

Supporting Information

Bond-alternated and bond-equalized hexazine derivatives

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Coordinates and energies (sum of electronic and zero point energy, E+ZPE) of the structures calculated using M06-2X, PBE0, ω B97XD, B3LYP, and TPSSh functionals. All the structures correspond to minima unless otherwise specified. Structure numbers are the same as those in the manuscript. Transition states are indicated by [TS].

M06-2X/Def2-TZVPP

1 (E+ZPE= -78.522091 a.u.)

6	0.000000000	0.661033000	0.000000000
1	0.921954000	1.227957000	0.000000000
1	-0.921913000	1.227998000	0.000000000
6	0.000000000	-0.661033000	0.000000000
1	-0.921954000	-1.227957000	0.000000000
1	0.921913000	-1.227998000	0.000000000

2 (E+ZPE= -110.601565 a.u.)

7	0.613960000	-0.119479000	0.000010000
7	-0.613901000	-0.119530000	-0.000022000
1	-1.012048000	0.836442000	0.000018000
1	1.011636000	0.836616000	0.000070000

3 (E+ZPE= -328.261692 a.u.)

7	0.000000000	0.000000000	-1.289903000
7	1.125744000	0.118764000	-0.641634000
7	1.125744000	-0.118764000	0.641634000
7	0.000000000	0.000000000	1.289903000
7	-1.125744000	0.118764000	0.641634000
7	-1.125744000	-0.118764000	-0.641634000

4 (E+ZPE= -137.217302 a.u.)

7	-1.175516000	0.344669000	-0.000059000
7	-0.147224000	-0.325878000	-0.000169000
1	-1.999792000	-0.268197000	0.000591000
1	-0.245039000	-1.348176000	0.000117000
5	1.322935000	0.172301000	-0.000033000
1	1.779144000	-0.370863000	0.984185000
1	1.780623000	-0.372746000	-0.982352000
1	1.329569000	1.366940000	-0.000782000

5 (E+ZPE= -408.048279 a.u.)

7	1.124241000	0.720050000	-0.000246000
7	1.172915000	-0.537593000	-0.000096000
7	0.061487000	-1.333740000	-0.000117000
7	-1.052016000	-0.747021000	-0.000071000
7	-1.185749000	0.613584000	0.000055000
7	-0.120931000	1.284541000	-0.000055000
5	-0.134262000	2.849105000	0.000098000
1	0.536390000	3.099119000	-0.975483000

1	-1.272334000	3.190560000	0.000084000
5	2.534613000	-1.308209000	0.000159000
1	2.415972000	-2.014346000	-0.975182000
1	3.399180000	-0.493139000	-0.000132000
5	-2.400314000	-1.540797000	0.000034000
1	-2.951524000	-1.085199000	0.976142000
1	-2.952431000	-1.084714000	-0.975273000
1	2.415884000	-2.013220000	0.976380000
1	0.536113000	3.098843000	0.975984000
1	-2.127068000	-2.697137000	-0.000258000

5 [TS] (E+ZPE= -408.041974 a.u.)

7	-1.308844000	0.509182000	0.000093000
7	-0.418518000	1.293898000	-0.000111000
7	1.095440000	0.878839000	0.000068000
7	1.329799000	-0.284604000	0.000041000
7	0.213394000	-1.388195000	0.000012000
7	-0.911328000	-1.009386000	0.000137000
5	-2.245840000	-1.871986000	-0.000065000
1	-2.782655000	-1.436114000	-0.988997000
1	-1.909188000	-3.013410000	0.000434000
5	-0.498385000	2.880927000	-0.000076000
1	0.149033000	3.128477000	-0.987778000
1	-1.655223000	3.160043000	-0.001060000
5	2.744238000	-1.008754000	-0.000051000
1	2.635517000	-1.692454000	0.988263000
1	2.635450000	-1.691996000	-0.988697000
1	0.147015000	3.127984000	0.989134000
1	-2.783743000	-1.435388000	0.987911000
1	3.564118000	-0.146209000	0.000072000

6 (E+ZPE= -414.014647 a.u.)

7	1.552192000	0.000534000	1.689146000
7	0.384413000	0.000528000	1.345787000
1	-0.360244000	0.000665000	2.057633000
1	1.630819000	0.000876000	2.715581000
5	-0.133573000	-0.000090000	-0.180127000
6	-1.011257000	-1.310350000	-0.245428000
6	1.113695000	-0.000649000	-1.126528000
6	-1.010820000	1.310438000	-0.246379000
7	-1.640074000	-2.268200000	-0.195903000
7	2.035275000	-0.001082000	-1.807629000
7	-1.639295000	2.268546000	-0.197484000

7 (E+ZPE=-1238.354495 a.u.)

7	-1.093747000	-0.768788000	0.000000000
7	0.022616000	-1.288620000	0.000001000
7	1.212644000	-0.562552000	0.000001000
7	1.104651000	0.664167000	0.000000000
7	-0.119166000	1.331741000	-0.000001000
7	-1.127529000	0.624833000	-0.000001000
5	-2.770052000	1.261890000	-0.000003000
5	0.292117000	-3.029719000	0.000003000
5	2.477960000	1.767819000	0.000000000
6	1.107313000	-3.138107000	1.327272000
7	1.689014000	-3.109718000	2.315531000
6	1.107315000	-3.138110000	-1.327264000
7	1.689017000	-3.109723000	-2.315522000
6	-1.137441000	-3.632701000	0.000003000
7	-2.206718000	-4.045045000	0.000003000
6	3.714650000	0.830876000	0.000001000
7	4.606060000	0.110619000	0.000002000
6	2.164541000	2.528074000	-1.327290000
7	1.849448000	3.017747000	-2.315607000
6	2.164540000	2.528076000	1.327288000
7	1.849445000	3.017750000	2.315604000
6	-2.577638000	2.801436000	-0.000005000
7	-2.400253000	3.933652000	-0.000006000
6	-3.271543000	0.610082000	-1.327264000
7	-3.537830000	0.092093000	-2.315503000
6	-3.271545000	0.610085000	1.327259000
7	-3.537833000	0.092098000	2.315498000

7[TS] (E+ZPE=-1238.355634 a.u.)

7	-0.699236000	-1.180557000	0.000003000
7	-1.312133000	-0.151446000	0.000004000
7	-0.672722000	1.195994000	0.000002000
7	0.524967000	1.212216000	-0.000001000
7	1.372176000	-0.015252000	-0.000003000
7	0.787370000	-1.060586000	-0.000002000
5	1.520683000	-2.678235000	-0.000006000
5	-3.079748000	0.022146000	0.000008000
5	1.559090000	2.656095000	-0.000002000
6	-3.217227000	0.832938000	-1.325975000
7	-3.205443000	1.422583000	-2.309855000
6	-3.217222000	0.832941000	1.325989000
7	-3.205434000	1.422588000	2.309868000
6	-3.601030000	-1.437871000	0.000010000
7	-3.954627000	-2.527962000	0.000012000
6	0.555322000	3.837561000	0.000001000
7	-0.212025000	4.688741000	0.000003000
6	2.330034000	2.369664000	1.325950000
7	2.834820000	2.064396000	2.309740000
6	2.330029000	2.369667000	-1.325957000
7	2.834812000	2.064401000	-2.309750000
6	3.045770000	-2.399862000	-0.000010000
7	4.166629000	-2.161108000	-0.000012000
6	0.887134000	-3.202563000	1.325974000

7	0.370449000	-3.486974000	2.309838000
6	0.887126000	-3.202559000	-1.325983000
7	0.370435000	-3.486966000	-2.309845000

8 (E+ZPE=-110.900667 a.u.)

7	-0.666609000	-0.157583000	-0.000001000
7	0.532712000	0.029644000	0.000005000
1	-1.185807000	0.735834000	-0.000001000
1	0.980171000	0.957794000	-0.000013000
1	1.142914000	-0.798057000	-0.000012000

9 (E+ZPE= -328.413152 a.u.)

7	1.025297000	0.867878000	-0.000025000
7	1.187190000	-0.425324000	-0.000289000
7	0.238947000	-1.321840000	-0.000067000
7	-0.961925000	-0.815424000	0.000137000
7	-1.264272000	0.453984000	0.000093000
7	-0.225256000	1.240721000	0.000144000
1	2.198290000	-0.788292000	0.000177000
1	-0.416346000	2.297877000	-0.000152000
1	-1.781819000	-1.509548000	0.000018000

9 [TS] (E+ZPE= -328.406983 a.u.)

7	0.075824000	1.433574000	0.000014000
7	-0.986155000	0.905544000	0.000012000
7	-1.279444000	-0.651122000	-0.000002000
7	-0.291172000	-1.306800000	-0.000012000
7	1.203657000	-0.782447000	-0.000012000
7	1.277306000	0.401244000	-0.000001000
1	-1.908011000	1.466196000	0.000021000
1	2.223711000	0.919305000	0.000001000
1	-0.315814000	-2.385455000	-0.000022000

10 (E+ZPE= -150.200032 a.u.)

7	-1.149644000	-0.360968000	0.000006000
7	-0.180458000	0.372959000	0.000149000
1	-2.026092000	0.181280000	-0.000344000
1	-0.283828000	1.398296000	-0.000263000
1	1.684307000	0.235190000	-0.890240000
1	1.684520000	0.235443000	0.889921000
1	1.129487000	-1.233299000	0.000109000
6	1.187053000	-0.150141000	-0.000044000

11 (E+ZPE= -446.464488 a.u.)

7	1.241831000	0.316795000	-0.000008000
7	0.972376000	-0.920697000	-0.000018000
7	-0.346615000	-1.233849000	-0.000006000
7	-1.283535000	-0.381756000	0.000001000
7	-0.895261000	0.917084000	0.000005000
7	0.311154000	1.302456000	0.000003000
6	2.666773000	0.766950000	0.000004000

7	1.241831000	0.316795000	-0.000008000
7	0.972376000	-0.920697000	-0.000018000
7	-0.346615000	-1.233849000	-0.000006000
7	-1.283535000	-0.381756000	0.000001000
7	-0.895261000	0.917084000	0.000005000
7	0.311154000	1.302456000	0.000003000
6	2.666773000	0.766950000	0.000004000
1	2.786051000	1.396038000	-0.897681000
1	2.786181000	1.395486000	0.898073000
1	3.291516000	-0.126152000	-0.000275000
6	-0.669175000	-2.692919000	-0.000001000
1	-0.184146000	-3.110706000	-0.897787000
1	-0.184163000	-3.110693000	0.897801000
1	-1.754959000	-2.787572000	-0.000008000
6	-1.997593000	1.925993000	0.000006000
1	-2.601761000	1.714882000	-0.897908000
1	-2.601853000	1.714789000	0.897832000
1	-1.536545000	2.913561000	0.000071000

11 [TS] (E+ZPE= -446.457645 a.u.)

7	0.442550000	1.287559000	0.000039000
7	-0.740139000	1.210735000	-0.000050000
7	-1.336400000	-0.260525000	-0.000063000
7	-0.678479000	-1.246315000	-0.000003000
7	0.893782000	-1.027053000	0.000038000
7	1.418514000	0.035621000	0.000074000
6	1.258380000	2.562576000	0.000044000
1	1.877308000	2.500884000	0.906071000
1	1.876623000	2.501295000	-0.906497000
1	0.548686000	3.391421000	0.000461000
6	-2.848529000	-0.191581000	-0.000114000
1	-3.104683000	0.374441000	0.906430000
1	-3.104595000	0.375060000	-0.906286000
1	-3.211317000	-1.220660000	-0.000471000
6	1.590234000	-2.370988000	0.000049000
1	1.227993000	-2.876007000	0.906452000
1	1.227834000	-2.876112000	-0.906228000
1	2.662849000	-2.170525000	-0.000048000

12 (E+ZPE= -2870.180561 a.u.)

16	2.149304000	2.403616000	-1.437836000
5	0.990848000	2.811689000	-0.000088000
5	2.683342000	1.297643000	0.000088000
16	2.149141000	2.403769000	1.437834000
16	-3.156307000	0.659132000	-1.438049000
5	-2.929988000	-0.547992000	-0.000141000
5	-2.466092000	1.674971000	-0.000224000
16	-3.156465000	0.659272000	1.437625000
16	1.007203000	-3.062982000	1.437988000
5	-0.217626000	-2.972961000	0.000135000
5	1.939549000	-2.263305000	0.000230000
16	1.007378000	-3.063128000	-1.437560000
1	0.163425000	3.654871000	-0.000180000
1	3.613327000	0.569160000	0.000179000

7	1.019186000	-0.845525000	0.000103000
7	-0.318616000	-1.285457000	0.000044000
7	-1.242068000	-0.459843000	-0.000050000
7	-0.954130000	0.918770000	-0.000102000
7	0.222578000	1.305719000	-0.000054000
7	1.272443000	0.367024000	0.000055000
1	-2.300494000	2.844657000	-0.000271000
1	-3.246202000	-1.686223000	-0.000102000
1	3.083401000	-1.968062000	0.000285000
1	-1.313426000	-3.414309000	0.000090000

12 [TS 1] (E+ZPE= -2870.179158 a.u.)

