Chemistry of Heterocyclic Compounds **2023**, *59*(3), 118–127

Prediction of the regioselectivity of the ruthenium-catalyzed [3+2] cycloadditions of benzyl azide with internal alkynes using conceptual DFT indices of reactivity

Youcef Yousfi[1], Wafaa Benchouk[1]*, Sidi Mohamed Mekelleche[1]

[1] *Laboratory of Applied Thermodynamics and Molecular Modeling, Department of Chemistry, Faculty of Science, University of Tlemcen, BP 119, Tlemcen 13000, Algeria; e-mail: wafaa.benchouk@mail.univ-tlemcen.dz*

SUPPLEMENTARY INFORMATION

Contents

Cartesian coordinates and energies for all optimized structures

Ruthenium(II) catalyzed benzyl azide with Internal Alkynes

All structures are optimized at B3LPY/6-31G(d) (LanL2DZ for Ru and Cl) level of theory

MC-1A **E**(Hartree)**=** -1395.554642

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.06626200	1.83851400	1.12040400
C	-2.21580900	2.27714700	-0.23050700
C	-1.01020900	3.01317500	-0.59352300
C	-0.14351600	3.01248200	0.52627100
C	-0.75697200	2.25176300	1.57800300
C	-0.47932200	-0.81231300	1.25920800
C	-1.32232600	-1.17710000	0.36880300
N	1.58615300	-0.95756200	-1.33978500
N	1.60573500	-1.87864000	-1.99045400
N	1.46570500	0.03582100	-0.60763800
Cl	-0.90302300	0.38599900	-2.63376700
Ru	-0.60175300	0.78419600	-0.15730100
C	-3.45119000	2.19104700	-1.07283500
C	-0.81398000	3.74137900	-1.88648900
C	-3.12072900	1.18947600	1.96310600
C	-0.25157300	2.16320500	2.98686200
C	1.15543500	3.74938700	0.64586800
H	-4.10633600	1.38450700	-0.74184000
H	-4.01504100	3.12988200	-1.01109800
H	-3.19874000	2.00590400	-2.11702300
H	-3.84114600	0.64522400	1.35199700
H	-2.68994600	0.48240200	2.67327000
H	-3.66761200	1.94770000	2.53515700
H	0.81271200	1.93397700	3.02587800
H	-0.42293900	3.11341600	3.50710500
H	-0.76772500	1.38394200	3.54758400
H	1.65125800	3.86361700	-0.31883600
H	0.97683000	4.75580400	1.04262900
H	1.84341100	3.25075400	1.32985900
H	-1.45855900	4.62728900	-1.92554400
H	0.21735600	4.07560400	-2.00898500
H	-1.06079100	3.09757900	-2.73250100
C	-2.25656800	-2.18795100	-0.07164900
C	-2.59310600	-2.35704400	-1.42567800
C	-2.86415800	-3.02753600	0.88564400
C	-3.48748700	-3.35202600	-1.80588100
H	-2.14424200	-1.70070500	-2.15948200
C	-3.76905900	-4.00699000	0.49787400
H	-2.63019100	-2.89299400	1.93440800
C	-4.07900300	-4.17779500	-0.85159200
H	-3.72856300	-3.47746100	-2.85549900
H	-4.23184800	-4.63944200	1.24742300
H	-4.78067100	-4.94691900	-1.15475000
C	0.42598600	-1.17946600	2.32655900
O	1.44033600	-0.54452900	2.59603000
C	0.06062200	-2.42609700	3.11849600
H	-0.83612200	-2.23964800	3.71789800
H	-0.15898000	-3.26385700	2.45221100
H	0.88617600	-2.68052000	3.78310200
C	2.73825800	0.69434500	-0.16012200
H	2.86482200	1.58937000	-0.77468900
H	2.53258800	0.98806200	0.86669800
C	3.96656600	-0.17767600	-0.22641300
C	4.28050500	-1.03421800	0.83570200
C	4.80454900	-0.14392000	-1.34532600
C	5.41433200	-1.83945300	0.77464800
H	3.63315700	-1.05812300	1.70548800
C	5.93862600	-0.95054200	-1.40532800
H	4.57027800	0.51914200	-2.17213600
C	6.24479300	-1.79945200	-0.34449100
H	5.65274000	-2.49613700	1.60382600
H	6.58187400	-0.91402200	-2.27717500
H	7.12852500	-2.42609600	-0.38846800

MC-1B **E**(Hartree)**=** -1395.552113

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.45116400	-1.92688200	0.71981500
C	1.30054300	-2.50475900	1.39976300
C	0.77184300	-1.52859600	2.27876400
C	1.56082600	-0.32828400	2.16039000
C	2.63392000	-0.60069400	1.23320400
C	1.13594500	1.36107700	-0.59654900
C	1.55693900	0.57968800	-1.49197600
N	-1.69974500	0.46678300	-1.22483100
N	-1.83338200	1.08549900	-2.15723900
N	-1.44358500	-0.13179200	-0.16224700
Cl	0.06287400	-2.32214200	-1.73568000
Ru	0.76855500	-0.69553200	0.07790800
C	0.84421500	-3.92059000	1.23645800
C	-0.35303900	-1.71755200	3.25088200
C	3.38564000	-2.66088000	-0.19248200
C	3.79865300	0.29291900	0.93502700
C	1.46201200	0.85957700	3.06966900
H	0.74550400	-4.17482700	0.17995300
H	1.57198400	-4.60331300	1.68972600
H	-0.11998200	-4.09644900	1.71550500
H	2.84296000	-3.36129000	-0.82785900
H	3.92091600	-1.96988900	-0.84440300
H	4.12487700	-3.22462900	0.38980000
H	3.56938800	1.33693400	1.15051700
H	4.65498300	0.00249400	1.55439900
H	4.09461000	0.22742900	-0.11302700
H	0.42847600	1.07548500	3.34572600
H	2.01810100	0.67269500	3.99667400
H	1.87273500	1.75871500	2.61218100
H	0.04572600	-1.95627600	4.24386000
H	-0.95487800	-0.81250600	3.35736400
H	-1.01217500	-2.53639800	2.96039800
C	-2.49603300	-1.12308500	0.25536000
H	-2.31947600	-2.03539000	-0.31811900
H	-2.26961500	-1.31988000	1.30089600
C	-3.90965900	-0.62297000	0.09515500
C	-4.45282500	0.28724500	1.00945500
C	-4.69592600	-1.05496100	-0.97650900
C	-5.75438500	0.75343800	0.85683200
H	-3.85197300	0.62821000	1.84654800
C	-6.00090400	-0.59000400	-1.13048600
H	-4.28488700	-1.76142200	-1.69000700
C	-6.53161200	0.31444900	-0.21485600
H	-6.16510600	1.45504600	1.57413500
H	-6.60105900	-0.93564100	-1.96437100
H	-7.54693700	0.67548900	-0.33296000
C	0.93333800	2.69706700	-0.08792700
C	1.80215800	3.72879700	-0.49324100
C	-0.11782500	3.01098900	0.78800300
C	1.61454100	5.02885600	-0.04008900
H	2.62034800	3.49518500	-1.16428100
C	-0.30287700	4.31585700	1.23338100
H	-0.78646200	2.22095700	1.10676100
C	0.56115800	5.32956400	0.82379400
H	2.29277400	5.81108600	-0.36260500
H	-1.12521900	4.54266800	1.90300300
H	0.41648200	6.34510500	1.17418600
C	2.29135200	0.25023500	-2.71681900
O	3.50608800	0.15171800	-2.67577800
C	1.48952800	0.02937300	-3.97103500
H	2.16415600	-0.10658800	-4.81636800
H	0.86974900	-0.86097400	-3.82728400
H	0.81488600	0.87137400	-4.14919400

MC-1C **E**(Hartree)**=** -1395.551214

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.87504800	-1.65058000	0.64035900
C	-2.09066300	-2.67926200	0.03235100
C	-1.88603100	-2.34170400	-1.35414300
C	-2.60957800	-1.11698200	-1.61182900
C	-3.20991200	-0.68839000	-0.38505500
C	-1.11391500	1.31605800	0.70932000
C	-0.70894200	0.58269500	1.64524800
N	1.51166400	0.40516500	-1.54423300
N	2.65780700	0.79688200	-1.55204900
N	0.39120200	0.15440800	-1.55328300
Cl	1.15535100	-1.95429900	0.51662500
Ru	-0.96959300	-0.72494900	-0.14364500
C	-1.59977500	-3.92694800	0.69446400
C	-1.19916400	-3.20861800	-2.36636000
C	-3.39808300	-1.62907400	2.04483600
C	-4.17622700	0.44176200	-0.20385300
C	-2.77665300	-0.47099700	-2.95341400
H	-1.56877900	-3.82046500	1.77826100
H	-2.27135200	-4.75939600	0.45244700
H	-0.59395800	-4.18088300	0.36147200
H	-2.86566000	-2.33691500	2.68001200
H	-3.29278500	-0.64564100	2.50526600
H	-4.45991000	-1.90177400	2.05725300
H	-4.04053300	1.22555400	-0.94882900
H	-5.20243300	0.06618600	-0.29347700
H	-4.07706900	0.89776900	0.78183600
H	-1.86913800	-0.55780400	-3.55301300
H	-3.58986900	-0.95244100	-3.50875000
H	-3.01880200	0.58824500	-2.86130400
H	-1.85276700	-4.02575900	-2.69400700
H	-0.91500900	-2.63779200	-3.25188300
H	-0.29150900	-3.64793500	-1.94927800
C	3.72373700	-0.24504000	-1.75942600
H	3.28963300	-1.23155300	-1.58677800
H	4.04489800	-0.16337400	-2.80117200
C	4.87986900	0.00690300	-0.82644800
C	4.81299100	-0.42835500	0.50115200
C	6.02059900	0.67907000	-1.26932500
C	5.87654300	-0.19486200	1.36799400
H	3.92584100	-0.94933600	0.84564000
C	7.08513200	0.91275600	-0.40136500
H	6.07733000	1.02106600	-2.29785200
C	7.01392400	0.47567100	0.91905500
H	5.81911400	-0.53939100	2.39439600
H	7.96753700	1.43337300	-0.75613100
H	7.84203500	0.65469800	1.59572900
C	-0.36312300	0.33239700	3.04531000
O	-1.24537400	0.34352300	3.88755700
C	1.08279200	0.07499600	3.37593100
H	1.40913000	-0.83341100	2.86109800
H	1.70733500	0.89108300	3.00068700
H	1.19465200	-0.02298800	4.45576500
C	-1.49487200	2.61052200	0.19613500
C	-1.48160700	2.91685300	-1.17282400
C	-1.89431600	3.60859800	1.10616200
C	-1.84354600	4.18472600	-1.61848600
H	-1.17917300	2.15471400	-1.87913000
C	-2.25827500	4.87054100	0.65407500
H	-1.91733800	3.37663900	2.16444000
C	-2.23411800	5.16553200	-0.70951700
H	-1.82026500	4.40667500	-2.67968200
H	-2.56327700	5.62738400	1.36817000
H	-2.51894700	6.15133600	-1.05902300

MC-1D **E**(Hartree)**=** -1395.552407

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.22484200	0.63475500	-0.68092000
C	2.93038600	-0.27640100	-1.74264200
C	2.88766300	-1.61205900	-1.20350300
C	3.21792400	-1.52247400	0.19991100
C	3.42024500	-0.14305000	0.52205300
C	0.64312400	0.60521700	1.61908700
C	0.27162300	1.34320600	0.65846700
N	-1.06020700	-2.15862300	0.71946400
N	-2.23572300	-2.31471100	0.97375900
N	0.06969800	-2.01402200	0.59228700
Cl	-0.45954500	-0.52682600	-2.01337100
Ru	1.30023200	-0.42830000	-0.17529900
C	2.74212400	0.06887600	-3.18638200
C	2.70381300	-2.86469800	-2.00678500
C	3.47205000	2.10815900	-0.80636600
C	3.93142000	0.39122500	1.82542500
C	3.37596200	-2.66639500	1.15422900
H	2.61590000	1.14184100	-3.33092800
H	3.62210100	-0.24685800	-3.75884800
H	1.86325800	-0.42903900	-3.59779300
H	2.93320200	2.53812400	-1.65089200
H	3.15766300	2.64298500	0.09113900
H	4.54042800	2.30640600	-0.95351400
H	3.65087600	-0.25065900	2.65926900
H	5.02555000	0.45713100	1.79514400
H	3.54905700	1.39324200	2.02729500
H	2.83456100	-3.54790300	0.80969000
H	4.43314700	-2.93929400	1.25208700
H	2.99136300	-2.40326600	2.14042300
H	3.64377000	-3.16742600	-2.48370800
H	2.36812200	-3.69307700	-1.38106100
H	1.95868300	-2.71960500	-2.79053300
C	-3.12625400	-2.67263900	-0.18577000
H	-2.55039500	-2.60993300	-1.11106900
H	-3.44642200	-3.70412600	-0.02147600
C	-4.31610900	-1.74667700	-0.22630200
C	-4.19751500	-0.48098800	-0.81047800
C	-5.53900400	-2.13382500	0.32541800
C	-5.29085200	0.37987600	-0.84010100
H	-3.24861200	-0.17892200	-1.24190800
C	-6.63329100	-1.27207000	0.29436500
H	-5.63601000	-3.11396500	0.78144200
C	-6.50991500	-0.01313200	-0.28861900
H	-5.19073800	1.35822200	-1.29652200
H	-7.57924200	-1.58373000	0.72303500
H	-7.36066100	0.65879200	-0.31514800
C	-0.33498500	2.55667400	0.16866500
C	-0.50182400	2.80499300	-1.20385100
C	-0.74283500	3.54494700	1.08818400
C	-1.05832500	4.00318600	-1.63847400
H	-0.22271500	2.03262700	-1.90752000
C	-1.29252800	4.74087500	0.64639500
H	-0.61967000	3.36624700	2.14891100
C	-1.45223500	4.97457500	-0.71987800
H	-1.18713200	4.17783100	-2.70080900
H	-1.59843600	5.49142100	1.36667000
H	-1.88378500	5.90780200	-1.06433900
C	0.68709100	0.20739100	3.01609800
O	1.21434700	-0.82493200	3.39917300
C	0.02368100	1.16188400	3.99745100
H	0.53001400	2.13179600	3.98259800
H	-1.02133400	1.32977400	3.72352600
H	0.08069300	0.73716900	4.99929800

MC-2A **E**(Hartree)**=** -1243.097015

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-1.90580700	1.60331600	1.70429100
C	-1.98298100	2.58882500	0.67354100
C	-0.70047500	3.28332300	0.62464400
C	0.13910900	2.71849400	1.61572700
C	-0.57049600	1.65058000	2.25950800
C	-0.57493000	-0.98383800	0.67172100
C	-1.43322400	-0.87950700	-0.26850600
N	1.34335200	-0.43108500	-1.76701300
N	1.19567500	-1.20241700	-2.57513800
N	1.41602100	0.37467000	-0.82254300
Cl	-0.86942100	1.77840800	-2.34353000
Ru	-0.53823100	1.04983100	0.05733300
C	-3.20247100	2.99113000	-0.09657900
C	-0.40741600	4.46744000	-0.24337400
C	-3.03205000	0.75889900	2.21656600
C	-0.10410000	0.92756400	3.48708200
C	1.50306900	3.19364400	2.01297000
H	-3.94847500	2.19594600	-0.10799600
H	-3.66124900	3.87674500	0.35973300
H	-2.94868700	3.22354400	-1.13092200
H	-3.80285100	0.61882400	1.45824000
H	-2.68724000	-0.23082200	2.51960500
H	-3.49734100	1.23543600	3.08705600
H	0.93033600	0.59656200	3.40049200
H	-0.18663300	1.58727200	4.35947700
H	-0.71152300	0.04474200	3.68623800
H	2.01572500	3.70369300	1.19645000
H	1.42237100	3.90644900	2.84226000
H	2.13216900	2.37103700	2.35885600
H	-0.99164700	5.33473400	0.08493200
H	0.64715900	4.74510300	-0.20513600
H	-0.66267800	4.25374800	-1.28325900
C	-2.42045600	-1.55860100	-1.07470800
C	-3.03297200	-0.94686800	-2.18040700
C	-2.79738700	-2.87174800	-0.72350100
C	-3.99365400	-1.63420700	-2.91548400
H	-2.72692900	0.05315900	-2.45842300
C	-3.76058100	-3.54660700	-1.46086000
H	-2.32339400	-3.34069000	0.12985000
C	-4.36205000	-2.93012200	-2.55963600
H	-4.45490200	-1.15503600	-3.77184800
H	-4.04399700	-4.55551800	-1.18154300
H	-5.11265800	-3.46024600	-3.13565600
C	0.24558000	-1.82993400	1.50493600
O	1.31642800	-1.53522600	2.00210700
O	-0.32494700	-3.05326200	1.68045900
C	0.44147900	-4.00673400	2.45358200
C	-0.37555900	-5.27942600	2.54715600
H	0.64889500	-3.57955800	3.43763900
H	1.40025600	-4.17335700	1.95638700
H	0.16917800	-6.02776600	3.12891000
H	-1.33303200	-5.09288000	3.03856100
H	-0.57038400	-5.69187200	1.55482200
C	2.72060700	1.08922900	-0.71012500
H	2.74843400	1.87979600	-1.46619900
H	2.67722200	1.55880300	0.26922700
C	3.92881800	0.18821400	-0.81845400
C	4.86515500	0.37818200	-1.83665700
C	4.12602600	-0.84086100	0.11158900
C	5.99233000	-0.43804900	-1.92325600
H	4.71336300	1.16822600	-2.56516300
C	5.24907100	-1.65667100	0.02033200
H	3.39203000	-1.00571600	0.89390800
C	6.18578800	-1.45601400	-0.99419800
H	6.71320800	-0.27995800	-2.71742000
H	5.39536700	-2.45089500	0.74389100
H	7.06052800	-2.09322100	-1.06065300

