1.247426
O -2.218758 1.926685 -4.801665
H -2.926461 1.285909 -4.732408
H -2.538361 2.569762 -5.434546
O -0.640195 -2.080833 -4.274251
H 0.160723 -2.604048 -4.306019
H -0.351713 -1.188538 -4.466136
O -4.286168 0.458837 -1.603137
H -3.941569 -0.423889 -1.467935
H -5.003323 0.535497 -0.973816
O 3.884830 -1.766551 -4.376698

H	3.540231	-0.883825	-4.511899	H	-2.773284	1.147866	-1.452734
H	4.601985	-1.843211	-5.006018	H	-2.421697	2.209241	-0.432065
O	0.238857	0.773119	-1.705583	O	0.464353	-2.330577	-0.572183
H	-0.049625	-0.119176	-1.513698	H	0.576752	-1.577221	-1.151885
H	-0.562061	1.296334	-1.673815	H	-0.445438	-2.598806	-0.700897
O	2.884624	0.726073	-4.500523	O	3.536189	-0.592565	-2.271389
H	2.986706	1.020721	-3.595540	H	4.137436	-0.792218	-2.988936
H	1.938709	0.724245	-4.647063	H	3.490291	-1.403047	-1.764196
O	0.127002	0.529164	-4.411307	O	3.795021	0.860096	0.086692
H	-0.626297	1.052140	-4.685661	H	2.918778	1.237788	0.162713
H	0.173435	0.654058	-3.463426	H	3.821482	0.490955	-0.796069
O	-2.096125	2.098841	-2.027210	O	-2.233405	-2.627511	-0.976663
H	-2.156954	2.193235	-2.977801	H	-2.631852	-2.347156	-0.152725
H	-2.874734	1.597248	-1.785539	H	-2.813447	-3.316103	-1.301665
O	-4.178838	0.139342	-4.349242	O	0.825695	-0.074578	-2.025801
H	-3.959286	-0.790610	-4.405975	H	1.733006	-0.180834	-2.311682
H	-4.365027	0.285826	-3.421821	H	0.876894	0.527772	-1.283652
O	-3.327659	-2.495746	-4.221659	O	3.591149	-1.269623	1.711335
H	-3.559663	-3.263840	-4.743616	H	4.333441	-1.306136	2.314579
H	-2.381887	-2.403928	-4.337057	H	3.744183	-0.481623	1.189923
O	2.926321	1.188032	-1.758175	O	-4.578432	0.669954	1.102423
H	1.980549	1.096214	-1.642777	H	-5.497848	0.914921	0.998030
H	3.158325	1.956126	-1.236218	H	-4.138811	1.060303	0.347046
O	1.694787	-3.406555	-3.952624	O	3.217773	-2.713713	-0.638612
H	1.755616	-3.500949	-3.002034	H	3.423523	-2.366232	0.229235
H	2.473396	-2.904962	-4.194295	H	2.267704	-2.830118	-0.631456
O	-0.528340	-1.836879	-1.568527	O	-3.294992	-1.761235	1.340869
H	0.224959	-2.359855	-1.294174	H	-2.682061	-1.554536	2.046435
H	-0.574773	-1.961772	-2.516408	H	-3.830647	-0.973196	1.249760
O	-3.285962	-2.033787	-1.479311	O	-2.526078	1.555250	2.730034
H	-2.340047	-2.031959	-1.332771	H	-3.333789	1.298825	2.284969
H	-3.388044	-2.328435	-2.384295	H	-2.134823	0.728563	3.012416
O	3.777500	-1.447056	-1.630592	O	1.068364	1.310491	0.306400
H	3.963689	-1.593540	-2.558013	H	0.329413	1.897739	0.465537
H	3.557948	-0.517104	-1.573860	H	0.924798	0.576709	0.904049
c. isomer 3				O	-1.950416	-0.189402	-2.287340
O	-1.446780	-0.941652	3.238139	H	-1.000407	-0.114008	-2.376952
H	-0.608959	-0.973458	2.776320	H	-2.087155	-1.054643	-1.901472
H	-1.271541	-1.357832	4.082129	O	0.843973	-1.000102	1.763482
O	-1.171798	2.811447	0.771281	H	0.649800	-1.539456	0.996914
H	-1.204342	3.749924	0.956844	H	1.779512	-1.130799	1.918134
H	-1.615158	2.404156	1.515444	d. isomer 4			
O	-3.166358	1.800469	-0.873221	O	4.739299	4.700644	1.699038

H	4.893068	3.816754	2.032693	O	0.970023	1.648351	-3.547615
H	5.536872	5.182187	1.918645	H	1.838429	2.042134	-3.463718
O	3.493010	2.545860	-3.182948	H	0.691775	1.868045	-4.436741
H	3.987023	1.756833	-2.960192				
H	3.651260	3.142595	-2.451445	e. isomer 5			
O	3.952325	1.329635	0.128216	O	-0.390596	3.858415	5.454789
H	4.297907	0.852223	-0.626028	H	-0.887014	3.350815	4.812805
H	3.844718	2.227722	-0.184983	H	-0.685891	3.527125	6.302893
O	1.439581	0.320728	0.221072	O	-1.499815	1.973920	3.732544
H	2.332974	0.662163	0.259837	H	-0.638323	1.573207	3.616383
H	1.123644	0.372190	1.123164	H	-1.853726	2.043342	2.845887
O	4.491138	0.108695	-2.281949	O	0.958710	0.877694	3.716555
H	3.613280	-0.266965	-2.348852	H	1.506848	1.549499	4.122086
H	5.065422	-0.553237	-2.667017	H	0.944104	0.163243	4.353406
O	2.495545	2.128920	3.962640	O	2.118235	2.918154	5.203024
H	1.778498	1.649122	3.548068	H	2.730165	3.622803	4.990317
H	2.432007	1.901201	4.890185	H	1.268530	3.352535	5.277501
O	4.892231	2.163036	2.569470	O	1.594872	1.382036	7.444868
H	4.674338	1.722958	1.747834	H	1.953225	1.929302	6.746073
H	4.110186	2.059898	3.111689	H	0.732385	1.756340	7.624441
O	2.355492	4.760834	3.114129	O	-1.007964	2.260790	7.658764
H	3.171642	4.860244	2.623978	H	-1.342459	2.024676	8.523978
H	2.394188	3.871865	3.466931	H	-1.410727	1.627449	7.064716
O	3.701525	3.888508	-0.737001	O	-1.915200	0.360118	5.936004
H	4.121662	4.310738	0.012292	H	-1.980049	0.870766	5.128993
H	2.803497	4.219675	-0.726656	H	-1.062909	-0.071816	5.878854
O	1.110407	4.616410	-0.662983	O	0.590922	-0.695241	6.000421
H	0.725447	4.924139	0.157591	H	1.035634	-0.046751	6.546247
H	0.645723	3.802020	-0.855519	H	0.420879	-1.429509	6.590480
O	0.416696	0.816965	2.734359	O	-2.676927	-1.085641	8.197808
H	-0.138488	1.501607	2.361172	H	-2.699720	-0.664323	7.338620
H	-0.198690	0.161948	3.063729	H	-2.430473	-0.385352	8.802033
O	0.045347	5.206588	1.809197	O	-1.687664	0.784846	9.926875
H	0.855115	5.083955	2.304646	H	-0.795760	0.441985	9.870428
H	-0.283839	6.058909	2.094535	H	-2.003146	0.493333	10.782283
O	-0.076121	2.184904	-1.050909	O	0.733631	-0.408676	9.697689
H	0.445385	1.517574	-0.604889	H	0.802091	-0.795521	10.570556
H	0.109031	2.052428	-1.980641	H	1.544119	0.089430	9.591703
O	-1.066784	2.694393	1.515736	O	-0.245508	-2.322618	8.070243
H	-0.784320	3.596693	1.665072	H	-1.144931	-1.999171	8.018738
H	-0.963955	2.563625	0.573102	H	0.209598	-1.680540	8.615080
O	1.919576	-0.676961	-2.345972	O	-2.330558	-0.662558	12.205753
H	1.634485	-0.533948	-1.443473	H	-2.715630	-1.357733	11.672194
H	1.486207	0.014048	-2.846902	H	-2.916977	-0.584870	12.958289

O	-3.169839	-2.585120	10.519506	H	-1.491521	2.199994	2.078053
H	-2.397973	-3.149096	10.470651	H	-1.381871	2.228825	3.587703
H	-3.233601	-2.189758	9.650106	O	-1.656622	3.108369	0.599132
O	-0.690796	-3.807260	10.301211	H	-2.533916	2.929719	0.260498
H	-0.480292	-3.405540	9.458275	H	-1.069656	2.875139	-0.120109
H	-0.451630	-4.727957	10.194677	O	2.178725	-4.126691	0.415424
O	0.232876	-1.763255	11.985578	H	2.917618	-4.617650	0.774908
H	-0.598445	-1.359863	12.235408	H	1.698151	-3.819272	1.184043
H	-0.017192	-2.576805	11.547588	O	1.987745	-0.787476	-3.994714

2. Coordinates of the initial structures for geometry optimization calculations.

(1) W20

O	0.381332	-0.452904	-0.383074
H	-0.442954	-0.837023	-0.681798
H	1.058557	-1.012080	-0.763761
O	-0.213563	1.962040	-1.480915
H	0.132760	1.174110	-1.062036
H	0.240751	2.005981	-2.322284
O	0.897605	1.681433	-3.982215
H	1.454794	2.252379	-4.511170
H	1.363248	0.845426	-3.959808
O	1.895693	-2.321916	-1.662489
H	1.115740	-2.733178	-2.035006
H	2.171286	-2.917322	-0.965515
O	-2.620026	-1.889645	1.384590
H	-2.499671	-2.834326	1.481157
H	-1.823940	-1.507314	1.753780
O	-1.762163	-4.511057	1.586163
H	-1.293836	-4.770931	0.792835
H	-2.166416	-5.319247	1.901822
O	-0.223879	-5.151849	-0.538580
H	0.665929	-4.922888	-0.270154
H	-0.354466	-4.682008	-1.362248
O	-2.622952	0.912874	-2.181538
H	-1.798614	1.346356	-1.960645
H	-3.274875	1.339202	-1.625235
O	-1.939692	-1.544895	-1.227256
H	-2.344205	-0.744648	-1.562227
H	-2.338549	-1.673329	-0.366645
O	-1.442561	0.342603	-4.651701
H	-0.690375	0.918256	-4.513599
H	-2.027885	0.532475	-3.918505
O	-1.515748	1.634128	2.849702

H	-1.491521	2.199994	2.078053
H	-1.381871	2.228825	3.587703
O	-1.656622	3.108369	0.599132
H	-2.533916	2.929719	0.260498
H	-1.069656	2.875139	-0.120109
O	2.178725	-4.126691	0.415424
H	2.917618	-4.617650	0.774908
H	1.698151	-3.819272	1.184043
O	1.987745	-0.787476	-3.994714
H	1.320429	-1.299174	-4.451975
H	2.171585	-1.288420	-3.200050
O	-0.249781	-2.047082	-5.055476
H	-0.752419	-1.240401	-4.942105
H	-0.440592	-2.324828	-5.951401
O	-3.884357	0.528610	1.907548
H	-3.140620	0.905182	2.377953
H	-3.643900	-0.388051	1.772846
O	-4.132959	2.146123	-0.234716
H	-4.992252	2.566497	-0.201044
H	-4.130864	1.544327	0.509643
O	-0.442302	-3.337103	-2.630476
H	-1.073352	-2.766683	-2.191580
H	-0.429359	-3.028422	-3.536446
O	0.613167	-3.371968	2.480275
H	-0.224819	-3.804537	2.316273
H	0.392459	-2.444095	2.561350
O	-0.296506	-0.760564	2.233712
H	0.068925	-0.580348	1.367563
H	-0.608598	0.089428	2.544109

(2) SWCNT-36

C	1.357000	0.000000	0.000000
C	0.678500	1.175200	0.000000
C	0.000000	1.357000	1.230600
C	-1.175200	0.678500	1.230600
C	-1.357000	0.000000	0.000000
C	-0.678500	-1.175200	0.000000
C	0.000000	-1.357000	1.230600
C	1.175200	-0.678500	1.230600
C	1.357000	0.000000	2.461200
C	0.678500	1.175200	2.461200
C	0.000000	1.357000	3.691900
C	-1.175200	0.678500	3.691900
C	-1.357000	0.000000	2.461200

C	-0.678500	-1.175200	2.461200	C	0.678500	1.175200	17.228700
C	0.000000	-1.357000	3.691900	C	0.000000	1.357000	18.459300
C	1.175200	-0.678500	3.691900	C	-1.175200	0.678500	18.459300
C	1.357000	0.000000	4.922500	C	-1.357000	0.000000	17.228700
C	0.678500	1.175200	4.922500	C	-0.678500	-1.175200	17.228700
C	0.000000	1.357000	6.153100	C	0.000000	-1.357000	18.459300
C	-1.175200	0.678500	6.153100	C	1.175200	-0.678500	18.459300
C	-1.357000	0.000000	4.922500	C	1.357000	0.000000	19.690000
C	-0.678500	-1.175200	4.922500	C	0.678500	1.175200	19.690000
C	0.000000	-1.357000	6.153100	C	0.000000	1.357000	20.920600
C	1.175200	-0.678500	6.153100	C	-1.175200	0.678500	20.920600
C	1.357000	0.000000	7.383700	C	-1.357000	0.000000	19.690000
C	0.678500	1.175200	7.383700	C	-0.678500	-1.175200	19.690000
C	0.000000	1.357000	8.614400	C	0.000000	-1.357000	20.920600
C	-1.175200	0.678500	8.614400	C	1.175200	-0.678500	20.920600
C	-1.357000	0.000000	7.383700	C	1.357000	0.000000	22.151200
C	-0.678500	-1.175200	7.383700	C	0.678500	1.175200	22.151200
C	0.000000	-1.357000	8.614400	C	0.000000	1.357000	23.381800
C	1.175200	-0.678500	8.614400	C	-1.175200	0.678500	23.381800
C	1.357000	0.000000	9.845000	C	-1.357000	0.000000	22.151200
C	0.678500	1.175200	9.845000	C	-0.678500	-1.175200	22.151200
C	0.000000	1.357000	11.075600	C	0.000000	-1.357000	23.381800
C	-1.175200	0.678500	11.075600	C	1.175200	-0.678500	23.381800
C	-1.357000	0.000000	9.845000	C	1.357000	0.000000	24.612400
C	-0.678500	-1.175200	9.845000	C	0.678500	1.175200	24.612400
C	0.000000	-1.357000	11.075600	C	0.000000	1.357000	25.843100
C	1.175200	-0.678500	11.075600	C	-1.175200	0.678500	25.843100
C	1.357000	0.000000	12.306200	C	-1.357000	0.000000	24.612400
C	0.678500	1.175200	12.306200	C	-0.678500	-1.175200	24.612400
C	0.000000	1.357000	13.536800	C	0.000000	-1.357000	25.843100
C	-1.175200	0.678500	13.536800	C	1.175200	-0.678500	25.843100
C	-1.357000	0.000000	12.306200	C	1.357000	0.000000	27.073700
C	-0.678500	-1.175200	12.306200	C	0.678500	1.175200	27.073700
C	0.000000	-1.357000	13.536800	C	0.000000	1.357000	28.304300
C	1.175200	-0.678500	13.536800	C	-1.175200	0.678500	28.304300
C	1.357000	0.000000	14.767500	C	-1.357000	0.000000	27.073700
C	0.678500	1.175200	14.767500	C	-0.678500	-1.175200	27.073700
C	0.000000	1.357000	15.998100	C	0.000000	-1.357000	28.304300
C	-1.175200	0.678500	15.998100	C	1.175200	-0.678500	28.304300
C	-1.357000	0.000000	14.767500	C	1.357000	0.000000	29.534900
C	-0.678500	-1.175200	14.767500	C	0.678500	1.175200	29.534900
C	0.000000	-1.357000	15.998100	C	0.000000	1.357000	30.765600
C	1.175200	-0.678500	15.998100	C	-1.175200	0.678500	30.765600
C	1.357000	0.000000	17.228700	C	-1.357000	0.000000	29.534900