16	-0.565731000	-3.168257000	1.438279000
5	-1.604706000	-2.512486000	0.000000000
5	0.631114000	-2.906006000	0.000000000
16	-0.565731000	-3.168257000	-1.438279000
16	-2.479896000	2.075278000	1.439066000
5	-1.385413000	2.637622000	0.000000000
5	-2.862182000	0.910358000	0.000000000
16	-2.479896000	2.075278000	-1.439066000
16	3.058118000	1.077882000	-1.438081000
5	2.336708000	2.033176000	0.000000000
5	2.947581000	-0.149793000	0.000000000
16	3.058118000	1.077882000	1.438081000
1	-2.779507000	-2.387213000	0.000000000
1	1.778967000	-3.183493000	0.000000000
7	1.275475000	-0.258497000	0.000000000
7	0.793401000	1.063557000	0.000000000
7	-0.423914000	1.265337000	0.000000000
7	-1.334771000	0.181329000	0.000000000
7	-0.903031000	-0.977676000	0.000000000
7	0.486359000	-1.214262000	0.000000000
1	-3.682757000	0.060387000	0.000000000
1	-0.682736000	3.588203000	0.000000000
1	3.394297000	-1.243444000	0.000000000
1	2.001910000	3.165784000	0.000000000

12 [Intermediate] (E+ZPE= -2870.248747 a.u.)

16	1.759117000	-3.047126000	1.437319000
5	0.523663000	-2.839546000	0.000000000
5	2.819058000	-3.297552000	0.000000000
16	1.759117000	-3.047126000	-1.437319000
16	-3.518250000	-0.000064000	1.437299000
5	-2.721045000	0.966364000	0.000000000
5	-4.264539000	-0.793400000	0.000000000
16	-3.518250000	-0.000064000	-1.437299000
16	1.759117000	3.047136000	-1.437306000
5	1.445027000	4.090043000	0.000000000
5	2.197421000	1.873550000	0.000000000
16	1.759117000	3.047136000	1.437306000
1	-0.505297000	-3.423993000	0.000000000
1	3.963582000	-3.591348000	0.000000000
7	1.019589000	0.790609000	0.000000000
7	-0.264938000	1.318762000	0.000000000

7	-1.194249000	0.487808000	0.000000000
7	-1.009379000	-0.888686000	0.000000000
7	0.174905000	-1.278005000	0.000000000
7	1.274569000	-0.429679000	0.000000000
1	-5.090618000	-1.638298000	0.000000000
1	-2.712911000	2.149693000	0.000000000
1	3.218165000	1.274864000	0.000000000
1	1.126179000	5.227848000	0.000000000

12 [TS2] (E+ZPE= -2870.243114 a.u.)

16	-1.236973000	-3.296221000	1.442775000
5	-1.928559000	-2.280325000	0.000108000
5	-0.703324000	-4.241727000	0.000014000
16	-1.237668000	-3.296515000	-1.442675000
16	-2.236105000	2.719503000	1.442872000
5	-1.010820000	2.810583000	0.000012000
5	-3.322070000	2.729198000	0.000305000
16	-2.236475000	2.720064000	-1.442536000
16	3.473846000	0.577010000	-1.442654000
5	4.026474000	1.511165000	0.000374000
5	2.938967000	-0.529820000	-0.000307000
16	3.473336000	0.576332000	1.442784000
1	-3.047588000	-1.893019000	0.000362000
1	-0.147694000	-5.285081000	-0.000011000
7	1.296093000	-0.406837000	-0.000380000
7	0.870201000	1.111950000	-0.000254000
7	-0.295757000	1.326189000	-0.000265000
7	-1.398141000	0.197890000	-0.000311000
7	-1.000684000	-0.918965000	-0.000214000
7	0.527634000	-1.309514000	-0.000385000
1	-4.503494000	2.768552000	0.000476000
1	-0.115665000	3.585784000	0.000067000
1	3.162870000	-1.692609000	-0.000546000
1	4.653463000	2.513258000	0.000731000

13 (E+ZPE= -2849.691862 a.u.)

16	-2.813223000	-1.782868000	-1.328372000
16	-2.813111000	-1.783043000	1.328374000
16	2.950708000	-1.544652000	-1.328515000
16	2.950775000	-1.544799000	1.328134000
16	-0.137490000	3.327665000	1.328504000
16	-0.137598000	3.327791000	-1.328123000
1	-1.340219000	-3.384862000	-0.000166000
1	-3.633223000	0.232814000	0.000168000
1	1.615032000	-3.262898000	-0.000253000
1	3.601544000	0.531842000	-0.000093000
1	-2.261340000	2.853079000	0.000256000
1	2.018337000	3.029924000	0.000089000
6	1.392082000	0.086619000	-0.000059000
6	0.672562000	1.221865000	0.000056000
6	-0.771121000	1.162244000	0.000112000
6	-1.394551000	-0.028509000	0.000056000
6	-0.621033000	-1.248908000	-0.000055000
6	0.721909000	-1.193451000	-0.000113000
6	1.839816000	-2.203962000	-0.000200000

6	2.859450000	-0.256314000	-0.000118000
6	0.988802000	2.695261000	0.000115000
6	-1.207752000	2.604503000	0.000201000
6	-2.828616000	-0.491447000	0.000086000
6	-1.651731000	-2.348138000	-0.000084000

14 (E+ZPE= -4589.699981 a.u.)

5	-1.425781000	-0.779308000	-0.000023000
5	-1.433748000	0.816530000	0.000029000
5	0.038141000	1.624515000	-0.000035000
5	1.424066000	0.833362000	0.000045000
5	1.387978000	-0.845526000	-0.000007000
5	0.009919000	-1.650231000	0.000054000
15	-2.782405000	-2.125975000	-0.000018000
15	-0.584376000	-3.361271000	0.000049000
15	3.232980000	-1.346380000	0.000012000
15	3.202821000	1.174650000	0.000045000
15	-0.450390000	3.472760000	-0.000061000
15	-2.618617000	2.186276000	-0.000005000
1	3.883449000	-2.595559000	0.000035000
1	4.022420000	2.320559000	0.000038000
1	0.306726000	4.660258000	-0.000064000
1	-4.020800000	2.322205000	-0.000024000
1	-4.189426000	-2.064118000	-0.000017000
1	-0.002153000	-4.644269000	0.000049000
16	-1.927471000	3.659977000	1.501181000
16	-1.927453000	3.659946000	-1.501291000
16	4.133396000	-0.160778000	1.501376000
16	4.133423000	-0.160803000	-1.501320000
16	-2.206054000	-3.499060000	1.501285000
16	-2.206046000	-3.499075000	-1.501272000

15 (E+ZPE= -553.790767 a.u.)

7	-0.512469000	-1.275283000	0.000123000
7	0.797735000	-1.016707000	-0.000001000
7	1.360497000	0.194036000	-0.000206000
7	0.481694000	1.199053000	-0.000059000
7	-0.848153000	1.081194000	0.000030000
7	-1.279503000	-0.182441000	-0.000053000
8	1.536157000	-1.957665000	0.000063000
8	-2.463644000	-0.351107000	-0.000007000
8	0.927660000	2.308903000	0.000089000

15 [TS] (E+ZPE= -553.729971 a.u.)

7	1.461426000	-0.004465000	0.000201000
7	0.460909000	1.393427000	-0.000017000
7	-0.726736000	1.267773000	-0.000156000
7	-1.437373000	-0.297680000	-0.000007000
7	-0.734708000	-1.263326000	-0.000042000
7	0.976512000	-1.095823000	0.000025000
8	1.233267000	2.294269000	-0.000005000
8	1.370372000	-2.215140000	-0.000057000
8	-2.603665000	-0.079047000	0.000060000

16 (E+ZPE= -1522.740526 a.u)

7	-1.015730000	-0.911232000	0.000279000
7	-1.183883000	0.386766000	0.000366000
7	-0.281320000	1.335248000	0.000081000
7	0.926881000	0.831883000	-0.000186000
7	1.297021000	-0.423996000	-0.000123000
7	0.256974000	-1.218610000	0.000095000
9	0.516485000	-2.451000000	-0.000133000
9	-2.380925000	0.778224000	-0.000325000
9	1.864485000	1.672730000	0.000060000

16 [T.S] (E+ZPE= -1522.740526 a.u)

7	0.356952000	1.456895000	0.000144000
7	1.224889000	0.667878000	0.000051000
7	1.083184000	-1.037190000	0.000040000
7	-0.034024000	-1.394505000	-0.000025000
7	-1.440031000	-0.419464000	-0.000083000
7	-1.191038000	0.726637000	0.000015000
9	-1.973167000	1.712668000	-0.000015000
9	2.469965000	0.852118000	-0.000057000
9	-0.496746000	-2.564982000	-0.000038000

17 (E+ZPE= -625.821353 a.u)

7	0.041777000	-1.367204000	0.000147000
7	-1.102356000	-0.682325000	-0.000045000
7	-1.204773000	0.647271000	0.000044000
7	-0.039666000	1.295769000	0.000101000
7	1.163049000	0.719681000	-0.000111000
7	1.142127000	-0.613672000	0.000017000
16	2.574350000	-1.383025000	-0.000017000
16	-2.485259000	-1.537388000	-0.000037000
16	-0.089160000	2.920623000	-0.000012000

17 [T.S] (E+ZPE= -625.791347 a.u)

7	0.370765000	1.420704000	-0.014103000
7	-1.205289000	0.789964000	0.033458000
7	-1.397656000	-0.383991000	0.174024000
7	-0.079581000	-1.437098000	-0.010750000
7	1.035707000	-1.020740000	-0.140922000
7	1.289283000	0.652529000	-0.013972000
16	2.894564000	0.887721000	0.034925000
16	-2.225665000	2.049725000	-0.041818000
16	-0.674686000	-2.946795000	-0.005242000

18 (E+ZPE= -566.772322 a.u)

7	-0.271158000	1.253744000	0.000231000
7	1.009925000	0.915713000	0.000077000
7	1.221426000	-0.392107000	-0.000047000

7	0.288140000	-1.332541000	-0.000120000
7	-0.950221000	-0.861750000	-0.000167000
7	-1.298054000	0.416692000	0.000067000
5	-0.572243000	2.647479000	0.000440000
5	2.578971000	-0.828229000	-0.000086000
5	-2.006673000	-1.819331000	-0.000331000
7	3.784992000	-1.215669000	-0.000048000
7	-2.945543000	-2.669699000	-0.000612000
7	-0.839547000	3.885674000	0.000604000

18 [T.S] (E+ZPE= -566.725512 a.u)

7	-0.518601000	-1.378763000	-0.015705000
7	-1.408807000	0.043545000	-0.018195000
7	-0.933485000	1.136706000	-0.051568000
7	0.741969000	1.197312000	0.014522000
7	1.449616000	0.239734000	0.079140000
7	0.665663000	-1.242643000	0.009566000
5	-2.767679000	-0.387902000	-0.001703000
5	1.047603000	2.589983000	0.003086000
5	1.720821000	-2.201477000	-0.004798000
7	1.218424000	3.836753000	-0.015857000
7	2.717315000	-2.969813000	-0.028891000
7	-3.932626000	-0.863263000	0.029428000

19 (E+ZPE= -494.165688 a.u)

7	-1.352244000	0.293168000	0.000009000
7	-0.869587000	-0.964559000	-0.000047000
7	0.422211000	-1.317842000	-0.000121000
7	1.270166000	-0.270717000	-0.000078000
7	0.930131000	1.024479000	-0.000015000
7	-0.400683000	1.235362000	-0.000061000
7	-1.681225000	-1.913021000	0.000087000
7	-0.816209000	2.412483000	0.000048000
7	2.497450000	-0.499358000	0.000119000
1	0.017799000	3.001220000	0.000089000
1	2.590274000	-1.516020000	0.000157000
1	-2.608142000	-1.485173000	0.000159000

19 [T.S] (E+ZPE= -566.772322 a.u)