MC-2B **E**(Hartree)**=** -1243.093188

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.21366000	0.18228800	-0.27772500
C	2.94628800	-1.13844000	-0.83253000
C	2.37519700	-1.93734400	0.18328100
C	2.26557200	-1.14435900	1.38394700
C	2.83721400	0.15661600	1.10408900
C	-0.12622600	1.04549400	1.36240800
C	-0.04905500	1.77410400	0.34174700
N	-1.27782700	-1.97804300	0.37670700
N	-1.46773500	-2.77599000	1.15963900
N	-1.00453700	-1.09148400	-0.43465000
Cl	0.73288000	0.64773100	-2.54995200
Ru	1.04507600	-0.05014300	-0.13756700
C	3.30012100	-1.56698700	-2.22157100
C	1.99169200	-3.38159500	0.06845500
C	3.94831800	1.27380200	-0.99331600
C	3.11520000	1.23667200	2.10422500
C	1.91520000	-1.69776000	2.73425400
H	2.97150200	-0.82672500	-2.95225800
H	4.38607200	-1.68729200	-2.31121700
H	2.83593600	-2.51920000	-2.48051200
H	3.58080700	1.38187300	-2.01458500
H	3.82717300	2.23373400	-0.48997900
H	5.02141900	1.05093500	-1.03455900
H	2.41193400	1.21174000	2.93675100
H	4.12399200	1.11834000	2.51620600
H	3.05305500	2.22649000	1.65102900
H	1.01138700	-2.31058300	2.70811800
H	2.72847700	-2.33165600	3.10714400
H	1.75889700	-0.90718000	3.46765900
H	2.83187100	-4.02040000	0.36535200
H	1.15138000	-3.63223400	0.71774000
H	1.72088100	-3.64769100	-0.95393600
C	-0.46299200	2.96805500	-0.40480600
O	-1.64487200	3.21637200	-0.56458900
C	0.62518200	3.85044400	-0.96231700
H	1.07753200	3.32647400	-1.80907000
H	0.19372000	4.79363300	-1.29670400
H	1.40694600	4.02927400	-0.21922400
C	-0.65384200	0.77650300	2.71723200
C	-1.60778900	1.88362100	3.19554500
H	0.17027200	0.66473500	3.42988400
H	-1.17603700	-0.18671000	2.71825300
H	-1.99655300	1.64683900	4.18961600
H	-1.09198300	2.84506900	3.24872000
H	-2.44945900	1.99161600	2.50962700
C	-2.05845200	-0.83732000	-1.49256600
H	-2.02398200	-1.67592700	-2.19327500
H	-1.68687600	0.04399600	-2.00779900
C	-3.44220500	-0.64855600	-0.92756400
C	-4.34834500	-1.71366600	-0.89965100
C	-3.83866500	0.59887700	-0.42799600
C	-5.62918600	-1.54355100	-0.37755300
H	-4.05541300	-2.67923600	-1.30059000
C	-5.11916300	0.76628100	0.09202000
H	-3.15054000	1.43826700	-0.45578700
C	-6.01558300	-0.30205600	0.12028100
H	-6.32365900	-2.37608000	-0.36679600
H	-5.42066300	1.73826300	0.46629800
H	-7.01356800	-0.16456200	0.52152600

MC-2C **E**(Hartree)**=** -1243.093553

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.95950300	-0.26367800	1.30997300
C	-2.51319700	-1.64145800	1.25013000
C	-2.60025900	-2.07733600	-0.09665500
C	-3.13278800	-0.99230200	-0.89810100
C	-3.39320700	0.10883900	-0.01252200

C	-0.82204300	1.52260400	-1.32450700
C	-0.76936100	1.92774700	-0.14765700
N	1.44188700	-1.16924100	-1.31957100
N	2.63912700	-1.08804500	-1.49607000
N	0.29582500	-1.19879100	-1.26860300
Cl	0.67139200	-0.36902900	1.67781200
Ru	-1.21103300	-0.27120000	-0.03909700
C	-2.06113000	-2.43909600	2.43327100
C	-2.26255500	-3.44115100	-0.61849700
C	-3.14516500	0.52828400	2.56786500
C	-4.06650600	1.39925200	-0.36483300
C	-3.55275700	-1.10700100	-2.33343600
H	-1.24582200	-1.93127200	2.95268400
H	-2.89125400	-2.57187300	3.13562400
H	-1.70769100	-3.42865300	2.14205700
H	-2.36705400	0.29008900	3.29460600
H	-3.10446800	1.60013800	2.37463400
H	-4.11591600	0.30031500	3.02516400
H	-3.98553500	1.61912200	-1.43035300
H	-5.13268400	1.33986100	-0.11727100
H	-3.63321100	2.23653900	0.18447400
H	-2.83648500	-1.68749400	-2.91815600
H	-4.52638900	-1.60546900	-2.41300800
H	-3.64890200	-0.12696500	-2.80190800
H	-3.16279400	-4.06433400	-0.67126900
H	-1.83811200	-3.38901100	-1.62258300
H	-1.54046900	-3.94842000	0.02178000
C	3.51317000	-1.79794700	-0.49705200
H	2.91154500	-2.05782500	0.37589400
H	3.86943800	-2.71035700	-0.98221000
C	4.67182900	-0.91595800	-0.10804100
C	4.49893100	0.07369600	0.86531800
C	5.92027100	-1.06901700	-0.71414200
C	5.56470700	0.89306200	1.22584500
H	3.52789400	0.19307800	1.33459300
C	6.98674100	-0.24828300	-0.35328500
H	6.05970900	-1.83431500	-1.47110200
C	6.80969800	0.73424800	0.61791000
H	5.42452500	1.65419800	1.98522100
H	7.95313500	-0.37752300	-0.82763200
H	7.63898400	1.37233300	0.90239600
C	-0.72435000	2.89060700	0.95431900
O	-1.74787200	3.43373400	1.33537800
C	0.61989200	3.15658400	1.57837500
H	0.97591100	2.22777500	2.03501200
H	1.34806000	3.43676100	0.81199700
H	0.52613600	3.94644400	2.32365000
C	-0.72627000	1.65490700	-2.79041300
C	-0.33687100	3.07681400	-3.22831600
H	-1.68461900	1.37399800	-3.24090900
H	0.00284600	0.93284100	-3.17291500
H	-0.28721400	3.13839300	-4.31865100
H	-1.06811700	3.80749500	-2.87587600
H	0.63976500	3.35257900	-2.82509200

MC-2D **E**(Hartree)**=** -1243.094852

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.99654900	-0.69462200	-0.99778400
C	2.44664000	-1.93567400	-0.47369700
C	2.32922200	-1.80595900	0.93339500
C	2.79665100	-0.49294100	1.31625800
C	3.25185800	0.17125400	0.11799500
C	0.66672900	1.99145100	0.39597700
C	0.64827100	1.91408800	-0.84561800
N	-1.56594900	-1.36599800	0.88475500
N	-2.35380000	-2.28988700	0.89724900
N	-0.77739700	-0.54114100	0.98064500
Cl	-0.38045700	-0.86810300	-2.05829100
Ru	1.08047300	-0.17251100	-0.07459200
C	2.15003300	-3.15257200	-1.29293700
C	1.83702700	-2.85892500	1.87979900
C	3.38202400	-0.47250500	-2.42840900

C	3.93968600	1.50089000	0.08418900
C	3.00911300	-0.01180800	2.72005600
H	3.08515400	-3.65428400	-1.56874300
H	1.53653000	-3.86848900	-0.74484700
H	1.61714300	-2.88969200	-2.20712400
H	2.59379100	-0.81630100	-3.10028800
H	3.55877500	0.58407900	-2.63316600
H	4.30243100	-1.01664700	-2.67138700
H	3.49912600	2.19395900	0.80262000
H	5.00001500	1.37598700	0.33282600
H	3.88290100	1.95858400	-0.90405800
H	2.28684600	-0.45477600	3.40860100
H	4.01078400	-0.28980200	3.07044300
H	2.91576400	1.07160800	2.79244100
H	2.67352400	-3.47351600	2.23197200
H	1.36285400	-2.41827500	2.75807600
H	1.11449900	-3.52367000	1.40467200
C	-3.41149500	-2.27721900	-0.17745100
H	-2.89623900	-2.32765800	-1.13891000
H	-3.96223400	-3.20169800	-0.01439000
C	-4.31893800	-1.07506000	-0.10764000
C	-4.04698300	0.05581700	-0.88517400
C	-5.42735600	-1.06750000	0.74568500
C	-4.87650300	1.17339200	-0.81040100
H	-3.18551600	0.05360300	-1.54521400
C	-6.25407700	0.04924700	0.81978300
H	-5.64333800	-1.94180300	1.35142900
C	-5.97939700	1.17252000	0.04035400
H	-4.66265600	2.04258100	-1.42218800
H	-7.11409100	0.04247400	1.48006100
H	-6.62590500	2.04133700	0.09414400
C	0.51064300	2.40748300	-2.22582900
C	-0.11062900	3.81245500	-2.29257100
H	-0.08513800	1.68836000	-2.79178100
H	1.50154700	2.41382200	-2.69520900
H	-0.17685700	4.14605300	-3.33165300
H	-1.11842300	3.81116700	-1.87093900
H	0.48829000	4.53881700	-1.73791300
C	0.60632500	2.57582000	1.73021900
O	1.60846100	2.97876100	2.29723600
C	-0.76330600	2.65377800	2.36684100
H	-0.67766200	3.07440100	3.36868300
H	-1.42113800	3.27749200	1.75431300
H	-1.21398400	1.65914200	2.40586600

MC-3A **E**(Hartree)**=** -1510.134555

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.54939300	-1.07311600	1.30378300
C	2.99774600	-1.54838100	0.03161200
C	2.16075400	-2.68463700	-0.33338000
C	1.21136400	-2.88196800	0.69562600
C	1.39979200	-1.86359800	1.69436300
C	0.39345500	1.07801600	0.87072900
C	1.08571400	1.44313800	-0.12341700
N	-1.59572900	-0.02173900	-1.69169300
N	-1.86696700	0.63043500	-2.57130700
N	-1.20213000	-0.69806300	-0.72961900
Cl	1.31613900	-0.45578000	-2.68361800
Ru	0.98739900	-0.69865600	-0.20101300
C	4.21773900	-1.11780900	-0.72381700
C	2.36816300	-3.53734900	-1.54595800
C	3.21378400	-0.03247000	2.15180000
C	0.73530700	-1.83447000	3.03885200
C	0.21687000	-4.00061900	0.77251500
H	4.58948900	-0.15495600	-0.37115100
H	5.02305700	-1.85157200	-0.59945800
H	3.99748400	-1.02187200	-1.78772700
H	3.82573800	0.64159200	1.55155000
H	2.48557200	0.57765400	2.68841200
H	3.86693500	-0.50902300	2.89160800
H	-0.32059100	-2.10137600	2.98152000
H	1.22417600	-2.54482300	3.71706800

H	0.79030800	-0.84783200	3.49699400
H	-0.13188900	-4.30192900	-0.21644800
H	0.67560500	-4.87954100	1.24049300
H	-0.65122600	-3.73096100	1.37492300
H	3.28728400	-4.12571800	-1.44211700
H	1.54222800	-4.23412900	-1.69539400
H	2.45265200	-2.91972300	-2.44196300
C	-0.47878100	1.39908100	1.97191100
O	-1.37030100	0.69815400	2.41669800
O	-0.18756300	2.61903200	2.49452900
C	-1.03697300	3.05539600	3.56884300
H	-0.62004100	4.00438000	3.89941100
H	-2.06152700	3.19351500	3.21794700
H	-1.03596900	2.32960000	4.38333200
C	-2.25648700	-1.46082700	0.02303500
H	-2.17151000	-2.50573900	-0.28551800
H	-1.95559300	-1.36698300	1.06456200
C	-3.66693100	-0.96460700	-0.17202400
C	-4.48129300	-1.50679400	-1.17148700
C	-4.17645100	0.05031000	0.64636500
C	-5.78213200	-1.04373100	-1.35437800
H	-4.09663500	-2.29809600	-1.80731900
C	-5.47746000	0.51117300	0.46387200
H	-3.54701600	0.46439000	1.42601400
C	-6.28167800	-0.03308800	-0.53626600
H	-6.40416400	-1.47292200	-2.13159800
H	-5.86605300	1.29393100	1.10575300
H	-7.29490000	0.32685600	-0.67555000
C	1.66984800	2.48725100	-0.98342800
C	1.11441000	3.89695900	-0.71683100
C	1.78936700	4.96419600	-1.58530300
H	2.75694500	2.47558700	-0.82345100
H	1.53292800	2.19574200	-2.02850100
H	1.23640900	4.14352300	0.34311000
H	0.03579900	3.89493700	-0.91070800
H	2.86882500	4.95959800	-1.38974000
H	1.67100700	4.69786300	-2.64213900
C	1.23477200	6.37132900	-1.34665900
H	1.36844900	6.67767100	-0.30436100
H	1.73691400	7.11015800	-1.97725000
H	0.16435500	6.41710600	-1.56986000

MC-3B **E**(Hartree)**=** -1510.126857

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	0.57116800	-1.73772300	2.33603200
C	-0.83639300	-1.95055600	2.01968300
C	-1.50484300	-0.70440900	2.12809500
C	-0.53922800	0.30258000	2.47049800
C	0.74120000	-0.34921300	2.63898200
C	1.37804600	1.22046400	0.05064300
C	2.07962500	0.20361600	-0.20418900
N	-0.28297400	0.43716100	-2.32985500
N	0.38719700	0.96902500	-3.06494900
N	-0.95182300	-0.08787400	-1.42123100
Cl	0.71049400	-2.62675800	-0.88636700
Ru	0.22547600	-0.58301000	0.52145500
C	-1.45155500	-3.28908200	1.75203400
C	-2.97652700	-0.46319600	1.99302200
C	1.59888000	-2.81544200	2.49185500
C	1.99633900	0.28280100	3.15929100
C	-0.86885300	1.70564300	2.88115100
H	-0.87559400	-3.83339400	1.00086500
H	-1.47302500	-3.88780900	2.66983900
H	-2.47810600	-3.19768500	1.39319600
H	1.49325100	-3.56863600	1.71097000
H	2.60944500	-2.41165800	2.42601800
H	1.48809000	-3.30362600	3.46802900
H	2.00835700	1.35846400	2.98038000
H	2.07464400	0.12217300	4.24065300
H	2.88209000	-0.14161100	2.68469900
H	-1.70349300	2.11223800	2.30848100

