Supporting Information

Optimized geometries and absolute energies.

B3LYP/6−31++G(d,p)

Compound **I**

E(RB3LYP) = −690.22332819 a.u.

C	0.45727800	2.57290900	−0.00002100
C	−0.63595400	1.69602800	−0.00008900
C	−0.44590500	0.30737100	−0.00010400
C	0.89592500	−0.17395600	−0.00004400
C	1.99782000	0.72589300	0.00001100
C	1.76132000	2.10486300	0.00002900
H	0.27458500	3.64605000	0.00000700
C	1.17817900	−1.61774900	−0.00009100
H	2.60715400	2.78340300	0.00008300
C	0.04921600	−2.54604800	−0.00007100
C	−1.21495800	−2.10065400	−0.00016900
H	0.29546300	−3.60331400	−0.00010700
H	−2.03529300	−2.81736300	−0.00034600
O	3.27496700	0.30323700	0.00004200
H	3.24572300	−0.69230800	0.00000500
O	−1.92367100	2.20224600	−0.00006900
H	−1.88811500	3.16712100	−0.00016000
O	2.34716700	−2.06177800	−0.00007000
C	−1.63794600	−0.65681200	−0.00000400
C	−2.51241800	−0.45341200	−1.27356100
H	−1.91888800	−0.61522800	−2.17851500
H	−3.34097600	−1.17035000	−1.27522700
H	−2.92734000	0.55473100	−1.30007000
C	−2.51176400	−0.45358900	1.27402000
H	−1.91778900	−0.61559700	2.17866000
H	−2.92659400	0.55458900	1.30094900
H	−3.34039400	−1.17044700	1.27605600

Compound **II**

E(RB3LYP) = −690.22456699 a.u.

C	−2.30527700	−1.03804500	−0.00038100
O	0.04894400	−2.64639200	0.00048600
H	0.89883800	−3.10173400	0.00135300
O	0.88380700	2.80687700	0.00066400
H	−0.00829600	3.25381600	0.00032300
C	−2.55066800	−1.90080300	−1.27397100
H	−3.57701700	−2.28477800	−1.27256700
H	−2.41266000	−1.30013600	−2.17826800
H	−1.86442300	−2.74748900	−1.30584000
H	−1.86557000	−2.74716700	1.30623700
C	−2.55130200	−1.90005200	1.27405200
H	−3.57778800	−2.28360700	1.27236400
H	−2.41288500	−1.29887800	2.17788700
O	−1.62782800	3.13546700	−0.00030700
C	3.13836400	1.25189300	0.00109000
H	3.23094000	1.92476600	−0.86373200
H	3.23229300	1.92108800	0.86868300
C	2.72559900	−1.72003900	0.00131600
H	2.65955600	−2.38283100	0.88162100
H	2.65754000	−2.38704500	−0.87559900
C	−1.79840400	1.89511600	−0.00036400
C	−3.15466700	1.34952600	−0.00067100
H	−3.96480800	2.07216600	−0.00078500
C	−3.36933000	0.02649100	−0.00069300
H	−4.39153400	−0.35014400	−0.00092600
C	4.26083600	0.25739700	−0.00186600
H	5.27138600	0.66063700	−0.00419400
C	4.08066500	−1.06503200	−0.00192600
H	4.93840200	−1.73395200	−0.00432500
C	1.76295200	0.62638700	0.00075100
C	1.55643700	−0.75344500	0.00063000
C	0.64555400	1.47940100	0.00037400
C	−0.67073100	0.95476300	−0.00004300
C	−0.88780500	−0.45224100	−0.00007900
C	0.24221600	−1.27503900	0.00028800

Compound **III**

E(RB3LYP) = −845.06112225 a.u.