7	0.657817000	-1.332863000	0.124453000
7	1.421827000	-0.425521000	0.016225000
7	0.825385000	1.236064000	0.124393000
7	-0.342394000	1.444054000	0.016199000
7	-1.483142000	0.096787000	0.124733000
7	-1.079441000	-1.018543000	0.016325000
7	2.646181000	-0.201190000	-0.112098000
7	-1.497384000	-2.190993000	-0.112109000
7	-1.148841000	2.392204000	-0.112183000
1	-2.514149000	-2.123609000	-0.200399000
1	-0.582138000	3.239040000	-0.200856000
1	3.096228000	-1.115423000	-0.200306000

20 (E+ZPE= -1354.004412 a.u)

7	-1.363477000	0.152429000	0.000003000
7	-0.526580000	1.185161000	-0.000008000
7	0.814137000	1.104811000	-0.000014000
7	1.289994000	-0.136385000	-0.000004000
7	0.550015000	-1.257388000	0.000009000
7	-0.762812000	-1.048894000	0.000010000
15	-1.110741000	2.766902000	-0.000017000
15	-1.841550000	-2.344718000	0.000023000
15	2.951790000	-0.421904000	-0.000005000
1	-0.777175000	-3.270473000	0.000028000
1	3.219224000	0.963206000	-0.000017000
1	-2.443466000	2.304923000	-0.000005000

20 [T.S] (E+ZPE= -1353.949881 a.u)

7	-0.268379000	-1.455206000	0.336570000
7	0.865927000	-1.117416000	0.139039000
7	1.393856000	0.495110000	0.341526000
7	0.534951000	1.308438000	0.140261000
7	-1.126061000	0.959543000	0.340482000
7	-1.400984000	-0.190995000	0.139388000
15	2.327538000	-1.891930000	-0.195187000
15	-2.802857000	-1.068683000	-0.195577000
15	0.475663000	2.960818000	-0.196718000
1	-3.541000000	0.121262000	-0.412055000
1	1.874711000	3.003929000	-0.416841000
1	1.665943000	-3.124585000	-0.419756000

21 (E+ZPE= -446.026259 a.u)

7	1.142106000	0.663383000	-0.359427000
7	1.115582000	-0.652371000	-0.012284000
7	0.002544000	-1.416656000	-0.000628000
7	-1.113206000	-0.656385000	0.012240000
7	-1.144201000	0.659110000	0.359978000
7	-0.002280000	1.287925000	0.000020000
6	-0.004810000	2.584578000	-0.000231000
6	2.256229000	-1.242299000	0.159284000
6	-2.251851000	-1.250279000	-0.158966000
1	2.247865000	-2.309134000	0.289990000
1	3.138167000	-0.632050000	0.103364000
1	0.934974000	3.078964000	-0.161523000
1	-0.946523000	3.075342000	0.160865000
1	-2.239813000	-2.317042000	-0.289992000
1	-3.135883000	-0.643122000	-0.102514000

21 [T.S] (E+ZPE= -445.937923 a.u)

7	0.316096000	-1.472993000	0.377570000
7	1.229009000	-0.753335000	0.060113000
7	1.117593000	1.010181000	0.377723000
7	0.037930000	1.440944000	0.060127000
7	-1.433669000	0.462753000	0.377888000
7	-1.266963000	-0.687613000	0.060160000
6	-2.000484000	-1.672861000	-0.352969000

6	2.449088000	-0.895885000	-0.352869000
6	-0.448600000	2.568795000	-0.353017000
1	3.071248000	-0.020672000	-0.356514000
1	2.784784000	-1.891663000	-0.590541000
1	-1.553642000	-2.649291000	-0.356853000
1	-3.030713000	-1.465632000	-0.590543000
1	0.245956000	3.357352000	-0.590774000
1	-1.517633000	2.670049000	-0.356713000

22 (E+ZPE= -1200.149147 a.u)

7	-0.664478000	0.983302000	-0.399877000
7	0.574392000	1.089025000	0.100982000
7	1.246060000	0.089101000	0.583461000
7	0.676711000	-1.122479000	0.218442000
7	-0.652956000	-1.275714000	0.201876000
7	-1.276405000	-0.153932000	-0.104821000
14	-3.063364000	-0.109014000	0.138615000
14	1.375169000	2.684260000	-0.180880000
14	1.726912000	-2.368951000	-0.257830000
1	2.491378000	2.535617000	0.787173000
1	0.354750000	3.584629000	0.407681000
1	-3.399770000	0.987904000	-0.798539000
1	-3.436682000	-1.401486000	-0.486377000
1	1.063924000	-3.675074000	-0.224201000
1	3.061083000	-2.184842000	0.315157000

22 [T.S] (E+ZPE= -1200.115851 a.u)

7	-0.679613000	1.180370000	-0.301051000
7	0.840341000	1.031902000	0.248688000
7	1.293709000	0.000318000	0.641632000
7	0.406208000	-1.338140000	0.198115000
7	-0.781666000	-1.290778000	0.110931000
7	-1.375183000	0.214465000	-0.145018000
14	-3.170350000	0.018318000	0.141626000
14	1.636998000	2.618997000	-0.246010000
14	1.700081000	-2.528277000	-0.304523000
1	2.798718000	2.551979000	0.686029000
1	0.637715000	3.491517000	0.424917000
1	-3.646252000	1.228333000	-0.584319000
1	-3.359613000	-1.125916000	-0.783722000
1	0.864282000	-3.761585000	-0.270362000
1	2.444382000	-2.497828000	0.979070000

PBE0/Def2tzvpp**1 (E+ZPE= -78.464337 a.u)**

6	0.000000000	0.661620000	0.000000000
1	0.922969000	1.230140000	0.000000000
1	-0.922962000	1.230148000	0.000000000
6	0.000000000	-0.661620000	0.000000000
1	-0.922969000	-1.230140000	0.000000000
1	0.922962000	-1.230148000	0.000000000

2 (E+ZPE= -110.532555 a.u)

7	0.585629000	0.188834000	0.000004000
7	-0.585629000	-0.188834000	-0.000028000
1	-1.173955000	0.659401000	0.000066000
1	1.173955000	-0.659401000	0.000098000

3 (E+ZPE= -328.036181 a.u)

7	0.000000000	0.000000000	-1.264168000
7	1.121294000	0.184100000	-0.630654000
7	1.121294000	-0.184100000	0.630654000
7	0.000000000	0.000000000	1.264168000
7	-1.121294000	0.184100000	0.630654000
7	-1.121294000	-0.184100000	-0.630654000

4 (E+ZPE= -137.120869 a.u)

7	-1.178705000	0.340456000	0.000036000
7	-0.137562000	-0.320630000	-0.000233000
1	-1.991168000	-0.286822000	0.000264000
1	-0.221503000	-1.343368000	0.000435000
5	1.304742000	0.177197000	0.000049000
1	1.780038000	-0.384670000	0.974648000
1	1.780451000	-0.384902000	-0.974188000
1	1.342339000	1.374994000	-0.000030000

5 (E+ZPE= -407.765507 a.u)

7	-0.366599000	-1.285326000	-0.000143000
7	-1.237958000	-0.353629000	-0.000155000
7	-0.929842000	0.960155000	0.000000000
7	0.312725000	1.248907000	0.000183000
7	1.296435000	0.325182000	0.000131000
7	0.925227000	-0.895277000	-0.000024000
5	1.960962000	-2.023690000	-0.000027000
1	1.627560000	-2.700644000	-0.957038000
1	3.052726000	-1.546420000	-0.000011000

6 (E+ZPE= -413.680349 a.u)

7	1.550666000	-0.000198000	1.700277000
7	0.383717000	-0.000073000	1.348016000
1	-0.366475000	-0.000613000	2.052414000
1	1.620934000	-0.000532000	2.726641000
5	-0.126715000	0.000030000	-0.171607000
6	-1.002522000	-1.305465000	-0.239295000
6	1.105871000	0.000293000	-1.128412000
6	-1.002770000	1.305369000	-0.238910000
7	-1.634028000	-2.266553000	-0.200921000
7	2.016367000	0.000491000	-1.830161000
7	-1.634489000	2.266306000	-0.200256000

7 (E+ZPE= -1237.341958 a.u)

7	1.296173000	0.300680000	-0.000003000
7	0.431345000	1.205465000	0.000013000
7	1.296173000	0.300680000	-0.000003000
7	0.431345000	1.205465000	0.000013000

7	-0.908491000	0.972156000	0.000000000
7	-1.259669000	-0.229196000	-0.000029000
7	-0.387687000	-1.272872000	-0.000057000
7	0.828301000	-0.976308000	-0.000080000
5	2.068933000	-2.165554000	-0.000043000
5	0.840996000	2.874464000	0.000112000
5	-2.909920000	-0.708921000	-0.000054000
6	0.137171000	3.308347000	1.323776000
7	-0.396308000	3.541301000	2.317407000
6	0.137554000	3.308424000	-1.323731000
7	-0.395642000	3.541435000	-2.317501000
6	2.389406000	2.926368000	0.000337000
7	3.539137000	2.947150000	0.000507000
6	-3.729078000	0.606089000	0.000058000
7	-4.321945000	1.591391000	0.000143000
6	-2.933964000	-1.535142000	-1.323874000
7	-2.869037000	-2.113447000	-2.317613000
6	-2.933938000	-1.535350000	1.323636000
7	-2.868989000	-2.113815000	2.317281000
6	1.339762000	-3.532518000	0.000383000
7	0.782905000	-4.538611000	0.000691000
6	2.796324000	-1.773429000	-1.324005000
7	3.264541000	-1.428156000	-2.317852000
6	2.796784000	-1.772840000	1.323491000
7	3.265342000	-1.427119000	2.317022000

8 (E+ZPE= -110.827660 a.u)

7	-0.667173000	-0.156957000	0.000000000
7	0.532951000	0.029480000	-0.000001000
1	-1.187127000	0.735154000	0.000001000
1	0.984962000	0.955223000	0.000002000
1	1.141720000	-0.798040000	0.000003000

9 (E+ZPE= -328.196049 a.u)

7	-1.291827000	-0.376031000	-0.000076000
7	-0.910747000	0.871418000	-0.000397000
7	0.320256000	1.306753000	-0.000052000
7	1.210056000	0.353014000	0.000177000
7	0.971562000	-0.930726000	0.000131000
7	-0.299302000	-1.224429000	0.000210000
1	-1.683584000	1.611908000	0.000258000
1	-0.554160000	-2.263971000	-0.000179000
1	2.237759000	0.652063000	-0.000033000

10 (E+ZPE= -150.099433 a.u)

7	-1.291827000	-0.376031000	-0.000076000
7	-0.910747000	0.871418000	-0.000397000
7	0.320256000	1.306753000	-0.000052000
7	1.210056000	0.353014000	0.000177000
7	0.971562000	-0.930726000	0.000131000
7	-0.299302000	-1.224429000	0.000210000
1	-1.683584000	1.611908000	0.000258000
1	-0.554160000	-2.263971000	-0.000179000
1	2.237759000	0.652063000	-0.000033000

11 (E+ZPE= -446.169938 a.u)

7	1.131525000	0.597480000	-0.000816000
7	1.150526000	-0.687808000	-0.000165000
7	-0.048319000	-1.278647000	0.000426000
7	-1.170911000	-0.652465000	0.000373000
7	-1.083200000	0.681177000	0.000209000
7	0.020392000	1.340253000	-0.000322000
6	2.402983000	1.320192000	0.000115000
1	2.401604000	1.984112000	-0.887647000
1	2.400679000	1.983827000	0.888092000
1	3.217729000	0.594009000	0.000463000
6	-0.058172000	-2.741123000	-0.000010000
1	0.517451000	-3.071186000	-0.888058000
1	0.517725000	-3.071632000	0.887690000
1	-1.094444000	-3.083601000	0.000035000
6	-2.344820000	1.420939000	0.000095000
1	-2.918836000	1.087198000	-0.887618000
1	-2.918629000	1.087679000	0.888126000
1	-2.123311000	2.489624000	-0.000220000

12 (E+ZPE= -2869.119184 a.u)