H	-1.15458500	1.72547700	3.94012800
H	-0.02243900	2.37928100	2.75384200
H	-3.44330900	-0.45051000	2.98534800
H	-3.18918300	0.49512600	1.51771900
H	-3.46725300	-1.23841800	1.40633700
C	3.31227800	-0.47953100	-0.57116000
O	4.14024600	-0.82921400	0.24215900
O	3.40849400	-0.68193700	-1.89040800
C	4.52936500	-1.48792900	-2.33330400
C	4.38889300	-1.66593700	-3.83069000
H	4.49736800	-2.44114800	-1.80209100
H	5.45787500	-0.97928000	-2.06274100
H	5.21694400	-2.27010100	-4.21133200
H	3.45145000	-2.17148700	-4.06957600
H	4.40240200	-0.70056200	-4.34148400
C	1.21050000	2.65364400	0.09521500
C	-0.04397400	3.26133200	-0.07154900
C	2.33612300	3.47813600	0.28496000
C	-0.16798900	4.64661700	-0.06417400
H	-0.91582900	2.63302400	-0.20699500
C	2.20463700	4.86149700	0.29722900
H	3.30849300	3.01912800	0.41933300
C	0.95361800	5.45289400	0.12111900
H	-1.14384500	5.09921900	-0.20191900
H	3.08233800	5.48125500	0.44362200
H	0.85467700	6.53231000	0.12949100
C	-2.04982800	-0.96803700	-1.91653000
H	-1.91840100	-1.12632000	-2.99191000
H	-1.89616800	-1.93468700	-1.43741300
C	-3.43280000	-0.41870600	-1.63966500
C	-3.70526500	0.95116900	-1.64695700
C	-4.48619100	-1.31323000	-1.42750100
C	-5.00218300	1.41719800	-1.44112800
H	-2.90077800	1.65900100	-1.81021300
C	-5.78437300	-0.84980700	-1.22806000
H	-4.28786000	-2.38044500	-1.41882900
C	-6.04598400	0.51865600	-1.23121800
H	-5.19729600	2.48383600	-1.44770900
H	-6.58961800	-1.55727500	-1.06459500
H	-7.05482400	0.88176800	-1.07177000

MC-3C **E**(Hartree)**=** -1510.129488

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.03644500	1.22060100	-1.28882200
C	-2.99350300	2.16124900	-0.18217800
C	-3.31284500	1.44662800	1.00692400
C	-3.53413600	0.06342600	0.67269300
C	-3.39859100	-0.06157700	-0.75607900
C	-0.49623100	-1.45595800	0.17419900
C	-0.44362900	-1.05490500	-1.01725800
N	0.94286100	1.09666900	1.91577500
N	2.12800300	1.09084300	2.16179500
N	-0.19180400	1.00432900	1.76394300
Cl	0.37649100	1.93447500	-1.09770100
Ru	-1.41673800	0.55290900	0.05572700
C	-2.74614100	3.63238900	-0.32171700
C	-3.41530700	2.02783900	2.38430700
C	-2.89392600	1.58270600	-2.73437900
C	-3.69589000	-1.29224200	-1.55623700
C	-4.06453000	-0.99422700	1.59489300
H	-1.86016800	3.81889500	-0.93168600
H	-3.60228300	4.12167300	-0.80008100
H	-2.59154700	4.10783900	0.64779800
H	-2.15282300	2.37209500	-2.86299700
H	-2.56403700	0.72879800	-3.32418600
H	-3.85243200	1.93941900	-3.13129500
H	-3.46315000	-2.20041400	-0.99794700
H	-4.76224800	-1.32104700	-1.80944000
H	-3.12209800	-1.30818200	-2.48213600
H	-3.76902900	-0.81416200	2.62967300
H	-5.16080900	-1.01360700	1.56616000
H	-3.70871800	-1.98716600	1.31726500

H	-4.44987400	2.32343700	2.59318300
H	-3.11720000	1.30775100	3.14782200
H	-2.78672800	2.91155400	2.49637000
C	2.92495200	2.27189700	1.67658800
H	2.30404600	2.86063600	0.99880300
H	3.17384100	2.86470100	2.56012400
C	4.17761000	1.79664500	0.98493600
C	4.11226400	1.33012900	-0.33256400
C	5.40706800	1.81231700	1.64611100
C	5.26686600	0.89273500	-0.97476200
H	3.15598800	1.31553500	-0.84563600
C	6.56216400	1.37325700	1.00222600
H	5.46216200	2.17052700	2.66923600
C	6.49298100	0.91317000	-0.31035000
H	5.21062000	0.54082100	-1.99885900
H	7.51253000	1.39204400	1.52388500
H	7.39089800	0.57365600	-0.81477900
C	-0.08870900	-1.25350700	-2.41475200
O	-0.77423100	-0.96383200	-3.36935400
O	1.11740400	-1.85365800	-2.52228200
C	1.58713700	-2.08986500	-3.87316300
C	2.96704400	-2.70638900	-3.77068800
H	1.60033400	-1.13695700	-4.40642500
H	0.87867700	-2.74738100	-4.38306700
H	3.36929900	-2.88254800	-4.77191900
H	3.64886100	-2.04231800	-3.23553500
H	2.93233400	-3.66177100	-3.24223500
C	-0.19854400	-2.42253800	1.19965100
C	-0.66009800	-2.28927100	2.51778300
C	0.58566900	-3.54561900	0.86784900
C	-0.35691500	-3.25271300	3.47471900
H	-1.24922200	-1.42033400	2.78048400
C	0.88101200	-4.50503300	1.82638400
H	0.95903900	-3.64162300	-0.14449900
C	0.41027800	-4.36400500	3.13302900
H	-0.71881500	-3.13445700	4.48996000
H	1.48607700	-5.36372300	1.55746400
H	0.64618700	-5.11357300	3.87987500

MC-3D **E**(Hartree)**=** -1510.132838

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.17043200	-0.37524400	1.30074500
C	-2.99151100	-1.78704900	1.11626900
C	-3.08032800	-2.08409000	-0.28177500
C	-3.37696300	-0.84698000	-0.97468200
C	-3.44795500	0.19683200	0.00460200
C	-0.68087100	1.34734000	-0.46557800
C	-0.18753800	1.07953800	0.66956700
N	0.90396700	-1.23107700	-1.97897000
N	2.07838400	-1.19157300	-2.27510100
N	-0.22359600	-1.18394600	-1.77469900
Cl	0.36331600	-2.15018400	1.06284600
Ru	-1.37066100	-0.64459800	-0.01994100
C	-2.77455400	-2.79484900	2.20020300
C	-3.02595800	-3.45358500	-0.88955900
C	-3.27331900	0.34681800	2.61079700
C	-3.89344100	1.60633600	-0.23801000
C	-3.67193000	-0.69872600	-2.43641700
H	-2.43425900	-2.32649500	3.12331100
H	-3.71669500	-3.31513500	2.41039900
H	-2.02601400	-3.53249900	1.91194700
H	-2.66386500	-0.12860000	3.37971400
H	-2.94141700	1.38206800	2.52180700
H	-4.31106900	0.35856200	2.96556100
H	-3.73097900	1.90448400	-1.27266500
H	-4.96408700	1.69539000	-0.01974200
H	-3.36646600	2.31277900	0.40570700
H	-3.20469800	-1.49585400	-3.01607400
H	-4.75276600	-0.74597600	-2.61485500
H	-3.29449500	0.25089600	-2.81629100
H	-4.01472200	-3.92751100	-0.87703400
H	-2.69012800	-3.41554400	-1.92671500

H	-2.33752200	-4.09896200	-0.34210900
C	2.93180900	-2.33247300	-1.78974100
H	2.34177400	-2.95592000	-1.11531600
H	3.20926100	-2.90881700	-2.67534600
C	4.16048300	-1.79932500	-1.09649800
C	4.07768500	-1.35488100	0.22745500
C	5.38452100	-1.73477600	-1.76507400
C	5.20766700	-0.85566600	0.86840300
H	3.12755000	-1.40592400	0.74928400
C	6.51579200	-1.23656200	-1.12208300
H	5.45387200	-2.07606100	-2.79310900
C	6.42802500	-0.79571100	0.19617600
H	5.13439000	-0.51432300	1.89478700
H	7.46240000	-1.19383000	-1.64921100
H	7.30736100	-0.40831800	0.69883700
C	0.60486800	1.50167400	1.79740200
C	0.77940700	0.70154400	2.93750800
C	1.19910900	2.77989800	1.76168000
C	1.52489400	1.17055600	4.01412100
H	0.35408200	-0.29254600	2.94582200
C	1.94104600	3.23954300	2.84157800
H	1.06505800	3.39332000	0.87915900
C	2.10562500	2.43716900	3.97170600
H	1.65720600	0.54244900	4.88804700
H	2.39392000	4.22414500	2.80347300
H	2.68688700	2.79763300	4.81333700
C	-0.82174600	2.21357400	-1.61441400
O	-1.48177000	1.98733600	-2.60851200
O	-0.10650300	3.35788300	-1.45282300
C	-0.15838300	4.29643700	-2.55399600
C	0.69940000	5.48730800	-2.17765900
H	-1.19939300	4.57969200	-2.72789500
H	0.20458700	3.79912400	-3.45644300
H	0.68901200	6.22159500	-2.98749200
H	0.32278800	5.96936100	-1.27273600
H	1.73362100	5.18277800	-2.00342500

MC-4A **E**(Hartree)**=** -1396.995451

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.14716700	-0.81095900	0.06153300
C	2.36992800	-2.04409200	0.07514200
C	1.52731300	-2.01863200	1.21261500
C	1.71936500	-0.77116800	1.89917500
C	2.76392200	-0.04608700	1.20730800
C	0.31358900	1.74784300	0.48368900
C	0.93896500	1.92435900	-0.60618400
N	-1.64396800	-0.07511500	-1.60662100
N	-2.02721900	0.35807700	-2.57540300
N	-1.13423200	-0.50016400	-0.55958900
Cl	1.24266900	-0.50268200	-2.68541900
Ru	1.06340000	-0.17024200	-0.19323400
C	2.54485100	-3.17235400	-0.89343000
C	0.63256500	-3.12983200	1.67119500
C	4.27143300	-0.52468600	-0.88636000
C	3.41341600	1.21096700	1.69906200
C	1.17252400	-0.43092000	3.25358200
H	2.54172500	-2.80350500	-1.92050300
H	3.49648400	-3.68562300	-0.71191900
H	1.74670800	-3.91053100	-0.80113700
H	3.97798100	-0.74449800	-1.91350500
H	4.57575600	0.52193300	-0.84347200
H	5.14599500	-1.13659300	-0.63458200
H	2.68148000	1.90804100	2.11022200
H	4.13631000	0.97858400	2.48923400
H	3.94853800	1.72570700	0.90034500
H	0.12531900	-0.71294300	3.36010800
H	1.74574200	-0.95138600	4.03095600
H	1.23543600	0.63766100	3.45625100
H	1.20062100	-3.83870500	2.28490600
H	-0.19113000	-2.76029800	2.28285600
H	0.21492500	-3.68730100	0.83154600
C	1.40425500	2.75419300	-1.73380300

C	0.78693600	4.15846900	-1.79617900
H	1.22388900	2.19961100	-2.65815400
H	2.49704800	2.82405800	-1.65830200
H	1.18559500	4.70599100	-2.65434000
H	-0.29837400	4.10303800	-1.91004800
H	1.00712200	4.73588300	-0.89493200
C	-0.59321000	2.20231400	1.51472000
O	-1.27306400	1.44235900	2.19485600
C	-0.67817700	3.70840800	1.71771900
H	-1.33265600	3.91795500	2.56365800
H	0.31240200	4.13352100	1.89857600
H	-1.07709300	4.18624500	0.81886100
C	-2.05604400	-1.21142900	0.39115000
H	-1.70812600	-0.89711600	1.37261600
H	-1.87289100	-2.28167700	0.26740300
C	-3.52118600	-0.89968200	0.21810100
C	-4.32100200	-1.68191900	-0.62143800
C	-4.09884700	0.17923200	0.89820400
C	-5.67395500	-1.39311500	-0.78303300
H	-3.88382100	-2.52406500	-1.14871000
C	-5.45188400	0.46565900	0.73735100
H	-3.48245900	0.78210100	1.55575800
C	-6.24106200	-0.31766100	-0.10331700
H	-6.28343400	-2.00803700	-1.43543400
H	-5.89202500	1.29925700	1.27314800
H	-7.29473200	-0.09299000	-0.22537600

MC-4B **E**(Hartree)**=** -1396.987538

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.29941300	-1.27266100	1.48666700
C	2.11609600	-2.30891500	0.51484100
C	0.83663900	-2.95115100	0.79028200
C	0.24630200	-2.29442200	1.89656700
C	1.11512800	-1.22645000	2.31541600
C	1.10386500	1.38871300	0.36449600
C	1.56481200	0.97930900	-0.72859400
N	-1.63684500	1.05746200	-0.78657300
N	-1.65976100	2.06244900	-1.29740400
N	-1.51180900	0.00104800	-0.13753800
Cl	0.24296800	-1.49251300	-2.22172000
Ru	0.63140800	-0.75136300	0.16418800
C	3.12201000	-2.79191100	-0.48424800
C	0.32041600	-4.15077700	0.05812700
C	3.54662100	-0.46299800	1.67158600
C	0.93330600	-0.43198900	3.57484600
C	-1.03222700	-2.65840000	2.58797400
H	3.83956600	-2.00942100	-0.72979900
H	3.67269700	-3.65382700	-0.08753400
H	2.63190400	-3.08905100	-1.41207800
H	4.01474400	-0.23460900	0.71354400
H	3.34354300	0.48466100	2.17209100
H	4.26892800	-1.01597300	2.28282200
H	-0.09979400	-0.10201200	3.70351200
H	1.19662100	-1.03802900	4.45056100
H	1.56902100	0.45303200	3.59190000
H	-1.65158200	-3.32148300	1.98332200
H	-0.81721300	-3.17973500	3.52803300
H	-1.62010700	-1.77209200	2.83798600
H	0.93538300	-5.02865200	0.28642800
H	-0.70870000	-4.38558400	0.33454700
H	0.34880500	-3.98212200	-1.02025500
C	-2.60048300	-1.00578000	-0.38842700
H	-2.35757200	-1.51352700	-1.32384200
H	-2.48891600	-1.71835700	0.42577500
C	-3.98825100	-0.41514900	-0.40569500
C	-4.67478400	-0.25505200	-1.61224800
C	-4.60748000	-0.01248500	0.78363000
C	-5.95650000	0.29286600	-1.63147500
H	-4.20370800	-0.56422700	-2.53930700
C	-5.88550500	0.53592900	0.76666000
H	-4.08279100	-0.13164000	1.72618900
C	-6.56318300	0.68910500	-0.44298200

H	-6.47864500	0.40904900	-2.57431600
H	-6.35590800	0.84048600	1.69485300
H	-7.56037100	1.11422300	-0.45664200
C	0.79616100	2.45536500	1.33734900
C	1.16726300	3.85563400	0.81309400
H	1.31771600	2.26333900	2.28225700
H	-0.27236000	2.41959500	1.58269400
C	0.80786400	4.97289000	1.79819700
H	2.24157800	3.88108300	0.59962300
H	0.66080900	4.02192300	-0.14267700
C	1.18077500	6.36553600	1.28180600
H	-0.26829300	4.93790700	2.00723400
H	1.31107200	4.79152700	2.75621200
H	0.91024900	7.14302700	2.00139300
H	2.25637200	6.44318300	1.09605800
H	0.66703400	6.58756800	0.34180200
C	2.21356500	1.21763800	-2.01338200
O	1.84886300	2.02768800	-2.82941200
O	3.29691300	0.42514700	-2.17302000
C	3.94379900	0.53121400	-3.45297000
H	4.79025900	-0.15088300	-3.40837400
H	3.25471900	0.23456700	-4.24477600
H	4.28148200	1.55302000	-3.63332300