C	-0.678500	-1.175200	29.534900	C	0.678500	1.175200	44.302400
C	0.000000	-1.357000	30.765600	C	0.000000	1.357000	45.533000
C	1.175200	-0.678500	30.765600	C	-1.175200	0.678500	45.533000
C	1.357000	0.000000	31.996200	C	-1.357000	0.000000	44.302400
C	0.678500	1.175200	31.996200	C	-0.678500	-1.175200	44.302400
C	0.000000	1.357000	33.226800	C	0.000000	-1.357000	45.533000
C	-1.175200	0.678500	33.226800	C	1.175200	-0.678500	45.533000
C	-1.357000	0.000000	31.996200	C	1.357000	0.000000	46.763600
C	-0.678500	-1.175200	31.996200	C	0.678500	1.175200	46.763600
C	0.000000	-1.357000	33.226800	C	0.000000	1.357000	47.994300
C	1.175200	-0.678500	33.226800	C	-1.175200	0.678500	47.994300
C	1.357000	0.000000	34.457400	C	-1.357000	0.000000	46.763600
C	0.678500	1.175200	34.457400	C	-0.678500	-1.175200	46.763600
C	0.000000	1.357000	35.688000	C	0.000000	-1.357000	47.994300
C	-1.175200	0.678500	35.688000	C	1.175200	-0.678500	47.994300
C	-1.357000	0.000000	34.457400	C	1.357000	0.000000	49.224900
C	-0.678500	-1.175200	34.457400	C	0.678500	1.175200	49.224900
C	0.000000	-1.357000	35.688000	C	0.000000	1.357000	50.455500
C	1.175200	-0.678500	35.688000	C	-1.175200	0.678500	50.455500
C	1.357000	0.000000	36.918700	C	-1.357000	0.000000	49.224900
C	0.678500	1.175200	36.918700	C	-0.678500	-1.175200	49.224900
C	0.000000	1.357000	38.149300	C	0.000000	-1.357000	50.455500
C	-1.175200	0.678500	38.149300	C	1.175200	-0.678500	50.455500
C	-1.357000	0.000000	36.918700	C	1.357000	0.000000	51.686100
C	-0.678500	-1.175200	36.918700	C	0.678500	1.175200	51.686100
C	0.000000	-1.357000	38.149300	C	0.000000	1.357000	52.916800
C	1.175200	-0.678500	38.149300	C	-1.175200	0.678500	52.916800
C	1.357000	0.000000	39.379900	C	-1.357000	0.000000	51.686100
C	0.678500	1.175200	39.379900	C	-0.678500	-1.175200	51.686100
C	0.000000	1.357000	40.610500	C	0.000000	-1.357000	52.916800
C	-1.175200	0.678500	40.610500	C	1.175200	-0.678500	52.916800
C	-1.357000	0.000000	39.379900	C	1.357000	0.000000	54.147400
C	-0.678500	-1.175200	39.379900	C	0.678500	1.175200	54.147400
C	0.000000	-1.357000	40.610500	C	0.000000	1.357000	55.378000
C	1.175200	-0.678500	40.610500	C	-1.175200	0.678500	55.378000
C	1.357000	0.000000	41.841200	C	-1.357000	0.000000	54.147400
C	0.678500	1.175200	41.841200	C	-0.678500	-1.175200	54.147400
C	0.000000	1.357000	43.071800	C	0.000000	-1.357000	55.378000
C	-1.175200	0.678500	43.071800	C	1.175200	-0.678500	55.378000
C	-1.357000	0.000000	41.841200	C	1.357000	0.000000	56.608600
C	-0.678500	-1.175200	41.841200	C	0.678500	1.175200	56.608600
C	0.000000	-1.357000	43.071800	C	0.000000	1.357000	57.839200
C	1.175200	-0.678500	43.071800	C	-1.175200	0.678500	57.839200
C	1.357000	0.000000	44.302400	C	-1.357000	0.000000	56.608600

C	-0.678500	-1.175200	56.608600	C	0.678500	1.175200	71.376100
C	0.000000	-1.357000	57.839200	C	0.000000	1.357000	72.606700
C	1.175200	-0.678500	57.839200	C	-1.175200	0.678500	72.606700
C	1.357000	0.000000	59.069900	C	-1.357000	0.000000	71.376100
C	0.678500	1.175200	59.069900	C	-0.678500	-1.175200	71.376100
C	0.000000	1.357000	60.300500	C	0.000000	-1.357000	72.606700
C	-1.175200	0.678500	60.300500	C	1.175200	-0.678500	72.606700
C	-1.357000	0.000000	59.069900	C	1.357000	0.000000	73.837300
C	-0.678500	-1.175200	59.069900	C	0.678500	1.175200	73.837300
C	0.000000	-1.357000	60.300500	C	0.000000	1.357000	75.067900
C	1.175200	-0.678500	60.300500	C	-1.175200	0.678500	75.067900
C	1.357000	0.000000	61.531100	C	-1.357000	0.000000	73.837300
C	0.678500	1.175200	61.531100	C	-0.678500	-1.175200	73.837300
C	0.000000	1.357000	62.761700	C	0.000000	-1.357000	75.067900
C	-1.175200	0.678500	62.761700	C	1.175200	-0.678500	75.067900
C	-1.357000	0.000000	61.531100	C	1.357000	0.000000	76.298600
C	-0.678500	-1.175200	61.531100	C	0.678500	1.175200	76.298600
C	0.000000	-1.357000	62.761700	C	0.000000	1.357000	77.529200
C	1.175200	-0.678500	62.761700	C	-1.175200	0.678500	77.529200
C	1.357000	0.000000	63.992300	C	-1.357000	0.000000	76.298600
C	0.678500	1.175200	63.992300	C	-0.678500	-1.175200	76.298600
C	0.000000	1.357000	65.223000	C	0.000000	-1.357000	77.529200
C	-1.175200	0.678500	65.223000	C	1.175200	-0.678500	77.529200
C	-1.357000	0.000000	63.992300	C	1.357000	0.000000	78.759800
C	-0.678500	-1.175200	63.992300	C	0.678500	1.175200	78.759800
C	0.000000	-1.357000	65.223000	C	0.000000	1.357000	79.990400
C	1.175200	-0.678500	65.223000	C	-1.175200	0.678500	79.990400
C	1.357000	0.000000	66.453600	C	-1.357000	0.000000	78.759800
C	0.678500	1.175200	66.453600	C	-0.678500	-1.175200	78.759800
C	0.000000	1.357000	67.684200	C	0.000000	-1.357000	79.990400
C	-1.175200	0.678500	67.684200	C	1.175200	-0.678500	79.990400
C	-1.357000	0.000000	66.453600	C	1.357000	0.000000	81.221100
C	-0.678500	-1.175200	66.453600	C	0.678500	1.175200	81.221100
C	0.000000	-1.357000	67.684200	C	0.000000	1.357000	82.451700
C	1.175200	-0.678500	67.684200	C	-1.175200	0.678500	82.451700
C	1.357000	0.000000	68.914800	C	-1.357000	0.000000	81.221100
C	0.678500	1.175200	68.914800	C	-0.678500	-1.175200	81.221100
C	0.000000	1.357000	70.145500	C	0.000000	-1.357000	82.451700
C	-1.175200	0.678500	70.145500	C	1.175200	-0.678500	82.451700
C	-1.357000	0.000000	68.914800	C	1.357000	0.000000	83.682300
C	-0.678500	-1.175200	68.914800	C	0.678500	1.175200	83.682300
C	0.000000	-1.357000	70.145500	C	0.000000	1.357000	84.912900
C	1.175200	-0.678500	70.145500	C	-1.175200	0.678500	84.912900
C	1.357000	0.000000	71.376100	C	-1.357000	0.000000	83.682300

C	-0.678500	-1.175200	83.682300	H	0.104209	0.432203	-9.398633
C	0.000000	-1.357000	84.912900	H	1.313209	1.009203	-8.224633
C	1.175200	-0.678500	84.912900	H	0.892209	-0.720797	-8.300633
C	1.357000	0.000000	86.143500	H	0.553209	1.146203	-5.601633
C	0.678500	1.175200	86.143500	H	-0.934791	0.272203	-5.202633
C	0.000000	1.357000	87.374200	H	0.464209	-0.632797	-5.811633
C	-1.175200	0.678500	87.374200	N	-4.103791	0.460203	-7.165633
C	-1.357000	0.000000	86.143500	C	-5.162791	-0.573797	-6.885633
C	-0.678500	-1.175200	86.143500	C	-4.798791	-2.076797	-6.969633
C	0.000000	-1.357000	87.374200	O	-5.613791	-2.869797	-7.438633
C	1.175200	-0.678500	87.374200	H	-3.737791	0.626203	-8.106633
H	0.658636	1.867802	-0.815357	H	-5.639791	-0.422797	-5.901633
H	1.946874	-0.363505	-0.815360	H	-6.016791	-0.420797	-7.561633
H	-0.658636	-1.867802	-0.815357	N	-3.608791	-2.469797	-6.497633
H	-1.946874	0.363505	-0.815360	C	-3.154791	-3.898797	-6.452633
H	0.363527	1.946857	88.189563	C	-3.757791	-4.714797	-5.237633
H	-1.867798	0.658608	88.189560	O	-4.933791	-4.534797	-4.910633
H	1.867798	-0.658608	88.189560	C	-1.584791	-3.878797	-6.674633
H	-0.363527	-1.946857	88.189563	C	-0.895791	-5.173797	-7.185633
				C	-0.732791	-3.377797	-5.475633
				C	-1.625791	-5.921797	-8.312633
				H	-2.994791	-1.677797	-6.318633
				H	-3.618791	-4.379797	-7.338633
				H	-1.410791	-3.153797	-7.498633
				H	0.075209	-4.839797	-7.588633
				H	-0.613791	-5.882797	-6.371633
				H	-1.116791	-2.437797	-5.047633
				H	-0.674791	-4.112797	-4.649633
				H	0.311209	-3.176797	-5.778633
				H	-1.881791	-5.249797	-9.154633
				H	-1.003791	-6.737797	-8.724633
				H	-2.567791	-6.382797	-7.960633
				N	-3.022791	-5.632797	-4.574633
				C	-3.596791	-6.434797	-3.451633
				C	-2.661791	-7.180797	-2.486633
				O	-2.781791	-8.393797	-2.316633
				H	-2.082791	-5.774797	-4.954633
				H	-4.269791	-5.812797	-2.829633
				H	-4.263791	-7.194797	-3.874633
				N	-1.793791	-6.434797	-1.804633
				C	-0.943791	-6.972797	-0.697633
				C	-1.068791	-6.138797	0.626367
				O	-1.543791	-6.659797	1.637367
				C	0.502209	-7.159797	-1.219633
(3) 1RPB(charge=-1)							
N	-0.250791	4.106203	-2.909633				
C	-1.465791	4.667203	-3.577633				
C	-1.759791	4.215203	-5.053633				
O	-1.955791	5.020203	-5.968633				
C	-1.489791	6.198203	-3.363633				
S	-3.212791	6.721203	-3.338633				
H	0.617209	3.914203	-3.421633				
H	-2.342791	4.259203	-3.041633				
H	-1.042791	6.493203	-2.394633				
H	-0.919791	6.731203	-4.146633				
N	-1.896791	2.899203	-5.254633				
C	-2.427791	2.282203	-6.513633				
C	-3.553791	1.217203	-6.190633				
O	-3.947791	1.085203	-5.030633				
C	-1.250791	1.922203	-7.472633				
C	-0.636791	0.520203	-7.333633				
C	0.475209	0.300203	-8.364633				
C	-0.094791	0.306203	-5.921633				
H	-1.670791	2.347203	-4.421633				
H	-2.971791	3.034203	-7.075633				
H	-1.604791	2.037203	-8.514633				
H	-0.452791	2.692203	-7.396633				
H	-1.452791	-0.197797	-7.523633				