16	-1.784896000	-2.711075000	-1.417126000
5	-0.531392000	-2.877500000	-0.000085000
5	-2.432915000	-1.625540000	0.000088000
16	-1.784715000	-2.711194000	1.417129000
16	3.240345000	-0.189887000	-1.417352000
5	2.757627000	0.978608000	-0.000137000
5	2.624480000	-1.294151000	-0.000223000
16	3.240527000	-0.190005000	1.416918000
16	-1.455641000	2.901099000	1.417329000
5	-0.191472000	2.919817000	0.000135000
5	-2.226277000	1.898695000	0.000222000
16	-1.455824000	2.901218000	-1.416899000
1	0.399794000	-3.614488000	-0.000175000
1	-3.477899000	-1.061379000	0.000178000
7	-1.121966000	0.697406000	0.000102000
7	0.111687000	1.316393000	0.000048000
7	1.165077000	0.622964000	-0.000049000
7	1.084315000	-0.754963000	-0.000101000
7	-0.042910000	-1.320521000	-0.000052000
7	-1.195776000	-0.561567000	0.000054000
1	2.658568000	-2.481204000	-0.000275000
1	2.930079000	2.153570000	-0.000099000
1	-3.330026000	1.460499000	0.000275000
1	0.819496000	3.542884000	0.000096000

13 (E+ZPE= -2848.629484 a.u)

16	1.648706000	-2.886892000	-1.325953000
16	1.648870000	-2.886797000	1.325955000
16	1.675641000	2.871253000	-1.326153000
16	1.675796000	2.871335000	1.325758000
16	-3.324435000	0.015590000	1.326129000
16	-3.324586000	0.015494000	-1.325736000
1	3.319163000	-1.488274000	-0.000153000

1	-0.404487000	-3.614995000	0.000155000
1	3.332940000	1.457171000	-0.000252000
1	-0.370648000	3.618641000	-0.000101000
1	-2.948455000	-2.130331000	0.000253000
1	-2.928443000	2.157809000	0.000098000
6	-0.021327000	1.393876000	-0.000051000
6	-1.189718000	0.726573000	0.000049000
6	-1.196459000	-0.715382000	0.000101000
6	-0.034372000	-1.393595000	0.000052000
6	1.217769000	-0.678478000	-0.000051000
6	1.224071000	0.667038000	-0.000102000
6	2.283269000	1.731104000	-0.000198000
6	0.384164000	2.839466000	-0.000121000
6	-2.640832000	1.111804000	0.000119000
6	-2.651112000	-1.087047000	0.000199000
6	0.357576000	-2.842914000	0.000080000
6	2.266981000	-1.752405000	-0.000078000

14 (E+ZPE= -4588.234133 a.u)

5	1.632972000	0.131104000	0.000004000
5	0.757026000	1.463698000	0.000017000
5	-0.930023000	1.348617000	0.000014000
5	-1.646099000	-0.076275000	-0.000003000
5	-0.702933000	-1.479777000	-0.000017000
5	0.889102000	-1.387469000	-0.000014000
15	3.465035000	-0.273228000	0.000002000
15	2.317136000	-2.525540000	-0.000025000
15	-1.969166000	-2.864186000	-0.000034000
15	-3.345733000	-0.743895000	-0.000013000
15	-1.495886000	3.137397000	0.000033000
15	1.028619000	3.269446000	0.000037000
1	-1.852418000	-4.275333000	-0.000049000
1	-4.647127000	-0.185138000	-0.000008000
1	-2.776358000	3.741850000	0.000037000
1	2.163181000	4.117154000	0.000048000
1	4.628739000	0.533467000	0.000012000
1	2.484046000	-3.931947000	-0.000040000
16	-0.335228000	4.115026000	-1.497628000
16	-0.335232000	4.114993000	1.497717000
16	-3.396123000	-2.347792000	-1.497702000
16	-3.396127000	-2.347825000	1.497641000
16	3.731345000	-1.767167000	-1.497688000
16	3.731341000	-1.767201000	1.497659000

15 (E+ZPE= -553.441917 a.u)

7	-1.236979000	-0.596597000	-0.000091000
7	-1.069094000	0.727978000	-0.000293000
7	0.101807000	1.369551000	-0.000044000
7	1.165002000	0.561861000	-0.000015000
7	1.135177000	-0.772957000	0.000025000
7	-0.095907000	-1.289838000	0.000090000
8	-2.059601000	1.402412000	0.000236000
8	-0.184740000	-2.484863000	-0.000033000
8	2.244334000	1.082454000	0.000083000

16 (E+ZPE= -1522.161173 a.u)

7	-0.919443000	1.013586000	-0.000043000
7	0.380713000	1.187139000	-0.000056000
7	1.337518000	0.289467000	-0.000101000
7	0.837741000	-0.923276000	-0.000252000
7	-0.418071000	-1.303053000	-0.000159000
7	-1.218456000	-0.263865000	-0.000152000
9	-2.443926000	-0.529000000	0.000197000
9	0.763832000	2.380996000	0.000175000
9	1.680093000	-1.851993000	0.000221000

17 (E+ZPE= -625.450135 a.u)

7	1.247151000	-0.567337000	0.000331000
7	0.125064000	-1.289441000	0.000532000
7	-1.114930000	-0.796411000	-0.000044000
7	-1.179232000	0.536409000	-0.000690000
7	-0.132246000	1.363776000	-0.000428000
7	1.054153000	0.753056000	-0.000048000
16	2.377050000	1.697962000	0.000036000
16	0.281984000	-2.907560000	-0.000376000
16	-2.659016000	1.209575000	0.000491000

18 (E+ZPE= -566.362067 a.u)

7	-1.025455000	-0.771200000	0.000317000
7	-1.257739000	0.535347000	0.000157000
7	-0.155138000	1.273663000	-0.000050000
7	1.092513000	0.821567000	-0.000216000
7	1.180601000	-0.502473000	-0.000286000
7	0.165246000	-1.356926000	0.000053000
5	-2.162087000	-1.625815000	0.000440000
5	-0.326948000	2.685324000	-0.000066000
5	2.489041000	-1.059508000	-0.000356000
7	-0.480816000	3.949714000	-0.000044000
7	3.660960000	-1.558468000	-0.000508000
7	-3.180176000	-2.391225000	0.000565000

19 (E+ZPE= -493.838897 a.u)

7	-1.376918000	0.086393000	-0.000039000
7	-0.713065000	-1.081306000	-0.000090000
7	0.613639000	-1.235634000	-0.000067000
7	1.292977000	-0.076871000	0.000040000
7	0.763278000	1.149246000	0.000031000
7	-0.579918000	1.158179000	-0.000041000
7	-1.374551000	-2.145612000	0.000071000
7	-1.170878000	2.263201000	0.000000000
7	2.545435000	-0.117593000	0.000065000
1	-0.431481000	2.966892000	0.000039000
1	2.785149000	-1.109776000	0.000040000
1	-2.353666000	-1.857131000	0.000134000

20 (E+ZPE= -1353.458736 a.u)

7	-1.365854000	-0.123015000	0.000004000
7	-0.751416000	1.052742000	-0.000007000
7	0.576397000	1.244374000	-0.000012000

7	1.287419000	0.124369000	-0.000004000
7	0.789473000	-1.121363000	0.000008000
7	-0.535985000	-1.177116000	0.000011000
15	-1.636779000	2.495170000	-0.000017000
15	-1.342522000	-2.665048000	0.000023000
15	2.979281000	0.169886000	-0.000007000
1	-0.109679000	-3.367662000	0.000026000
1	2.971385000	1.588877000	-0.000017000
1	-2.861638000	1.778720000	-0.000009000

21 (E+ZPE= -445.719012 a.u)

7	1.156207000	0.669297000	-0.300890000
7	1.114141000	-0.650016000	-0.010062000
7	0.001155000	-1.403404000	-0.000465000
7	-1.113055000	-0.651864000	0.010036000
7	-1.157149000	0.667301000	0.301246000
7	-0.001037000	1.286565000	0.000014000
6	-0.002220000	2.588993000	-0.000161000
6	2.255327000	-1.259817000	0.135543000
6	-2.253317000	-1.263465000	-0.135282000
1	2.237352000	-2.331427000	0.229814000
1	3.144330000	-0.656644000	0.091499000
1	0.944808000	3.083541000	-0.122628000
1	-0.950140000	3.081842000	0.122241000
1	-2.233665000	-2.335028000	-0.229759000
1	-3.143258000	-0.661703000	-0.090920000

22 (E+ZPE= -1199.636609 a.u)

7	-0.758777000	1.021140000	-0.336639000
7	0.500789000	1.145466000	0.101622000
7	1.240597000	0.142025000	0.506793000
7	0.718916000	-1.071787000	0.183524000
7	-0.574538000	-1.285931000	0.062767000
7	-1.284773000	-0.171914000	-0.123824000
14	-3.041736000	-0.309569000	0.161123000
14	1.244894000	2.747999000	-0.167764000
14	1.879698000	-2.325473000	-0.241760000
1	2.433311000	2.650352000	0.723940000
1	0.217002000	3.659984000	0.404531000
1	-3.552017000	0.874927000	-0.581316000
1	-3.375059000	-1.574103000	-0.549988000
1	1.184097000	-3.599057000	0.076802000
1	3.037182000	-2.046487000	0.643959000

B3LYP/Def2tzvpp**1 (E+ZPE= -78.578344 a.u)**

6	0.000000000	0.662508000	0.000000000
1	0.921117000	1.231308000	0.000000000
1	-0.921110000	1.231315000	0.000000000
6	0.000000000	-0.662508000	0.000000000
1	-0.921117000	-1.231308000	0.000000000
1	0.921110000	-1.231315000	0.000000000

2 (E+ZPE= -110.665000 a.u)

7	0.588166000	0.188746000	0.000024000
7	-0.588166000	-0.188746000	-0.000008000
1	-1.177563000	0.659919000	-0.000074000
1	1.177563000	-0.659919000	-0.000042000

3 (E+ZPE= -328.396169 a.u)

7	0.000000000	0.000000000	-1.276853000
7	1.128455000	0.178165000	-0.635950000
7	1.128455000	-0.178165000	0.635950000
7	0.000000000	0.000000000	1.276853000
7	-1.128455000	0.178165000	0.635950000
7	-1.128455000	-0.178165000	-0.635950000

4 (E+ZPE= -137.304838 a.u)

7	-1.183981000	0.342037000	0.000011000
7	-0.138857000	-0.323085000	-0.000133000
1	-1.999803000	-0.282477000	0.000196000
1	-0.226323000	-1.346635000	0.000273000
5	1.312818000	0.177130000	0.000034000
1	1.787262000	-0.380260000	0.973764000
1	1.787365000	-0.380050000	-0.973751000
1	1.347273000	1.371111000	0.000201000

5 (E+ZPE= -408.282429 a.u)

7	-1.006223000	-0.893828000	-0.000029000
7	-1.246217000	0.361193000	0.000029000
7	-0.270964000	1.318332000	0.000007000
7	0.935905000	0.898652000	0.000007000
7	1.277202000	-0.424508000	0.000034000
7	0.310309000	-1.259847000	-0.000030000
5	0.577645000	-2.779267000	-0.000022000
1	-0.060309000	-3.170678000	-0.957745000
1	1.751127000	-2.961316000	-0.000029000
5	-2.695747000	0.889372000	0.000017000
1	-2.715727000	1.637734000	-0.957569000
1	-3.440139000	-0.035876000	-0.000155000
5	2.118094000	1.889895000	-0.000003000
1	2.776087000	1.533144000	0.957690000
1	2.776075000	1.533106000	-0.957695000
1	-2.715825000	1.637468000	0.957807000
1	-0.060342000	-3.170731000	0.957648000
1	1.689011000	2.997188000	-0.000041000

6 (E+ZPE= -414.189124 a.u)

7	-1.575831000	0.000322000	1.694299000
7	-0.400987000	0.000187000	1.351867000
1	0.341117000	0.000932000	2.066191000
1	-1.659675000	0.000806000	2.720415000
5	0.131969000	-0.000052000	-0.174954000
6	1.007142000	1.308740000	-0.230818000
6	-1.091365000	-0.000502000	-1.145613000

6	1.007561000	-1.308580000	-0.230153000
7	1.636309000	2.271398000	-0.185537000
7	-1.993895000	-0.000835000	-1.857991000
7	1.637074000	-2.270989000	-0.184399000

7 (E+ZPE= -1238.858713 a.u)