MC-4C **E**(Hartree)**=** -1396.989743

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.04706300	-2.23240300	-0.82521400
C	-1.03554900	-2.87659400	-0.04596100
C	0.20341700	-2.84106700	-0.80997800
C	-0.06156900	-2.17522000	-2.03908700
C	-1.44009500	-1.76406300	-2.05040700
C	-1.86747900	0.99957300	-0.25040400
C	-1.81649000	0.52162500	0.90154900
N	1.50280900	1.57238300	-0.24251700
N	2.00788700	2.53923500	0.28584700
N	0.98038300	0.73379000	-0.82512300
Cl	0.89773500	-0.76302200	1.86367500
Ru	-0.47924800	-0.76014900	-0.28101700
C	-1.22276700	-3.59080700	1.25628900
C	1.48496600	-3.49302300	-0.39063600
C	-3.49944000	-2.13680000	-0.47103300
C	-2.16629300	-1.18878800	-3.22978300
C	0.91740800	-1.93913700	-3.14840400
H	-2.09329800	-3.21224500	1.79089000
H	-1.36051100	-4.66559800	1.08647000
H	-0.35538900	-3.44873300	1.90175500
H	-3.63879000	-2.08502900	0.60866000
H	-3.96157600	-1.24827700	-0.90389400
H	-4.04059700	-3.01309200	-0.84619000
H	-1.54783100	-0.47951800	-3.78309900
H	-2.45872100	-1.98426200	-3.92596700
H	-3.07798600	-0.67290000	-2.92662900
H	1.94107700	-1.88548100	-2.77688900
H	0.86757700	-2.75446500	-3.87945500
H	0.70590200	-1.00753800	-3.67569100
H	1.41429700	-4.58221600	-0.49314200
H	2.32468400	-3.15436700	-0.99916700
H	1.71264300	-3.25939600	0.65065700
C	3.10607200	2.26112400	1.28097200
C	4.31932200	1.61700600	0.65781600
C	5.29505700	2.39614400	0.02708700
C	4.47055600	0.22643800	0.68915700
C	6.40594900	1.79836700	-0.56027700
H	5.18337100	3.47534700	-0.00050900
C	5.58482300	-0.37072600	0.10189600
H	3.71179500	-0.37936500	1.17386900
C	6.55295000	0.41216600	-0.52273600
H	7.15926100	2.41215900	-1.04145600
H	5.69801300	-1.44852900	0.13853000
H	7.42130600	-0.05390300	-0.97507400
H	3.34177900	3.24083600	1.69207000
H	2.68146200	1.63142000	2.06503300

C	-2.24031000	1.99576300	-1.26891700
H	-1.32303200	2.45005600	-1.66342500
H	-2.71551400	1.50307200	-2.12454100
C	-3.16689000	3.09219300	-0.70924000
C	-3.50518200	4.16721900	-1.74767400
H	-2.68815900	3.54973400	0.16223500
H	-4.08933800	2.62680700	-0.34435700
C	-4.43289600	5.25557500	-1.20038000
H	-2.57642500	4.62667000	-2.10705900
H	-3.97082000	3.69620900	-2.62234200
H	-4.65010000	6.01181600	-1.95954300
H	-5.38646800	4.83300900	-0.86923500
H	-3.98143400	5.76358700	-0.34308800
C	-2.12381100	0.57791700	2.32587100
O	-2.02254000	1.56985100	3.00544100
O	-2.56435000	-0.60965300	2.79381500
C	-2.80795700	-0.65212800	4.21049200
H	-3.55177700	0.09241100	4.49815800
H	-3.17188400	-1.65718000	4.41332900
H	-1.88091900	-0.46465800	4.75386800

MC-4D **E**(Hartree)**=** -1396.994527

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.50011000	-2.63884600	-1.00261900
C	0.11665200	-2.81369800	-1.35399600
C	-0.65851400	-2.87277200	-0.15625400
C	0.25645300	-2.77742900	0.96577000
C	1.58389700	-2.66218800	0.43789800
C	1.86069600	0.36597500	0.84968300
C	1.93944600	0.68909900	-0.36085400
N	-1.47566600	1.30753600	0.90237600
N	-1.88266900	2.45071800	0.95599200
N	-1.05620800	0.24347700	0.95628900
Cl	-0.72292700	0.38847500	-2.08883900
Ru	0.38890700	-0.87842900	-0.17856900
C	-0.42299100	-2.92895200	-2.74459000
C	-2.13383100	-3.12450600	-0.07092900
C	2.66341100	-2.66477700	-1.94855900
C	2.85468400	-2.71005400	1.22945900
C	-0.10826400	-2.91737400	2.41292600
H	0.26660600	-2.51089800	-3.47689200
H	-0.58745700	-3.98488000	-2.99039000
H	-1.36668500	-2.39465900	-2.84938600
H	2.41588800	-2.19715000	-2.90245900
H	3.52491900	-2.13914500	-1.53362600
H	2.97532000	-3.69603600	-2.15432600
H	2.69666600	-2.38833000	2.25755200
H	3.23877000	-3.73676400	1.24584200
H	3.62775100	-2.07658300	0.79108200
H	-1.14138500	-2.61431800	2.58862900
H	-0.00757800	-3.96086700	2.73478500
H	0.52938500	-2.29372400	3.03956400
H	-2.34191800	-4.19748500	0.01863100
H	-2.57460600	-2.62785000	0.79466800
H	-2.64823800	-2.75737500	-0.95988200
C	-2.88694500	2.84220600	-0.09781700
C	-4.17995700	2.07082400	-0.00495600
C	-5.18151900	2.46590500	0.88822700
C	-4.38312600	0.93872300	-0.80145300
C	-6.36832000	1.74572200	0.98300000
H	-5.02935000	3.34251600	1.50969000
C	-5.57329900	0.21909800	-0.70646300
H	-3.60506800	0.62681000	-1.49070000
C	-6.56648700	0.62026000	0.18384600
H	-7.14010300	2.06388300	1.67497000
H	-5.72534000	-0.65253200	-1.33325200
H	-7.49305100	0.06134800	0.25379700
H	-3.04660700	3.90517300	0.07384600
H	-2.41407400	2.70094200	-1.07182000

C	2.22253000	0.52618700	2.24318900
O	1.81654300	-0.13725900	3.17397900
O	3.10787800	1.54231300	2.39813500
C	3.52820400	1.79268200	3.75029300
H	4.02091500	0.91417500	4.17065300
H	4.22339100	2.62704600	3.68606400
H	2.67343200	2.05304100	4.37663700
C	2.44338700	1.46736600	-1.50091500
C	3.37586700	2.62370600	-1.09764300
C	3.88613700	3.40987100	-2.30983400
H	4.22223100	2.22899900	-0.52540100
H	2.83703400	3.29450100	-0.42021900
C	4.80430500	4.57386900	-1.92608900
H	4.42128100	2.73030300	-2.98459700
H	3.03024800	3.79088900	-2.87953100
H	5.15103900	5.11640500	-2.80986600
H	4.28615000	5.28847400	-1.27924000
H	5.68760800	4.21949300	-1.38570800
H	1.58123500	1.83326600	-2.06625100
H	2.96073600	0.78021100	-2.18299700

MC-5A **E**(Hartree)**=** -1357,072087

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.20749700	1.84956500	0.42989100
C	-1.27195600	2.76866300	-0.18313000
C	-0.09317900	2.78407400	0.60047500
C	-0.28291100	1.90791500	1.74857700
C	-1.60814500	1.36851100	1.65704100
C	-0.40032300	-1.47467500	0.63355300
C	-1.54138900	-1.36732000	0.10630600
N	2.14528100	0.19462800	-1.69881200
N	2.38563700	0.16840000	-2.80779100
N	1.76569600	0.20064000	-0.50742100
Cl	-0.77701000	0.26213600	-2.53425500
Ru	-0.45810000	0.58825800	-0.05898000
C	-1.53556000	3.54650300	-1.43766900
C	1.11273300	3.64163900	0.33599000
C	-3.63320100	1.67427000	-0.00455900
C	-2.30094600	0.55545100	2.70998600
C	0.62324700	1.80669600	2.94419600
H	-1.77689200	2.87399200	-2.26769100
H	-2.38010100	4.23276300	-1.29113100
H	-0.66737200	4.14236900	-1.73154100
H	-3.71174000	1.63724600	-1.09465600
H	-4.06906500	0.75327700	0.38827700
H	-4.24743300	2.51492300	0.34960900
H	-1.58939700	-0.03811800	3.29239000
H	-2.83328300	1.21410200	3.40987500
H	-3.03229900	-0.13023800	2.27517500
H	1.66201300	2.03253300	2.68798600
H	0.32070900	2.51543800	3.72810800
H	0.60796700	0.80310300	3.37885100
H	0.93841000	4.66805900	0.68652200
H	1.99867800	3.27200800	0.85891000
H	1.34814000	3.69338000	-0.73121800
C	-2.86817400	-1.84601400	-0.20695000
C	-3.50302100	-1.59124600	-1.43759700
C	-3.54837200	-2.61817100	0.76017700
C	-4.77461000	-2.10346400	-1.68798800
H	-2.97551700	-1.00101400	-2.17891500
C	-4.82052500	-3.12342300	0.50065500
H	-3.06544700	-2.81768900	1.71285000
C	-5.43987200	-2.86788800	-0.72532500
H	-5.24930000	-1.90462200	-2.64540600
H	-5.32780100	-3.71741400	1.25665900
H	-6.43233600	-3.26145800	-0.92832900
C	0.66035300	-2.37569600	1.13969700
O	1.31473600	-1.91458500	2.33016400
H	0.62691900	-1.77880600	3.00054400

H	0.23634400	-3.37832800	1.30641300
H	1.45677200	-2.47293200	0.39656800
C	2.88264100	0.31753900	0.49764000
H	3.12669500	1.38205600	0.59609600
H	2.43179300	-0.03179500	1.42508600
C	4.12623300	-0.47695000	0.17022800
C	5.09643500	0.03875600	-0.70149500
C	4.33203900	-1.74019900	0.74410600
C	6.23841000	-0.70010300	-1.01272300
H	4.96274600	1.02778000	-1.13477500
C	5.47657000	-2.47721700	0.43630800
H	3.60200100	-2.13117500	1.44757900
C	6.42842300	-1.96204300	-0.44616800
H	6.98007700	-0.28848900	-1.69173800
H	5.62718200	-3.45295700	0.89042600
H	7.31848800	-2.53768400	-0.68552500

MC-5B **E**(Hartree)**=** -1357,079987

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.66909500	-1.27966500	0.73938100
C	2.10800900	-2.47340000	0.17616600
C	0.95463600	-2.84644600	0.99048200
C	0.81321300	-1.88268400	2.02041600
C	1.83518900	-0.88048000	1.85469300
C	1.32868800	1.20895900	-0.60701100
C	1.38207400	0.48300400	-1.64537700
N	-1.64610200	0.91780700	-0.85788900
N	-1.71045000	1.71423600	-1.66583000
N	-1.40199300	0.10747900	0.06110100
Cl	-0.51066300	-2.06032700	-1.97770000
Ru	0.68843000	-0.83135000	-0.10415100
C	2.67888800	-3.31670900	-0.92572200
C	0.14658500	-4.09351800	0.78713900
C	3.95644700	-0.62178600	0.33832500
C	2.16045700	0.19274900	2.85300100
C	-0.18981300	-1.89674600	3.13697000
H	3.41540700	-2.76245700	-1.51407300
H	3.18145400	-4.20218100	-0.51131300
H	1.89044100	-3.65195600	-1.60509300
H	3.91461000	0.46235800	0.47317700
H	4.78504700	-1.00589400	0.94895600
H	1.26195900	0.57364300	3.34749600
H	2.82258100	-0.20522300	3.63564800
H	2.66548800	1.04326700	2.39068800
H	-1.03869000	-2.54926900	2.91648000
H	0.27346400	-2.26363800	4.06325000
H	-0.57461000	-0.89304000	3.34617800
H	0.74490400	-4.98158500	1.03198200
H	-0.74470300	-4.11012600	1.42121800
H	-0.17918900	-4.17586000	-0.25447600
C	1.60559300	0.37198000	-3.10701600
H	2.44152400	-0.30875100	-3.30463900
H	0.72072200	-0.07057200	-3.58153200
O	1.96878000	1.61974200	-3.69845100
H	1.20944000	2.21419600	-3.58862000
H	4.19719900	-0.81461000	-0.71039500
C	-2.55309100	-0.77878900	0.45216600
H	-2.46677600	-1.68006400	-0.16197400
H	-2.34693000	-1.03857100	1.49201300
C	-3.91021400	-0.13566000	0.30750800
C	-4.67880600	-0.36966200	-0.84058000
C	-4.41432200	0.71339900	1.30284600
C	-5.92961400	0.23226500	-0.99002800
H	-4.29300700	-1.02729100	-1.61588800
C	-5.66326000	1.31586700	1.15476100
H	-3.82483900	0.89922500	2.19818000
C	-6.42320900	1.07547300	0.00693200
H	-6.51737700	0.04106700	-1.88359100
H	-6.04530500	1.96918200	1.93452700
H	-7.39733400	1.54308100	-0.10811500
C	1.51868900	2.48530700	0.04378600
C	0.82113700	2.85715200	1.20735900

C	2.41526600	3.41239000	-0.53225000
C	1.01555400	4.11351900	1.77997800
H	0.12219300	2.15264300	1.64718300
C	2.60501000	4.66431000	0.04655600
H	2.93475500	3.13523400	-1.44522300
C	1.90990700	5.02038700	1.20677500
H	0.46520100	4.38620800	2.67696300
H	3.29762400	5.36659800	-0.41029200
H	2.06201400	5.99746700	1.65722600

MC-5C **E**(Hartree)**=** -1357,084312

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.21775000	-0.60955100	0.86586400
C	-2.78635200	-1.96892300	0.76334200
C	-2.64580800	-2.28756700	-0.65400200
C	-2.99438700	-1.12600700	-1.39954900
C	-3.31362100	-0.06828900	-0.47469000
C	-0.63636800	1.35466800	0.75644000
C	-0.20993400	0.49556700	1.57083400
N	1.35760900	-0.03892900	-1.59814800
N	2.53855000	0.25299900	-1.61980800
N	0.21006200	-0.18263700	-1.60989000
Cl	0.60109000	-2.46046400	0.44848500
Ru	-1.18085200	-0.66900900	-0.03670900
C	-2.63615400	-2.96111300	1.87827100
C	-2.29977400	-3.64326900	-1.19489900
C	-3.59457800	0.12040200	2.12097400
C	-3.90479500	1.26426000	-0.83292100
C	-3.02172300	-1.00512900	-2.89471800
H	-2.57469800	-2.46727800	2.85191000
H	-3.49962900	-3.64047400	1.90294000
H	-1.73091900	-3.56052500	1.74883900
H	-3.26706700	1.16389500	2.09164600
H	-4.68464500	0.11464400	2.25656500
H	-3.51268600	1.64616500	-1.77946800
H	-4.99617100	1.18082600	-0.93566000
H	-3.69981900	2.01682600	-0.06804600
H	-4.02361500	-1.23514400	-3.28219700
H	-2.76774100	0.00855400	-3.21783400
H	-2.31551400	-1.69331400	-3.36670400
H	-3.14932300	-4.33166800	-1.08603200
H	-2.04232400	-3.59845000	-2.25686800
H	-1.44376200	-4.06717600	-0.66239900
C	3.51642600	-0.88415900	-1.54038300
H	3.01384600	-1.74033400	-1.07642100
H	3.79258200	-1.14961200	-2.56735900
C	4.73426300	-0.46029400	-0.75559300
C	4.61398300	-0.09033900	0.59175900
C	5.99608400	-0.45444400	-1.35895700
C	5.74708800	0.27463700	1.31787000
H	3.63976900	-0.08309300	1.07543500
C	7.13067000	-0.09439000	-0.62831100
H	6.09356900	-0.73535100	-2.40548300
C	7.00704900	0.27161400	0.71233900
H	5.64389600	0.55750300	2.36194400
H	8.10600800	-0.09668200	-1.10780900
H	7.88762100	0.55402900	1.28357400
C	-0.85457300	2.70343900	0.28589300
C	-0.91267000	3.02903300	-1.08163600
C	-0.99248800	3.74250900	1.23055400
C	-1.08647800	4.35019000	-1.48981600
H	-0.81397000	2.23718400	-1.81680800
C	-1.17449100	5.05962500	0.81613400
H	-0.95105800	3.50267200	2.28908500
C	-1.22078800	5.37063900	-0.54551800
H	-1.11893700	4.58339700	-2.55087800
H	-1.27828100	5.84601200	1.55915600
H	-1.36144100	6.39888000	-0.86702100
C	0.52170700	0.07438300	2.80243800
H	-3.14710400	-0.34371500	3.00394200
O	1.79867100	-0.47909800	2.55433200
H	1.64393800	-1.27235300	1.99917400