C	−2.30527700	−1.03804500	−0.00038100
O	0.04894400	−2.64639200	0.00048600
H	0.89883800	−3.10173400	0.00135300
O	0.88380700	2.80687700	0.00066400
H	−0.00829600	3.25381600	0.00032300
C	−2.55066800	−1.90080300	−1.27397100
H	−3.57701700	−2.28477800	−1.27256700
H	−2.41266000	−1.30013600	−2.17826800
H	−1.86442300	−2.74748900	−1.30584000
H	−1.86557000	−2.74716700	1.30623700
C	−2.55130200	−1.90005200	1.27405200
H	−3.57778800	−2.28360700	1.27236400
H	−2.41288500	−1.29887800	2.17788700
O	−1.62782800	3.13546700	−0.00030700
C	3.13836400	1.25189300	0.00109000
H	3.23094000	1.92476600	−0.86373200
H	3.23229300	1.92108800	0.86868300
C	2.72559900	−1.72003900	0.00131600
H	2.65955600	−2.38283100	0.88162100
H	2.65754000	−2.38704500	−0.87559900
C	−1.79840400	1.89511600	−0.00036400
C	−3.15466700	1.34952600	−0.00067100
H	−3.96480800	2.07216600	−0.00078500
C	−3.36933000	0.02649100	−0.00069300
H	−4.39153400	−0.35014400	−0.00092600
C	4.26083600	0.25739700	−0.00186600
H	5.27138600	0.66063700	−0.00419400
C	4.08066500	−1.06503200	−0.00192600
H	4.93840200	−1.73395200	−0.00432500
C	1.76295200	0.62638700	0.00075100
C	1.55643700	−0.75344500	0.00063000
C	0.64555400	1.47940100	0.00037400
C	−0.67073100	0.95476300	−0.00004300
C	−0.88780500	−0.45224100	−0.00007900
C	0.24221600	−1.27503900	0.00028800

Compound**IV**

E(RB3LYP) = −883.12882130 a.u.

O	−1.81194500	3.11747500	0.04999100
O	0.71017000	2.86503400	−0.08706500
H	−0.18939800	3.28981900	−0.03493900
O	−0.02735800	−2.65942700	−0.10552300
H	0.84190800	−3.07694800	−0.14691100
C	3.50895000	−0.95522600	1.07444500
H	3.73230700	−1.65684500	1.86989300
C	3.67821300	0.37410400	1.07543700
H	4.07263400	0.99191400	1.87376900
C	1.58411800	0.67299900	−0.17645300
C	1.39757400	−0.70982800	−0.18099500
C	0.50050900	1.53298200	−0.09676800
C	−0.80953500	0.95833800	−0.03074500
C	−1.00498900	−0.45355100	−0.03364000
C	0.13266900	−1.28341500	−0.10516300
C	−3.30156000	1.30497200	0.11277800
H	−4.12134000	2.01469100	0.16569900
C	−3.49419100	−0.02080700	0.11002300
H	−4.50770300	−0.41672800	0.16265600
C	−1.95624000	1.87394300	0.04421000
C	3.09534500	0.91969900	−0.24150900
H	3.39837100	1.92479000	−0.53096100
C	3.47626100	−0.26724400	−1.18150900
H	3.00939000	−0.20322600	−2.16944600
H	4.55617500	−0.41213100	−1.27550800
C	2.80812600	−1.32647300	−0.24778500
H	2.88196500	−2.37365700	−0.55310700
C	−2.41123600	−1.06221600	0.03991600
C	−2.70898900	−1.91846500	−1.22775600
H	−2.63014600	−1.30703600	−2.13190800
H	−2.01128900	−2.75296000	−1.30465000
H	−3.72683900	−2.32085800	−1.17500200
C	−2.56735300	−1.94241200	1.31641900
H	−3.58432100	−2.34719000	1.36735300
H	−1.86376400	−2.77523300	1.30069800
H	−2.39092400	−1.34745400	2.21770800

Compound **V**

E(RB3LYP) = −846.28279889 a.u.