7	1.337577000	-0.134566000	-0.021545000
7	0.611435000	-1.142359000	-0.005995000
7	-0.785400000	-1.091398000	0.002860000
7	-1.295018000	0.041513000	0.006140000
7	-0.552369000	1.225654000	0.018461000
7	0.683425000	1.100569000	-0.000370000
5	1.802854000	2.465488000	-0.003278000
5	1.234158000	-2.794155000	0.005898000
5	-3.036921000	0.328478000	-0.002529000
6	0.582817000	-3.306570000	-1.312687000
7	0.075871000	-3.602021000	-2.303837000
6	0.578831000	-3.273031000	1.335925000
7	0.066375000	-3.537464000	2.333231000
6	2.773340000	-2.643662000	0.006394000
7	3.916187000	-2.514203000	0.006495000
6	-3.676343000	-1.079404000	-0.029325000
7	-4.136023000	-2.133506000	-0.049816000
6	-3.152477000	1.123456000	1.331803000
7	-3.152087000	1.691432000	2.333906000
6	-3.126725000	1.160621000	-1.316618000
7	-3.102747000	1.755081000	-2.303044000
6	0.903710000	3.723448000	0.024596000
7	0.221086000	4.648873000	0.046196000
6	2.582679000	2.136161000	1.304234000
7	3.098223000	1.827534000	2.286939000
6	2.534452000	2.158902000	-1.344110000
7	3.013156000	1.865061000	-2.349870000

8 (E+ZPE= -110.957142 a.u)

7	-0.669831000	-0.156750000	0.000001000
7	0.535346000	0.029417000	0.000001000
1	-1.192648000	0.734719000	-0.000006000
1	0.989491000	0.955723000	0.000001000
1	1.144552000	-0.799111000	-0.000006000

9 (E+ZPE= -328.549693 a.u)

7	1.035764000	0.874230000	-0.000078000
7	1.193434000	-0.429603000	-0.000385000
7	0.239227000	-1.334102000	-0.000044000
7	-0.968765000	-0.818733000	0.000173000
7	-1.274991000	0.459878000	0.000126000
7	-0.224667000	1.248330000	0.000202000
1	2.201767000	-0.793385000	0.000248000
1	-0.413792000	2.303463000	-0.000171000
1	-1.787983000	-1.510079000	-0.000033000

10 (E+ZPE= -150.281490 a.u)

7	-1.157409000	-0.359855000	-0.000025000
7	-0.178536000	0.372208000	0.000121000
1	-2.032294000	0.184389000	-0.000128000
1	-0.274151000	1.399292000	0.000069000
1	1.690183000	0.237491000	-0.888550000
1	1.690307000	0.237388000	0.888407000
1	1.143897000	-1.235822000	-0.000122000
6	1.188945000	-0.151534000	-0.000058000

11 (E+ZPE= -446.682876 a.u)

7	-1.122595000	0.635339000	0.000027000
7	-0.053432000	1.349083000	-0.000013000
7	1.111521000	0.654512000	-0.000042000
7	1.195080000	-0.628278000	-0.000024000
7	0.011077000	-1.289844000	0.000009000
7	-1.141634000	-0.720818000	0.000035000
6	-2.442597000	1.309964000	0.000031000
1	-2.988484000	0.944697000	-0.890261000
1	-2.988513000	0.944634000	0.890274000
1	-2.277417000	2.387271000	0.000060000
6	2.355764000	1.460357000	-0.000058000
1	2.312343000	2.115759000	-0.890335000
1	2.312360000	2.115775000	0.890206000
1	3.206155000	0.778661000	-0.000061000
6	0.086821000	-2.770318000	0.000035000
1	0.676118000	-3.060448000	-0.890235000
1	0.676140000	-3.060417000	0.890301000
1	-0.928751000	-3.165907000	0.000057000

12 (E+ZPE= -2870.609025 a.u)

16	-2.433363000	-2.213258000	-1.417836000
5	-1.229425000	-2.671492000	-0.000087000
5	-2.775471000	-0.971533000	0.000090000
16	-2.433216000	-2.213421000	1.417840000
16	3.133545000	-1.000300000	-1.418065000
5	2.928163000	0.271241000	-0.000136000
5	2.229465000	-1.917819000	-0.000225000
16	3.133696000	-1.000463000	1.417625000
16	-0.700328000	3.213644000	1.418087000
5	0.546178000	2.889639000	0.000135000
5	-1.698941000	2.400168000	0.000222000
16	-0.700471000	3.213799000	-1.417655000
1	-0.516378000	-3.614101000	-0.000178000
1	-3.646375000	-0.172490000	0.000181000
7	-0.920213000	0.961805000	0.000103000
7	0.436730000	1.257517000	0.000050000
7	1.293172000	0.316055000	-0.000048000
7	0.870758000	-1.006972000	-0.000101000
7	-0.372788000	-1.277943000	-0.000051000
7	-1.307311000	-0.250638000	0.000056000
1	1.973080000	-3.071604000	-0.000278000
1	3.387764000	1.360146000	-0.000098000
1	-2.871754000	2.253740000	0.000274000
1	1.673568000	3.244490000	0.000097000

13 (E+ZPE= -2850.061163 a.u)

16	-0.994998000	-3.192510000	-1.343024000
16	-0.994818000	-3.192565000	1.343027000
16	3.262188000	0.734673000	-1.343230000
16	3.262365000	0.734616000	1.342827000
16	-2.267286000	2.457830000	1.343248000
16	-2.267461000	2.457881000	-1.342850000
1	1.182413000	-3.444824000	-0.000149000
1	-2.930084000	-2.163263000	0.000152000
1	3.338497000	-1.455895000	-0.000253000
1	2.392214000	2.746406000	-0.000102000
1	-3.574514000	0.698396000	0.000251000
1	-0.408489000	3.619222000	0.000101000
6	1.007634000	0.968882000	-0.000048000
6	-0.278840000	1.369800000	0.000048000
6	-1.342842000	0.388229000	0.000099000
6	-1.046815000	-0.926349000	0.000052000
6	0.335225000	-1.357039000	-0.000050000
6	1.325658000	-0.443376000	-0.000099000
6	2.828917000	-0.500153000	-0.000199000
6	2.341489000	1.664495000	-0.000121000
6	-0.981369000	2.700024000	0.000120000
6	-2.612222000	1.195494000	0.000198000
6	-1.847593000	-2.199839000	0.000079000
6	0.270780000	-2.859978000	-0.000076000

14 (E+ZPE= -4590.450597 a.u)

5	-0.957977000	1.326490000	-0.000003000
5	0.625762000	1.525921000	-0.000017000
5	1.627704000	0.166486000	-0.000014000
5	1.008571000	-1.304802000	0.000003000
5	-0.669731000	-1.492796000	0.000017000
5	-1.634334000	-0.220939000	0.000014000
15	-2.452252000	2.519388000	-0.000002000
15	-3.403376000	0.120146000	0.000025000
15	-0.955761000	-3.383326000	0.000034000
15	1.597583000	-3.007405000	0.000012000
15	3.407948000	0.863910000	-0.000033000
15	1.805799000	2.887303000	-0.000037000
1	-2.155421000	-4.126284000	0.000049000
1	2.841070000	-3.675775000	0.000008000
1	4.651106000	0.196238000	-0.000037000
1	1.762902000	4.298390000	-0.000048000
1	-2.495929000	3.929811000	-0.000012000
1	-4.603813000	-0.622758000	0.000041000
16	3.422548000	2.332599000	1.520040000
16	3.422525000	2.332575000	-1.520130000
16	0.308935000	-4.130182000	1.520106000
16	0.308913000	-4.130206000	-1.520044000
16	-3.731418000	1.797568000	1.520092000
16	-3.731441000	1.797543000	-1.520064000

15 (E+ZPE= -554.016899 a.u)

7	-1.284893000	-0.521611000	-0.000104000
7	-1.029045000	0.801277000	-0.000213000

7	0.190718000	1.373536000	-0.000017000
7	1.208442000	0.490545000	-0.000061000
7	1.094163000	-0.851932000	-0.000023000
7	-0.179399000	-1.291809000	-0.000014000
8	-1.980527000	1.542082000	0.000193000
8	-0.345218000	-2.486224000	0.000060000
8	2.325757000	0.944137000	0.000125000

16 (E+ZPE= -1522.981799 a.u)

7	-1.184487000	-0.709343000	-0.000026000
7	-1.097230000	0.610100000	-0.000047000
7	-0.022064000	1.380465000	-0.000052000
7	1.076978000	0.645182000	-0.000113000
7	1.206545000	-0.671122000	-0.000076000
7	0.020249000	-1.255280000	-0.000079000
9	0.040423000	-2.522278000	0.000102000
9	-2.204567000	1.226136000	0.000126000
9	2.164151000	1.296141000	0.000078000

17 (E+ZPE= -626.064067 a.u)

7	-0.813510000	-1.116509000	0.000113000
7	-1.299259000	0.138304000	-0.000005000
7	-0.560182000	1.262773000	-0.000004000
7	0.769405000	1.056047000	-0.000045000
7	1.373680000	-0.146261000	-0.000163000
7	0.529857000	-1.194350000	-0.000030000
16	1.193909000	-2.691332000	0.000021000
16	-2.927726000	0.311716000	-0.000039000
16	1.733822000	2.379614000	0.000076000

18 (E+ZPE= -567.046017 a.u)

7	-1.223827000	-0.418484000	0.000302000
7	-1.038496000	0.906695000	0.000152000
7	0.249499000	1.269086000	-0.000047000
7	1.304482000	0.446006000	-0.000210000
7	0.974316000	-0.850624000	-0.000272000
7	-0.265988000	-1.352724000	0.000053000
5	-2.570204000	-0.878743000	0.000438000
5	0.524083000	2.665218000	-0.000064000
5	2.046114000	-1.786482000	-0.000360000
7	0.770036000	3.915687000	-0.000049000
7	3.006109000	-2.624679000	-0.000516000
7	-3.776126000	-1.290959000	0.000575000

19 (E+ZPE= -494.375962 a.u)

7	-1.304328000	0.487853000	-0.000010000
7	-1.004797000	-0.834458000	-0.000061000
7	0.229669000	-1.373510000	-0.000221000
7	1.225072000	-0.452933000	-0.000453000
7	1.074667000	0.885644000	-0.000261000
7	-0.220287000	1.287401000	-0.000235000
7	-1.951194000	-1.665296000	0.000294000
7	-0.466598000	2.522423000	0.000349000

7	2.417795000	-0.857122000	0.000365000
1	0.442383000	2.988109000	0.000501000
1	2.366609000	-1.877167000	0.000682000
1	-2.808988000	-1.110949000	0.000446000

20 (E+ZPE= -1354.266632 a.u)

7	-1.323378000	0.398826000	0.000003000
7	-0.307495000	1.267482000	-0.000007000
7	1.007095000	0.946660000	-0.000011000
7	1.251429000	-0.367452000	-0.000003000
7	0.316301000	-1.345513000	0.000008000
7	-0.943921000	-0.900050000	0.000010000
15	-0.590609000	2.947428000	-0.000017000
15	-2.257265000	-1.985172000	0.000024000
15	2.847866000	-0.962230000	-0.000007000
1	-1.388849000	-3.105463000	0.000027000
1	3.383761000	0.350023000	-0.000018000
1	-1.995001000	2.755388000	-0.000009000

21 (E+ZPE= -446.231141 a.u)

7	1.159299000	0.671380000	-0.328134000
7	1.122254000	-0.656284000	-0.010780000
7	0.001042000	-1.418835000	-0.000501000
7	-1.121273000	-0.657952000	0.010750000
7	-1.160103000	0.669569000	0.328506000
7	-0.000929000	1.296368000	0.000009000
6	-0.002012000	2.602616000	-0.000165000
6	2.268585000	-1.261396000	0.146589000
6	-2.266806000	-1.264660000	-0.146301000
1	2.259871000	-2.331011000	0.250548000
1	3.156854000	-0.659742000	0.100024000
1	0.940511000	3.100854000	-0.130844000
1	-0.945354000	3.099313000	0.130451000
1	-2.256620000	-2.334242000	-0.250468000
1	-3.155898000	-0.664252000	-0.099399000

22 (E+ZPE= -1200.442900 a.u)

7	-0.751396000	1.022656000	-0.358506000
7	0.513170000	1.148525000	0.105377000
7	1.244991000	0.138342000	0.527528000
7	0.715531000	-1.088588000	0.193872000
7	-0.587131000	-1.295134000	0.082413000
7	-1.294593000	-0.168441000	-0.126877000
14	-3.061094000	-0.292264000	0.159768000
14	1.265810000	2.757744000	-0.169544000
14	1.879787000	-2.342306000	-0.250940000
1	2.450362000	2.664425000	0.721727000
1	0.246717000	3.672412000	0.404620000
1	-3.565973000	0.894127000	-0.575190000
1	-3.412030000	-1.546116000	-0.553440000
1	1.183205000	-3.617394000	0.040074000
1	3.030676000	-2.093418000	0.645579000