H	0.68421500	0.96093300	3.42829700
H	-0.10790400	-0.62429600	3.37537400

MC-5D **E**(Hartree)**=** -1357,079478

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.13970800	-0.06396100	-0.68195600
C	2.59658400	-0.86260600	-1.74428900
C	2.27062800	-2.15696600	-1.22004800
C	2.66359400	-2.17505500	0.17898100
C	3.19148600	-0.88584100	0.51222900
C	0.52757700	0.43517100	1.76933100
C	0.69930400	1.35886200	0.94059000
N	-1.65200800	-1.91875300	0.56290800
N	-2.84197100	-1.80480100	0.78607300
N	-0.50045100	-2.03792300	0.50523800
Cl	-0.77772400	0.04074300	-1.71531000
Ru	1.04649700	-0.67895500	-0.07773000
C	2.41055500	-0.43106000	-3.16772800
C	1.76195300	-3.32403000	-2.01674100
C	3.73134100	1.30751500	-0.82701100
C	3.79566100	-0.48671500	1.82719900
C	2.63362500	-3.37968700	1.07537500
H	2.42983500	0.65715100	-3.26148800
H	3.21528200	-0.84004900	-3.79434100
H	1.45275700	-0.77689000	-3.56440900
H	3.19778600	1.90373800	-1.57114200
H	3.70195100	1.86237400	0.11356300
H	4.78232600	1.23667800	-1.14080800
H	3.28421200	-0.96964700	2.66403000
H	4.85941000	-0.75895000	1.86419900
H	3.72425200	0.59339100	1.98131700
H	3.52343900	-4.00188600	0.90736800
H	2.62682700	-3.09651200	2.13176900
H	1.75678800	-4.00519600	0.88171100
H	2.59089800	-3.88266500	-2.47381100
H	1.20020100	-4.02238400	-1.38921300
H	1.09814500	-2.99256100	-2.82036700
C	-3.75999100	-1.83301100	-0.40749500
H	-3.15958600	-1.69893200	-1.31195900
H	-4.22694000	-2.82385100	-0.41862400
C	-4.80188700	-0.74981600	-0.27522300
C	-4.47470900	0.57723700	-0.58821300
C	-6.09493700	-1.05383200	0.16419400
C	-5.43430900	1.58149000	-0.46217500
H	-3.46981600	0.81287300	-0.93106500
C	-7.05535700	-0.04808500	0.28784200
H	-6.35230500	-2.08207600	0.40911100
C	-6.72520900	1.27162100	-0.02486800
H	-5.17474700	2.60736500	-0.70937400
H	-8.05789600	-0.29546000	0.62666000
H	-7.47146200	2.05617000	0.06968500
C	0.09610500	-0.15508900	3.06202300
O	0.74350900	-1.37992900	3.38636700
H	0.65290000	-1.94663300	2.60212900
H	0.33257100	0.53631100	3.87821600
H	-0.99878300	-0.28219600	3.04930200
C	0.87027600	2.72188000	0.49703500
C	0.54434000	3.14950200	-0.80343700
C	1.38872600	3.66185200	1.41329600
C	0.72862000	4.48255400	-1.16722800
H	0.13757300	2.42678100	-1.50281500
C	1.56829800	4.99151300	1.03913500
H	1.64599500	3.33698900	2.41764400
C	1.23987200	5.40797800	-0.25360200
H	0.46727300	4.80089600	-2.17321300
H	1.96701900	5.70260500	1.75809200
H	1.38133700	6.44520600	-0.54552000

MC-6A **E**(Hartree)**=** -1283.618469

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.90298100	-1.39517300	0.00425300
C	1.89133900	-2.42534900	0.19420200
C	1.17674300	-2.11994600	1.37873000
C	1.69183800	-0.89456100	1.92960300
C	2.79257900	-0.47258500	1.09304700
C	0.72269200	1.85096100	0.16525400
C	1.38338300	1.73233900	-0.88619000
N	-1.63069600	0.49879700	-1.40290200
N	-1.89028300	1.23433600	-2.21489000
N	-1.26308900	-0.23378600	-0.46387400
Cl	0.84188000	-0.93529100	-2.62924800
Ru	0.98976100	-0.35785300	-0.16570900
C	1.74735400	-3.64542500	-0.66189500
C	0.13534200	-2.97902800	2.02954400
C	3.97660000	-1.43786500	-1.03980900
C	3.74968100	0.63657100	1.40445000
C	1.38373600	-0.37233100	3.30266800
H	1.74840100	-3.37726500	-1.71962100
H	2.57686400	-4.33848200	-0.47840900
H	0.81837200	-4.17889100	-0.45395500
H	3.56521700	-1.71677200	-2.01047800
H	4.46568300	-0.46929300	-1.15193000
H	4.74607400	-2.16935200	-0.76422500
H	3.25260700	1.48333900	1.87692200
H	4.52724800	0.27818000	2.08919600
H	4.24475600	1.00489200	0.50566000
H	0.33252000	-0.49232800	3.56783100
H	1.97766900	-0.91237500	4.05089300
H	1.61656500	0.68665600	3.39643400
H	0.61270100	-3.67127700	2.73315900
H	-0.58173800	-2.38816900	2.60311600
H	-0.41345800	-3.58134100	1.30453800
C	-0.06080500	2.61627400	1.19017700
O	-0.83248600	1.71589200	2.01026400
H	-0.66147300	0.83490600	1.65201100
C	-2.22526500	-1.32892100	-0.14036400
H	-2.10705100	-2.12314800	-0.88332600
H	-1.87764700	-1.71181500	0.81697900
C	-3.66593000	-0.88021000	-0.04360400
C	-4.65157900	-1.51014000	-0.80575300
C	-4.03334000	0.15441600	0.82689100
C	-5.98743000	-1.12713200	-0.69356800
H	-4.37381900	-2.30431500	-1.49104800
C	-5.36579500	0.53969800	0.93331600
H	-3.27423500	0.66813000	1.40849500
C	-6.34644000	-0.10238300	0.17684900
H	-6.74289900	-1.62544700	-1.29037500
H	-5.63979400	1.34243800	1.60850900
H	-7.38405300	0.19965000	0.26317700
C	2.10900800	2.16925600	-2.09421900
C	1.96201600	3.67306400	-2.37507300
H	1.75561400	1.57851700	-2.94208300
H	3.16879500	1.91075100	-1.97947000
H	2.52802600	3.94666500	-3.26978000
H	0.91549800	3.93671800	-2.54410000
H	2.33448100	4.27410400	-1.54127500
C	-1.03845500	3.58280500	0.49797100
H	-1.72867500	3.04296900	-0.14998300
H	-1.62009200	4.10730600	1.26080900
H	-0.50111200	4.31858100	-0.10428400
C	0.87087500	3.41025000	2.12062500
H	1.57145700	2.74791000	2.62871500
H	1.43886000	4.15846800	1.56313100
H	0.26876100	3.91548400	2.88009600

MC-6B **E**(Hartree)**=** -1283.614529

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.72524800	-1.34206600	0.47381800
C	2.45816800	-1.59194400	-0.90916000
C	1.26284300	-2.42365600	-0.98772200
C	0.80550800	-2.65754800	0.32997800
C	1.67009500	-1.96400600	1.24500200
C	1.18153800	1.20723600	1.44117300
C	1.43398300	1.70850200	0.31848700
N	-1.73823500	1.25239100	0.40176000
N	-1.94097500	2.33019800	0.67121700
N	-1.39946700	0.07478800	0.20381300
Cl	0.22377900	0.42633900	-2.44678000
Ru	0.85135400	-0.34269200	-0.09997000
C	3.34014800	-1.26763300	-2.07526500
C	0.71467400	-2.99910500	-2.25684700
C	3.95246000	-0.69285500	1.03615300
C	1.65965700	-2.16881000	2.73133800
C	-0.33337300	-3.53453700	0.75289800
H	4.04073100	-0.46679000	-1.83935700
H	3.92424500	-2.15021800	-2.36374700
H	2.74769300	-0.95112300	-2.93440900
H	3.73130800	-0.10167800	1.92529000
H	4.68951300	-1.45592200	1.31280600
H	0.65478500	-2.09754700	3.15180300
H	2.04740200	-3.16582700	2.97485400
H	2.29073300	-1.44524900	3.24557300
H	-0.98714100	-3.78973000	-0.08161900
H	0.04954300	-4.47508600	1.16596100
H	-0.93677800	-3.06297200	1.53216900
H	1.38415900	-3.77657500	-2.64260100
H	-0.26675900	-3.45208400	-2.10687100
H	0.61306000	-2.22440400	-3.01903900
C	1.90792500	2.93411500	-0.39687000
O	2.47531600	3.75637100	0.65355000
H	2.69579000	4.60462900	0.25260600
H	4.41889800	-0.02580900	0.31137900
C	-2.38177900	-0.74335900	-0.59156400
H	-2.09539000	-0.63570400	-1.63935000
H	-2.18562000	-1.76753200	-0.28122700
C	-3.82689200	-0.37762700	-0.36727100
C	-4.50934600	0.40207500	-1.30563800
C	-4.50549100	-0.80439800	0.78010100
C	-5.84513900	0.74464300	-1.10497700
H	-3.99055400	0.73744300	-2.19744700
C	-5.83870200	-0.46222600	0.98298700
H	-3.98533000	-1.41066000	1.51483700
C	-6.51136200	0.31317000	0.03900800
H	-6.36374600	1.34670000	-1.84234700
H	-6.35486300	-0.80247400	1.87365000
H	-7.55100200	0.57792500	0.19517800
C	1.09199700	1.29497200	2.91607300
C	-0.29360800	1.00266300	3.51063500
H	1.40097900	2.31345900	3.17911000
H	1.82666200	0.62573600	3.37518000
H	-0.24977900	1.01683700	4.60294400
H	-1.02049800	1.75327500	3.19405000
H	-0.65798500	0.02335100	3.19266200
C	2.99617700	2.60062500	-1.42589400
H	2.60017800	1.94534400	-2.20241600
H	3.35605400	3.52386100	-1.89271400
H	3.84065900	2.11631900	-0.93180200
C	0.74658600	3.68945100	-1.05877900
H	1.13201800	4.59404100	-1.54372700
H	0.26380300	3.06885100	-1.81356500
H	0.01371200	3.98161900	-0.30577700

MC-6C **E**(Hartree)**=** -1283.627580

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.24136100	0.49117200	0.55346300
C	3.27880300	-0.21485300	-0.68927700
C	2.95128800	-1.60899900	-0.41853600
C	2.69663700	-1.73646400	0.97015900
C	2.84027500	-0.44087500	1.58504300
C	0.21450900	1.49330700	1.12562700
C	0.17681500	1.78251400	-0.08274800
N	-1.39423800	-1.89676600	0.20335700
N	-2.18222000	-2.72216600	-0.21197600
N	-0.61753700	-1.20008200	0.67227200
Cl	0.23757800	-0.73696300	-2.27169700
Ru	1.21475500	-0.24164900	0.06353800
C	3.75889400	0.29505000	-2.01300400
C	2.98288200	-2.70592500	-1.43718500
C	3.65146600	1.91358200	0.77913000
C	2.87243400	-0.19245900	3.06388000
C	2.36445900	-3.00229100	1.70094000
H	3.74712900	1.38413600	-2.05474400
H	4.78864100	-0.03522500	-2.19525000
H	3.13314300	-0.07976400	-2.82443500
H	3.02820700	2.40000600	1.53103900
H	4.69108300	1.95804300	1.12371600
H	2.06430500	-0.70912100	3.58564200
H	3.81894800	-0.54783100	3.48917600
H	2.79297500	0.86974900	3.29532900
H	1.87009900	-3.72546800	1.05139100
H	3.27911900	-3.46990300	2.08389100
H	1.71045000	-2.81384500	2.55405400
H	4.01828700	-2.93914800	-1.71184300
H	2.52563200	-3.62070400	-1.05784300
H	2.44349500	-2.41433000	-2.33973500
C	-3.24918100	-2.19741100	-1.13785000
H	-2.74555800	-1.71806000	-1.98023000
H	-3.75492200	-3.09374300	-1.49190500
C	-4.21309000	-1.25692300	-0.45751400
C	-4.01300400	0.12711700	-0.50791900
C	-5.30896400	-1.76288200	0.25066400
C	-4.90171700	0.98593000	0.13822100
H	-3.16937400	0.54596500	-1.04774000
C	-6.19326600	-0.90415800	0.89579000
H	-5.46928300	-2.83548900	0.29298100
C	-5.99071900	0.47442700	0.83959400
H	-4.74240500	2.05686500	0.08259800
H	-7.04226400	-1.30796600	1.43610000
H	-6.68265100	1.14557100	1.33630800
C	-0.27117900	2.61585400	-1.25249500
O	-1.31541700	1.94546300	-1.96081800
H	-0.94397200	1.10052200	-2.27505200
H	3.57726000	2.49960000	-0.13698800
C	-0.12053300	1.56738700	2.56088900
C	-1.21494600	2.60310100	2.86967400
H	0.77776800	1.80169000	3.14157600
H	-0.44630600	0.57750000	2.89548800
H	-1.42481100	2.61985700	3.94284900
H	-0.90659600	3.60614100	2.56728800
H	-2.13988500	2.35788300	2.34395400
C	-0.89972100	3.91537900	-0.72980400
H	-0.16735300	4.51555000	-0.18595200
H	-1.27453300	4.49211000	-1.57867700
H	-1.73671000	3.68786400	-0.06872300
C	0.89108400	2.92648500	-2.20676200
H	0.51888100	3.53919200	-3.03120200
H	1.68833500	3.47289300	-1.69429400
H	1.29859300	2.00139800	-2.61450700

MC-6D **E**(Hartree)**=** -1283.620372

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.79034700	-1.24935800	1.25111900
C	-2.44911400	-2.26279000	0.26534500
C	-2.72171400	-1.73289900	-1.02172500
C	-3.22506100	-0.38741100	-0.87130300
C	-3.30713200	-0.11626100	0.54198500
C	-0.73219100	1.82680600	0.02753900
C	-0.48675200	1.40959200	1.17576400
N	1.40414300	-0.45705900	-1.66471500
N	2.58973900	-0.28422500	-1.86969800
N	0.26502300	-0.51337300	-1.55042000
Cl	0.74683100	-1.53979100	1.29156200
Ru	-1.17005600	-0.40005500	0.02592700
C	-1.97035700	-3.64190500	0.59909500
C	-2.54188100	-2.43899200	-2.33125700
C	-2.77713500	-1.46831700	2.73339500
C	-3.92946600	1.10015900	1.15407200
C	-3.80637500	0.45707200	-1.96677400
H	-1.12612800	-3.60254800	1.28956900
H	-2.77609700	-4.21931100	1.06708400
H	-1.64738300	-4.18323700	-0.29072800
H	-1.85148400	-1.95517800	3.04538600
H	-2.86118700	-0.52688400	3.27822600
H	-3.61748200	-2.10337600	3.03878100
H	-3.82234600	1.96321800	0.49784700
H	-5.00007400	0.93258000	1.31870700
H	-3.47908900	1.34555900	2.11704400
H	-3.35417700	0.22057600	-2.93199000
H	-4.88462900	0.27587600	-2.05970500
H	-3.64962700	1.51959500	-1.78078300
H	-3.49885800	-2.84293800	-2.68091400
H	-2.16816000	-1.76151800	-3.10083200
H	-1.83903200	-3.26816600	-2.24783100
C	3.50951600	-1.38980200	-1.42806400
H	2.93974300	-2.11620800	-0.84544500
H	3.88758600	-1.86471500	-2.33679900
C	4.64565200	-0.82281800	-0.61399600
C	4.46113200	-0.54952600	0.74563300
C	5.88308400	-0.55660800	-1.20333300
C	5.50460600	-0.02061000	1.49989100
H	3.49887600	-0.75669000	1.20290800
C	6.92695300	-0.02622100	-0.44795500
H	6.03165300	-0.76608800	-2.25792900
C	6.73853800	0.24248700	0.90560700
H	5.35571200	0.18274800	2.55455200
H	7.88492000	0.17400400	-0.91482700
H	7.55046700	0.65231600	1.49617500
C	-0.84946700	2.92179800	-0.98934500
O	-2.22609700	3.35887700	-1.08359200
H	-2.47481400	3.70008000	-0.21749200
C	-0.07172600	1.45486100	2.59077500
C	0.51203900	2.80915800	3.02243300
H	0.64914300	0.65233300	2.75920800
H	-0.93769400	1.20563700	3.21582700
H	0.79962100	2.77339200	4.07688000
H	1.40089100	3.05674400	2.43803600
H	-0.21182200	3.61914000	2.89902600
C	0.02142800	4.11205100	-0.54659000
H	-0.27518800	4.45978100	0.44624500
H	1.07546300	3.83081100	-0.50548800
H	-0.10268000	4.93383500	-1.25599400
C	-0.47257100	2.49191300	-2.40590000
H	-1.06953900	1.63741000	-2.72091200
H	-0.65762300	3.32418300	-3.08835100
H	0.58385300	2.22320800	-2.45874800