C	−2.25800000	−1.08847600	−0.09268000
O	0.12797200	−2.64852200	0.15836100
H	0.97942300	−3.09753900	0.10370900
O	0.90525500	2.80097000	−0.08938900
H	0.01121400	3.24276200	−0.06688900
C	−2.37175200	−2.18483700	−1.18220800
H	−3.42542400	−2.46689800	−1.29495100
H	−2.02116100	−1.80819900	−2.14954400
H	−1.80120200	−3.07821900	−0.93455100
H	−1.90946600	−2.47549300	1.56562400
C	−2.62181700	−1.69631600	1.28555100
H	−3.62202300	−2.14396000	1.24599400
H	−2.62045400	−0.93927300	2.07679500
O	−1.59660100	3.11051100	0.04781300
C	3.17399800	1.27266700	−0.07477700
H	3.25772600	1.90422300	−0.97110700
H	3.26433500	1.98309700	0.75976800
C	2.78903600	−1.69716800	0.09618400
H	2.72933800	−2.29661100	1.02052500
H	2.72518800	−2.42526300	−0.73153800
C	−1.75967500	1.87512200	0.07899000
C	4.30606100	0.28979100	−0.03472600
H	5.31262400	0.70147600	−0.06873400
C	4.13801000	−1.03211000	0.04055100
H	5.00171800	−1.69272400	0.06806800
C	1.80510500	0.63365800	−0.04096300
C	1.61080500	−0.74427300	0.03217800
C	0.67715200	1.47330200	−0.06237200
C	−0.63752200	0.93698400	−0.03719200
C	−0.84139200	−0.47837400	−0.03191300
C	0.29974600	−1.28033300	0.04622500
C	−3.29374500	−0.00436700	−0.47952700
H	−3.20049800	0.20773100	−1.55289100
H	−4.29963600	−0.41324300	−0.33006200
C	−3.13785900	1.30575700	0.28677500
H	−3.86878900	2.05881400	−0.02110000
H	−3.27483200	1.14948600	1.36602500

Compound **VI**

E(RB3LYP) = −847.50719150 a.u.

C	2.27878400	−1.10237600	0.15101800
O	−0.07525500	−2.64318200	−0.34606800
H	−0.92711700	−3.06588900	−0.50689900
O	−0.83319400	2.82752700	−0.07307100
H	0.06521000	3.25404800	0.00137500
C	2.28667600	−2.22219100	1.22278600
H	3.32415200	−2.51441800	1.42504200
H	1.85164900	−1.86367100	2.16230300
H	1.73667700	−3.10647300	0.90576000
H	2.07424800	−2.45533800	−1.55861000
C	2.76168200	−1.68563300	−1.20133400
H	3.75243400	−2.13986400	−1.08091500
H	2.83405600	−0.91364300	−1.97450800
O	1.67062800	3.10280100	0.03890500
C	−3.14850200	1.19211100	−0.31629900
H	−3.16232900	2.25923000	−0.08731600
H	−3.50937300	1.09093100	−1.35107300
C	−2.81194500	−1.54746000	−0.45688400
H	−3.19626200	−1.41580300	−1.47868300
H	−2.64255600	−2.62512300	−0.33988300
C	1.82196500	1.86594500	−0.00246500
C	−1.74061700	0.65867900	−0.22840000
C	−1.55210100	−0.72336900	−0.29814100
C	−0.62403600	1.49628000	−0.09501600
C	0.68394600	0.93932600	−0.00695000
C	0.87691300	−0.47820800	−0.02296800
C	−0.25572600	−1.27795200	−0.21936600
C	3.28481800	−0.03803400	0.65239900
H	3.09715500	0.15335500	1.71726900
H	4.29626300	−0.45495200	0.58521700
C	3.20876500	1.28774400	−0.09723500
H	3.91424200	2.02789400	0.29088800
H	3.44130700	1.15250700	−1.16285800
C	−3.90077900	−1.11981300	0.55754100
H	−4.83935200	−1.61732000	0.28961600
H	−3.61673000	−1.50354100	1.54340200
C	−4.09465700	0.42032400	0.63005400
H	−5.13087800	0.68673100	0.39495100
H	−3.91134500	0.76192900	1.65434000

Compound **VII**

E(RB3LYP) = −843.87349516 a.u.