ω B97xd/Def2tzvpp**1 (E+ZPE= -78.539279 a.u)**

6	0.000000000	0.661033000	0.000000000
1	0.921954000	1.227957000	0.000000000
1	-0.921913000	1.227998000	0.000000000
6	0.000000000	-0.661033000	0.000000000
1	-0.921954000	-1.227957000	0.000000000
1	0.921913000	-1.227998000	0.000000000

2 (E+ZPE= -110.620744 a.u)

7	0.585806000	0.188214000	0.000003000
7	-0.585806000	-0.188214000	-0.000030000
1	-1.172408000	0.658303000	0.000078000
1	1.172408000	-0.658303000	0.000110000

3 (E+ZPE= -328.265698 a.u)

7	0.000000000	0.000000000	-1.281382000
7	1.124662000	0.150522000	-0.636763000
7	1.124662000	-0.150522000	0.636763000
7	0.000000000	0.000000000	1.281382000
7	-1.124662000	0.150522000	0.636763000
7	-1.124662000	-0.150522000	-0.636763000

4 (E+ZPE= -137.240417 a.u)

7	-1.177870000	0.343041000	-0.000030000
7	-0.143981000	-0.323751000	0.000208000
1	-1.996657000	-0.274445000	-0.000293000
1	-0.234768000	-1.344535000	-0.000396000
5	1.316257000	0.172878000	-0.000074000
1	1.780763000	-0.376026000	0.983896000
1	1.780772000	-0.376401000	-0.983826000
1	1.341566000	1.371990000	-0.000254000

5 (E+ZPE= -408.085626 a.u)

7	-0.342671000	1.291271000	-0.000006000
7	0.874814000	0.948187000	0.000012000
7	1.289619000	-0.348856000	0.000026000
7	0.383792000	-1.231704000	0.000012000
7	-0.946933000	-0.942411000	-0.000019000
7	-1.258600000	0.283503000	-0.000022000
5	-2.744419000	0.736285000	-0.000047000
1	-2.793961000	1.459717000	-0.973951000
1	-3.425387000	-0.242502000	-0.000066000
5	2.009851000	2.008580000	0.000017000
1	2.661122000	1.689805000	-0.973904000
1	1.502666000	3.087701000	0.000014000
5	0.734558000	-2.744866000	0.000028000
1	0.132795000	-3.149449000	0.973936000
1	0.132845000	-3.149457000	-0.973908000
1	2.661128000	1.689805000	0.973932000
1	-2.793994000	1.459697000	0.973872000
1	1.922692000	-2.845242000	0.000059000

6 (E+ZPE= -414.009661 a.u)

7	1.576713000	-0.000118000	1.685842000
7	0.405045000	-0.000040000	1.350726000
1	-0.330802000	-0.000420000	2.068232000
1	1.664319000	-0.000341000	2.709421000
5	-0.131631000	0.000017000	-0.169176000
6	-1.010703000	-1.310707000	-0.229950000
6	1.094918000	0.000145000	-1.143867000
6	-1.010798000	1.310683000	-0.229737000
7	-1.640187000	-2.269827000	-0.185453000
7	1.996538000	0.000244000	-1.853240000
7	-1.640374000	2.269734000	-0.185081000

7 (E+ZPE= -1238.311678 a.u)

7	0.917975000	0.958305000	0.000000000
7	-0.292453000	1.251806000	0.000001000
7	-1.288931000	0.315988000	0.000001000
7	-0.937900000	-0.879000000	0.000000000
7	0.370811000	-1.274081000	-0.000001000
7	1.230224000	-0.372610000	-0.000001000
5	3.025272000	-0.710356000	-0.000003000
5	-0.897294000	2.974722000	0.000003000
5	-2.127662000	-2.264498000	0.000000000
6	-1.708826000	2.930776000	1.328991000
7	-2.273028000	2.817008000	2.322515000
6	-1.708828000	2.930779000	-1.328983000
7	-2.273031000	2.817012000	-2.322507000
6	0.407674000	3.811097000	0.000003000
7	1.385831000	4.410909000	0.000003000
6	-3.504454000	-1.552547000	0.000001000
7	-4.513003000	-1.005378000	0.000003000
6	-1.683782000	-2.945224000	-1.329008000
7	-1.303186000	-3.376901000	-2.322564000
6	-1.683779000	-2.945226000	1.329006000
7	-1.303182000	-3.376905000	2.322561000
6	3.096792000	-2.258671000	-0.000005000
7	3.126897000	-3.405695000	-0.000006000
6	3.392764000	0.014422000	-1.329008000
7	3.576233000	0.559894000	-2.322565000
6	3.392767000	0.014420000	1.329003000
7	3.576237000	0.559890000	2.322560000

8 (E+ZPE= -110.918678 a.u)

7	-0.667167000	-0.156848000	0.000000000
7	0.533420000	0.029447000	0.000000000
1	-1.186637000	0.733644000	-0.000002000
1	0.981634000	0.954807000	0.000000000
1	1.141238000	-0.796646000	-0.000002000

9 (E+ZPE= -328.437693 a.u)

7	-0.941220000	-0.961199000	-0.000039000
7	-1.222269000	0.313019000	0.000371000
7	-0.361815000	1.295706000	-0.000067000
7	0.882223000	0.901988000	-0.000137000

7	1.303033000	-0.334517000	0.000101000
7	0.340050000	-1.215002000	-0.000217000
1	-2.255918000	0.578489000	-0.000995000
1	0.626995000	-2.242906000	0.000554000
1	1.628916000	1.664460000	0.000363000

10 (E+ZPE= -150.226056 a.u)

7	-1.151254000	-0.359437000	-0.000011000
7	-0.178095000	0.371540000	-0.000227000
1	-2.023468000	0.184479000	0.000454000
1	-0.276766000	1.394631000	0.000271000
1	1.684371000	0.235586000	-0.888731000
1	1.684134000	0.235521000	0.889077000
1	1.135556000	-1.234189000	0.000046000
6	1.183603000	-0.150126000	0.000091000

11 (E+ZPE= -446.512824 a.u)

7	-1.265722000	-0.200777000	0.000215000
7	-0.875136000	1.014246000	-0.000029000
7	0.458930000	1.196462000	-0.000276000
7	1.315907000	0.250747000	-0.000165000
7	0.806732000	-0.995703000	-0.000040000
7	-0.440790000	-1.264917000	0.000131000
6	-2.715859000	-0.495297000	0.000056000
1	-2.911948000	-1.112229000	-0.893514000
1	-2.912103000	-1.112164000	0.893635000
1	-3.253344000	0.453052000	-0.000039000
6	0.929036000	2.599511000	-0.000007000
1	0.492855000	3.077958000	-0.893529000
1	0.492792000	3.077693000	0.893628000
1	2.019067000	2.590680000	0.000042000
6	1.786893000	-2.104259000	0.000065000
1	2.419198000	-1.965715000	-0.893545000
1	2.419286000	-1.965494000	0.893578000
1	1.234332000	-3.043904000	0.000209000

12 (E+ZPE= -2870.271041 a.u)

16	2.637142000	-1.856182000	-1.436309000
5	2.905338000	-0.649730000	-0.000089000
5	1.592920000	-2.516431000	0.000088000
16	2.637272000	-1.856000000	1.436307000
16	0.289182000	3.211643000	-1.436519000
5	-0.889662000	2.841665000	-0.000141000
5	1.382955000	2.636448000	-0.000223000
16	0.289301000	3.211814000	1.436095000
16	-2.926308000	-1.355209000	1.436525000
5	-2.974451000	-0.120314000	0.000135000
5	-2.016682000	-2.191513000	0.000229000
16	-2.926435000	-1.355399000	-1.436096000
1	3.652743000	0.270850000	-0.000181000
1	0.978690000	-3.530749000	0.000180000
7	-0.722867000	-1.109090000	0.000102000
7	-1.313189000	0.165254000	0.000044000
7	-0.598966000	1.180184000	-0.000051000
7	0.799736000	1.054219000	-0.000103000
7	1.321434000	-0.071812000	-0.000055000

7	0.513129000	-1.220397000	0.000054000
1	2.568468000	2.611412000	-0.000270000
1	-2.060583000	3.028886000	-0.000104000
1	-1.593468000	-3.299218000	0.000284000
1	-3.545349000	0.919013000	0.000092000

13 (E+ZPE= -2849.782630 a.u)

16	-3.122453000	1.145797000	-1.326914000
16	-3.122517000	1.145618000	1.326918000
16	0.568954000	-3.276840000	-1.327154000
16	0.568887000	-3.277005000	1.326758000
16	2.553556000	2.130978000	1.327142000
16	2.553611000	2.131147000	-1.326749000
1	-3.496556000	-1.000472000	-0.000152000
1	-2.020176000	3.024837000	0.000155000
1	-1.609597000	-3.261504000	-0.000253000
1	2.614749000	-2.528098000	-0.000101000
1	0.882332000	3.528545000	0.000252000
1	3.629401000	0.236708000	0.000099000
6	0.913447000	-1.050162000	-0.000051000
6	1.375944000	0.210223000	0.000049000
6	0.452760000	1.316339000	0.000101000
6	-0.870035000	1.086769000	0.000052000
6	-1.366261000	-0.265883000	-0.000051000
6	-0.506044000	-1.296674000	-0.000102000
6	-0.631417000	-2.797365000	-0.000199000
6	1.537371000	-2.420727000	-0.000121000
6	2.738418000	0.851876000	0.000119000
6	1.327961000	2.541791000	0.000198000
6	-2.107207000	1.945623000	0.000080000
6	-2.865064000	-0.120998000	-0.000077000

14 (E+ZPE= -4590.04462 a.u) non-planar

5	1.589274000	-0.475466000	-0.014162000
5	0.387690000	-1.566973000	0.337024000
5	-1.206401000	-1.137135000	-0.008554000
5	-1.548768000	0.449450000	0.342932000
5	-0.380814000	1.613100000	-0.010634000
5	1.163970000	1.117449000	0.340817000
15	3.266523000	-0.633831000	-0.822639000
15	2.649060000	1.686438000	1.390692000
15	-1.082970000	3.144051000	-0.820240000
15	-2.787362000	1.451617000	1.388600000
15	-2.186296000	-2.507715000	-0.816872000
15	0.142138000	-3.143493000	1.379552000
1	-0.144565000	4.191350000	-0.794570000
1	-2.321390000	0.969489000	2.637361000
1	-3.561885000	-2.216565000	-0.783921000
1	0.336025000	-2.506048000	2.630497000
1	3.703017000	-1.970603000	-0.796214000
1	1.996448000	1.521090000	2.637993000
16	-2.036799000	-2.784080000	1.343136000
16	-1.619833000	-3.821891000	-2.087542000
16	-1.394307000	3.165159000	1.339100000
16	-2.506345000	3.301040000	-2.090078000
16	3.435813000	-0.377085000	1.337897000
16	4.118421000	0.520178000	-2.089680000

15 (E+ZPE= -553.818160 a.u)

7	1.247631000	0.580766000	-0.000117000
7	1.060681000	-0.743772000	-0.000234000
7	-0.120847000	-1.370830000	0.000004000
7	-1.174469000	-0.546685000	-0.000042000
7	-1.126763000	0.790073000	-0.000016000
7	0.113787000	1.290442000	0.000020000
8	2.040803000	-1.430997000	0.000197000
8	0.218882000	2.482873000	0.000043000
8	-2.259702000	-1.051871000	0.000097000

16 (E+ZPE= -1522.778201 a.u)

7	-0.145414000	1.360459000	-0.000030000
7	1.008721000	0.735822000	-0.000036000
7	1.250921000	-0.554308000	-0.000068000
7	0.132879000	-1.241474000	-0.000176000
7	-1.105484000	-0.806153000	-0.000105000
7	-1.141607000	0.505657000	-0.000106000
9	-2.288491000	1.013952000	0.000135000
9	2.022361000	1.474893000	0.000136000
9	0.266118000	-2.488847000	0.000135000

17 (E+ZPE= -625.871502 a.u)

7	0.625556000	-1.219140000	0.000157000
7	-0.703915000	-1.090731000	0.000098000
7	-1.368520000	0.067891000	0.000018000
7	-0.592542000	1.155017000	-0.000090000
7	0.743166000	1.151354000	-0.000160000
7	1.296652000	-0.064234000	0.000003000
16	2.916469000	-0.144766000	-0.000004000
16	-1.583665000	-2.453258000	-0.000105000
16	-1.332978000	2.597955000	0.000097000

18 (E+ZPE= -566.76673 a.u)