MC-7A **E**(Hartree)**=** -1303.049767

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.27262800	-2.75187300	-0.90101000
C	-0.15831200	-3.02056400	-0.97127600
C	-0.66644300	-3.03128800	0.35055900
C	0.40890300	-2.73883700	1.25974900
C	1.62191200	-2.61546200	0.48056300
C	1.27639000	0.38993200	1.37362900
C	1.74654900	0.66978000	0.25112200
N	-1.27803300	1.59904600	0.37322700
N	-0.96349900	2.66198900	0.58367900
N	-1.51514200	0.38469800	0.23505600
Cl	0.06473600	0.05722100	-2.43243500
Ru	0.31711500	-0.95710200	-0.11027600
C	-0.90109100	-3.32116400	-2.23698600
C	-2.06405600	-3.36488000	0.77615900
C	2.20740400	-2.81112400	-2.07008300
C	3.00949400	-2.49503600	1.03199300
C	0.31913200	-2.85912000	2.75260100
H	-0.68800500	-2.56540600	-2.99554500
H	-0.60574000	-4.30009600	-2.63178300
H	-1.98073600	-3.34027200	-2.07879800
H	1.79144300	-2.28156000	-2.92799600
H	3.17118400	-2.35772400	-1.83530000
H	2.39031700	-3.85310200	-2.36045400
H	3.03653900	-1.88206000	1.93401300
H	3.40444800	-3.48554000	1.28639300
H	3.68763400	-2.04105200	0.30867500
H	-0.55988700	-2.34977100	3.15402600
H	0.25354600	-3.91323100	3.04934200
H	1.19800700	-2.44057200	3.24271100
H	-2.10887200	-4.39958800	1.13632600
H	-2.40272300	-2.72495000	1.59425000
H	-2.77589300	-3.27797700	-0.04547700
C	1.06796000	0.57763700	2.82064200
C	2.57186000	1.44903500	-0.69603900
H	1.52671500	-0.22059400	3.41117800
H	1.51225100	1.52763400	3.13450500
H	0.00525900	0.59861100	3.07759500
N	3.29533900	2.55587400	-0.05860400
C	3.65310200	3.58771800	-1.04036700
C	2.47544900	4.48536100	-1.42053800
H	4.09274200	3.13440500	-1.94863200
H	4.43548800	4.21075900	-0.60154700
H	2.79833300	5.25268900	-2.13050400
H	1.66408500	3.92369600	-1.88869400
H	2.07276500	4.97707200	-0.53221400
C	4.45015300	2.07547300	0.70644800
C	4.91126600	3.05256100	1.78803900
H	5.29654200	1.82655200	0.03741000
H	4.15346400	1.14117000	1.18916200
H	5.74280100	2.62421100	2.35563800
H	5.25559900	4.00195900	1.37086600
H	4.09259400	3.26832700	2.47871100
H	3.25931400	0.76182900	-1.22443400
H	1.91029800	1.83621800	-1.47045800
C	-2.77573200	0.08628700	-0.52813700
H	-2.53395900	0.17533200	-1.58921500
H	-2.97235400	-0.96066400	-0.30877100
C	-3.94863600	0.95167400	-0.13994100
C	-4.37458600	1.98425100	-0.97976500
C	-4.62433700	0.74045600	1.06782800
C	-5.45691200	2.78744800	-0.62380700
H	-3.85803500	2.15594000	-1.91824000
C	-5.70346100	1.54167300	1.42591000
H	-4.30181600	-0.05818900	1.72814700
C	-6.12248900	2.56759700	0.57886200
H	-5.77855000	3.58292000	-1.28634800
H	-6.22091500	1.36530400	2.36225800
H	-6.96498900	3.19096500	0.85629200

MC-7B **E**(Hartree)**=** -1303.048308

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.59868800	2.91445100	0.12488200
C	0.31291500	3.19725500	-0.49967600
C	0.20614100	2.39395600	-1.66145200
C	1.38752700	1.58127400	-1.77169300
C	2.27042500	1.94262200	-0.68530200
C	1.48233500	-0.94416300	0.33974500
C	1.59707100	-0.43957700	1.47368500
N	-1.49286200	-1.14472900	0.90777200
N	-1.43533000	-2.02686900	1.60800800
N	-1.42882700	-0.20758100	0.09060500
Cl	-0.64968800	1.69162600	2.40548300
Ru	0.48980400	1.03853900	0.22517900
C	-0.64925700	4.23982500	-0.01961900
C	-0.89329900	2.42494700	-2.67985300
C	2.15450000	3.66359000	1.29710900
C	3.68404400	1.47544900	-0.51563400
C	1.74944100	0.76660400	-2.97870500
H	-0.82744100	4.13334100	1.05186600
H	-0.25004600	5.24361400	-0.20612000
H	-1.61279600	4.16749900	-0.52690200
H	1.41489400	3.73398600	2.09588700
H	3.03844300	3.17120500	1.70421600
H	2.44544300	4.67874400	1.00087900
H	3.79603500	0.41583700	-0.74933200
H	4.35167000	2.04111800	-1.17592700
H	4.02984500	1.61877200	0.50832600
H	0.92349600	0.13321600	-3.30991600
H	2.01835700	1.42230700	-3.81628400
H	2.60945100	0.12427800	-2.78759900
H	-0.57512900	3.00261400	-3.55586300
H	-1.14984200	1.42311700	-3.03281700
H	-1.79820300	2.89598600	-2.29439500
C	1.98852200	-0.37119700	2.88970100
H	2.76676900	0.38335800	3.03976400
H	1.13828400	-0.08116100	3.50793400
H	2.37664600	-1.33838400	3.22560900
C	-2.73263400	0.51252000	-0.10954100
H	-2.86338600	1.18132200	0.74401700
H	-2.56310300	1.11521800	-0.99831500
C	-3.91674700	-0.40378600	-0.29562400
C	-4.08002800	-1.12419000	-1.48494700
C	-4.86585200	-0.55118600	0.71914400
C	-5.17072900	-1.96974100	-1.65671500
H	-3.34661100	-1.01931000	-2.27797300
C	-5.96132900	-1.39634600	0.54805700
H	-4.74717000	0.00142100	1.64519800
C	-6.11544200	-2.10622800	-0.63933000
H	-5.28797600	-2.51968600	-2.58375900
H	-6.69180700	-1.49903000	1.34243800
H	-6.96732100	-2.76313200	-0.77386800
C	1.61859000	-2.00782100	-0.68108700
H	2.14809700	-1.60491000	-1.54566500
H	0.61435700	-2.28698100	-1.05623500
C	1.57566800	-3.97506600	0.75311700
C	2.44188000	-4.83108500	1.67635200
H	0.83949300	-4.61054800	0.22632500
H	1.00022800	-3.27929300	1.36527200
H	1.81241300	-5.36920100	2.39078700
H	3.02635400	-5.57575900	1.12947100
H	3.13857900	-4.20048900	2.23340800
C	2.86684500	-3.98298900	-1.31984400
C	4.13302900	-3.40625700	-1.95389200
H	2.08654400	-4.12623100	-2.09147700
H	3.09907900	-4.97869800	-0.93718400
H	4.48920900	-4.05997400	-2.75556100
H	3.96493100	-2.41810200	-2.39000800
H	4.92128300	-3.31167200	-1.20378900
N	2.36136500	-3.18009600	-0.20020700

MC-7C **E**(Hartree)**=** -1303.047967

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.51700100	-1.88799500	0.96024400
C	-2.07910200	-2.51827100	-0.27832700
C	-2.49747600	-1.69852400	-1.35939100
C	-3.16442000	-0.53925500	-0.82404800
C	-3.21170500	-0.68886300	0.61308400
C	-1.05666700	1.69923400	0.43090200
C	-0.61510500	1.15820800	1.46735900
N	1.52593800	0.03985300	-1.50172400
N	2.70941900	0.30566100	-1.56212200
N	0.38572200	-0.09294300	-1.49361900
Cl	0.92790700	-1.66031100	1.09531800
Ru	-1.08671400	-0.50102200	0.01887100
C	-1.40324000	-3.85232200	-0.35938500
C	-2.29255900	-1.97990100	-2.81692100
C	-2.37721000	-2.49779300	2.32119500
C	-3.95673900	0.21214600	1.54772600
C	-3.91746800	0.49035000	-1.61295000
H	-0.57693200	-3.91040400	0.35088300
H	-2.11405500	-4.65527100	-0.13107000
H	-0.99964100	-4.03998900	-1.35540700
H	-1.35605500	-2.84718500	2.48219500
H	-2.61256300	-1.77876200	3.10704300
H	-3.05799200	-3.35002500	2.43356400
H	-3.89476400	1.25272600	1.22941600
H	-5.01611000	-0.06909600	1.57766500
H	-3.56651300	0.14938200	2.56396900
H	-3.53004100	0.58005500	-2.62927200
H	-4.97701400	0.21700600	-1.68989700
H	-3.85492400	1.47381700	-1.14515700
H	-3.17410400	-2.47696100	-3.23818500
H	-2.12953300	-1.06111900	-3.38294800
H	-1.43263200	-2.62928900	-2.98314000
C	3.66177100	-0.84294900	-1.36863600
H	3.11962300	-1.67776800	-0.92057900
H	4.02288400	-1.12772500	-2.36065700
C	4.80888400	-0.41523700	-0.48926400
C	4.65882900	-0.41674200	0.90156300
C	6.02311400	-0.00758000	-1.04496400
C	5.71260600	-0.01907300	1.71925700
H	3.71481400	-0.73386300	1.33257000
C	7.07780500	0.39088700	-0.22626000
H	6.14492800	-0.00248200	-2.12353800
C	6.92349000	0.38536400	1.15792700
H	5.58990100	-0.02821800	2.79658100
H	8.01754200	0.70277100	-0.66835200
H	7.74381900	0.69246100	1.79722800
C	-0.04972000	1.05730600	2.82180600
N	-1.56807400	2.75129500	-0.28450800
C	-1.64659400	4.02730900	0.45548400
H	-0.65696500	4.31763100	0.83635000
H	-1.94685400	4.78858000	-0.27001100
C	-1.16882800	2.87897400	-1.69503600
H	-1.90865800	3.52161900	-2.18389300
H	-1.25368300	1.88828400	-2.14220900
C	-2.65271600	3.99981300	1.60176700
H	-2.66816700	4.97037200	2.10545700
H	-3.65922500	3.79032300	1.23105100
H	-2.39345800	3.24046400	2.34113000
C	0.23955300	3.43648600	-1.93210000
H	0.46667900	3.43528100	-3.00229300
H	0.33461600	4.46597000	-1.57677100
H	0.99774800	2.83512300	-1.42577100
H	-0.74178600	0.55817700	3.50930100
H	0.86813100	0.46820000	2.81254700
H	0.17391200	2.05367900	3.21909300

MC-7D **E**(Hartree)**=** -1303.050197

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-2.98487800	-0.47159900	1.48998100
C	-2.72749000	-1.88144200	1.23718800
C	-3.06070100	-2.14968600	-0.11736500
C	-3.51064100	-0.92580600	-0.73363300
C	-3.50042600	0.09886100	0.28212100
C	-0.91271400	1.11225800	-1.49001800
C	-0.61509600	1.51490600	-0.35598700
N	1.09864400	-1.78055500	-1.35190700
N	2.29164700	-1.84786300	-1.56512700
N	-0.04117500	-1.68215800	-1.26402200
Cl	0.51851200	-0.77168100	1.62848200
Ru	-1.40964500	-0.57352100	-0.04567000
C	-2.26995800	-2.86131300	2.27379700
C	-2.98140200	-3.47782800	-0.80667900
C	-2.87190600	0.18507200	2.83181200
C	-4.02319200	1.49210900	0.11267000
C	-4.13033100	-0.81724300	-2.09532100
H	-1.38960900	-2.48455800	2.79792800
H	-3.06313500	-3.03911600	3.00925000
H	-2.00781300	-3.82305300	1.83066600
H	-1.94175100	-0.10279200	3.32433900
H	-2.87976300	1.27248000	2.74650200
H	-3.70914900	-0.10573000	3.47772400
H	-3.79416400	1.88964200	-0.87720400
H	-5.11210700	1.50592400	0.23727300
H	-3.59541500	2.17334300	0.84886600
H	-3.60289300	-1.42762000	-2.83124900
H	-5.17378200	-1.15517500	-2.07398500
H	-4.13193300	0.21251200	-2.45570800
H	-3.95215500	-3.98564200	-0.76935700
H	-2.70625300	-3.36564300	-1.85674100
H	-2.24479400	-4.13041700	-0.33728400
C	3.10479700	-2.60497300	-0.55034400
H	2.50304900	-2.74657600	0.34960300
H	3.33817800	-3.57721600	-0.99256900
C	4.36938500	-1.84757500	-0.23587100
C	4.33852400	-0.78957400	0.67876400
C	5.57577300	-2.18260500	-0.85351300
C	5.50184800	-0.08316300	0.96995300
H	3.39974700	-0.52813800	1.15641000
C	6.74013300	-1.47478600	-0.56213000
H	5.60532200	-3.00134800	-1.56549600
C	6.70423500	-0.42375200	0.35087500
H	5.47038300	0.73294500	1.68302900
H	7.67238700	-1.74481100	-1.04560900
H	7.60955300	0.12713300	0.58077700
C	-1.00902400	1.09595700	-2.95656100
C	-0.08177900	2.43389700	0.66987000
H	-2.04064000	0.98032200	-3.29941500
H	-0.61461400	2.03216000	-3.36529200
H	-0.43081500	0.27104300	-3.38170700
N	0.52212100	3.64216400	0.09629000
C	1.45062800	4.26885400	1.04557000
C	2.80201900	3.55823800	1.11918600
H	1.00090100	4.33404600	2.05428900
H	1.61789100	5.29805800	0.72025100
H	3.46382400	4.07646600	1.81977100
H	2.70475200	2.52455900	1.45844800
H	3.27599700	3.54411300	0.13532400
C	-0.49184100	4.57511000	-0.40548200
C	0.04518400	5.53144100	-1.47030600
H	-0.95124000	5.14948500	0.42189900
H	-1.29257400	3.97875900	-0.84913600
H	-0.75706100	6.17621700	-1.84143500
H	0.83438800	6.18085400	-1.08382300
H	0.45737000	4.96775800	-2.31050200
H	-0.88389800	2.68578600	1.39046100
H	0.66594300	1.88448500	1.24090000

MC-8A **E**(Hartree)**=** -1208.372000

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.46747300	-2.46756900	-0.13735200
C	0.13839700	-2.56241200	0.44919600
C	0.13158100	-1.80240500	1.64273800
C	1.42390300	-1.19388300	1.81167800
C	2.26341400	-1.64676200	0.72417000
C	1.98606400	1.40949900	-0.35672700
C	2.04249400	0.78445200	-1.43779200
N	-1.07503100	1.89694800	-1.04630700
N	-1.07605400	2.56066400	-1.95815700
N	-0.96669900	1.12801400	-0.07447300
Cl	-0.49629000	-0.90322700	-2.40002400
Ru	0.67938400	-0.43166800	-0.19397300
C	-0.96999300	-3.42104400	-0.07710600
C	-1.00180200	-1.72458000	2.62102300
C	1.93711500	-3.26632600	-1.31492400
C	3.74159300	-1.43429500	0.60731300
C	1.89563100	-0.52050100	3.06705100
H	-1.08639200	-3.28479200	-1.15354900
H	-0.75661300	-4.47882100	0.11788400
H	-1.92430900	-3.18153500	0.39445900
H	1.20390300	-3.23752200	-2.12181500
H	2.88128900	-2.88645100	-1.70794700
H	2.09519600	-4.31269400	-1.02615400
H	4.04727000	-0.47532400	1.02331800
H	4.27967600	-2.22336800	1.14578400
H	4.06869200	-1.45844400	-0.43269900
H	1.12622300	0.11641800	3.50791100
H	2.17034100	-1.26843600	3.82160600
H	2.77434900	0.09848100	2.88994900
H	-0.98045600	-2.59431200	3.28817900
H	-0.93430500	-0.83773900	3.25405500
H	-1.97368100	-1.72013500	2.12435500
C	2.35479100	2.63553100	0.43403200
C	2.42865400	3.82037100	-0.56004400
C	1.33382400	2.97050000	1.53613100
C	3.74914800	2.45102900	1.07425600
H	3.17491400	3.63286300	-1.33566000
H	1.46627400	3.98140600	-1.05029100
H	2.70767100	4.73928600	-0.03381200
H	1.19418900	2.12832200	2.21480500
H	1.67993600	3.83099200	2.11673100
H	0.36256800	3.22564500	1.10860600
H	4.06020500	3.37751000	1.56728700
H	3.74323700	1.66039700	1.82632500
H	4.49545200	2.19773300	0.31801300
C	2.47984800	0.55848900	-2.82701600
H	3.12614900	-0.32255200	-2.89245600
H	1.62193500	0.37436600	-3.47413600
H	3.03952100	1.42361200	-3.19873900
C	-2.02832300	1.28900600	0.94835000
H	-1.68909900	0.68098600	1.78478600
H	-2.04562100	2.32902100	1.29334700
C	-3.41908300	0.86532700	0.50988000
C	-3.62262900	-0.06943800	-0.50920100
C	-4.52487400	1.40004600	1.17906800
C	-4.91834000	-0.46156900	-0.84424300
H	-2.77723000	-0.47605500	-1.05488600
C	-5.81596700	0.99960500	0.84679700
H	-4.37673100	2.13704300	1.96295700
C	-6.01563600	0.06534400	-0.16801800
H	-5.06483600	-1.17981000	-1.64311500
H	-6.66429300	1.42431300	1.37188500
H	-7.02058400	-0.24200900	-0.43478400