C	−4.03846400	−1.11479000	−0.04046600
C	−2.76026500	−1.63911000	−0.05252300
C	−1.61827900	−0.79386000	−0.00917000
C	−1.83504200	0.61604300	0.01681200
C	−3.15481300	1.13181900	0.02958000
C	−4.24191900	0.28235900	0.00838700
C	−0.27695600	−1.30095600	0.01136900
C	−0.70316900	1.48676500	0.01388600
C	0.59936200	0.95990800	−0.00635900
C	0.82510200	−0.46584300	0.00127800
C	2.25422300	−1.03084000	0.00207500
C	3.30472100	0.04807000	−0.02109600
C	3.07909400	1.36914700	−0.03251900
C	1.71950700	1.90336300	−0.01875600
H	−4.89291100	−1.78412300	−0.07902800
H	−2.65004000	−2.71755300	−0.12721000
H	−3.28522000	2.20762400	0.05345400
H	−5.25056100	0.68351800	0.01881500
H	4.33082800	−0.31772900	−0.02823100
H	3.88357600	2.09782600	−0.04808800
O	−0.07775700	−2.67013000	0.01070100
H	−0.86172500	−3.11391000	0.35612900
O	−0.94080600	2.80442600	0.02519600
H	−0.03959300	3.24966000	0.01248400
C	2.52064700	−1.86907600	1.28748100
H	3.55489900	−2.23141000	1.28970300
H	2.37108000	−1.25912000	2.18363200
H	1.85329800	−2.73018600	1.33071900
H	1.83430300	−2.76730700	−1.27630100
C	2.50628000	−1.90874200	−1.25952700
H	3.53872100	−2.27637700	−1.25808400
H	2.35350300	−1.32454200	−2.17213000
O	1.54102100	3.14546500	−0.01571700

Compound **VIII**

E(RB3LYP) = −995.33124708 a.u.

C	3.59857300	−0.89359100	−0.00010800
C	2.28888400	−1.33804500	−0.00006200
C	1.25504100	−0.39580600	−0.00008600
C	1.43219800	0.99448200	−0.00006000
C	2.78695900	1.45812600	−0.00009700
C	3.81490900	0.50273300	−0.00012900
C	0.02051400	−1.06260400	−0.00015700
C	0.20456900	1.74325200	0.00005000
H	4.43681000	−1.58350400	−0.00008600
H	4.83935300	0.86338200	−0.00018300
O	0.24499000	−2.43656200	0.00004400
O	0.26780500	3.07508800	0.00032600
H	−0.69194600	3.40185700	0.00042900
C	−2.65421700	−1.98118700	−1.26691200
H	−3.63124400	−2.47648600	−1.27480500
H	−2.56526900	−1.38251800	−2.17832300
H	−1.87853700	−2.75000000	−1.27428100
H	−1.87780300	−2.74482500	1.28030000
C	−2.65484700	−1.97734800	1.26933600
H	−3.63094800	−2.47447000	1.27696000
H	−2.56857900	−1.37593400	2.17918300
O	−2.21359300	3.14245000	0.00037300
C	1.64377600	−2.66810200	0.00005400
O	2.08884000	−3.78686700	0.00012600
C	3.13915800	2.92323500	−0.00015400
H	2.71962100	3.43062300	−0.87410100
H	2.72053200	3.43041100	0.87437900
H	4.22360700	3.05749600	−0.00065600
C	−2.25945800	1.88666400	−0.00020100
C	−3.56174300	1.21833600	−0.00116600
H	−4.42925700	1.87090000	−0.00188500
C	−3.67095300	−0.11846100	−0.00158300
H	−4.65984600	−0.57515800	−0.00275800
C	−1.16738800	−0.37963900	−0.00031600
C	−1.04752500	1.06767200	−0.00017400
C	−2.52025600	−1.08715800	−0.00008700

MP2/6−31++G(d,p)

Compound **I**

E(MP2) = −688.20266692a.u.