7	-0.131275000	-1.277658000	-0.000381000
7	-1.247308000	-0.558803000	-0.000183000
7	-1.040861000	0.752506000	0.000039000
7	0.139711000	1.359598000	0.000238000
7	1.172115000	0.525176000	0.000536000
7	1.107561000	-0.800766000	0.000093000
5	-0.276407000	-2.690031000	0.000327000
5	-2.191379000	1.584467000	-0.000086000
5	2.467881000	1.105580000	-0.000294000
7	-3.218357000	2.327133000	-0.000161000
7	3.624579000	1.623545000	-0.001048000
7	-0.406232000	-3.950742000	0.000906000

19 (E+ZPE= -446.051542 a.u)

7	1.137381000	0.658875000	-0.372626000
7	1.114001000	-0.653713000	-0.014424000
7	0.000926000	-1.417601000	-0.000582000
7	-1.113126000	-0.655194000	0.014384000
7	-1.138001000	0.657250000	0.373039000

7	-0.000810000	1.285996000	0.000003000
6	-0.001814000	2.583311000	-0.000178000
6	2.255452000	-1.240553000	0.164555000
6	-2.253934000	-1.243410000	-0.164212000
1	2.252588000	-2.307470000	0.298801000
1	3.138104000	-0.630560000	0.107838000
1	0.937537000	3.079435000	-0.162007000
1	-0.941925000	3.078011000	0.161580000
1	-2.249818000	-2.310291000	-0.298707000
1	-3.137301000	-0.634497000	-0.107053000

20 (E+ZPE= -1354.048674 a.u)

7	-0.824280000	-1.098995000	0.000002000
7	-1.289417000	0.146222000	-0.000006000
7	-0.539593000	1.263311000	-0.000010000
7	0.771361000	1.043554000	-0.000002000
7	1.363867000	-0.164350000	0.000008000
7	0.518051000	-1.189793000	0.000008000
15	-2.943939000	0.449695000	-0.000016000
15	1.082546000	-2.774357000	0.000023000
15	1.861409000	2.324675000	-0.000007000
1	2.428181000	-2.339415000	0.000028000
1	0.812061000	3.272607000	-0.000019000
1	-3.240406000	-0.933033000	-0.000009000

21 (E+ZPE= -446.051542 a.u)

7	1.137381000	0.658875000	-0.372626000
7	1.114001000	-0.653713000	-0.014424000
7	0.000926000	-1.417601000	-0.000582000
7	-1.113126000	-0.655194000	0.014384000
7	-1.138001000	0.657250000	0.373039000
7	-0.000810000	1.285996000	0.000003000
6	-0.001814000	2.583311000	-0.000178000
6	2.255452000	-1.240553000	0.164555000
6	-2.253934000	-1.243410000	-0.164212000
1	2.252588000	-2.307470000	0.298801000
1	3.138104000	-0.630560000	0.107838000
1	0.937537000	3.079435000	-0.162007000
1	-0.941925000	3.078011000	0.161580000
1	-2.249818000	-2.310291000	-0.298707000
1	-3.137301000	-0.634497000	-0.107053000

22 (E+ZPE= -1200.204169 a.u)

7	-0.604746000	0.956082000	-0.441567000
7	0.619467000	1.054161000	0.103788000
7	1.246834000	0.055049000	0.640589000
7	0.653036000	-1.144889000	0.246053000
7	-0.697462000	-1.254166000	0.283898000
7	-1.269025000	-0.136259000	-0.096508000
14	-3.081517000	0.013607000	0.126785000
14	1.458716000	2.635161000	-0.190506000
14	1.631473000	-2.401875000	-0.268461000
1	2.556771000	2.466694000	0.806344000
1	0.455042000	3.560585000	0.404326000
1	-3.303678000	1.044571000	-0.927591000

1	-3.467320000	-1.285400000	-0.503699000
1	0.959822000	-3.698755000	-0.378861000
1	3.041222000	-2.254040000	0.096271000

TPSSH/Def2tzvpp

1 (E+ZPE= -78.574742 a.u)

6	0.000000000	0.663530000	0.000000000
1	0.922232000	1.233566000	0.000000000
1	-0.922231000	1.233567000	0.000000000
6	0.000000000	-0.663530000	0.000000000
1	-0.922232000	-1.233566000	0.000000000
1	0.922231000	-1.233567000	0.000000000

2 (E+ZPE= -110.662230 a.u)

7	0.590362000	0.189343000	0.000026000
7	-0.590362000	-0.189343000	-0.000006000
1	-1.175064000	0.665892000	-0.000087000
1	1.175064000	-0.665892000	-0.000055000

3 (E+ZPE= -328.409625 a.u)

7	0.000000000	0.000000000	-1.257494000
7	1.127729000	0.215835000	-0.632375000
7	1.127729000	-0.215835000	0.632375000
7	0.000000000	0.000000000	1.257494000
7	-1.127729000	0.215835000	0.632375000
7	-1.127729000	-0.215835000	-0.632375000

4 (E+ZPE= -137.303618 a.u)

7	-1.187619000	0.343510000	-0.000014000
7	-0.138504000	-0.323740000	0.000157000
1	-2.001216000	-0.288369000	-0.000236000
1	-0.226439000	-1.349075000	-0.000333000
5	1.316932000	0.178475000	-0.000051000
1	1.787633000	-0.383327000	0.975612000
1	1.787648000	-0.383834000	-0.975423000
1	1.350574000	1.373842000	-0.000368000

5 (E+ZPE= -408.294232 a.u)

7	1.273379000	-0.453919000	-0.000080000
7	0.281258000	-1.268675000	0.000001000
7	-1.029805000	-0.875827000	0.000011000
7	-1.239395000	0.390768000	0.000059000
7	-0.243569000	1.329715000	0.000083000
7	0.958120000	0.877921000	-0.000055000
5	2.166874000	1.846673000	-0.000023000
1	2.814253000	1.473552000	-0.961578000
1	1.755976000	2.963270000	0.000197000
5	0.515889000	-2.799842000	0.000024000
1	-0.131095000	-3.173984000	-0.961398000
1	1.688343000	-3.002277000	0.000088000
5	-2.682746000	0.953182000	-0.000002000
1	-2.683259000	1.700711000	0.961306000

1	-2.683291000	1.700447000	-0.961519000
1	-0.131177000	-3.173919000	0.961422000
1	2.814525000	1.473246000	0.961224000
1	-3.444267000	0.039009000	0.000124000

6 (E+ZPE= -414.177828 a.u)

7	1.579090000	0.000136000	1.701113000
7	0.399679000	0.000160000	1.356254000
1	-0.344079000	0.000191000	2.071559000
1	1.655330000	0.000233000	2.730486000
5	-0.129601000	-0.000024000	-0.173614000
6	-1.008356000	-1.311583000	-0.227863000
6	1.097400000	-0.000155000	-1.145328000
6	-1.008277000	1.311583000	-0.228114000
7	-1.642875000	-2.277163000	-0.190401000
7	2.000008000	-0.000253000	-1.865607000
7	-1.642737000	2.277209000	-0.190809000

7 (E+ZPE= -1238.836721 a.u)

7	0.989597000	-0.898078000	0.165375000
7	1.255661000	0.327068000	0.054024000
7	0.290174000	1.319855000	0.030739000
7	-0.901393000	0.926638000	-0.046000000
7	-1.262924000	-0.403320000	-0.203420000
7	-0.342078000	-1.239480000	-0.016095000
5	-0.616215000	-2.956319000	0.033168000
5	2.868224000	0.941468000	-0.039919000
5	-2.253394000	2.005702000	0.006206000
6	2.974584000	1.750176000	1.293037000
7	3.024614000	2.325015000	2.295426000
6	2.686056000	1.795006000	-1.343675000
7	2.480799000	2.387887000	-2.317427000
6	3.793872000	-0.298877000	-0.164124000
7	4.484789000	-1.220041000	-0.257840000
6	-1.660509000	3.408296000	0.311216000
7	-1.220438000	4.450488000	0.546287000
6	-2.823048000	1.790166000	-1.434793000
7	-3.202079000	1.608144000	-2.512960000
6	-3.068111000	1.344474000	1.168872000
7	-3.614246000	0.824704000	2.046839000
6	-2.144951000	-3.151055000	-0.149085000
7	-3.281453000	-3.301691000	-0.291746000
6	0.280809000	-3.446352000	-1.148472000
7	0.938661000	-3.766895000	-2.043987000
6	-0.050278000	-3.206904000	1.473080000
7	0.371228000	-3.320843000	2.545981000

8 (E+ZPE= -110.959330 a.u)

7	-0.672001000	-0.157014000	0.000001000
7	0.536435000	0.029211000	0.000000000
1	-1.187539000	0.740985000	-0.000004000
1	0.992877000	0.955493000	0.000002000
1	1.143619000	-0.801856000	-0.000002000

9 (E+ZPE= -328.575688 a.u)

7	-0.743647000	1.140558000	0.000034000
7	0.573317000	1.131900000	0.000521000
7	1.359597000	0.073732000	0.000122000
7	0.693611000	-1.062451000	-0.000175000
7	-0.615938000	-1.214287000	-0.000160000
7	-1.266938000	-0.069452000	-0.000334000
1	1.058662000	2.088581000	-0.000439000
1	-2.338119000	-0.127471000	0.000186000
1	1.279450000	-1.961110000	0.000192000

10 (E+ZPE= -150.285346 a.u)

7	-1.158033000	-0.361816000	-0.000020000
7	-0.177376000	0.374894000	0.000105000
1	-2.031225000	0.189537000	-0.000107000
1	-0.273635000	1.403074000	0.000079000
1	1.689608000	0.237076000	-0.890137000
1	1.689712000	0.236974000	0.890012000
1	1.134637000	-1.237834000	-0.000116000
6	1.189793000	-0.153395000	-0.000054000

11 (E+ZPE= -446.714054 a.u)

7	1.289124000	-0.056816000	-0.000083000
7	0.658441000	-1.185686000	-0.000036000
7	-0.693738000	-1.087967000	0.000029000
7	-1.356079000	0.022620000	0.000047000
7	-0.595365000	1.144769000	0.000067000
7	0.697606000	1.163047000	-0.000002000
6	2.775065000	-0.068851000	0.000028000
1	3.095347000	0.504038000	-0.892189000
1	3.095242000	0.504099000	0.892240000
1	3.102416000	-1.109322000	0.000081000
6	-1.447167000	-2.368790000	-0.000067000
1	-1.111145000	-2.932523000	-0.892330000
1	-1.111150000	-2.932641000	0.892123000
1	-2.511913000	-2.132041000	-0.000059000
6	-1.327891000	2.437667000	0.000025000
1	-1.984169000	2.428517000	-0.892190000
1	-1.984140000	2.428572000	0.892263000
1	-0.590459000	3.241366000	-0.000012000

12 (E+ZPE= -2870.678550 a.u)

16	1.053158000	-3.115832000	-1.416564000
5	1.953428000	-2.209288000	-0.000085000
5	-0.212292000	-2.941384000	0.000089000
16	1.053361000	-3.115761000	1.416568000
16	2.171712000	2.470019000	-1.416747000
5	0.936578000	2.796306000	-0.000138000
5	2.653450000	1.286762000	-0.000225000
16	2.171921000	2.470091000	1.416306000
16	-3.224973000	0.645813000	1.416767000
5	-2.441172000	1.654574000	0.000136000
5	-2.890000000	-0.587049000	0.000224000
16	-3.225177000	0.645744000	-1.416331000

1	3.104639000	-1.935203000	-0.000174000
1	-1.293653000	-3.422078000	0.000178000
7	-1.253185000	-0.459396000	0.000102000
7	-0.979679000	0.906478000	0.000049000
7	0.228755000	1.314961000	-0.000049000
7	1.274883000	0.395157000	-0.000102000
7	1.024437000	-0.855611000	-0.000052000
7	-0.295219000	-1.301691000	0.000054000
1	3.610382000	0.590570000	-0.000278000
1	0.123672000	3.656304000	-0.000100000
1	-3.228274000	-1.721060000	0.000276000
1	-2.316707000	2.831403000	0.000099000

13 (E+ZPE= -2850.113711 a.u)