O	1.339209	-7.761797	-0.230633	O	-1.126791	7.515203	2.885367
H	-1.791791	-5.468797	-2.135633	C	1.593209	7.080203	1.827367
H	-1.291791	-7.987797	-0.413633	C	2.333209	8.041203	2.771367
H	0.499209	-7.804797	-2.121633	C	3.602209	7.708203	3.257367
H	0.938209	-6.198797	-1.543633	C	1.743209	9.247203	3.163367
H	1.283209	-7.228797	0.569367	C	4.270209	8.568203	4.125367
N	-0.624791	-4.868797	0.644367	C	2.411209	10.106203	4.034367
C	-0.647791	-3.989797	1.852367	C	3.674209	9.766203	4.513367
C	-1.065791	-2.507797	1.508367	H	-0.296791	4.801203	0.995367
O	-1.740791	-2.280797	0.504367	H	1.403209	5.616203	3.383367
C	0.720209	-4.218797	2.552367	H	2.343209	6.610203	1.160367
S	2.090209	-4.273797	1.381367	H	0.950209	7.649203	1.130367
H	-0.215791	-4.551797	-0.242633	H	4.071209	6.778203	2.964367
H	-1.438791	-4.328797	2.551367	H	0.758209	9.515203	2.805367
H	0.938209	-3.465797	3.331367	H	5.250209	8.306203	4.498367
H	0.716209	-5.183797	3.092367	H	1.948209	11.034203	4.337367
N	-0.726791	-1.501797	2.340367	H	4.192209	10.433203	5.188367
C	-1.085791	-0.058797	2.117367	N	-0.960791	5.785203	4.325367
C	0.185209	0.804203	1.788367	C	-2.051791	6.195203	5.260367
O	1.257209	0.603203	2.380367	C	-3.476791	6.394203	4.645367
C	-1.862791	0.434203	3.376367	O	-3.939791	7.517203	4.433367
C	-2.430791	1.858203	3.327367	C	-1.552791	7.378203	6.124367
O	-1.781791	2.813203	3.732367	H	-0.484791	4.883203	4.391367
N	-3.636791	2.081203	2.870367	H	-2.160791	5.359203	5.978367
H	-0.123791	-1.808797	3.113367	H	-0.590791	7.158203	6.623367
H	-1.795791	0.029203	1.270367	H	-1.402791	8.288203	5.512367
H	-2.679791	-0.270797	3.624367	H	-2.279791	7.641203	6.914367
H	-1.201791	0.414203	4.260367	N	-4.179791	5.285203	4.350367
H	-4.077791	1.336203	2.321367	C	-5.536791	5.351203	3.720367
H	-3.834791	3.080203	2.775367	C	-5.672791	5.625203	2.198367
N	0.034209	1.771203	0.858367	O	-6.766791	5.440203	1.667367
C	1.134209	2.693203	0.448367	H	-3.686791	4.412203	4.568367
C	1.401209	3.829203	1.477367	H	-6.063791	4.401203	3.921367
O	2.434209	3.770203	2.151367	H	-6.155791	6.112203	4.234367
C	1.057209	3.146203	-1.045633	N	-4.610791	6.054203	1.497367
C	-0.234791	3.798203	-1.592633	C	-4.679791	6.400203	0.042367
O	-1.199791	3.996203	-0.848633	C	-4.916791	5.211203	-0.963633
H	-0.905791	1.833203	0.450367	O	-5.645791	5.374203	-1.944633
H	2.063209	2.095203	0.461367	C	-3.405791	7.224203	-0.252633
H	1.921209	3.801203	-1.252633	S	-3.459791	8.046203	-1.861633
H	1.263209	2.269203	-1.682633	H	-3.772791	6.183203	2.086367
N	0.522209	4.846203	1.611367	H	-5.540791	7.083203	-0.102633
C	0.758209	5.979203	2.555367	H	-3.249791	8.030203	0.493367
C	-0.547791	6.492203	3.256367	H	-2.506791	6.583203	-0.212633

N	-4.324791	4.028203	-0.728633	C	2.812209	-4.891797	-5.628633
C	-4.578791	2.818203	-1.554633	H	3.095209	-2.404797	-3.656633
C	-3.698791	1.615203	-1.171633	H	2.721209	-5.304797	-2.793633
O	-3.588791	1.255203	0.001367	H	4.717209	-4.235797	-4.866633
H	-3.771791	4.018203	0.133367	H	5.394209	-6.485797	-3.954633
H	-5.631791	2.503203	-1.424633	H	3.785209	-7.141797	-4.317633
H	-4.487791	3.040203	-2.636633	H	4.869209	-6.630797	-5.634633
N	-3.115791	0.962203	-2.178633	H	1.946209	-5.527797	-5.363633
C	-2.386791	-0.325797	-2.002633	H	2.436209	-3.864797	-5.772633
C	-0.841791	-0.240797	-2.265633	H	3.172209	-5.224797	-6.621633
O	-0.329791	0.716203	-2.848633	N	5.462209	-3.527797	-1.923633
C	-3.058791	-1.366797	-2.943633	C	6.532209	-3.398797	-0.897633
C	-4.509791	-1.783797	-2.643633	C	5.863209	-2.695797	0.331367
C	-5.584791	-1.032797	-3.131633	O	5.521209	-1.508797	0.323367
C	-4.762791	-2.984797	-1.979633	C	7.786209	-2.635797	-1.446633
C	-6.886791	-1.507797	-3.019633	C	8.893209	-2.488797	-0.375633
C	-6.068791	-3.462797	-1.868633	C	8.447209	-3.307797	-2.674633
C	-7.127791	-2.725797	-2.393633	H	5.128209	-2.694797	-2.394633
O	-8.406791	-3.201797	-2.308633	H	6.893209	-4.410797	-0.612633
H	-3.382791	1.299203	-3.111633	H	7.467209	-1.614797	-1.743633
H	-2.520791	-0.684797	-0.969633	H	8.535209	-1.930797	0.512367
H	-2.990791	-1.002797	-3.981633	H	9.254209	-3.468797	-0.009633
H	-2.442791	-2.285797	-2.968633	H	9.771209	-1.932797	-0.753633
H	-5.421791	-0.076797	-3.601633	H	7.745209	-3.395797	-3.523633
H	-3.939791	-3.557797	-1.579633	H	9.316209	-2.731797	-3.046633
H	-7.702791	-0.939797	-3.447633	H	8.805209	-4.330797	-2.447633
H	-6.248791	-4.419797	-1.409633	N	5.632209	-3.507797	1.354367
H	-8.376791	-4.096797	-1.966633	C	4.867209	-3.121797	2.563367
N	-0.091791	-1.282797	-1.865633	C	5.540209	-2.095797	3.534367
C	1.370209	-1.393797	-2.107633	O	6.512209	-2.394797	4.232367
C	1.811209	-2.887797	-2.202633	C	4.494209	-4.446797	3.257367
O	1.335209	-3.740797	-1.446633	S	3.504209	-5.456797	2.146367
C	2.130209	-0.693797	-0.962633	H	5.855209	-4.465797	1.077367
H	-0.612791	-2.045797	-1.417633	H	3.905209	-2.684797	2.226367
H	1.639209	-0.870797	-3.049633	H	5.387209	-5.005797	3.598367
H	1.879209	-1.102797	0.033367	H	3.881209	-4.252797	4.159367
H	3.228209	-0.757797	-1.081633	N	4.951209	-0.892797	3.608367
H	1.896209	0.378203	-0.939633	C	5.376209	0.177203	4.570367
N	2.773209	-3.191797	-3.087633	C	5.079209	-0.095797	6.093367
C	3.459209	-4.532797	-3.104633	O	5.800209	0.383203	6.970367
C	4.639209	-4.591797	-2.047633	C	4.773209	1.539203	4.107367
O	4.785209	-5.590797	-1.340633	C	5.288209	2.099203	2.764367
C	3.922209	-4.939797	-4.551633	C	4.712209	1.688203	1.557367
C	4.517209	-6.367797	-4.619633	C	6.321209	3.042203	2.741367

C	5.158209	2.212203	0.347367	H	1.548645	1.341311	-1.094888
C	6.767209	3.568203	1.529367	H	1.602715	1.868937	-2.554520
C	6.184209	3.153203	0.334367	O	1.451700	0.895188	-4.144950
H	4.208209	-0.752797	2.917367	H	1.992122	1.075289	-4.918955
H	6.474209	0.257203	4.524367	H	1.513943	-0.085142	-3.983928
H	3.666209	1.485203	4.086367	O	1.382588	-2.620116	-1.062727
H	4.967209	2.295203	4.893367	H	0.399469	-2.654589	-1.086616
H	3.908209	0.965203	1.553367	H	1.631770	-3.212298	-0.329504
H	6.781209	3.372203	3.662367	O	-1.349593	0.302494	2.696136
H	4.704209	1.889203	-0.578633	H	-1.623744	-0.559868	3.060433
H	7.565209	4.297203	1.517367	H	-0.366565	0.293560	2.749858
H	6.529209	3.561203	-0.604633	O	-1.549408	-2.403442	3.419221
N	4.034209	-0.878797	6.387367	H	-1.574693	-2.976833	2.605497
C	3.707209	-1.381797	7.748367	H	-2.110251	-2.834437	4.069748
C	4.184209	-2.855797	7.931367	O	-1.365665	-4.000497	1.282739
O	4.111209	-3.734797	7.073367	H	-0.412500	-4.197835	1.265461
C	2.206209	-1.101797	8.043367	H	-1.556147	-3.612868	0.410432
C	1.142209	-1.812797	7.183367	O	-1.351789	2.276517	-1.538013
C	0.383209	-1.197797	6.165367	H	-0.369849	2.305960	-1.593319
C	0.686209	-3.119797	7.242367	H	-1.595077	3.051853	-0.998606
N	-0.544791	-2.089797	5.588367	O	-1.405155	0.015910	-0.016315
C	-0.332791	-3.274797	6.268367	H	-1.557533	0.848845	-0.515353
C	1.067209	-4.214797	8.059367	H	-1.554531	0.180112	0.941017
C	-0.974791	-4.522797	6.101367	O	-1.413630	0.868297	-4.023921
C	0.423209	-5.439797	7.874367	H	-0.468733	1.022406	-4.200708
C	-0.582791	-5.591797	6.911367	H	-1.618288	1.422437	-3.251172
O	4.691209	-3.091797	9.174367	O	1.535858	3.117418	2.782814
H	3.622209	-1.253797	5.529367	H	1.569157	3.490945	1.860104
H	4.259209	-0.814797	8.515367	H	2.122397	3.662547	3.314174
H	2.002209	-1.296797	9.112367	O	1.387655	4.177251	0.335316
H	2.045209	-0.009797	7.967367	H	0.440402	4.388459	0.264071
H	0.493209	-0.159797	5.881367	H	1.574277	3.593043	-0.420974
H	-1.315791	-1.885797	4.942367	O	1.506829	-4.037346	1.363925
H	1.867209	-4.108797	8.781367	H	2.039661	-4.793111	1.625329
H	-1.747791	-4.649797	5.359367	H	1.533599	-3.400859	2.128528
H	0.713209	-6.288797	8.478367	O	1.376759	-1.753440	-3.788187
H	-1.059791	-6.553797	6.788367	H	0.428035	-1.940953	-3.900121

3. Coordinates of the optimized structures.

(1) W20 HF/cc-pVTZ

O	1.337770	-0.075822	-0.061124	H	-1.555871	-0.803171	-3.868302
H	0.352101	-0.059885	-0.052778	H	-2.056769	-2.134888	-4.521245
H	1.548436	-0.965328	-0.424263	O	-1.335411	3.141147	2.815222
O	1.415211	2.149227	-1.639161	H	-0.380777	3.186393	3.000779
				H	-1.559779	2.197689	2.895104

O	-1.485519	4.284227	0.405013	O	1.605048	4.098862	0.554063
H	-2.020574	5.079387	0.473173	H	1.585023	3.930629	-0.426978
H	-1.522280	3.843559	1.296849	H	2.182838	4.855174	0.686123
O	-1.381895	-2.481768	-1.108774	O	1.383280	3.672652	-2.082954
H	-1.527234	-1.588675	-0.728342	H	0.432834	3.825539	-2.238278
H	-1.603416	-2.395034	-2.054821	H	1.529729	2.754119	-2.368538
O	1.324436	-2.385387	3.461752	O	1.485181	-2.524082	3.341808
H	0.367609	-2.400720	3.639497	H	2.015601	-2.997176	3.989950
H	1.537986	-1.445413	3.326330	H	1.484766	-1.570506	3.633468
O	1.415268	0.320443	2.641837	O	1.359976	-3.683853	-2.180565
H	1.552520	0.175212	1.679743	H	0.413622	-3.902357	-2.167388
H	1.642791	1.255501	2.803748	H	1.607690	-3.535167	-1.252589
(2) W20 GEBF(5)-HF/cc-pVTZ				O	-1.520499	-3.632285	-2.230315
O	1.377338	-0.151312	0.049594	H	-1.572534	-2.820324	-2.801765
H	0.392138	-0.123757	0.037195	H	-2.156853	-4.257174	-2.587135
H	1.582773	-1.097681	0.216396	O	-1.286639	4.150633	0.610516
O	1.390239	0.857263	-2.501680	H	-0.336736	4.275746	0.773422
H	1.546588	0.520418	-1.591610	H	-1.538048	3.405285	1.187285
H	1.547732	0.082630	-3.074777	O	-1.438088	3.838497	-2.025514
O	1.415189	-1.597818	-3.856567	H	-2.046058	4.489910	-2.386181
H	1.980751	-1.814762	-4.603240	H	-1.479873	3.932653	-1.033784
H	1.488568	-2.358931	-3.220411	O	-1.351695	-2.684252	0.399794
O	1.416433	-2.864428	0.571496	H	-1.445503	-1.722903	0.226648
H	0.436264	-2.873709	0.577574	H	-1.554520	-3.118381	-0.450881
H	1.663837	-2.873426	1.515170	O	1.241372	-0.013956	4.196109
O	-1.362596	1.760209	2.099135	H	0.288967	0.103915	4.364245
H	-1.650370	1.233607	2.870277	H	1.467093	0.706543	3.579289
H	-0.379817	1.748411	2.143525	O	1.394424	1.737100	2.016446
O	-1.609098	-0.069550	4.168586	H	1.554615	1.057178	1.324273
H	-1.588303	-0.985081	3.771777	H	1.632376	2.588840	1.600126
H	-2.217500	-0.113754	4.911230	(3) SWCNT-36 EBF(3)-B3LYP(3L)/6-31G			
O	-1.345537	-2.536548	3.203279	C	-1.236061	1.038293	-46.150379
H	-0.390299	-2.715219	3.290756	C	-1.591968	-0.267940	-46.150368
H	-1.522584	-2.708704	2.259673	C	-0.985318	-0.993644	-44.978948
O	-1.355701	1.089740	-2.506760	C	0.344365	-1.355846	-44.979002
H	-0.372986	1.064181	-2.543548	C	1.235270	-1.038093	-46.150427
H	-1.576243	2.039583	-2.479703	C	1.591176	0.268141	-46.150425
O	-1.347342	0.022733	-0.003187	C	0.984570	0.993840	-44.978981
H	-1.521205	0.461257	-0.866663	C	-0.345112	1.356041	-44.978984
H	-1.524914	0.665695	0.719560	C	-0.992724	0.987304	-43.645961
O	-1.441060	-1.475573	-3.830477	C	-1.356343	-0.347301	-43.645967
H	-0.487212	-1.455477	-4.020780	C	-0.991402	-1.011070	-42.342600
H	-1.634512	-0.602121	-3.449525	C	0.340843	-1.373995	-42.342647