C	0.42855200	2.57543400	−0.01876000
C	−0.65134100	1.68470200	0.00355300
C	−0.44841200	0.29495800	−0.01081700
C	0.89673600	−0.17009100	0.03189900
C	1.98659800	0.73839000	−0.00755400
C	1.73778000	2.11275700	0.00888900
H	0.23673800	3.64409000	−0.01329700
C	1.18386800	−1.61400400	−0.00331900
H	2.57720800	2.79547800	−0.00808200
C	0.05901400	−2.54407800	−0.01029900
C	−1.21063800	−2.09794600	−0.00989600
H	0.30356200	−3.59906900	−0.01959200
H	−2.02766000	−2.81539900	−0.01494900
O	3.28380100	0.34012600	0.00540900
H	3.27091200	−0.64836600	−0.00498200
O	−1.94868200	2.16941600	−0.00639700
H	−1.91480900	3.13635800	−0.00241400
O	2.35773900	−2.06080600	−0.01156000
C	−1.62932900	−0.66141700	0.00103900
C	−2.50846800	−0.45572200	−1.25363700
H	−1.91599300	−0.61565100	−2.15609400
H	−3.32936000	−1.17660100	−1.24723200
H	−2.92539300	0.54802700	−1.27499400
C	−2.47380000	−0.46201700	1.28026900
H	−1.85641300	−0.62389400	2.16542400
H	−2.89016500	0.54197100	1.31421300
H	−3.29485700	−1.18262800	1.29418100

Compound **II**

E(MP2) = −688.19562204 a.u.

C	3.65661900	−0.17111700	−0.19748100
C	1.30024100	0.64572600	0.04887800
C	0.85783800	−0.67837600	0.09705900
C	3.23080800	−1.44392000	−0.18631200
H	4.69541000	0.04519500	−0.42248900
C	0.34919400	1.68705000	0.03907200
C	−0.52330800	−0.96055800	0.03998300
H	3.93048700	−2.24372400	−0.40429500
C	−1.47425500	0.08460500	0.03820000
C	−1.00891900	1.41829900	−0.02489400
H	−1.71547800	2.23996400	−0.03633900
C	1.81783200	−1.83912600	0.12452700
H	1.47145500	−2.59793300	−0.58190300
H	1.76853000	−2.32421600	1.10740800
C	2.76393900	0.99595500	0.10608800
H	2.95903900	1.81471000	−0.59146000
H	2.99867200	1.40295500	1.09781800
C	−2.91027300	−0.22317000	−0.03811200
O	−3.31884000	−1.40560800	−0.04003000
C	−3.91847700	0.89871800	−0.09891700
H	−3.85486700	1.52041600	0.79511600
H	−3.73929300	1.53380100	−0.96681500
H	−4.91115500	0.46181400	−0.16638700
O	−0.87866400	−2.27208100	0.06964800
H	−1.86538800	−2.28983600	0.02825000
O	0.85875400	2.97148300	0.02337900
H	0.12514100	3.60197400	0.02857400

Compound**III**

E(MP2) = −842.55329444 a.u.