16	-1.630705000	2.916970000	-1.334811000
16	-1.630867000	2.916878000	1.334814000
16	-1.710728000	-2.870672000	-1.335032000
16	-1.710888000	-2.870760000	1.334630000
16	3.341495000	-0.046245000	1.334999000
16	3.341654000	-0.046152000	-1.334600000
1	-3.314728000	1.529917000	-0.000148000
1	0.432761000	3.625029000	0.000151000
1	-3.355758000	-1.437679000	-0.000253000
1	0.332300000	-3.635662000	-0.000104000
1	2.982357000	2.105648000	0.000254000
1	2.923020000	-2.187300000	0.000101000
6	0.007272000	-1.399297000	-0.000049000
6	1.188235000	-0.739046000	0.000048000
6	1.208193000	0.705924000	0.000099000
6	0.045935000	1.398547000	0.000051000
6	-1.215406000	0.693357000	-0.000050000
6	-1.234101000	-0.659512000	-0.000099000
6	-2.307657000	-1.714603000	-0.000199000
6	-0.409949000	-2.845561000	-0.000122000
6	2.638763000	-1.141167000	0.000120000
6	2.669289000	1.067774000	0.000199000
6	-0.331096000	2.855792000	0.000078000
6	-2.259368000	1.777746000	-0.000076000

14 (E+ZPE= -4590.254268 a.u)

5	-1.250465000	1.066045000	-0.000004000
5	0.246599000	1.633741000	-0.000017000
5	1.548370000	0.549917000	-0.000014000
5	1.291479000	-1.030419000	0.000003000
5	-0.298010000	-1.615900000	0.000017000
5	-1.538168000	-0.603244000	0.000014000
15	-2.981245000	1.825139000	-0.000002000
15	-3.363172000	-0.683426000	0.000025000
15	-0.090008000	-3.494343000	0.000034000
15	2.273434000	-2.570818000	0.000013000
15	3.071212000	1.669183000	-0.000033000
15	1.089746000	3.254287000	-0.000037000
1	-1.023017000	-4.555996000	0.000050000
1	3.648509000	-2.900046000	0.000008000
1	4.457096000	1.391820000	-0.000037000
1	0.687517000	4.609811000	-0.000048000

1	-3.434151000	3.163978000	-0.000012000
1	-4.335867000	-1.709624000	0.000040000
16	2.719083000	3.138356000	1.505810000
16	2.719067000	3.138327000	-1.505900000
16	1.358448000	-3.923890000	1.505881000
16	1.358432000	-3.923919000	-1.505820000
16	-4.077464000	0.785547000	1.505870000
16	-4.077480000	0.785518000	-1.505841000

15 (E+ZPE= -554.040310 a.u)

7	1.382650000	0.162876000	-0.000113000
7	0.779866000	-1.045629000	-0.000223000
7	-0.550276000	-1.278843000	-0.000021000
7	-1.295470000	-0.152586000	-0.000073000
7	-0.832369000	1.115950000	-0.000029000
7	0.515603000	1.198198000	-0.000030000
8	1.503234000	-2.015405000	0.000209000
8	0.993785000	2.309542000	0.000079000
8	-2.497022000	-0.294107000	0.000140000

16 (E+ZPE= -1523.002486 a.u)

7	-1.372885000	-0.203232000	-0.000040000
7	-0.812069000	1.023799000	-0.000376000
7	0.510449000	1.290615000	0.000015000
7	1.292678000	0.191409000	0.000380000
7	0.862457000	-1.087337000	0.000011000
7	-0.480583000	-1.215176000	-0.000026000
16	-1.082984000	-2.738040000	0.000016000
16	-1.829748000	2.306883000	0.000196000
16	2.912711000	0.431123000	-0.000197000

17 (E+ZPE= -626.098001 a.u)

7	-0.884335000	-1.073691000	0.000224000
7	-1.238315000	0.206524000	0.000494000
7	-0.487683000	1.302707000	-0.000023000
7	0.798008000	0.969147000	-0.000577000
7	1.372024000	-0.229010000	-0.000264000
7	0.440310000	-1.175665000	-0.000030000
9	0.884702000	-2.362963000	0.000041000
9	-2.488744000	0.415298000	-0.000298000
9	1.604035000	1.947656000	0.000393000

18 (E+ZPE= -567.064831 a.u)

7	-1.293925000	0.055000000	0.000056000
7	-0.640555000	1.227092000	0.000027000
7	0.694582000	1.093064000	-0.000023000
7	1.382975000	-0.058810000	-0.000056000
7	0.599339000	-1.148054000	0.000008000
7	-0.742411000	-1.168268000	0.000064000
5	-2.720263000	0.115711000	0.000399000
5	1.460338000	2.297947000	-0.000067000
5	1.259926000	-2.413659000	-0.000338000
7	2.146895000	3.377952000	-0.000082000
7	1.851954000	-3.548243000	-0.000698000
7	-3.998856000	0.170269000	0.000707000

19 (E+ZPE= -494.396933 a.u)

7	-1.351944000	-0.351267000	-0.000043000
7	-0.343007000	-1.258700000	-0.000064000
7	0.980189000	-0.995187000	0.000102000
7	1.261578000	0.332295000	0.000425000
7	0.371766000	1.346446000	0.000266000
7	-0.918576000	0.926401000	0.000132000
7	-0.640826000	-2.488342000	-0.000144000
7	-1.834564000	1.799139000	-0.000302000
7	2.475383000	0.689211000	-0.000220000
1	-1.345225000	2.699227000	-0.000373000
1	3.010225000	-0.184605000	-0.000509000
1	-1.664993000	-2.514602000	-0.000187000

20 (E+ZPE= -1354.279971 a.u)

7	-1.102927000	0.841369000	0.000004000
7	0.157906000	1.293710000	-0.000007000
7	1.280080000	0.534402000	-0.000011000
7	1.041412000	-0.783708000	-0.000003000
7	-0.177232000	-1.375923000	0.000007000
7	-1.199402000	-0.510150000	0.000010000
15	0.477852000	2.968060000	-0.000017000
15	-2.809412000	-1.070172000	0.000024000
15	2.331655000	-1.897770000	-0.000007000
1	-2.369571000	-2.416680000	0.000027000
1	3.277467000	-0.843285000	-0.000018000
1	-0.908184000	3.260298000	-0.000009000
5	-1.250465000	1.066045000	-0.000004000
5	0.246599000	1.633741000	-0.000017000
5	1.548370000	0.549917000	-0.000014000
5	1.291479000	-1.030419000	0.000003000
5	-0.298010000	-1.615900000	0.000017000
5	-1.538168000	-0.603244000	0.000014000
15	-2.981245000	1.825139000	-0.000002000
15	-3.363172000	-0.683426000	0.000025000
15	-0.090008000	-3.494343000	0.000034000
15	2.273434000	-2.570818000	0.000013000
15	3.071212000	1.669183000	-0.000033000
15	1.089746000	3.254287000	-0.000037000
1	-1.023017000	-4.555996000	0.000050000
1	3.648509000	-2.900046000	0.000008000
1	4.457096000	1.391820000	-0.000037000
1	0.687517000	4.609811000	-0.000048000
1	-3.434151000	3.163978000	-0.000012000
1	-4.335867000	-1.709624000	0.000040000
16	2.719083000	3.138356000	1.505810000
16	2.719067000	3.138327000	-1.505900000
16	1.358448000	-3.923890000	1.505881000
16	1.358432000	-3.923919000	-1.505820000
16	-4.077464000	0.785547000	1.505870000
16	-4.077480000	0.785518000	-1.505841000

21 (E+ZPE= -446.247632 a.u)

7	1.167449000	0.675789000	-0.313639000
7	1.121506000	-0.655188000	-0.008363000
7	0.001111000	-1.421507000	-0.000507000

7	-1.120467000	-0.656957000	0.008336000
7	-1.168326000	0.673862000	0.314016000
7	-0.000988000	1.295706000	0.000008000
6	-0.002133000	2.606305000	-0.000169000
6	2.271052000	-1.266060000	0.141526000
6	-2.269146000	-1.269540000	-0.141233000
1	2.256196000	-2.337884000	0.232188000
1	3.158436000	-0.661105000	0.094258000
1	0.944909000	3.100842000	-0.121150000
1	-0.950034000	3.099204000	0.120760000
1	-2.252710000	-2.341322000	-0.232107000
1	-3.157414000	-0.665911000	-0.093643000

22 (E+ZPE= -1200.450633 a.u)

7	-0.785210000	1.014002000	-0.350473000
7	0.485241000	1.166169000	0.097367000
7	1.257988000	0.172002000	0.494440000
7	0.748353000	-1.067310000	0.180161000
7	-0.551296000	-1.307946000	0.076887000
7	-1.290490000	-0.196698000	-0.123220000
14	-3.054954000	-0.382157000	0.162953000
14	1.184166000	2.803832000	-0.163171000
14	1.944563000	-2.309780000	-0.244165000
1	2.374088000	2.725273000	0.721911000
1	0.139537000	3.666544000	0.444263000
1	-3.583271000	0.796146000	-0.569001000
1	-3.351731000	-1.632812000	-0.580077000
1	1.266504000	-3.580235000	0.109498000
1	3.069933000	-2.002983000	0.668630000

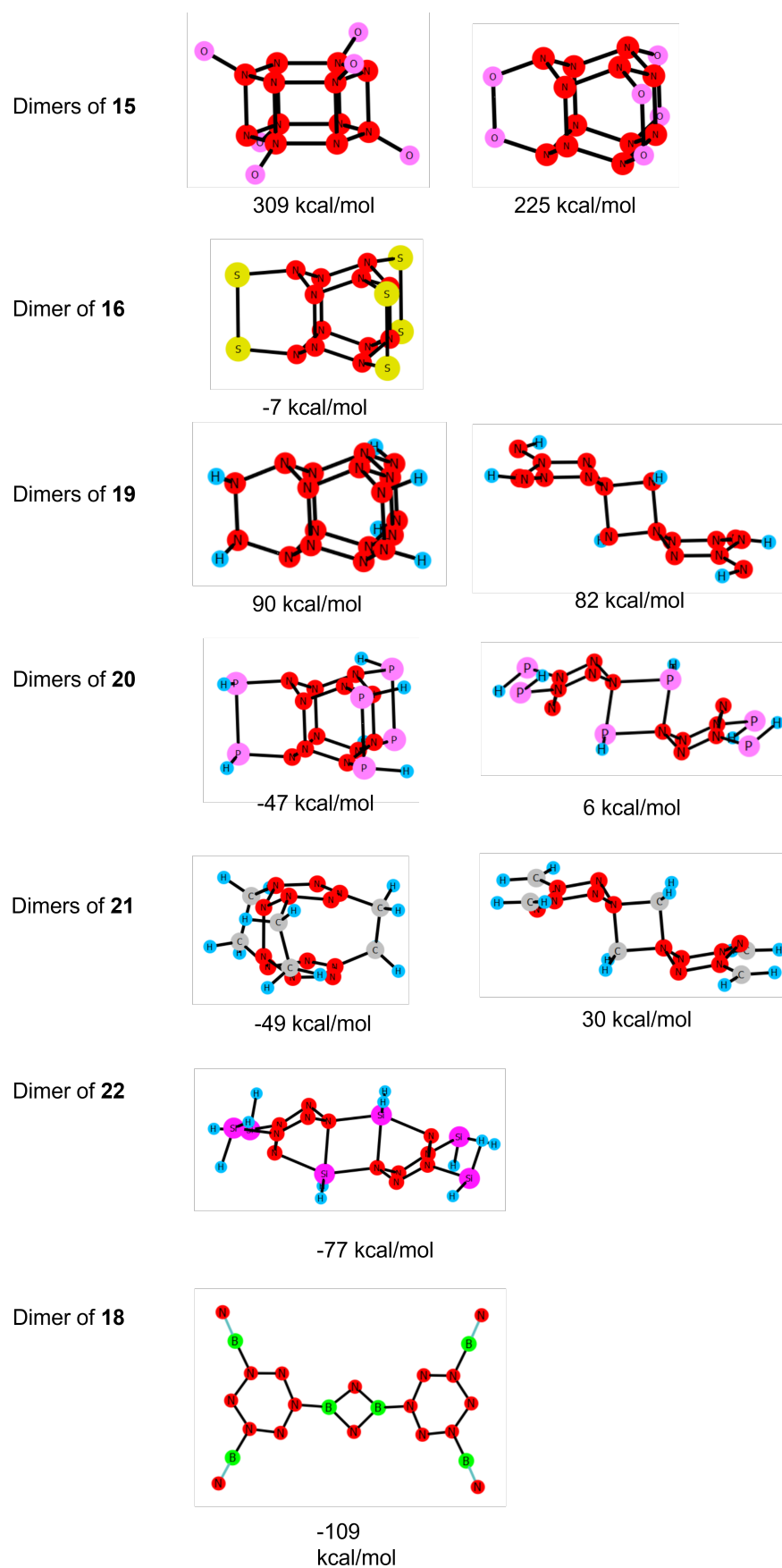


Fig. S1: Dimers of structures **15-22** and the corresponding Gibbs energy of dimerization.