C	0.992029	-0.987115	-43.646003	C	-1.009274	0.991418	-28.011680
C	1.355648	0.347490	-43.646018	C	-1.372607	-0.342779	-28.011696
C	0.990758	1.011251	-42.342634	C	-0.991443	-1.009336	-26.708822
C	-0.341488	1.374176	-42.342626	C	0.342769	-1.372640	-26.708848
C	-1.010955	0.992046	-41.040935	C	1.009253	-0.991401	-28.011732
C	-1.374436	-0.342110	-41.040933	C	1.372586	0.342796	-28.011746
C	-0.991804	-1.008801	-39.738116	C	0.991471	1.009337	-26.708847
C	0.342493	-1.372310	-39.738151	C	-0.342741	1.372641	-26.708820
C	1.010364	-0.991874	-41.040984	C	-1.009291	0.991435	-25.405961
C	1.373846	0.342282	-41.040988	C	-1.372659	-0.342762	-25.405960
C	0.991268	1.008963	-39.738150	C	-0.991404	-1.009360	-24.103108
C	-0.343029	1.372472	-39.738124	C	0.342808	-1.372658	-24.103126
C	-1.009346	0.991585	-38.434908	C	1.009364	-0.991447	-25.406005
C	-1.372782	-0.342600	-38.434895	C	1.372733	0.342749	-25.406002
C	-0.991719	-1.009186	-37.131965	C	0.991520	1.009335	-24.103130
C	0.342472	-1.372625	-37.131989	C	-0.342693	1.372633	-24.103104
C	1.008867	-0.991435	-38.434963	C	-1.009263	0.991414	-22.800243
C	1.372304	0.342750	-38.434952	C	-1.372609	-0.342782	-22.800231
C	0.991298	1.009322	-37.131998	C	-0.991343	-1.009365	-21.497374
C	-0.342893	1.372761	-37.131958	C	0.342871	-1.372655	-21.497393
C	-1.009455	0.991549	-35.829025	C	1.009416	-0.991449	-22.800277
C	-1.372820	-0.342668	-35.829013	C	1.372762	0.342747	-22.800266
C	-0.991600	-1.009258	-34.526117	C	0.991530	1.009321	-21.497392
C	0.342613	-1.372624	-34.526143	C	-0.342683	1.372612	-21.497377
C	1.009093	-0.991428	-35.829084	C	-1.009257	0.991407	-20.194515
C	1.372458	0.342790	-35.829073	C	-1.372549	-0.342814	-20.194506
C	0.991298	1.009362	-34.526149	C	-0.991310	-1.009429	-18.891649
C	-0.342915	1.372728	-34.526108	C	0.342917	-1.372719	-18.891672
C	-1.009447	0.991479	-33.223200	C	1.009475	-0.991458	-20.194541
C	-1.372732	-0.342746	-33.223205	C	1.372767	0.342763	-20.194534
C	-0.991498	-1.009274	-31.920322	C	0.991556	1.009372	-18.891665
C	0.342718	-1.372579	-31.920356	C	-0.342671	1.372663	-18.891662
C	1.009204	-0.991392	-33.223262	C	-1.009276	0.991400	-17.588805
C	1.372489	0.342833	-33.223264	C	-1.372532	-0.342831	-17.588803
C	0.991314	1.009344	-31.920352	C	-0.991230	-1.009356	-16.285920
C	-0.342902	1.372648	-31.920320	C	0.342979	-1.372642	-16.285939
C	-1.009425	0.991446	-30.617418	C	1.009547	-0.991461	-17.588823
C	-1.372708	-0.342766	-30.617437	C	1.372803	0.342770	-17.588826
C	-0.991467	-1.009333	-29.314568	C	0.991524	1.009292	-16.285934
C	0.342746	-1.372618	-29.314603	C	-0.342686	1.372579	-16.285932
C	1.009297	-0.991395	-30.617477	C	-1.009229	0.991371	-14.983031
C	1.372581	0.342817	-30.617493	C	-1.372455	-0.342860	-14.983034
C	0.991395	1.009366	-29.314596	C	-0.991234	-1.009465	-13.680162
C	-0.342818	1.372652	-29.314570	C	0.342995	-1.372755	-13.680171

C	1.009543	-0.991437	-14.983046	C	-1.009143	0.991272	0.651441
C	1.372770	0.342793	-14.983053	C	-1.372363	-0.342952	0.651442
C	0.991567	1.009395	-13.680174	C	-0.991133	-1.009485	1.954309
C	-0.342662	1.372686	-13.680165	C	0.343092	-1.372731	1.954300
C	-1.009221	0.991373	-12.377292	C	1.009621	-0.991434	0.651428
C	-1.372468	-0.342870	-12.377297	C	1.372841	0.342790	0.651440
C	-0.991241	-1.009459	-11.074420	C	0.991613	1.009312	1.954315
C	0.342996	-1.372741	-11.074422	C	-0.342611	1.372560	1.954310
C	1.009572	-0.991446	-12.377307	C	-1.009102	0.991306	3.257178
C	1.372820	0.342797	-12.377313	C	-1.372340	-0.342921	3.257174
C	0.991609	1.009381	-11.074429	C	-0.991184	-1.009447	4.560056
C	-0.342629	1.372664	-11.074413	C	0.343031	-1.372767	4.560056
C	-1.009195	0.991392	-9.771546	C	1.009580	-0.991485	3.257174
C	-1.372492	-0.342833	-9.771553	C	1.372818	0.342742	3.257179
C	-0.991240	-1.009381	-8.468667	C	0.991656	1.009263	4.560065
C	0.342974	-1.372681	-8.468669	C	-0.342558	1.372584	4.560058
C	1.009579	-0.991475	-9.771562	C	-1.009159	0.991378	5.862912
C	1.372876	0.342751	-9.771568	C	-1.372441	-0.342849	5.862906
C	0.991639	1.009290	-8.468673	C	-0.991223	-1.009437	7.165782
C	-0.342574	1.372592	-8.468658	C	0.342983	-1.372773	7.165792
C	-1.009139	0.991402	-7.165776	C	1.009621	-0.991563	5.862921
C	-1.372477	-0.342805	-7.165782	C	1.372903	0.342663	5.862919
C	-0.991262	-1.009439	-5.862914	C	0.991672	1.009251	7.165793
C	0.342963	-1.372729	-5.862920	C	-0.342534	1.372588	7.165785
C	1.009555	-0.991499	-7.165794	C	-1.009121	0.991352	8.468662
C	1.372892	0.342707	-7.165795	C	-1.372424	-0.342862	8.468654
C	0.991691	1.009331	-5.862917	C	-0.991232	-1.009472	9.771548
C	-0.342533	1.372622	-5.862906	C	0.342992	-1.372772	9.771569
C	-1.009122	0.991370	-4.560049	C	1.009550	-0.991533	8.468683
C	-1.372455	-0.342841	-4.560051	C	1.372853	0.342681	8.468675
C	-0.991179	-1.009398	-3.257175	C	0.991640	1.009297	9.771561
C	0.343045	-1.372649	-3.257184	C	-0.342585	1.372598	9.771553
C	1.009565	-0.991487	-4.560069	C	-1.009232	0.991343	11.074408
C	1.372898	0.342724	-4.560062	C	-1.372515	-0.342895	11.074404
C	0.991634	1.009268	-3.257175	C	-0.991229	-1.009478	12.377292
C	-0.342590	1.372520	-3.257168	C	0.343016	-1.372718	12.377318
C	-1.009158	0.991311	-1.954302	C	1.009612	-0.991507	11.074441
C	-1.372416	-0.342911	-1.954300	C	1.372895	0.342730	11.074432
C	-0.991120	-1.009457	-0.651436	C	0.991579	1.009325	12.377306
C	0.343103	-1.372681	-0.651447	C	-0.342665	1.372567	12.377294
C	1.009623	-0.991451	-1.954320	C	-1.009281	0.991320	13.680148
C	1.372881	0.342771	-1.954308	C	-1.372557	-0.342914	13.680153
C	0.991593	1.009305	-0.651433	C	-0.991246	-1.009461	14.983032
C	-0.342630	1.372530	-0.651432	C	0.342990	-1.372667	14.983060

C	1.009599	-0.991457	13.680189	C	-1.009437	0.991427	29.314566
C	1.372874	0.342776	13.680186	C	-1.372693	-0.342794	29.314569
C	0.991529	1.009339	14.983047	C	-0.991483	-1.009357	30.617438
C	-0.342707	1.372546	14.983031	C	0.342736	-1.372612	30.617474
C	-1.009222	0.991308	16.285905	C	1.009307	-0.991389	29.314600
C	-1.372485	-0.342908	16.285918	C	1.372562	0.342832	29.314604
C	-0.991311	-1.009470	17.588807	C	0.991315	1.009405	30.617459
C	0.342926	-1.372703	17.588829	C	-0.342904	1.372660	30.617456
C	1.009467	-0.991413	16.285950	C	-1.009429	0.991417	31.920321
C	1.372730	0.342803	16.285954	C	-1.372709	-0.342805	31.920320
C	0.991518	1.009383	17.588822	C	-0.991544	-1.009308	33.223222
C	-0.342719	1.372616	17.588798	C	0.342687	-1.372573	33.223246
C	-1.009327	0.991384	18.891635	C	1.009223	-0.991359	31.920356
C	-1.372599	-0.342846	18.891648	C	1.372503	0.342863	31.920357
C	-0.991359	-1.009400	20.194522	C	0.991300	1.009378	33.223243
C	0.342866	-1.372679	20.194535	C	-0.342931	1.372642	33.223224
C	1.009494	-0.991454	18.891681	C	-1.009469	0.991478	34.526113
C	1.372767	0.342777	18.891686	C	-1.372816	-0.342740	34.526105
C	0.991487	1.009348	20.194539	C	-0.991638	-1.009240	35.829043
C	-0.342737	1.372628	20.194506	C	0.342584	-1.372586	35.829056
C	-1.009307	0.991413	21.497363	C	1.009183	-0.991395	34.526154
C	-1.372588	-0.342804	21.497367	C	1.372531	0.342823	34.526145
C	-0.991399	-1.009359	22.800251	C	0.991311	1.009337	35.829065
C	0.342800	-1.372695	22.800261	C	-0.342912	1.372683	35.829029
C	1.009397	-0.991449	21.497406	C	-1.009455	0.991547	37.131956
C	1.372678	0.342768	21.497404	C	-1.372872	-0.342650	37.131952
C	0.991451	1.009338	22.800269	C	-0.991700	-1.009063	38.434924
C	-0.342748	1.372675	22.800236	C	0.342494	-1.372473	38.434941
C	-1.009350	0.991448	24.103099	C	1.009082	-0.991433	37.132005
C	-1.372635	-0.342768	24.103098	C	1.372499	0.342763	37.131996
C	-0.991437	-1.009337	25.405974	C	0.991279	1.009196	38.434946
C	0.342765	-1.372687	25.405992	C	-0.342914	1.372605	38.434907
C	1.009364	-0.991455	24.103138	C	-1.009143	0.991588	39.738103
C	1.372650	0.342761	24.103133	C	-1.372620	-0.342719	39.738113
C	0.991414	1.009342	25.405992	C	-0.992194	-1.010596	41.040949
C	-0.342787	1.372693	25.405971	C	0.341972	-1.374043	41.040981
C	-1.009384	0.991445	26.708818	C	1.008672	-0.991433	39.738161
C	-1.372663	-0.342773	26.708818	C	1.372150	0.342873	39.738161
C	-0.991434	-1.009272	28.011697	C	0.991671	1.010774	41.040970
C	0.342771	-1.372576	28.011731	C	-0.342494	1.374222	41.040940
C	1.009326	-0.991429	26.708852	C	-1.011477	0.991156	42.342585
C	1.372605	0.342790	26.708852	C	-1.374369	-0.341099	42.342609
C	0.991339	1.009299	28.011716	C	-0.987502	-0.992280	43.645971
C	-0.342866	1.372604	28.011712	C	0.347112	-1.355867	43.646015

C	1.010900	-0.990951	42.342650	C	-1.181481	0.777680	-39.737143
C	1.373792	0.341303	42.342661	C	-1.280119	-0.601704	-39.737135
C	0.986871	0.992513	43.645991	C	-0.777527	-1.181757	-38.433947
C	-0.347743	1.356100	43.645968	C	0.601730	-1.280402	-38.433931
C	-0.994107	0.985055	44.978932	C	1.181955	-0.777655	-37.130989
C	-1.356285	-0.344633	44.978967	C	1.280609	0.601596	-37.130988
C	-1.038545	-1.235547	46.150390	C	0.777750	1.181757	-38.433932
C	0.267694	-1.591429	46.150417	C	-0.601507	1.280403	-38.433946
C	0.993418	-0.984792	44.979001	C	-1.181762	0.777659	-37.131020
C	1.355595	0.344896	44.979020	C	-1.280416	-0.601593	-37.131017
C	1.037806	1.235837	46.150406	C	-0.777596	-1.181876	-35.828097
C	-0.268434	1.591717	46.150366	C	0.601658	-1.280538	-35.828080
H	-2.261454	-0.723778	-46.872064	C	1.181949	-0.777680	-34.525178
H	-1.581720	1.770675	-46.872169	C	1.280637	0.601571	-34.525181
H	2.260640	0.723980	-46.872140	C	0.777758	1.181882	-35.828083
H	1.580910	-1.770474	-46.872226	C	-0.601496	1.280546	-35.828101
H	-1.770980	-1.581354	46.872056	C	-1.181820	0.777692	-34.525214
H	0.723486	-2.261043	46.872025	C	-1.280508	-0.601559	-34.525212
H	-0.724262	2.261333	46.871949	C	-0.777649	-1.181859	-33.222330
H	1.770204	1.581647	46.872108	C	0.601598	-1.280550	-33.222312
(4) SWCNT-36 EBF(3)-B3LYP(4L)/6-31G							
C	-0.779429	-1.413339	-46.149308	C	1.181903	-0.777687	-31.919438
C	0.570969	-1.509926	-46.149231	C	1.280604	0.601558	-31.919441
C	1.165658	-0.774108	-44.977993	C	0.777744	1.181877	-33.222316
C	1.263872	0.600503	-44.977998	C	-0.601503	1.280569	-33.222336
C	0.779793	1.413362	-46.149287	C	-1.181842	0.777712	-31.919475
C	-0.570604	1.509951	-46.149228	C	-1.280543	-0.601533	-31.919472
C	-1.165313	0.774126	-44.978005	C	-0.777692	-1.181861	-30.616610
C	-1.263527	-0.600486	-44.978021	C	0.601551	-1.280564	-30.616590
C	-0.776439	-1.164498	-43.644967	C	1.181860	-0.777690	-29.313737
C	0.603272	-1.263097	-43.644939	C	1.280582	0.601550	-29.313738
C	1.183961	-0.776748	-42.341563	C	0.777719	1.181892	-30.616597
C	1.282446	0.600525	-42.341554	C	-0.601523	1.280595	-30.616613
C	0.776762	1.164509	-43.644949	C	-1.181864	0.777727	-29.313771
C	-0.602949	1.263108	-43.644942	C	-1.280586	-0.601513	-29.313767
C	-1.183661	0.776754	-42.341580	C	-0.777738	-1.181832	-28.010915
C	-1.282145	-0.600519	-42.341577	C	0.601500	-1.280563	-28.010898
C	-0.777603	-1.183501	-41.039943	C	1.181816	-0.777720	-26.708051
C	0.601651	-1.282107	-41.039924	C	1.280568	0.601515	-26.708052
C	1.181731	-0.777679	-39.737120	C	0.777704	1.181872	-28.010902
C	1.280370	0.601705	-39.737109	C	-0.601533	1.280604	-28.010916
C	0.777880	1.183503	-41.039926	C	-1.181876	0.777764	-26.708078
C	-0.601374	1.282110	-41.039932	C	-1.280629	-0.601471	-26.708077
				C	-0.777802	-1.181801	-25.405230
				C	0.601426	-1.280580	-25.405217