C	−2.29112000	−1.04119100	−0.00865700
O	0.04072600	−2.64429800	0.02289100
H	0.89609400	−3.09169100	−0.02614500
O	0.90067100	2.81232400	0.02642600
H	0.01771100	3.26158600	0.00475300
C	−2.51554500	−1.91904100	−1.26131300
H	−3.53808700	−2.30416700	−1.26037000
H	−2.37183000	−1.32399100	−2.16491600
H	−1.82538800	−2.75874800	−1.27439100
H	−1.84442700	−2.71432800	1.32035500
C	−2.53016100	−1.87170100	1.27319600
H	−3.55442200	−2.25226000	1.27929300
H	−2.38860900	−1.24530800	2.15563000
O	−1.64477000	3.13667200	−0.02521100
C	3.12263500	1.25543600	0.03910900
H	3.17047700	1.97552500	−0.78393600
H	3.24633800	1.86073800	0.94454000
C	2.71777900	−1.72043100	0.04660200
H	2.68569800	−2.29547100	0.98281900
H	2.62283900	−2.45488100	−0.76586300
C	−1.80468300	1.88953900	−0.01435800
C	−3.15544600	1.33645600	−0.03545100
H	−3.97076100	2.04910300	−0.05703900
C	−3.36017400	0.00622200	−0.03583300
H	−4.37820300	−0.37579300	−0.05199500
C	4.23951000	0.26609000	−0.07421300
H	5.24498900	0.66431800	−0.16011000
C	4.06146300	−1.06314600	−0.07568300
H	4.91962100	−1.72137700	−0.15759300
C	1.75634000	0.62487900	0.05282100
C	1.55421900	−0.75767400	0.00031700
C	0.64248200	1.47673500	0.00965200
C	−0.67202800	0.95494600	0.04228200
C	−0.89160700	−0.44874700	−0.01070100
C	0.24215700	−1.27351300	0.02258500

Compound**IV**

E(MP2) = −880.52521607a.u.

O	−1.82615100	3.11925800	0.02966500
O	0.73151400	2.87211200	−0.07087400
H	−0.15847600	3.30337000	−0.03559500
O	−0.03206500	−2.66000700	−0.11517700
H	0.84674200	−3.06492000	−0.12891400
C	3.47593200	−0.97077500	1.06206900
H	3.68776600	−1.67616700	1.85400300
C	3.64241600	0.36925800	1.08353600
H	4.01799300	0.97401000	1.89724000
C	1.58006600	0.67028600	−0.17003600
C	1.39619700	−0.71291500	−0.21113200
C	0.49632300	1.53338200	−0.09986400
C	−0.80463300	0.95933800	−0.00203700
C	−1.00674200	−0.45330300	−0.04978300
C	0.13185500	−1.28375400	−0.10504600
C	−3.29965300	1.29303700	0.09938900
H	−4.12504100	1.99299300	0.14272400
C	−3.48276700	−0.03988000	0.09866300
H	−4.49250700	−0.44051200	0.14867200
C	−1.95968200	1.86894800	0.03442600
C	3.08000600	0.92212700	−0.22635200
H	3.37764900	1.93045100	−0.50315400
C	3.46746000	−0.24785900	−1.17095800
H	3.00496000	−0.17312600	−2.15721200
H	4.54706400	−0.38478500	−1.25502000
C	2.80047300	−1.32037400	−0.26524000
H	2.88295300	−2.35872700	−0.59003500
C	−2.39529200	−1.06554100	0.04094300
C	−2.68791300	−1.93754800	−1.20165600
H	−2.61074800	−1.33390300	−2.10771100
H	−1.98953900	−2.76823100	−1.26717700
H	−3.70288300	−2.33735700	−1.13843200
C	−2.52859000	−1.91235100	1.32781300
H	−3.54015200	−2.31971500	1.39748700
H	−1.82003200	−2.73728100	1.32089700
H	−2.34486400	−1.28944700	2.20491200

Compound **V**

E(MP2) = −843.76071778 a.u.