MC-8B **E**(Hartree)**=** -1208.377527

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.62787500	-0.99218500	-1.16897100
C	1.70462300	-2.11873100	-1.10478100
C	1.54610200	-2.47880400	0.25234900
C	2.34496700	-1.59415200	1.05894000
C	3.05358200	-0.70078300	0.16508000
C	1.10526100	1.30218500	1.52022100
C	0.92462500	1.91303500	0.43963700
N	-1.70191000	0.25744200	1.62713800
N	-2.00570600	0.96751600	2.45470700
N	-1.25227800	-0.46356700	0.72946900
Cl	-0.33870000	0.26784300	-2.19150400
Ru	0.91676900	-0.24328900	-0.02619300
C	1.12602900	-2.81171900	-2.29917500
C	0.73680200	-3.61751000	0.79411000
C	3.17151900	-0.41248900	-2.43830600
C	4.14470400	0.25115500	0.54834700
C	2.62889100	-1.81707800	2.51548500
H	0.67531300	-2.09205300	-2.98491700
H	1.91084400	-3.35660200	-2.83625900
H	0.35807000	-3.53383300	-2.01654600
H	2.37490600	-0.26520600	-3.16848100
H	3.64910500	0.55237200	-2.26587000
H	3.92076600	-1.08525000	-2.87371800
H	3.98433300	0.67979000	1.53790600
H	5.11158500	-0.26553100	0.55950200
H	4.21633300	1.07827900	-0.15831200
H	1.71568200	-1.97071700	3.09480900
H	3.25218200	-2.71022600	2.64462000
H	3.16825500	-0.98130800	2.95853800
H	1.37917000	-4.48630900	0.98069100
H	0.26383100	-3.35439300	1.74251600
H	-0.04360100	-3.92982200	0.09958400
C	1.31526900	1.26835600	2.98383300
C	0.75774000	3.22647300	-0.26693400
H	2.36196800	1.08105000	3.23981400
H	1.03845200	2.23416900	3.41780100
H	0.71740600	0.49802800	3.47656900
C	1.22350200	4.33854200	0.70233200
H	1.12457700	5.31825800	0.22427300
H	0.61842400	4.34487000	1.61282300
H	2.27043800	4.20166800	0.98603900
C	-0.72763800	3.45718500	-0.62121200
H	-0.84236200	4.43654200	-1.09733000
H	-1.08317100	2.68920400	-1.30685200
H	-1.34831000	3.44248600	0.27904000
C	1.61265300	3.27391500	-1.54818300
H	2.67356100	3.14474100	-1.31331100
H	1.30852700	2.49016400	-2.24165100
H	1.49301400	4.24540500	-2.03830000
C	-2.23126400	-1.41525500	0.10003900
H	-1.79083800	-1.61479300	-0.87431400
H	-2.23150100	-2.33474900	0.69309800
C	-3.63099100	-0.87056700	-0.03931200
C	-3.92310300	0.06905800	-1.03600100
C	-4.65004700	-1.29597500	0.81709000
C	-5.21482700	0.56856400	-1.16776200
H	-3.12984100	0.39608100	-1.69971300
C	-5.94412600	-0.79579200	0.68293900
H	-4.43306500	-2.02856600	1.58854500
C	-6.22727200	0.13804900	-0.30996700
H	-5.43345100	1.29294700	-1.94427400
H	-6.72728800	-1.13614800	1.35099100
H	-7.23323400	0.52823500	-0.41727000

MC-8C **E**(Hartree)**=** -1208.376420

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.42350400	0.23518600	0.30790600
C	-2.83715000	-0.28356000	1.50180500
C	-2.45572300	-1.66459100	1.24789100
C	-2.81037900	-1.97338000	-0.09454800
C	-3.38015100	-0.80067800	-0.69922000
C	-1.01839300	1.22956100	-1.72888000
C	-0.65283400	1.82821300	-0.70041800
N	1.35371600	-1.35558300	-1.23716800
N	2.55342700	-1.33223800	-1.42081500
N	0.20806900	-1.35355300	-1.17579000
Cl	0.61187300	-0.20177100	1.64949100
Ru	-1.28091900	-0.27190500	-0.07890300
C	-2.76120200	0.37557800	2.84403700
C	-1.90171100	-2.59774000	2.28068000
C	-4.08016300	1.57044800	0.13719300
C	-4.07414500	-0.75843700	-2.02793600
C	-2.64713100	-3.29946200	-0.77268900
H	-2.93860600	1.44874000	2.77832800
H	-3.51699900	-0.04889800	3.51570800
H	-1.77883800	0.22381200	3.29435100
H	-3.77377800	2.27012500	0.91462900
H	-3.83301800	2.01925400	-0.82665600
H	-5.17018900	1.46715700	0.19128800
H	-3.55004600	-1.34736600	-2.78333000
H	-5.08905300	-1.16555900	-1.94067100
H	-4.16741400	0.26241100	-2.40018500
H	-1.83087400	-3.87529000	-0.33563100
H	-3.56441300	-3.89183300	-0.67607500
H	-2.43951100	-3.18124400	-1.83743200
H	-2.66726000	-2.84441500	3.02551700
H	-1.56011300	-3.53337800	1.83532600
H	-1.05348000	-2.14222200	2.79500300
C	3.39960900	-1.95722100	-0.34376800
H	2.79450000	-2.07686500	0.55659800
H	3.70515500	-2.93981800	-0.71381100
C	4.60417800	-1.09446700	-0.06914000
C	4.52219200	-0.05979400	0.86792600
C	5.80505400	-1.30666900	-0.74993000
C	5.62938300	0.74577500	1.12043000
H	3.58814800	0.10759300	1.39402900
C	6.91199700	-0.49925100	-0.49909800
H	5.87419800	-2.10736800	-1.47947900
C	6.82525800	0.52839900	0.43765100
H	5.55812800	1.54329000	1.85143300
H	7.84036000	-0.67373200	-1.03149500
H	7.68679900	1.15624200	0.63619400
C	-1.19384100	1.02017500	-3.17633700
C	-0.06560900	3.03388400	-0.03121300
H	-2.23115600	0.80703500	-3.44233600
H	-0.88197200	1.91559200	-3.72463700
H	-0.58985100	0.17904400	-3.52899500
C	-0.46503900	4.26790100	-0.87524900
H	-0.03266200	5.17354100	-0.43826700
H	-0.09906000	4.17813600	-1.90126700
H	-1.55089200	4.38903000	-0.90774000
C	1.47425300	2.90360800	-0.01986200
H	1.91650000	3.79919100	0.42893900
H	1.77728800	2.03217000	0.55875700
H	1.86399700	2.80067500	-1.03585300
C	-0.57678000	3.21326100	1.40927400
H	-1.66248700	3.34133100	1.42636200
H	-0.31300100	2.34873300	2.01790200
H	-0.12728600	4.10798200	1.85127400

MC-8D **E**(Hartree)**=** -1208.377202

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.26792000	-0.74321300	0.87627700
C	-2.63157200	-1.98350700	0.55577000
C	-2.33562900	-1.99128600	-0.84830600
C	-2.85072800	-0.75774300	-1.40922300
C	-3.41981100	0.01153500	-0.34873800
C	-0.79535800	1.91190800	0.54325200
C	-0.85517300	1.31158200	1.62803000
N	1.41794300	-0.09661500	-1.51577500
N	2.61451100	0.07175100	-1.65046800
N	0.27292200	-0.12740300	-1.44957600
Cl	0.69746300	-1.44472100	1.25452600
Ru	-1.22566500	-0.28377600	0.03619300
C	-2.34350000	-3.10639900	1.50265800
C	-1.76797600	-3.14852900	-1.61513700
C	-3.88960900	-0.37210500	2.18841900
C	-4.21092800	1.27846100	-0.46721800
C	-2.86888900	-0.42146100	-2.86964800
H	-2.41645500	-2.78530500	2.54168900
H	-3.06156300	-3.92025300	1.34756400
H	-1.33596900	-3.49551700	1.35340100
H	-3.39710400	-0.86780100	3.02541200
H	-3.84847100	0.70467700	2.36118300
H	-4.94581100	-0.66727200	2.20522100
H	-4.07279400	1.75395900	-1.43836500
H	-5.28118400	1.06913700	-0.35353000
H	-3.93166600	1.99930200	0.30388400
H	-1.93905800	-0.71809500	-3.35787900
H	-3.69010100	-0.94730100	-3.37064100
H	-3.00568500	0.64701100	-3.03710400
H	-2.55811300	-3.84843700	-1.91364800
H	-1.26206600	-2.81569300	-2.52310500
H	-1.04244900	-3.69971200	-1.01482200
C	3.48782800	-1.11988200	-1.36776100
H	2.89122900	-1.88380600	-0.86540400
H	3.83197100	-1.49908400	-2.33353400
C	4.65905600	-0.70825700	-0.51197100
C	4.49022900	-0.54097600	0.86696400
C	5.91480600	-0.48498400	-1.07945700
C	5.56763600	-0.15955100	1.66100900
H	3.51346900	-0.71322100	1.30768300
C	6.99326900	-0.10342200	-0.28372100
H	6.05075400	-0.61123600	-2.14893400
C	6.82042500	0.05980200	1.08842900
H	5.43019600	-0.03664600	2.72954100
H	7.96518200	0.06432800	-0.73432600
H	7.65854300	0.35466000	1.71020500
C	-0.50314900	3.14638100	-0.25881600
C	-1.16776300	4.34148900	0.46600800
C	1.02721200	3.36932700	-0.28927700
C	-1.03781000	3.07429000	-1.69964800
H	-2.25378100	4.22566100	0.50018900
H	-0.80187800	4.42820400	1.49162500
H	-0.93908100	5.27419900	-0.05934700
H	1.54835900	2.54976900	-0.78639400
H	1.25793800	4.29339700	-0.82924800
H	1.42717200	3.45414800	0.72341700
H	-0.81731300	4.00840200	-2.22492200
H	-0.57909000	2.25394900	-2.25328800
H	-2.11917400	2.92703000	-1.70898200
C	-0.72732700	1.06884300	3.07199000
H	-1.67434400	0.75958000	3.52067600
H	0.00398200	0.27785700	3.24734700
H	-0.39479500	1.98258500	3.57643300

Prediction

MC-9A **E**(Hartree)**=** -1470.805660

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.09708300	-1.61576000	1.39127300
C	2.33792300	-2.26419200	0.14121400
C	1.19375000	-3.12507700	-0.13876900
C	0.26920000	-2.98588100	0.92279600
C	0.78678600	-2.02217200	1.85387100
C	0.44840800	0.93859900	0.98761600
C	1.29388300	1.17243400	0.05900500
N	-1.55775300	0.54673200	-1.62244900
N	-1.58831700	1.33310400	-2.42992900
N	-1.42196800	-0.29621100	-0.72264600
Cl	1.01030500	-0.90454900	-2.60339600
Ru	0.65363000	-0.87218500	-0.10598900
C	3.60414200	-2.24443000	-0.65808400
C	1.10616300	-4.07345500	-1.29336100
C	3.06600400	-0.77067000	2.15940700
C	0.20972500	-1.73208800	3.20745800
C	-0.99926300	-3.76242500	1.10626700
H	4.21602500	-1.37433700	-0.41825100
H	4.19847700	-3.14212500	-0.44910400
H	3.38476200	-2.21394400	-1.72567100
H	3.79260800	-0.29507800	1.50038300
H	2.55944800	0.02168000	2.71236900
H	3.61554300	-1.38701400	2.88006500
H	-0.87036700	-1.58947500	3.17611500
H	0.42614100	-2.56229700	3.89078500
H	0.64087600	-0.83007800	3.64112600
H	-1.43998700	-4.05608100	0.15274400
H	-0.79760300	-4.68038400	1.67085700
H	-1.74300200	-3.19572300	1.66817200
H	1.80894500	-4.90325400	-1.15452000
H	0.10614900	-4.49807300	-1.39264700
H	1.35082900	-3.56726300	-2.22887600
C	2.17772800	2.14623900	-0.53803600
C	2.85622000	1.90403800	-1.74331700
C	2.38704100	3.37093400	0.13010600
C	3.71722000	2.86389600	-2.26573300
H	2.67743600	0.97213800	-2.26311700
C	3.25113900	4.32026300	-0.39805700
H	1.86400300	3.55449300	1.06056100
C	3.91942200	4.07013300	-1.59805600
H	4.23065600	2.66867300	-3.20059800
H	3.40540300	5.25801800	0.12449200
H	4.59259100	4.81419400	-2.00967500
C	-0.43507400	1.45026900	2.00181000
O	-1.47646200	0.94338200	2.38037700
O	0.03190700	2.61820700	2.52478800
C	-0.80502100	3.23610500	3.51666500
C	-2.68035600	-0.89034600	-0.16259400
H	-2.76557700	-1.89813700	-0.57690400
H	-2.48838400	-0.95881300	0.90661400
C	-3.93355900	-0.09606300	-0.42897000
C	-4.74910800	-0.39887200	-1.52341300
C	-4.29047800	0.96115800	0.41660200
C	-5.90337600	0.34014600	-1.77232000
H	-4.48108900	-1.21833000	-2.18276100
C	-5.44445100	1.69864700	0.16715600
H	-3.65866900	1.19234100	1.26731200
C	-6.25206800	1.39045500	-0.92680200
H	-6.52874600	0.09510500	-2.62322300
H	-5.71653300	2.51299600	0.82933600
H	-7.15100400	1.96572600	-1.11787200
H	-1.00296800	2.54794000	4.33965800
H	-0.24785400	4.10259000	3.86692700
H	-1.75479500	3.54857900	3.07840500

MC-10A **E**(Hartree)**=** -1447.417880

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.19203400	-1.73794500	1.12497800
C	2.40840500	-2.12488800	-0.23198600
C	1.27822000	-2.95126200	-0.64428100
C	0.38473300	-3.04916000	0.44810400
C	0.90959000	-2.26960200	1.53498200
C	0.43084500	0.72519800	1.26554300
C	1.21158900	1.23932200	0.38256600
N	-1.61437000	0.78798100	-1.44105000
N	-1.69550900	1.66582900	-2.14259000
N	-1.43483200	-0.15473900	-0.65230400
Cl	1.01536100	-0.31271200	-2.61013800
Ru	0.67406400	-0.75959700	-0.16272800
C	3.65416900	-1.92100000	-1.03663700
C	1.17619300	-3.66135900	-1.95680600
C	3.16035200	-1.02350000	2.01678700
C	0.37826600	-2.27056300	2.93605100
C	-0.85679100	-3.88514400	0.50907800
H	4.24680000	-1.08940500	-0.65459400
H	4.27630800	-2.82321300	-0.99643100
H	3.41567400	-1.71100900	-2.07929200
H	3.88173200	-0.44384100	1.44070200
H	2.65248700	-0.33598800	2.69503800
H	3.71627800	-1.74621600	2.62444600
H	-0.70741100	-2.19061500	2.96617300
H	0.66857500	-3.20180800	3.43720200
H	0.77934500	-1.44328700	3.52063300
H	-1.33315800	-3.98068800	-0.46735000
H	-0.60934200	-4.89613900	0.85322700
H	-1.58589000	-3.47614700	1.20931300
H	1.91500800	-4.46936700	-2.00700500
H	0.18941400	-4.10342900	-2.10022600
H	1.36196700	-2.97344100	-2.78343300
C	1.95712500	2.40464500	-0.01090300
C	2.61161800	2.48443800	-1.25284300
C	2.05057600	3.48800000	0.88982600
C	3.34014100	3.62095200	-1.58321300
H	2.51711800	1.65852500	-1.94553600
C	2.78336200	4.61612800	0.54855600
H	1.54221300	3.41992600	1.84366100
C	3.43003700	4.68549200	-0.68679600
H	3.83753700	3.67806500	-2.54478700
H	2.85128400	5.44427400	1.24502100
H	4.00103500	5.56921000	-0.94986000
C	-2.67351100	-0.85684600	-0.17178300
H	-2.79170200	-1.75599300	-0.78233500
H	-2.42960400	-1.14469500	0.84833300
C	-3.92567800	-0.01785200	-0.20680900
C	-4.82375900	-0.12698400	-1.27283100
C	-4.19742400	0.88849200	0.82552700
C	-5.97644700	0.65442900	-1.31034500
H	-4.62213700	-0.82848900	-2.07628700
C	-5.34874600	1.66933500	0.78599800
H	-3.50687000	0.97064100	1.65810700
C	-6.23940500	1.55439400	-0.28073100
H	-6.66631500	0.55963700	-2.14116700
H	-5.55261400	2.36599300	1.59113700
H	-7.13616300	2.16311400	-0.30794500
N	-0.39093000	1.06135200	2.34945000
O	-0.10804000	2.06856000	3.00825400
O	-1.36383800	0.33037400	2.60535900