C	1.181761	-0.777761	-24.102372	C	-1.181858	0.777833	-11.074053
C	1.280570	0.601467	-24.102370	C	-1.280747	-0.601391	-11.074059
C	0.777717	1.181846	-25.405218	C	-0.777943	-1.181808	-9.771234
C	-0.601511	1.280625	-25.405228	C	0.601281	-1.280692	-9.771233
C	-1.181867	0.777805	-24.102389	C	1.181699	-0.777883	-8.468404
C	-1.280675	-0.601423	-24.102390	C	1.280586	0.601341	-8.468398
C	-0.777861	-1.181797	-22.799552	C	0.777784	1.181768	-9.771227
C	0.601370	-1.280606	-22.799542	C	-0.601440	1.280652	-9.771226
C	1.181745	-0.777781	-21.496708	C	-1.181860	0.777837	-8.468403
C	1.280565	0.601449	-21.496700	C	-1.280747	-0.601387	-8.468402
C	0.777738	1.181839	-22.799540	C	-0.777928	-1.181811	-7.165579
C	-0.601493	1.280648	-22.799546	C	0.601294	-1.280690	-7.165574
C	-1.181880	0.777818	-21.496714	C	1.181703	-0.777861	-5.862740
C	-1.280701	-0.601412	-21.496713	C	1.280572	0.601361	-5.862737
C	-0.777864	-1.181797	-20.193879	C	0.777765	1.181761	-7.165574
C	0.601366	-1.280605	-20.193871	C	-0.601458	1.280641	-7.165572
C	1.181753	-0.777765	-18.891037	C	-1.181871	0.777809	-5.862744
C	1.280555	0.601466	-18.891028	C	-1.280739	-0.601412	-5.862742
C	0.777718	1.181828	-20.193867	C	-0.777914	-1.181823	-4.559911
C	-0.601512	1.280636	-20.193866	C	0.601308	-1.280674	-4.559908
C	-1.181905	0.777787	-18.891034	C	1.181716	-0.777854	-3.257072
C	-1.280707	-0.601444	-18.891037	C	1.280576	0.601372	-3.257074
C	-0.777851	-1.181841	-17.588214	C	0.777743	1.181772	-4.559909
C	0.601380	-1.280616	-17.588212	C	-0.601480	1.280623	-4.559912
C	1.181740	-0.777760	-16.285377	C	-1.181894	0.777804	-3.257080
C	1.280542	0.601466	-16.285371	C	-1.280753	-0.601422	-3.257079
C	0.777695	1.181855	-17.588203	C	-0.777924	-1.181821	-1.954247
C	-0.601536	1.280629	-17.588201	C	0.601303	-1.280685	-1.954247
C	-1.181898	0.777763	-16.285369	C	1.181706	-0.777864	-0.651410
C	-1.280700	-0.601463	-16.285376	C	1.280571	0.601365	-0.651414
C	-0.777863	-1.181829	-14.982545	C	0.777742	1.181774	-1.954247
C	0.601362	-1.280626	-14.982550	C	-0.601485	1.280638	-1.954254
C	1.181743	-0.777813	-13.679714	C	-1.181893	0.777820	-0.651419
C	1.280574	0.601413	-13.679712	C	-1.280758	-0.601408	-0.651418
C	0.777704	1.181822	-14.982535	C	-0.777941	-1.181817	0.651418
C	-0.601522	1.280620	-14.982538	C	0.601287	-1.280685	0.651420
C	-1.181902	0.777796	-13.679705	C	1.181695	-0.777860	1.954252
C	-1.280733	-0.601430	-13.679715	C	1.280569	0.601366	1.954251
C	-0.777913	-1.181809	-12.376890	C	0.777750	1.181778	0.651415
C	0.601313	-1.280661	-12.376894	C	-0.601478	1.280646	0.651412
C	1.181699	-0.777867	-11.074059	C	-1.181888	0.777826	1.954246
C	1.280588	0.601356	-11.074055	C	-1.280763	-0.601400	1.954251
C	0.777754	1.181783	-12.376882	C	-0.777939	-1.181812	3.257079
C	-0.601471	1.280636	-12.376884	C	0.601286	-1.280684	3.257080

C	1.181695	-0.777850	4.559911	C	-1.181860	0.777769	17.588221
C	1.280556	0.601372	4.559909	C	-1.280644	-0.601462	17.588219
C	0.777744	1.181783	3.257074	C	-0.777786	-1.181841	18.891041
C	-0.601481	1.280655	3.257074	C	0.601445	-1.280647	18.891027
C	-1.181887	0.777826	4.559910	C	1.181817	-0.777804	20.193863
C	-1.280748	-0.601396	4.559914	C	1.280623	0.601426	20.193860
C	-0.777932	-1.181795	5.862745	C	0.777772	1.181813	18.891031
C	0.601289	-1.280667	5.862742	C	-0.601458	1.280619	18.891041
C	1.181698	-0.777852	7.165574	C	-1.181811	0.777775	20.193884
C	1.280574	0.601371	7.165570	C	-1.280617	-0.601455	20.193880
C	0.777744	1.181775	5.862738	C	-0.777781	-1.181830	21.496716
C	-0.601477	1.280646	5.862741	C	0.601449	-1.280646	21.496703
C	-1.181878	0.777834	7.165580	C	1.181842	-0.777809	22.799540
C	-1.280755	-0.601388	7.165580	C	1.280645	0.601421	22.799537
C	-0.777936	-1.181792	8.468409	C	0.777808	1.181800	21.496706
C	0.601288	-1.280671	8.468399	C	-0.601423	1.280615	21.496713
C	1.181716	-0.777861	9.771224	C	-1.181799	0.777779	22.799555
C	1.280589	0.601364	9.771222	C	-1.280603	-0.601451	22.799553
C	0.777765	1.181777	8.468400	C	-0.777751	-1.181830	24.102387
C	-0.601459	1.280655	8.468403	C	0.601477	-1.280636	24.102378
C	-1.181872	0.777847	9.771239	C	1.181857	-0.777773	25.405222
C	-1.280746	-0.601378	9.771238	C	1.280637	0.601454	25.405217
C	-0.777913	-1.181790	11.074063	C	0.777809	1.181801	24.102377
C	0.601311	-1.280672	11.074053	C	-0.601419	1.280607	24.102383
C	1.181735	-0.777841	12.376877	C	-1.181788	0.777748	25.405229
C	1.280587	0.601385	12.376879	C	-1.280568	-0.601480	25.405229
C	0.777772	1.181776	11.074053	C	-0.777707	-1.181854	26.708071
C	-0.601452	1.280657	11.074062	C	0.601528	-1.280611	26.708065
C	-1.181857	0.777825	12.376898	C	1.181892	-0.777736	28.010908
C	-1.280709	-0.601400	12.376899	C	1.280630	0.601501	28.010903
C	-0.777861	-1.181827	13.679716	C	0.777787	1.181832	26.708061
C	0.601364	-1.280665	13.679707	C	-0.601448	1.280589	26.708064
C	1.181779	-0.777804	14.982529	C	-1.181804	0.777719	28.010910
C	1.280587	0.601421	14.982534	C	-1.280542	-0.601518	28.010912
C	0.777759	1.181810	13.679706	C	-0.777668	-1.181863	29.313760
C	-0.601466	1.280647	13.679720	C	0.601571	-1.280592	29.313756
C	-1.181859	0.777784	14.982553	C	1.181923	-0.777712	30.616605
C	-1.280668	-0.601441	14.982555	C	1.280631	0.601530	30.616599
C	-0.777801	-1.181824	16.285379	C	0.777762	1.181853	29.313750
C	0.601424	-1.280638	16.285367	C	-0.601477	1.280582	29.313751
C	1.181825	-0.777794	17.588197	C	-1.181824	0.777709	30.616603
C	1.280608	0.601436	17.588197	C	-1.280532	-0.601534	30.616606
C	0.777744	1.181801	16.285368	C	-0.777650	-1.181869	31.919462
C	-0.601482	1.280614	16.285382	C	0.601594	-1.280573	31.919461

C	1.181921	-0.777692	33.222325	C	-1.413236	0.779647	46.149305
C	1.280614	0.601555	33.222321	C	-1.509837	-0.570748	46.149232
C	0.777754	1.181873	31.919452	H	1.147726	-2.078671	-46.870821
C	-0.601490	1.280577	31.919454	H	-1.431167	-1.894200	-46.870988
C	-1.181813	0.777703	33.222323	H	-1.147350	2.078715	-46.870812
C	-1.280506	-0.601544	33.222328	H	1.431541	1.894218	-46.870961
C	-0.777630	-1.181874	34.525202	H	1.894705	-1.431355	46.870680
C	0.601621	-1.280563	34.525201	H	2.079287	1.147534	46.870454
C	1.181938	-0.777665	35.828090	H	-2.079061	-1.147466	46.870479
C	1.280602	0.601589	35.828087	H	-1.894458	1.431422	46.870713
C	0.777743	1.181893	34.525192				
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C	-1.181819	0.777691	35.828091	(5) 1RPB(charge=-1) GEBF(5)-HF/6-31G			
C	-1.280483	-0.601563	35.828096	N	-0.241919	3.766950	-2.775337
C	-0.777595	-1.181841	37.131011	C	-1.475019	4.300706	-3.354261
C	0.601656	-1.280497	37.131005	C	-1.630568	3.909038	-4.825205
C	1.181823	-0.777619	38.433938	O	-1.841045	4.782471	-5.666813
C	1.280471	0.601637	38.433933	C	-1.593002	5.817081	-3.175014
C	0.777721	1.181875	37.131000	S	-3.403706	6.329878	-3.364404
C	-0.601531	1.280530	37.131002	H	0.505472	3.513933	-3.378869
C	-1.181688	0.777659	38.433943	H	-2.292002	3.843494	-2.820436
C	-1.280335	-0.601597	38.433945	H	-1.277505	6.088935	-2.182724
C	-0.777607	-1.181582	39.737138	H	-1.019484	6.355125	-3.909083
C	0.601776	-1.280222	39.737123	N	-1.614235	2.597606	-5.145526
C	1.183582	-0.777717	41.039930	C	-2.041818	2.192098	-6.474438
C	1.282189	0.601536	41.039921	C	-2.958884	0.975688	-6.383630
C	0.777754	1.181628	39.737126	O	-3.377652	0.536056	-5.307241
C	-0.601630	1.280267	39.737123	C	-0.908984	2.064142	-7.518594
C	-1.183422	0.777768	41.039940	C	0.046265	0.852220	-7.437963
C	-1.282030	-0.601486	41.039937	C	0.631413	0.574321	-8.832564
C	-0.776665	-1.183783	42.341578	C	1.179520	1.058466	-6.423490
C	0.600609	-1.282268	42.341564	H	-1.393020	1.893918	-4.463775
C	1.164596	-0.776572	43.644952	H	-2.673068	2.996809	-6.837697
C	1.263198	0.603141	43.644931	H	-1.372529	2.077083	-8.503338
C	0.776839	1.183837	42.341565	H	-0.338303	2.984508	-7.466904
C	-0.600434	1.282323	42.341568	H	-0.517336	-0.030261	-7.143134
C	-1.164403	0.776631	43.644967	H	-0.148463	0.335335	-9.549703
C	-1.263006	-0.603082	43.644951	H	1.174583	1.439183	-9.203601
C	-0.774015	-1.165457	44.978009	H	1.321174	-0.262523	-8.806348
C	0.600591	-1.263668	44.978010	H	1.780410	1.919182	-6.702583
C	1.413465	-0.779582	46.149283	H	0.805390	1.199357	-5.421141
C	1.510065	0.570813	46.149207	H	1.835048	0.192097	-6.419382
C	0.774226	1.165519	44.977995	N	-3.365214	0.446130	-7.557619
C	-0.600380	1.263730	44.978017	C	-4.376720	-0.595471	-7.652682
				C	-3.750044	-1.971060	-7.825340