C	−2.24075700	−1.08607400	−0.11253000
O	0.11567000	−2.64451800	0.18396300
H	0.97361300	−3.08759400	0.14054400
O	0.91784100	2.81067600	−0.07867200
H	0.03292900	3.25285700	−0.09597700
C	−2.32930700	−2.14789700	−1.22354800
H	−3.37871200	−2.41826700	−1.36898800
H	−1.94992200	−1.74265900	−2.16443000
H	−1.76984300	−3.04626000	−0.98137900
H	−1.91290100	−2.51504200	1.49423400
C	−2.61294600	−1.72110100	1.23810700
H	−3.61733200	−2.14972500	1.18124000
H	−2.59913500	−0.98382100	2.04287300
O	−1.63380700	3.10556400	−0.00402700
C	3.15713000	1.27934900	−0.01531800
H	3.19528900	1.98065900	−0.85457700
H	3.27908300	1.90546800	0.87625600
C	2.78360200	−1.69270900	0.15631300
H	2.77010000	−2.19005300	1.13630800
H	2.68711500	−2.49170600	−0.59241400
C	−1.77325700	1.86502200	0.08223800
C	4.28180000	0.29660700	−0.11161900
H	5.28011600	0.69955400	−0.24545200
C	4.11730900	−1.03254400	−0.04013000
H	4.97944300	−1.68669100	−0.11212300
C	1.79712100	0.63554400	0.01569000
C	1.60955400	−0.74798500	0.04867100
C	0.67211000	1.47267900	−0.05536900
C	−0.63720500	0.93640800	−0.02414800
C	−0.84257400	−0.47457500	−0.03415800
C	0.30053200	−1.27753900	0.07495100
C	−3.26813600	−0.00442700	−0.48239400
H	−3.15023000	0.24908700	−1.54203200
H	−4.27196000	−0.42363600	−0.36744600
C	−3.12470300	1.26707100	0.34001200
H	−3.87933800	2.01447300	0.09237500
H	−3.20757300	1.05261200	1.41027500

Compound **VI**

E(MP2) = −844.97057376a.u.

C	2.25260400	−1.10165500	0.16801600
O	−0.07202900	−2.64301300	−0.34772600
H	−0.91966500	−3.05316900	−0.56516200
O	−0.84702600	2.84078100	−0.08497600
H	0.03933400	3.26617800	0.02297100
C	2.23578900	−2.18056600	1.26607200
H	3.26659900	−2.46343500	1.49652100
H	1.78107900	−1.78528900	2.17735800
H	1.69197400	−3.07069000	0.96471500
H	2.05290600	−2.50263900	−1.48276700
C	2.73561200	−1.72028500	−1.15511600
H	3.72719800	−2.16018200	−1.01746200
H	2.79868100	−0.97077100	−1.94607400
O	1.70060700	3.09503700	0.08093900
C	−3.13976400	1.18180000	−0.32849100
H	−3.15269900	2.25364900	−0.13697500
H	−3.55810500	1.02605900	−1.32998500
C	−2.81730900	−1.52896200	−0.48658000
H	−3.21111500	−1.37003100	−1.49654800
H	−2.65909200	−2.60664800	−0.38890900
C	1.83106000	1.85415600	−0.01566500
C	−1.73305200	0.66234800	−0.27435300
C	−1.55489900	−0.72480200	−0.31720400
C	−0.62225800	1.49908500	−0.10894300
C	0.67849500	0.93900000	−0.01985500
C	0.87083200	−0.47564600	−0.02183000
C	−0.26111000	−1.27611100	−0.24210100
C	3.25498100	−0.03797700	0.64202700
H	3.04916800	0.20151600	1.69148900
H	4.26078200	−0.46670100	0.60707500
C	3.19355100	1.24586400	−0.17027000
H	3.93190400	1.98189000	0.14993000
H	3.36267700	1.04539800	−1.23299800
C	−3.87844200	−1.10554000	0.55048400
H	−4.84013300	−1.52665800	0.24850200
H	−3.62249000	−1.56301300	1.50825900
C	−3.98083400	0.42810400	0.71264300
H	−5.02273100	0.74949800	0.64995800
H	−3.62023800	0.71971600	1.70120100

Compound **VII**

E(MP2) = −841.38495769a.u.