MC-11A **E**(Hartree)**=** -1335.135189

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	2.02349600	1.74403300	-1.25946000
C	2.40061200	2.02729400	0.08978600
C	1.34784000	2.84697500	0.67981200

C	0.33972500	3.03857600	-0.29296800
C	0.71408300	2.32468600	-1.48368200
C	0.31305500	-0.80770400	-1.36925800
C	1.15797400	-1.26947100	-0.52846000
N	-1.61392200	-0.88487300	1.41444300
N	-1.66531200	-1.78393700	2.09118900
N	-1.45927400	0.08185300	0.64857300
Cl	1.10641900	0.11017100	2.50376400
Ru	0.64535600	0.71011300	0.10855900
C	3.72014400	1.73815900	0.73605600
C	1.40932200	3.46061300	2.04277400
C	2.87762700	1.08714600	-2.29966000
C	0.01798400	2.41958400	-2.80833000
C	-0.87932100	3.89708100	-0.14158900
H	4.22023400	0.89162700	0.26424400
H	4.38204000	2.60865500	0.65307100
H	3.59118600	1.50310700	1.79284500
H	3.58331700	0.38668200	-1.85231700
H	2.27940600	0.53589600	-3.02593800
H	3.45276800	1.84439700	-2.84450700
H	-1.06709400	2.46951900	-2.70180400
H	0.33867800	3.32650500	-3.33471300
H	0.23923300	1.56814500	-3.45036300
H	-1.24984200	3.90063700	0.88428700
H	-0.64333700	4.93360400	-0.40903800
H	-1.68866700	3.57312900	-0.79665800
H	2.18756300	4.23168400	2.07286500
H	0.46396000	3.93025500	2.31713900
H	1.64174400	2.70498800	2.79562000
C	1.98680300	-2.40811200	-0.20876100
C	2.82694300	-2.42832000	0.91556100
C	1.97493000	-3.52412200	-1.07064800
C	3.63180900	-3.53480700	1.16789200
H	2.81216200	-1.58470000	1.59212600
C	2.78176000	-4.62286000	-0.81186100
H	1.32901000	-3.51498600	-1.94105300
C	3.61443800	-4.63138500	0.30890100
H	4.27160100	-3.54164000	2.04316700
H	2.76275900	-5.47470400	-1.48240400
H	4.24281400	-5.49170400	0.51093100
C	-2.71463400	0.79813000	0.24575400
H	-2.86305700	1.62469200	0.94661600
H	-2.47977000	1.21668900	-0.73145400
C	-3.94654000	-0.06922100	0.17520500
C	-4.85451400	-0.09268200	1.23799100
C	-4.19162300	-0.86548900	-0.95012000
C	-5.99104100	-0.89628500	1.18119300
H	-4.67406900	0.52408900	2.11277900
C	-5.32708000	-1.66833800	-1.00538900
H	-3.49599500	-0.85574500	-1.78280200
C	-6.22815100	-1.68523200	0.05857700
H	-6.68876500	-0.90435900	2.01074900
H	-5.50925000	-2.27880600	-1.88237800
H	-7.11259600	-2.31046100	0.01135500
C	-0.54596800	-0.91226300	-2.43501500
N	-1.30275400	-0.94604300	-3.31974200

MC-12C **E**(Hartree)**=** -1400.162658

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	1.98574800	-1.99447400	1.15480200
C	0.88087400	-2.80211200	0.75020200
C	-0.28311100	-2.37946400	1.51682100
C	0.12157300	-1.32385400	2.37878800
C	1.51258400	-1.05323000	2.14606900
C	1.96254200	0.80557200	-0.43127900
C	1.77703000	0.07785900	-1.43671100
N	-1.59692500	1.45823400	-0.61014700
N	-2.23746100	2.10479800	-1.41289400
N	-0.93754000	0.95167000	0.17825100
Cl	-1.17933800	-1.51293700	-1.63672100

Ru	0.44990400	-0.71110900	0.17597800
C	0.90807900	-3.98708700	-0.16428500
C	-1.62219400	-3.04871500	1.47585100
C	3.41315600	-2.15181400	0.73181900
C	2.38024200	-0.16367800	2.98364300
C	-0.74273300	-0.61415700	3.37568300
H	1.79749900	-3.99108700	-0.79462000
H	0.90646100	-4.91440900	0.42115400
H	0.03499700	-3.99046300	-0.81807500
H	3.49142800	-2.67253500	-0.22245000
H	3.90532500	-1.18408200	0.62369200
H	3.96956000	-2.73067500	1.47811500
H	1.84973400	0.72723800	3.32132400
H	2.71999400	-0.70670900	3.87411400
H	3.26426700	0.17000800	2.44108000
H	-1.78740600	-0.60045100	3.06350100
H	-0.68961400	-1.11337600	4.35015800
H	-0.42278000	0.41930300	3.51567500
H	-1.58117000	-4.02027500	1.98229700
H	-2.38546500	-2.44766200	1.97252100
H	-1.94040400	-3.21014600	0.44476100
C	-3.49435600	1.46177000	-1.93781500
C	-4.51764700	1.19202200	-0.86303000
C	-5.38580600	2.20198000	-0.43509100
C	-4.59451500	-0.07146400	-0.26728800
C	-6.31786900	1.95494800	0.56830900
H	-5.33115000	3.18447500	-0.89290800
C	-5.52979400	-0.31833900	0.73650900
H	-3.91897500	-0.85466600	-0.59536200
C	-6.39164900	0.69244200	1.15593000
H	-6.98991600	2.74351800	0.88797300
H	-5.58885300	-1.30376300	1.18520300
H	-7.12145100	0.49752200	1.93386000
H	-3.86736500	2.17360000	-2.67193500
H	-3.20269700	0.53946600	-2.44401400
C	2.54998500	1.91764200	0.27966200
C	1.79365200	2.75090600	1.12106600
C	3.91868500	2.20570800	0.11575600
C	2.37887100	3.84038100	1.75696700
H	0.74284400	2.53604300	1.26696400
C	4.50028100	3.29201500	0.76105100
H	4.51789200	1.57150300	-0.52625600
C	3.73444800	4.11614500	1.58384900
H	1.77332500	4.47638100	2.39346200
H	5.55612700	3.49557000	0.61942500
H	4.18912000	4.96262800	2.08565600
C	2.03451100	-0.18247200	-2.89154100
C	0.93165000	0.49801500	-3.73486300
C	3.40156800	0.44683600	-3.24969500
C	2.07284900	-1.69037000	-3.20532800
H	-0.04426100	0.07213200	-3.50574200
H	0.90275600	1.57319600	-3.53975200
H	1.14117200	0.34811500	-4.79904200
H	4.21089700	-0.01817100	-2.68012800
H	3.60961500	0.30043600	-4.31420300
H	3.40761400	1.52012100	-3.04560500
H	2.27876500	-1.83941500	-4.26990200
H	2.86664000	-2.18614700	-2.63897200
H	1.12003500	-2.15946600	-2.96234300

MC-13C **E**(Hartree)**=** -1494.835620

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	3.17345000	-0.91758200	-0.26353500
C	2.68570400	-1.75297800	-1.31754900
C	2.03972500	-2.90860600	-0.70597600
C	2.12302800	-2.75949500	0.70180400
C	2.78820400	-1.51556200	0.99480700
N	-1.75475000	-2.00479800	0.76346400
N	-2.62114500	-2.85829000	0.76377500

N	-0.89338400	-1.25912100	0.86544000
Cl	-0.61931900	-1.36697300	-2.18209900
Ru	0.96290700	-0.97636700	-0.20544400
C	2.92542900	-1.59568800	-2.78769300
C	1.48358400	-4.07585500	-1.46166600
C	4.02243700	0.30703700	-0.41032900
C	3.25373700	-1.06987200	2.34822200
C	1.62149500	-3.73349600	1.72508800
H	3.24957200	-0.58404700	-3.03487400
H	3.70783100	-2.28711200	-3.12248800
H	2.01559400	-1.80397800	-3.35286900
H	3.74848700	1.07381300	0.31586700
H	5.07807500	0.05649600	-0.25473100
H	2.56026200	-1.36563800	3.13658700
H	4.22788200	-1.51841400	2.57925000
H	3.36469400	0.01278600	2.40207000
H	0.76995100	-4.30574000	1.35465500
H	2.41084100	-4.44700600	1.98845100
H	1.31574000	-3.22999800	2.64367300
H	2.29504900	-4.70486900	-1.84615800
H	0.85039200	-4.69906700	-0.82831000
H	0.87883500	-3.73680400	-2.30404000
C	-3.71008300	-2.69510200	-0.26478300
H	-3.23693800	-2.72485800	-1.24866100
H	-4.32806600	-3.58189300	-0.13620400
C	-4.51557100	-1.43243600	-0.08797700
C	-4.18306700	-0.28130500	-0.80987300
C	-5.58543900	-1.38936700	0.81213200
C	-4.91418800	0.89220400	-0.63373400
H	-3.34975000	-0.31000000	-1.50442400
C	-6.31450600	-0.21716600	0.98698600
H	-5.84755900	-2.27912000	1.37575200
C	-5.97951600	0.92651100	0.26282300
H	-4.65090400	1.77810200	-1.20053700
H	-7.14534700	-0.19590700	1.68337900
H	-6.54903700	1.83946400	0.39647200
H	3.92704800	0.74440800	-1.40450000
N	0.18576400	3.30714800	-1.72288400
C	-1.15869100	3.53856000	-1.17511400
C	0.41696000	4.04574400	-2.97129100
C	0.43640800	1.86796300	-1.90946600
C	-1.30913100	4.89716300	-0.49184000
C	1.89679400	4.31318300	-3.24699500
C	0.69388600	1.16521700	-0.63596100
C	0.93565100	1.68305000	1.92496600
C	0.84679300	1.11468600	0.60419300
C	0.51328300	0.99995500	3.07657000
C	1.44261600	2.99026100	2.06694100
C	0.58970800	1.60530700	4.32665100
C	1.51836000	3.58712700	3.32012900
C	1.09416000	2.89830600	4.45643200
H	-1.92890400	3.42194500	-1.96073100
H	-1.34782500	2.75691300	-0.43653200
H	-0.04056300	3.52358700	-3.83186800
H	-0.09574500	5.00624700	-2.89044400
H	-0.38488700	1.36207000	-2.43922700
H	1.31676700	1.74391600	-2.54654300
H	-0.59285700	4.99245600	0.32701800
H	-1.15131000	5.73132900	-1.18054500
H	-2.31733500	4.99977500	-0.07990400
H	2.34036300	4.87411800	-2.42114500
H	2.46762000	3.38932400	-3.37068000
H	2.01326500	4.89454100	-4.16641200
H	0.11468900	-0.00109200	2.97549000
H	1.75705000	3.52573100	1.17891500
H	0.25144900	1.06533700	5.20435600
H	1.90890400	4.59497500	3.41004200
H	1.15445700	3.36574200	5.43271900

MC-14C **E**(Hartree)**=** -1680.403925

Atomic Symbol	Coordinates (Angstroms) X	Y	Z
C	-3.22576500	-0.23413300	0.39772800
C	-2.92863000	-1.58171500	0.77147600
C	-2.51239600	-2.29603800	-0.42886100
C	-2.55754800	-1.38043200	-1.51594900
C	-2.96203500	-0.09362300	-1.01775900
N	1.49505500	-1.46713800	-1.40209000
N	2.27946700	-2.30792600	-1.79105300
N	0.71018700	-0.67425100	-1.14723100
Cl	0.34580000	-2.27391900	1.44772900
Ru	-1.07074000	-0.64071600	0.07867100
C	-3.14506700	-2.21906000	2.10912200
C	-2.21223400	-3.76240200	-0.49290000
C	-3.81239500	0.82970200	1.27331600
C	-3.30879300	1.09809700	-1.85807200
C	-2.25607000	-1.69531500	-2.94985500
H	-3.25082600	-1.47175100	2.89653400
H	-4.05897400	-2.82471600	2.09756900
H	-2.30505700	-2.86368800	2.37094500
H	-3.39321400	1.81135300	1.04721300
H	-4.89694800	0.88622500	1.12549400
H	-2.64934500	1.19468200	-2.72157100
H	-4.33617400	1.00961700	-2.23211900
H	-3.24008100	2.02738100	-1.29305200
H	-1.53783100	-2.51089900	-3.04198700
H	-3.17147500	-1.99924300	-3.47074600
H	-1.85256700	-0.82805800	-3.47438600
H	-3.13611100	-4.34682200	-0.41046100
H	-1.73197700	-4.03279900	-1.43454000
H	-1.54341600	-4.05700600	0.31739800
C	3.42193300	-2.62985400	-0.85976700
H	2.98645000	-3.09809100	0.02579600
H	4.00717400	-3.36784700	-1.40476300
C	4.24994100	-1.42574500	-0.49129800
C	3.90980100	-0.65757900	0.62772300
C	5.34016600	-1.04028400	-1.27806000
C	4.64632800	0.48033400	0.95040500
H	3.06533400	-0.95381400	1.24127100
C	6.08036900	0.09209900	-0.95131400
H	5.60949200	-1.63058600	-2.14822300
C	5.73244700	0.85527800	0.16271100
H	4.36461800	1.07175500	1.81402800
H	6.92755500	0.37930700	-1.56420300
H	6.30687600	1.73956700	0.41520700
H	-3.63171500	0.62635700	2.32928100
C	-0.49557500	2.67301600	-0.42861900
C	-0.05632200	2.60826900	-1.76106600
C	-0.91011300	3.91748200	0.08310300
C	-0.02571900	3.75196200	-2.55114000
C	-0.88203300	5.05568900	-0.71525800
C	-0.44125900	4.97907900	-2.03551300
C	-0.51277100	1.51697500	0.43158500
C	0.05174600	0.73535600	2.89808600
C	-0.35691000	0.89056800	1.50160100
H	0.27147000	1.65672900	-2.15852800
H	-1.24024500	3.98004100	1.11328600
H	0.32627200	3.68582800	-3.57480400
H	-1.20170700	6.00633900	-0.30287500
H	-0.41898500	5.86782000	-2.65585700
H	-0.83196400	0.69269700	3.53961400
H	0.61177700	-0.18986900	3.02008100
S	1.09779200	2.18395300	3.43143700
H	1.24137700	1.78322400	4.71252300

Table S1. Global electronic properties (chemical potential μ, chemical hardness η, global electrophilicity ω and global nucleophilicity N, all in eV) of predicted series 1 activated complexes.

	ε_{HOMO}	ε_{LUMO}	**μ**	**η**	**ω**	**N**
MC-9A	-0,19123	-0,06458	-3.38	3.49	1.76	3.90
MC-10A	-0,20517	-0,09230	-4.05	3.07	2.67	3.52
MC-11A	-0,20012	-0,07579	-3.75	3.38	2.08	3.66

Table S2. Global electronic properties (chemical potential μ, chemical hardness η, global electrophilicity ω and global nucleophilicity N, all in eV) of predicted series 1 activated complexes.

	ε_{HOMO}	ε_{LUMO}	**μ**	**η**	**ω**	**N**
MC-12C	-0.18843	-0.06027	-3.38	3.49	1.64	3.98
MC-13C	-0.18587	-0.05891	-3.33	3.45	1.60	4.05
MC-14C	-0.19187	-0.06214	-3.45	3.53	1.69	3.88