O	-3.231705	-2.289440	-8.898365	O	-1.254728	-2.136659	0.194063
H	-2.970215	0.767935	-8.407613	C	0.366595	-4.394479	2.541190
H	-5.000646	-0.546253	-6.775402	S	1.935478	-4.347748	1.500897
H	-4.980765	-0.403586	-8.527631	H	-0.274120	-4.625597	-0.217540
N	-3.797113	-2.765268	-6.747958	H	-1.725651	-4.183955	2.289342
C	-3.253731	-4.113405	-6.661902	H	0.504206	-3.788471	3.422624
C	-3.775440	-4.653164	-5.330132	H	0.220352	-5.415479	2.851359
O	-4.374704	-3.902178	-4.557084	N	-0.817163	-1.584699	2.331780
C	-1.699882	-4.100766	-6.778939	C	-1.058976	-0.161175	2.118595
C	-1.054245	-5.461680	-7.112221	C	0.228258	0.544708	1.693074
C	-1.049225	-3.461663	-5.546600	O	1.316382	0.169313	2.132850
C	-1.586560	-6.151019	-8.376307	C	-1.579043	0.439871	3.444152
H	-4.230544	-2.441105	-5.912698	C	-2.072647	1.874723	3.442793
H	-3.666943	-4.709602	-7.466842	O	-1.886027	2.587124	4.441182
H	-1.512474	-3.464520	-7.633924	N	-2.763673	2.321765	2.391855
H	0.002930	-5.265123	-7.257594	H	-0.396216	-1.844942	3.195956
H	-1.105428	-6.137908	-6.263909	H	-1.796007	-0.070854	1.340527
H	-1.500286	-2.507904	-5.310164	H	-2.406866	-0.179202	3.773184
H	-1.125089	-4.096246	-4.668942	H	-0.801761	0.379130	4.192422
H	0.004733	-3.294418	-5.728468	H	-2.988854	1.788493	1.578585
H	-1.659288	-5.450065	-9.200148	H	-3.065723	3.268054	2.393260
H	-0.922823	-6.954040	-8.677770	N	0.074524	1.605461	0.867087
H	-2.568509	-6.591261	-8.235471	C	1.187318	2.465576	0.507737
N	-3.578776	-5.948557	-5.019354	C	1.382347	3.614704	1.499754
C	-4.104568	-6.510526	-3.780118	O	2.483329	3.762113	2.027664
C	-3.005901	-7.037101	-2.875011	C	1.155896	2.928380	-0.964012
O	-2.562722	-8.171041	-3.049700	C	-0.142707	3.514743	-1.458213
H	-3.134582	-6.564756	-5.656923	O	-1.078382	3.764904	-0.681349
H	-4.688938	-5.745792	-3.298261	H	-0.841379	1.874378	0.571517
H	-4.743114	-7.351295	-4.009641	H	2.087865	1.887146	0.621830
N	-2.569564	-6.230587	-1.882023	H	1.947539	3.657088	-1.112273
C	-1.697889	-6.736417	-0.813980	H	1.394368	2.090436	-1.600898
C	-1.809026	-5.816397	0.404059	N	0.352975	4.441738	1.776108
O	-2.682100	-6.028151	1.245740	C	0.553190	5.528780	2.719299
C	-0.268572	-6.984376	-1.279803	C	-0.801531	5.953853	3.243234
O	0.405985	-7.484523	-0.118494	O	-1.724731	6.153388	2.438440
H	-2.959621	-5.322251	-1.798846	C	1.254607	6.730983	2.029994
H	-2.098649	-7.683727	-0.485032	C	1.874885	7.723078	2.985151
H	-0.283927	-7.727543	-2.063108	C	3.097684	7.430762	3.589483
H	0.198193	-6.086568	-1.657693	C	1.264560	8.941077	3.262430
H	1.352726	-7.491699	-0.188849	C	3.689288	8.335629	4.457047
N	-0.949922	-4.778679	0.497016	C	1.853245	9.847059	4.134226
C	-0.845849	-3.971968	1.693731	C	3.065789	9.545559	4.733951
C	-0.947325	-2.488297	1.343292	H	-0.486718	4.416753	1.238816

H	1.179618	5.163759	3.517764	C	-1.001814	-0.472918	-2.688165
H	2.030269	6.309160	1.406740	O	-0.598083	0.495409	-3.361159
H	0.538175	7.218401	1.378143	C	-3.232448	-1.732155	-2.686722
H	3.588857	6.504192	3.359027	C	-4.586467	-1.856377	-2.020269
H	0.335023	9.192591	2.786038	C	-5.742241	-1.422612	-2.666347
H	4.638537	8.109166	4.902421	C	-4.715776	-2.405236	-0.749460
H	1.372513	10.786946	4.330110	C	-6.984327	-1.524920	-2.067751
H	3.527016	10.252401	5.396621	C	-5.957732	-2.517430	-0.136835
N	-0.940461	6.113580	4.563536	C	-7.088643	-2.073098	-0.799728
C	-2.068829	6.763882	5.241119	O	-8.351873	-2.150378	-0.255680
C	-3.435383	6.384554	4.673347	H	-3.420350	0.903650	-3.251060
O	-4.294264	7.248335	4.510120	H	-2.304592	-0.690831	-1.062108
C	-1.897483	8.281406	5.284243	H	-3.362206	-1.592772	-3.748979
H	-0.162638	5.895979	5.140755	H	-2.668241	-2.644367	-2.548917
H	-2.055987	6.380600	6.256121	H	-5.668467	-1.004602	-3.652653
H	-0.950195	8.535234	5.742022	H	-3.840613	-2.737358	-0.227314
H	-1.925434	8.694483	4.285817	H	-7.873071	-1.194088	-2.566178
H	-2.697011	8.734266	5.852999	H	-6.041472	-2.946181	0.844408
N	-3.687119	5.081299	4.434348	H	-8.393737	-2.505674	0.624173
C	-5.007497	4.662801	4.011398	N	-0.205943	-1.502634	-2.369889
C	-5.358036	4.874836	2.546141	C	1.203218	-1.547146	-2.703738
O	-6.478016	4.554062	2.157559	C	1.674144	-2.989551	-2.744409
H	-2.989824	4.382752	4.596722	O	1.103870	-3.882225	-2.115055
H	-5.122720	3.610143	4.224002	C	2.051664	-0.800553	-1.660407
H	-5.762779	5.201288	4.567019	H	-0.521754	-2.156058	-1.683288
N	-4.419704	5.389868	1.719718	H	1.331711	-1.093268	-3.677093
C	-4.752215	5.846352	0.371092	H	2.039941	-1.309853	-0.709772
C	-5.071589	4.698768	-0.577358	H	3.084034	-0.699567	-1.965158
O	-6.098335	4.702950	-1.247771	H	1.634220	0.179512	-1.523288
C	-3.558278	6.693724	-0.082714	N	2.806523	-3.199011	-3.457059
S	-3.741605	7.703961	-1.656372	C	3.503402	-4.476474	-3.551989
H	-3.557198	5.715836	2.104641	C	4.561983	-4.645054	-2.458605
H	-5.648858	6.448250	0.394549	O	4.876486	-5.775139	-2.086526
H	-3.393237	7.468512	0.652468	C	4.124673	-4.624183	-4.968379
H	-2.653968	6.112209	-0.142390	C	4.878813	-5.949949	-5.146080
N	-4.166615	3.699753	-0.678539	C	3.047053	-4.504445	-6.056229
C	-4.421802	2.591538	-1.564051	H	3.143396	-2.452072	-4.020438
C	-3.466526	1.461532	-1.289906	H	2.785242	-5.265779	-3.390888
O	-3.036220	1.236458	-0.140920	H	4.836375	-3.808849	-5.098871
H	-3.277656	3.743489	-0.228401	H	5.685500	-6.070428	-4.440451
H	-5.427001	2.225568	-1.395420	H	4.206719	-6.791694	-5.021924
H	-4.370301	2.897682	-2.601342	H	5.290740	-5.995990	-6.148454
N	-3.130776	0.687329	-2.319998	H	2.310530	-5.294122	-5.954006
C	-2.414125	-0.549725	-2.122686	H	2.527288	-3.555645	-6.031396

H	3.502292	-4.601000	-7.035378	H	5.997385	1.483462	-0.454830
N	5.145931	-3.524370	-1.992341	H	7.989511	4.351583	1.995341
C	6.102221	-3.486860	-0.890040	H	7.694344	3.262478	-0.199846
C	5.398541	-2.731163	0.232246	N	4.328608	-0.946665	6.430739
O	4.830399	-1.663982	-0.032824	C	4.116372	-1.462628	7.767829
C	7.408512	-2.762653	-1.292764	C	4.374865	-2.989008	7.715607
C	8.375176	-2.646839	-0.102773	O	4.558513	-3.486703	6.566518
C	8.088075	-3.466654	-2.472156	C	2.728821	-1.150324	8.365539
H	4.740296	-2.645708	-2.212280	C	1.514494	-1.557856	7.573778
H	6.315356	-4.506270	-0.605722	C	0.654266	-0.686887	7.003241
H	7.126515	-1.759519	-1.603641	C	0.952586	-2.890033	7.348869
H	7.949158	-2.121357	0.740919	N	-0.409474	-1.363400	6.401558
H	8.686368	-3.631180	0.235876	C	-0.246004	-2.718388	6.635241
H	9.267794	-2.110968	-0.405746	C	1.344182	-4.184271	7.710962
H	7.433655	-3.527221	-3.332601	C	-1.061648	-3.789387	6.274931
H	8.979052	-2.923697	-2.769151	C	0.540828	-5.250118	7.348535
H	8.387390	-4.474825	-2.205188	C	-0.652131	-5.057773	6.639792
N	5.385783	-3.272838	1.452652	O	4.327894	-3.578508	8.819661
C	4.620507	-2.697114	2.536298	H	4.505127	-1.690907	5.795218
C	5.372506	-1.567407	3.231524	H	4.849013	-1.035103	8.443813
O	6.596660	-1.564579	3.325886	H	2.706871	-1.626753	9.338549
C	4.264049	-3.754142	3.584420	H	2.677291	-0.079867	8.528056
S	3.415572	-5.270098	2.850006	H	0.701599	0.380208	6.976764
H	5.898704	-4.102641	1.627589	H	-1.273446	-0.930848	6.185779
H	3.719213	-2.287820	2.106942	H	2.254684	-4.346936	8.254298
H	5.136129	-4.156985	4.079967	H	-1.986907	-3.636350	5.749438
H	3.633817	-3.359973	4.360237	H	0.835704	-6.246658	7.616235
N	4.565663	-0.629845	3.766406	H	-1.259297	-5.906538	6.380546
C	5.017928	0.472666	4.602090				
C	4.520003	0.311715	6.049507	(6) IRPB(charge=-1) GEBF(6)-HF/6-31G			
O	4.389006	1.303730	6.779694	N	-0.277408	3.790857	-2.804593
C	4.621251	1.826792	3.991673	C	-1.456295	4.401999	-3.410056
C	5.479454	2.218793	2.806531	C	-1.650480	3.945211	-4.855782
C	5.328471	1.611324	1.560241	O	-1.817382	4.786583	-5.738753
C	6.451883	3.205841	2.941520	C	-1.429271	5.929392	-3.332943
C	6.124198	1.981795	0.488404	S	-3.184333	6.593206	-3.553136
C	7.246131	3.586183	1.867267	H	0.443559	3.437924	-3.390513
C	7.082940	2.974618	0.634289	H	-2.312166	4.057038	-2.849651
H	3.592388	-0.654321	3.548488	H	-1.075074	6.244106	-2.366559
H	6.096901	0.401476	4.648824	H	-0.816121	6.355274	-4.108821
H	3.582379	1.789706	3.686774	N	-1.715948	2.623438	-5.118618
H	4.698099	2.573861	4.767850	C	-2.178824	2.202266	-6.431109
H	4.598674	0.840133	1.422164	C	-3.122510	1.015606	-6.303422
H	6.585902	3.680423	3.896018	O	-3.508169	0.579754	-5.212034

C	-1.069383	2.040612	-7.500462	O	-3.075436	-8.258326	-2.302584
C	-0.202508	0.765973	-7.505380	H	-2.593249	-6.254262	-5.307858
C	0.532652	0.662579	-8.851787	H	-4.658230	-5.886344	-3.238034
C	0.801531	0.724701	-6.347941	H	-4.433048	-7.401451	-4.088655
H	-1.507084	1.934778	-4.420216	N	-2.192764	-6.202603	-1.949923
H	-2.798251	3.015772	-6.792391	C	-1.407221	-6.620008	-0.788010
H	-1.538194	2.134766	-8.477533	C	-1.653013	-5.686709	0.398446
H	-0.430567	2.911205	-7.411375	O	-2.624297	-5.881299	1.129253
H	-0.848633	-0.105109	-7.425028	C	0.051948	-6.814867	-1.178223
H	-0.161459	0.601337	-9.683857	O	0.761812	-7.183255	0.007797
H	1.171362	1.525643	-9.011334	H	-2.138486	-5.261208	-2.263395
H	1.159334	-0.222445	-8.882466	H	-1.806331	-7.568893	-0.471536
H	1.467295	1.580957	-6.395923	H	0.094181	-7.611906	-1.912078
H	0.319335	0.714099	-5.383273	H	0.464585	-5.919722	-1.618843
H	1.413290	-0.171035	-6.422529	H	1.705005	-7.096802	-0.077013
N	-3.588037	0.507316	-7.461910	N	-0.785603	-4.675735	0.604589
C	-4.579256	-0.552964	-7.522311	C	-0.781722	-3.892966	1.817848
C	-3.898113	-1.902037	-7.677029	C	-0.961914	-2.410066	1.491826
O	-3.329490	-2.180914	-8.737435	O	-1.322575	-2.060012	0.359979
H	-3.208778	0.816890	-8.324282	C	0.445061	-4.237662	2.676593
H	-5.198701	-0.506083	-6.643223	S	1.995789	-3.948824	1.656235
H	-5.194526	-0.393255	-8.394773	H	-0.019835	-4.547122	-0.016896
N	-3.930138	-2.706174	-6.605404	H	-1.658875	-4.183611	2.385442
C	-3.311885	-4.025103	-6.529682	H	0.500617	-3.673460	3.593104
C	-3.797843	-4.617537	-5.202442	H	0.405054	-5.286075	2.919271
O	-4.700839	-4.055930	-4.585423	N	-0.813047	-1.502142	2.472709
C	-1.778680	-3.934899	-6.766452	C	-1.114037	-0.091332	2.253552
C	-1.103781	-5.241319	-7.236802	C	0.133733	0.672331	1.802781
C	-1.036541	-3.294620	-5.589833	O	1.237708	0.375231	2.254783
C	-1.801033	-5.945268	-8.409340	C	-1.639011	0.498212	3.580289
H	-4.480892	-2.455087	-5.814348	C	-2.426869	1.787889	3.526485
H	-3.739009	-4.645018	-7.310710	O	-2.261947	2.644173	4.406485
H	-1.697984	-3.263169	-7.608001	N	-3.358892	1.913926	2.577342
H	-0.103274	-4.965525	-7.556557	H	-0.379686	-1.748146	3.335070
H	-0.957521	-5.937150	-6.414870	H	-1.858051	-0.042607	1.476899
H	-1.474031	-2.339647	-5.328373	H	-2.314305	-0.234701	4.006978
H	-1.038335	-3.925931	-4.708830	H	-0.823626	0.647623	4.272132
H	-0.003365	-3.112863	-5.860931	H	-3.405047	1.352159	1.758139
H	-2.066786	-5.235876	-9.185275	H	-3.945675	2.712964	2.573506
H	-1.148214	-6.690950	-8.847885	N	-0.059924	1.700231	0.940231
H	-2.708765	-6.458344	-8.110159	C	1.059399	2.535679	0.528559
N	-3.277480	-5.788439	-4.762766	C	1.292596	3.731396	1.454438
C	-3.923029	-6.537359	-3.688405	O	2.415436	3.894850	1.929491
C	-3.005153	-7.069222	-2.600459	C	1.036410	2.913843	-0.964423