C	4.03065300	−1.11064100	−0.07625100
C	2.75058400	−1.63560000	−0.08305300
C	1.61159700	−0.78762300	−0.04323200
C	1.82500300	0.61982600	0.05936300
C	3.14286100	1.14007100	0.04803700
C	4.22868000	0.28498000	0.01773200
C	0.27970000	−1.29517000	0.02449500
C	0.69678200	1.48569300	0.01608400
C	−0.60337000	0.95862700	0.02428200
C	−0.83047800	−0.46126300	−0.01283100
C	−2.23973800	−1.03754200	0.00716500
C	−3.29810200	0.02096800	−0.05048000
C	−3.08507800	1.34941500	−0.07290800
C	−1.73241200	1.89566300	−0.03874300
H	4.88346200	−1.77662800	−0.12841000
H	2.63680500	−2.70711600	−0.20301700
H	3.27666600	2.21232800	0.09953400
H	5.23426700	0.68734500	0.02209700
H	−4.31917500	−0.35281700	−0.06978700
H	−3.89606900	2.06616800	−0.11268200
O	0.08143700	−2.66658100	0.01727700
H	0.85183100	−3.09002700	0.42076300
O	0.95160500	2.81385100	0.04168700
H	0.06268300	3.26008100	0.01281600
C	−2.47987500	−1.94866500	−1.21767400
H	−3.50928800	−2.31532200	−1.20475400
H	−2.32727600	−1.38435100	−2.13934600
H	−1.80639100	−2.80205100	−1.20943800
H	−1.81053000	−2.67456600	1.38004600
C	−2.48666600	−1.82545200	1.31359400
H	−3.51513100	−2.19417100	1.33406700
H	−2.33461100	−1.17560800	2.17704800
O	−1.56905200	3.14360500	−0.04301600

Compound **VIII**

E(MP2) = −992.43761434 a.u.

C	3.59518100	−0.88821200	0.00293300
C	2.28512700	−1.32734700	0.00528000
C	1.25099200	−0.38996500	−0.05389100
C	1.42109500	1.00016100	0.02246500
C	2.77102100	1.46783300	−0.00090700
C	3.79805300	0.51268600	0.02431200
C	0.02257700	−1.05775200	−0.00482500
C	0.19698900	1.74257600	−0.01852300
H	4.43364200	−1.57385000	0.03080600
H	4.81887900	0.87850000	0.02262900
O	0.23357200	−2.43306300	−0.01685800
O	0.27784600	3.08994300	−0.01631900
H	−0.66566900	3.41944700	−0.02736100
C	−2.62632600	−2.02189000	−1.21284200
H	−3.59069700	−2.53488100	−1.19432300
H	−2.55963100	−1.44067300	−2.13393900
H	−1.83509200	−2.77068200	−1.20705300
H	−1.81736700	−2.69379700	1.32520700
C	−2.60185700	−1.93738400	1.30714100
H	−3.57066200	−2.44039400	1.35060700
H	−2.50077100	−1.29816600	2.18563500
O	−2.24803900	3.13357900	−0.03194200
C	1.64322400	−2.66203000	−0.01886500
O	2.09521900	−3.78502600	−0.02927300
C	3.11779100	2.93218500	0.02552700
H	2.70885400	3.44739900	−0.84306500
H	2.69578100	3.41686200	0.90536500
H	4.19999600	3.05982500	0.03538400
C	−2.27381600	1.87497700	−0.01744900
C	−3.56657000	1.19119800	−0.02020800
H	−4.44088700	1.83036200	−0.03623700
C	−3.66168000	−0.15228600	−0.00582800
H	−4.64455600	−0.61745500	−0.00544700
C	−1.17246000	−0.37521800	−0.01799200
C	−1.04737000	1.06522500	0.02528700
C	−2.50207200	−1.09575100	0.01620500