C	-0.200277	3.598694	-1.474914	C	-4.617458	6.000827	0.198446
O	-1.105211	3.966343	-0.713324	C	-4.984536	4.842530	-0.721728
H	-0.973407	1.879362	0.577716	O	-5.929404	4.930018	-1.497948
H	1.954481	1.951878	0.675001	C	-3.348399	6.733586	-0.257515
H	1.894734	3.548887	-1.164318	S	-3.471460	7.858035	-1.752998
H	1.169760	2.019809	-1.556072	H	-3.556261	6.006138	2.025473
N	0.282835	4.585528	1.728517	H	-5.468964	6.665564	0.168232
C	0.539813	5.714187	2.610851	H	-3.053751	7.429935	0.512913
C	-0.778952	6.161547	3.218621	H	-2.529652	6.048858	-0.397035
O	-1.681340	6.603743	2.493699	N	-4.180257	3.758672	-0.698934
C	1.226761	6.881491	1.860492	C	-4.438975	2.629841	-1.557560
C	1.934414	7.846623	2.782825	C	-3.446006	1.530621	-1.277894
C	3.201596	7.531115	3.272490	O	-2.943334	1.397904	-0.142972
C	1.351004	9.051374	3.158875	H	-3.398787	3.711895	-0.089630
C	3.868235	8.403493	4.117564	H	-5.435277	2.238062	-1.375024
C	2.016323	9.925058	4.009286	H	-4.415146	2.916808	-2.602630
C	3.276882	9.603979	4.488261	N	-3.146772	0.697617	-2.271909
H	-0.559412	4.546753	1.199805	C	-2.399368	-0.519323	-2.039897
H	1.208196	5.371126	3.384194	C	-0.954126	-0.385104	-2.516076
H	1.951572	6.439278	1.190851	O	-0.582744	0.551315	-3.248885
H	0.488733	7.394217	1.258115	C	-3.118268	-1.715798	-2.705395
H	3.663020	6.606213	2.982377	C	-4.529153	-1.936958	-2.202384
H	0.379521	9.310461	2.780267	C	-5.619361	-1.401855	-2.886761
H	4.847796	8.154991	4.476992	C	-4.777848	-2.742418	-1.098735
H	1.556700	10.854781	4.286571	C	-6.916650	-1.675993	-2.498599
H	3.798414	10.284725	5.133746	C	-6.078146	-3.027840	-0.696747
N	-0.907756	6.040543	4.546379	C	-7.143012	-2.501789	-1.408788
C	-1.986108	6.603783	5.365260	O	-8.457852	-2.765197	-1.087046
C	-3.374420	6.433762	4.751905	H	-3.479021	0.861048	-3.201046
O	-4.168311	7.371074	4.745348	H	-2.369578	-0.695252	-0.979990
C	-1.720687	8.063794	5.723604	H	-3.141818	-1.556830	-3.773814
H	-0.153631	5.635031	5.047061	H	-2.527453	-2.604108	-2.525438
H	-1.989761	6.013202	6.275604	H	-5.449132	-0.783424	-3.747713
H	-0.759661	8.161073	6.213085	H	-3.952809	-3.162679	-0.556345
H	-1.730329	8.681343	4.836896	H	-7.757505	-1.284613	-3.034859
H	-2.491657	8.430478	6.385718	H	-6.256731	-3.664625	0.150648
N	-3.707310	5.201115	4.318513	H	-8.583837	-3.363180	-0.359982
C	-5.040307	4.912492	3.846634	N	-0.121513	-1.345101	-2.098365
C	-5.257575	4.953016	2.341128	C	1.289011	-1.410784	-2.429926
O	-6.259092	4.411249	1.871892	C	1.698314	-2.869174	-2.556160
H	-3.065798	4.437945	4.410439	O	1.093495	-3.761499	-1.959208
H	-5.350589	3.936469	4.188547	C	2.169748	-0.770257	-1.342753
H	-5.727468	5.634988	4.265542	H	-0.437131	-1.964595	-1.378954
N	-4.348662	5.593242	1.578254	H	1.439773	-0.903809	-3.372979

H	2.033949	-1.266118	-0.392127	H	4.011511	-3.470935	4.351839
H	3.221624	-0.819879	-1.583867	N	4.740975	-0.704023	3.801775
H	1.896260	0.263295	-1.228068	C	5.092582	0.416989	4.657495
N	2.808144	-3.109957	-3.292621	C	4.543472	0.222650	6.080783
C	3.458272	-4.415645	-3.372880	O	4.432772	1.197266	6.838690
C	4.517676	-4.587148	-2.284407	C	4.611801	1.743219	4.038554
O	4.656754	-5.673851	-1.728261	C	5.395469	2.121458	2.802551
C	4.060004	-4.649911	-4.781434	C	5.142137	1.523498	1.570151
C	4.763276	-6.012531	-4.874452	C	6.410923	3.069459	2.878082
C	2.976441	-4.546007	-5.863919	C	5.885788	1.858982	0.449894
H	3.175579	-2.365107	-3.839352	C	7.149319	3.420350	1.756536
H	2.713037	-5.169803	-3.180260	C	6.887453	2.816000	0.536247
H	4.800682	-3.872811	-4.963488	H	3.776259	-0.780956	3.567060
H	5.582676	-6.104729	-4.177840	H	6.172076	0.427470	4.740393
H	4.068043	-6.819460	-4.673161	H	3.557455	1.655410	3.797033
H	5.154571	-6.150861	-5.875720	H	4.704286	2.513800	4.789572
H	2.192072	-5.277543	-5.698000	H	4.373497	0.784133	1.481611
H	2.517025	-3.565595	-5.898175	H	6.624530	3.535362	3.821416
H	3.407917	-4.740028	-6.840098	H	5.688603	1.359803	-0.481495
N	5.307215	-3.518253	-2.034956	H	7.925273	4.158989	1.835668
C	6.299993	-3.470299	-0.966191	H	7.457893	3.081198	-0.335212
C	5.647541	-2.700325	0.177476	N	4.265631	-1.032110	6.417461
O	5.076377	-1.632699	-0.074940	C	3.968702	-1.559203	7.734545
C	7.597260	-2.766056	-1.425943	C	4.222029	-3.082854	7.681312
C	8.588666	-2.621311	-0.258806	O	4.412758	-3.578411	6.532337
C	8.242118	-3.511017	-2.600271	C	2.547555	-1.251371	8.252549
H	5.013573	-2.628552	-2.362839	C	1.379925	-1.752404	7.445249
H	6.514284	-4.488740	-0.680395	C	0.564750	-0.965525	6.712704
H	7.317388	-1.767551	-1.755743	C	0.809788	-3.099235	7.386086
H	8.185439	-2.039382	0.558625	N	-0.479632	-1.714654	6.157210
H	8.876434	-3.595096	0.128809	C	-0.354478	-3.021063	6.606841
H	9.491285	-2.127285	-0.601132	C	1.169945	-4.329255	7.947651
H	7.573424	-3.568736	-3.450152	C	-1.184034	-4.118678	6.390629
H	9.144635	-3.000657	-2.919389	C	0.354461	-5.424211	7.731222
H	8.515741	-4.522682	-2.316650	C	-0.813412	-5.319849	6.964438
N	5.674959	-3.241512	1.398941	O	4.166323	-3.673004	8.784229
C	4.904587	-2.704456	2.499262	H	4.441188	-1.767919	5.772973
C	5.609833	-1.572636	3.239660	H	4.658970	-1.133391	8.451866
O	6.829453	-1.501967	3.336417	H	2.497471	-1.669242	9.250937
C	4.547088	-3.817631	3.486471	H	2.461257	-0.174121	8.347922
S	3.521489	-5.177810	2.668138	H	0.631463	0.087489	6.543440
H	6.181575	-4.080646	1.551377	H	-1.334567	-1.312606	5.864392
H	4.003119	-2.289900	2.077066	H	2.075589	-4.421722	8.514257
H	5.427543	-4.325949	3.856225	H	-2.087716	-4.032042	5.814781

H	0.622829	-6.373347	8.156664
H	-1.427793	-6.188304	6.817666

H	19.852481	1.018197	0.877318
H	18.531643	-1.117652	-0.870651

4. Coordinates for electric properties calculations

(I) dotriacontane

C	19.805866	0.378823	0.000178
C	18.531600	-0.465018	-0.000115
C	17.255090	0.378081	0.000164
C	15.975006	-0.459434	-0.000127
C	14.698996	0.384549	0.000153
C	13.418878	-0.453176	-0.000137
C	12.142861	0.390790	0.000143
C	10.862721	-0.446912	-0.000146
C	9.586692	0.397040	0.000135
C	8.306546	-0.440654	-0.000153
C	7.030512	0.403292	0.000129
C	5.750363	-0.434398	-0.000156
C	4.474329	0.409546	0.000126
C	3.194180	-0.428143	-0.000156
C	1.918145	0.415800	0.000124
C	0.638000	-0.421895	-0.000149
C	-0.638038	0.422037	0.000110
C	-1.918178	-0.415658	-0.000065
C	-3.194218	0.428261	-0.000059
C	-4.474353	-0.409444	-0.000063
C	-5.750393	0.434477	-0.000044
C	-7.030525	-0.403230	0.000030
C	-8.306562	0.440692	-0.000190
C	-9.586689	-0.397022	0.000053
C	-10.862723	0.446905	-0.000154
C	-12.142844	-0.390814	0.000168
C	-13.418867	0.453124	-0.000280
C	-14.698968	-0.384621	0.000211
C	-15.974986	0.459334	-0.000224
C	-17.255053	-0.378198	0.000349
C	-18.531572	0.464871	-0.000347
C	-19.805822	-0.378986	0.000419
H	-19.852399	-1.017925	0.877881
H	-14.700574	-1.037926	0.871197
H	-4.475936	-1.063266	0.870548
H	0.636403	-1.075973	0.870268
H	20.693090	-0.246986	-0.000030
H	19.852490	1.018793	-0.876528

H	17.257726	1.031717	0.871051
H	17.257735	1.032308	-0.870279
H	15.973479	-1.112916	-0.871004
H	15.973470	-1.113507	0.870307
H	14.700641	1.038620	-0.870254
H	14.700632	1.038030	0.871004
H	13.417295	-1.106670	-0.870988
H	13.417287	-1.107260	0.870270
H	12.144465	1.044289	0.870990
H	12.144472	1.044878	-0.870262
H	10.861129	-1.100414	-0.870992
H	10.861122	-1.101003	0.870258
H	9.588298	1.051132	-0.870269
H	9.588292	1.050544	0.870980
H	8.304951	-1.094160	-0.870998
H	8.304945	-1.094748	0.870250
H	7.032112	1.056799	0.870973
H	7.032116	1.057386	-0.870274
H	5.748766	-1.087906	-0.871001
H	5.748762	-1.088493	0.870246
H	4.475930	1.063640	-0.870278
H	4.475929	1.063056	0.870968
H	3.192581	-1.081654	-0.870997
H	3.192579	-1.082235	0.870250
H	1.919744	1.069316	0.870962
H	1.919742	1.069887	-0.870286
H	0.636410	-1.075422	-0.870979
H	-0.636465	1.076076	-0.870338
H	-0.636417	1.075615	0.870904
H	-1.919713	-1.069374	-0.870755
H	-1.919821	-1.069558	0.870487
H	-3.192634	1.082072	0.870560
H	-3.192634	1.082069	-0.870681
H	-4.475948	-1.063238	-0.870696
H	-5.748833	1.088263	-0.870682
H	-5.748776	1.088306	0.870562
H	-7.032066	-1.057190	-0.870476
H	-7.032158	-1.056883	0.870768
H	-8.304973	1.094747	0.870246
H	-8.304988	1.094252	-0.870997
H	-9.588293	-1.051059	-0.870396

H	-9.588266	-1.050596	0.870850	C	0.133253	0.324462	0.240563
H	-10.861174	1.100442	-0.870978	O	0.341887	1.390771	0.829480
H	-10.861102	1.100977	0.870268	N	-1.091124	-0.096697	-0.142897
H	-12.144398	-1.045015	-0.870156	H	-1.241189	-0.979649	-0.627833
H	-12.144475	-1.044215	0.871092	C	-2.324901	0.637335	0.147437
H	-13.417282	1.107415	0.869976	C	-3.483568	-0.339872	-0.190823
H	-13.417312	1.106429	-0.871276	O	-3.265140	-1.409857	-0.769241
H	-14.700616	-1.038881	-0.870057	N	-4.711386	0.072353	0.191606
H	-15.973511	1.112604	-0.871264	H	-4.869242	0.959048	0.667055
H	-15.973421	1.113635	0.870042	C	-5.938254	-0.676819	-0.089176
H	-17.257642	-1.032795	-0.869819	C	-7.105862	0.292953	0.239003
H	-17.257716	-1.031477	0.871507	O	-6.897634	1.371495	0.805053
H	-18.531601	1.118572	0.869391	N	-8.330430	-0.134822	-0.137526
H	-18.531646	1.117046	-0.871231	H	-8.480518	-1.027734	-0.603534
H	-20.693056	0.246810	-0.000065	C	-9.562568	0.608329	0.135623
H	-19.852481	-1.019397	-0.875965	C	-10.723596	-0.373557	-0.178137
(2) β -strand acetyl(ala) ₁₀ NH ₂				O	-10.510318	-1.456246	-0.733433
C	19.402172	0.699285	0.029799	N	-11.950764	0.049539	0.197711
C	18.238889	-0.208126	-0.288508	H	-12.104313	0.945132	0.656653
O	18.412171	-1.275953	-0.881556	C	-13.176828	-0.707539	-0.063903
N	17.007717	0.238073	0.111294	C	-14.346138	0.267324	0.236098
H	16.889771	1.106059	0.626212	O	-14.146768	1.357749	0.780620
C	15.781659	-0.518634	-0.130092	N	-15.570334	-0.169113	-0.139310
C	14.609950	0.433887	0.225555	H	-15.716627	-1.072551	-0.584543
O	14.798597	1.489028	0.839493	C	-16.798422	0.582414	0.121123
N	13.389367	0.012283	-0.179811	C	-17.966199	-0.397434	-0.161175
H	13.253932	-0.855679	-0.693441	O	-17.774663	-1.490702	-0.687448
C	12.151384	0.734404	0.116665	N	-19.198694	0.034879	0.228478
C	10.994941	-0.236568	-0.242392	C	15.663972	-1.801296	0.658395
O	11.208976	-1.286924	-0.856628	H	15.730442	-0.777389	-1.198517
N	9.767987	0.160193	0.162951	C	11.990453	2.037674	-0.627503
H	9.613295	1.028097	0.672244	H	12.118152	0.955001	1.194242
C	8.541805	-0.583275	-0.133026	C	8.406545	-1.891575	0.606619
C	7.371989	0.369421	0.234049	H	8.508525	-0.799291	-1.211460
O	7.576818	1.425989	0.841386	C	4.752962	1.981212	-0.597711
N	6.148317	-0.048264	-0.157047	H	4.884205	0.896862	1.223519
H	6.001282	-0.921822	-0.659358	C	1.160380	-1.936014	0.643179
C	4.913080	0.677926	0.145581	H	1.272324	-0.864276	-1.186861
C	3.755818	-0.294678	-0.209909	C	-2.482477	1.927632	-0.618526
O	3.974854	-1.352620	-0.809871	H	-2.353076	0.874889	1.221431
N	2.527970	0.107973	0.182746	C	-6.082791	-1.959817	0.691437
H	2.369736	0.984351	0.676878	H	-5.964988	-0.926796	-1.160393
C	1.301429	-0.636741	-0.110719	C	-9.718126	1.880173	-0.661125
				H	-9.589242	0.871913	1.203596

C	-13.321934	-1.969280	0.750863	O	-3.382000	-3.578000	2.573000
H	-13.201472	-0.986772	-1.127939	N	-1.179000	-3.867000	2.735000
C	-16.955801	1.834898	-0.706799	C	-0.951000	-2.506000	3.309000
H	-16.819394	0.872425	1.182673	C	0.473000	-2.470000	3.895000
H	16.556800	-2.448419	0.463332	S	0.907000	-1.032000	4.906000
H	14.750137	-2.360802	0.342818	C	-1.142000	-1.487000	2.187000
H	15.601219	-1.605248	1.755875	O	-2.012000	-0.643000	2.289000
H	12.878435	2.693739	-0.440425	N	-0.339000	-1.593000	1.156000
H	11.078587	2.573061	-0.267194	C	-0.461000	-0.637000	0.005000
H	11.897028	1.873976	-1.728205	C	0.698000	-0.854000	-0.986000
H	9.305433	-2.531294	0.414857	S	0.514000	-0.165000	-2.650000
H	7.503518	-2.441993	0.246476	C	-1.794000	-0.813000	-0.726000
H	8.312839	-1.733827	1.708179	O	-2.163000	0.040000	-1.510000
H	5.644083	2.634609	-0.416101	N	-2.482000	-1.904000	-0.455000
H	3.845281	2.520172	-0.231912	C	-3.809000	-2.159000	-1.116000
H	4.652080	1.817903	-1.697842	C	-4.435000	-3.424000	-0.515000
H	2.059265	-2.579357	0.463957	O	-5.642000	-3.600000	-1.244000
H	0.258642	-2.489458	0.284318	C	-4.682000	-0.924000	-0.810000
H	1.060607	-1.765460	1.742313	O	-5.558000	-0.547000	-1.563000
H	-1.589859	2.582218	-0.448932	N	-4.364000	-0.357000	0.326000
H	-3.388704	2.475027	-0.261706	C	-5.029000	0.857000	0.867000
H	-2.584436	1.745305	-1.715572	C	-5.439000	0.614000	2.318000
H	-5.184335	-2.607927	0.527880	C	-6.279000	-0.669000	2.419000
H	-6.984345	-2.519585	0.342037	O	-5.656000	-1.705000	2.588000
H	-6.184961	-1.766207	1.786527	O	-7.488000	-0.540000	2.321000
H	-8.824566	2.537301	-0.506991	C	-3.893000	1.901000	0.798000
H	-10.623617	2.437236	-0.317715	O	-2.765000	1.563000	1.101000
H	-9.820064	1.671802	-1.753529	N	-4.167000	3.126000	0.413000
H	-12.423819	-2.621913	0.604152	C	-3.083000	4.128000	0.193000
H	-14.223838	-2.537796	0.416837	C	-5.530000	3.671000	0.152000
H	-13.423435	-1.746641	1.840479	C	-3.769000	5.318000	-0.481000
H	-16.059392	2.493214	-0.575663	C	-5.286000	5.127000	-0.288000
H	-17.856680	2.403536	-0.371434	C	-2.362000	4.522000	1.491000
H	-17.065702	1.599371	-1.792936	O	-1.439000	5.313000	1.457000
H	-19.346725	0.953517	0.621320	N	-2.804000	3.958000	2.590000
H	-19.999726	-0.542620	0.010082	C	-2.182000	4.251000	3.918000
H	19.496293	0.847917	1.132449	C	-2.868000	3.357000	4.985000
H	20.340084	0.227643	-0.352574	C	-2.632000	1.850000	4.673000
H	19.272350	1.693968	-0.460793	C	-3.451000	0.957000	5.618000
				N	-4.909000	1.205000	5.369000
				C	-5.808000	0.254000	5.450000
(3) 1CNL (charge=1)				N	-5.476000	-0.970000	5.761000
N	-3.900000	-6.026000	1.526000	N	-7.050000	0.574000	5.209000
C	-2.485000	-5.678000	1.841000	C	-0.673000	3.947000	3.827000
C	-2.389000	-4.263000	2.423000				

O	0.141000	4.590000	4.458000	H	-4.419000	-5.164000	1.267000
N	-0.381000	2.955000	3.021000	H	-3.924000	-6.697000	0.732000
C	1.015000	2.493000	2.781000	H	-4.343000	-6.459000	2.361000
C	0.975000	0.984000	2.702000	H	-2.101000	-6.385000	2.561000
S	2.135000	0.024000	3.704000	H	-1.900000	-5.730000	0.935000
C	1.525000	3.099000	1.461000	H	-0.417000	-4.466000	2.590000
O	2.487000	3.841000	1.430000	H	-1.676000	-2.297000	4.076000
N	0.824000	2.733000	0.415000	H	0.608000	-3.349000	4.505000
C	1.117000	3.185000	-0.979000	H	1.185000	-2.533000	3.086000
C	0.759000	4.687000	-1.070000	H	0.335000	-2.303000	1.157000
C	2.570000	2.950000	-1.458000	H	-0.429000	0.371000	0.383000
O	3.124000	3.779000	-2.156000	H	1.559000	-0.365000	-0.567000
N	3.155000	1.836000	-1.081000	H	0.938000	-1.898000	-1.063000
C	4.566000	1.546000	-1.516000	H	-2.126000	-2.557000	0.182000
C	5.312000	0.724000	-0.408000	H	-3.667000	-2.251000	-2.184000
C	4.477000	-0.455000	0.086000	H	-3.800000	-4.286000	-0.656000
C	4.567000	-1.776000	-0.246000	H	-4.669000	-3.297000	0.530000
C	3.471000	-0.295000	0.975000	H	-6.227000	-2.870000	-1.028000
N	2.991000	-1.500000	1.153000	H	-3.644000	-0.755000	0.858000
C	3.577000	-2.458000	0.467000	H	-5.862000	1.140000	0.241000
C	5.412000	-2.488000	-1.097000	H	-4.559000	0.501000	2.932000
C	3.433000	-3.835000	0.329000	H	-6.015000	1.450000	2.688000
C	5.267000	-3.866000	-1.235000	H	-2.335000	3.667000	-0.441000
C	4.279000	-4.539000	-0.523000	H	-6.120000	3.622000	1.057000
C	4.587000	0.779000	-2.850000	H	-6.004000	3.106000	-0.637000
O	5.283000	-0.203000	-3.015000	H	-3.451000	6.254000	-0.045000
N	3.797000	1.278000	-3.772000	H	-3.531000	5.328000	-1.536000
C	3.664000	0.689000	-5.147000	H	-5.650000	5.806000	0.470000
C	5.078000	0.730000	-5.820000	H	-5.806000	5.328000	-1.214000
C	4.996000	0.452000	-7.344000	H	-3.557000	3.333000	2.543000
C	6.396000	0.601000	-7.970000	H	-2.322000	5.297000	4.151000
N	6.854000	2.015000	-7.788000	H	-2.467000	3.591000	5.960000
C	8.054000	2.398000	-8.151000	H	-3.926000	3.573000	4.992000
N	8.891000	1.549000	-8.686000	H	-2.897000	1.636000	3.650000
N	8.382000	3.646000	-7.959000	H	-1.586000	1.613000	4.809000
C	3.097000	-0.749000	-5.130000	H	-3.214000	-0.078000	5.416000
O	2.941000	-1.353000	-6.173000	H	-3.228000	1.180000	6.651000
N	2.799000	-1.252000	-3.953000	H	-5.202000	2.109000	5.133000
C	2.240000	-2.635000	-3.787000	H	-4.522000	-1.206000	5.946000
C	0.809000	-2.665000	-4.392000	H	-6.181000	-1.676000	5.813000
S	-0.469000	-1.626000	-3.640000	H	-7.285000	1.517000	4.972000
C	3.127000	-3.710000	-4.449000	H	-7.765000	-0.124000	5.259000
O	4.014000	-4.268000	-3.836000	H	-1.102000	2.481000	2.552000
O	2.734000	-4.133000	-5.579000	H	1.653000	2.811000	3.594000

H	-0.030000	0.685000	2.953000	H	3.08940757	4.74161904	7.94427047
H	1.122000	0.687000	1.678000	O	2.27289673	7.80578152	7.36093417
H	0.066000	2.129000	0.557000	H	1.45639512	8.27719960	7.69427709
H	0.462000	2.635000	-1.638000	H	3.08939835	8.27719960	7.69427709
H	-0.286000	4.827000	-0.839000	O	0.02750038	9.10216171	8.27761339
H	1.351000	5.261000	-0.374000	H	0.02749115	10.04498189	7.94427047
H	0.941000	5.054000	-2.070000	H	-0.78901046	8.63075961	7.94427047
H	2.669000	1.199000	-0.517000	O	0.02750038	11.69492209	7.36093417
H	5.083000	2.476000	-1.639000	H	0.84400199	12.16634017	7.69427709
H	6.255000	0.351000	-0.782000	H	-0.78900124	12.16634017	7.69427709
H	5.519000	1.369000	0.434000	O	4.51829309	1.32388057	8.27761339
H	3.166000	0.639000	1.417000	H	5.33480393	0.85247847	7.94427047
H	2.241000	-1.677000	1.758000	H	4.51830231	2.26670075	7.94427047
H	6.184000	-1.975000	-1.652000	O	4.51829309	3.91664095	7.36093417
H	2.665000	-4.356000	0.882000	H	4.51830231	3.91664628	6.36092047
H	5.924000	-4.412000	-1.895000	H	5.33480393	4.38805370	7.69426202
H	4.167000	-5.608000	-0.633000	O	6.76368945	5.21302114	8.27761339
H	3.268000	2.073000	-3.553000	H	7.58020029	4.74160839	7.94428554
H	2.983000	1.312000	-5.708000	H	6.76369867	5.21301581	9.27762709
H	5.516000	1.703000	-5.650000	O	6.76368945	7.80578152	7.36093417
H	5.720000	-0.013000	-5.370000	H	6.76368022	6.86296134	7.69427709
H	4.652000	-0.552000	-7.530000	H	5.94717860	8.27718362	7.69427709
H	4.313000	1.147000	-7.810000	O	4.51829309	9.10216171	8.27761339
H	7.098000	-0.065000	-7.487000	H	4.51829309	10.04498722	7.94428554
H	6.360000	0.376000	-9.025000	H	4.51829309	9.10217236	9.27762709
H	6.245000	2.669000	-7.389000	O	4.51829309	11.69492209	7.36093417
H	8.621000	0.597000	-8.825000	H	3.70179147	12.16634017	7.69427709
H	9.803000	1.854000	-8.958000	H	5.33479471	12.16634017	7.69427709
H	7.725000	4.277000	-7.548000	O	9.00908580	1.32388057	8.27761339
H	9.290000	3.970000	-8.225000	H	9.82559664	0.85247847	7.94427047
H	2.942000	-0.705000	-3.152000	H	9.00909503	2.26670075	7.94427047
H	2.184000	-2.850000	-2.729000	O	9.00908580	3.91664095	7.36093417
H	0.858000	-2.398000	-5.436000	H	9.00909503	3.91664628	6.36092047
H	0.451000	-3.683000	-4.341000	H	9.82559664	4.38805370	7.69426202
				O	9.00908580	9.10216171	8.27761339
(4) (H ₂ O) ₃₂				H	8.19257496	8.63074896	7.94428554
O	0.02750038	1.32388057	8.27761339	H	9.00907658	9.10215639	9.27762709
H	0.02749115	2.26670075	7.94427047	O	9.00908580	11.69492209	7.36093417
H	-0.78901046	0.85247847	7.94427047	H	9.00908580	11.69491144	6.36092047
O	0.02750038	3.91664095	7.36093417	H	9.00908580	10.75209659	7.69426202
H	0.02750960	3.91664628	6.36092047	O	0.02750038	1.32388057	11.02765106
H	0.84401122	4.38805370	7.69426202	H	0.02749115	1.32387524	10.02763736
O	2.27289673	5.21302114	8.27761339	H	-0.78901046	0.85246781	11.36097892
H	2.27290596	6.15584132	7.94427047	O	0.02750038	3.91664095	11.94433029

H	0.02750960	2.97382077	11.61098737
H	0.84401122	4.38804305	11.61098737
O	2.27289673	5.21302114	11.02765106
H	2.27289673	5.21303179	10.02763736
H	2.27289673	6.15584665	11.36097892
O	2.27289673	7.80578152	11.94433029
H	2.27290596	7.80578685	12.94434399
H	3.08940757	8.27719428	11.61100243
O	0.02750038	9.10216171	11.02765106
H	0.02750960	9.10215639	10.02763736
H	0.84401122	8.63074896	11.36097892
O	0.02750038	11.69492209	11.94433029
H	0.02750960	10.75210191	11.61098737
H	0.84401122	12.16632420	11.61098737
O	4.51829309	1.32388057	11.02765106
H	4.51830231	1.32387524	10.02763736
H	5.33480393	0.85246781	11.36097892
O	4.51829309	3.91664095	11.94433029
H	3.70178225	4.38804305	11.61098737
H	4.51828386	2.97382077	11.61098737
O	6.76368945	5.21302114	11.02765106
H	5.94718783	4.74160306	11.36099398
H	7.58019106	4.74160306	11.36099398
O	6.76368945	7.80578152	11.94433029
H	6.76368945	7.80577087	12.94434399
H	6.76368945	6.86295601	11.61100243
O	4.51829309	9.10216171	11.02765106
H	5.33480393	8.63075961	11.36099398
H	4.51830231	10.04498189	11.36099398
O	4.51829309	11.69492209	11.94433029
H	4.51830231	11.69492742	12.94434399
H	5.33480393	12.16633485	11.61100243
O	9.00908580	1.32388057	11.02765106
H	9.00908580	1.32389122	10.02763736
H	9.00908580	2.26670608	11.36097892
O	9.00908580	3.91664095	11.94433029
H	9.00909503	3.91664628	12.94434399
H	9.82559664	4.38805370	11.61100243
O	9.00908580	9.10216171	11.02765106
H	8.19258419	8.63074363	11.36099398
H	9.82558742	8.63074363	11.36099398
O	9.00908580	11.69492209	11.94433029
H	9.00909503	10.75210191	11.61098737
H	9.82559664	12.16632420	11.61098737