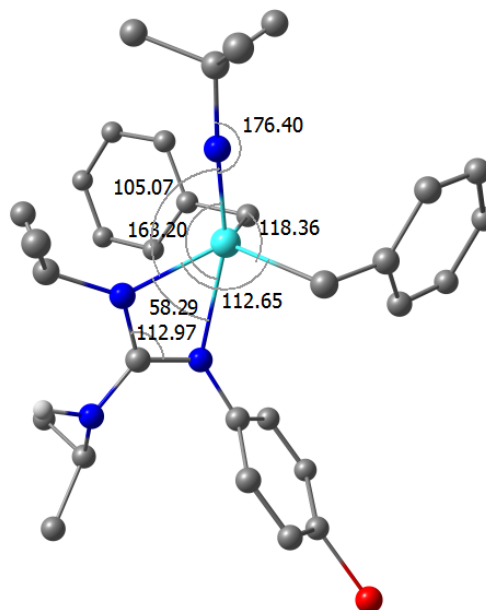
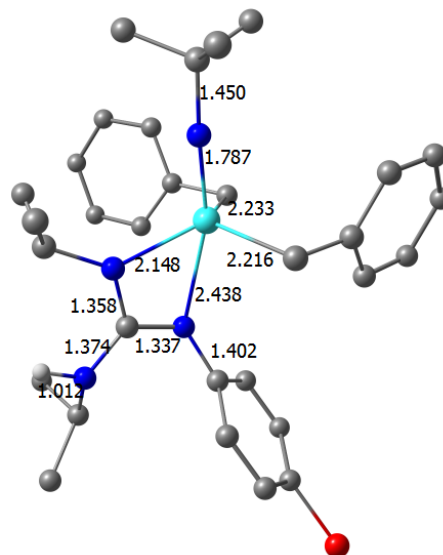
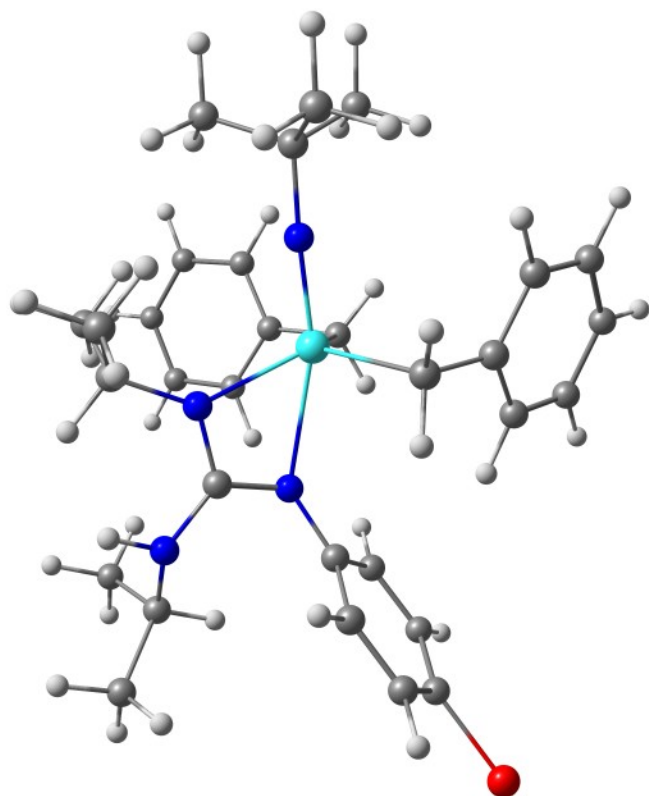


Supporting Information: Optimized geometries and Cartesian coordinates.

(1a)

E(gas) = -4053.39277511

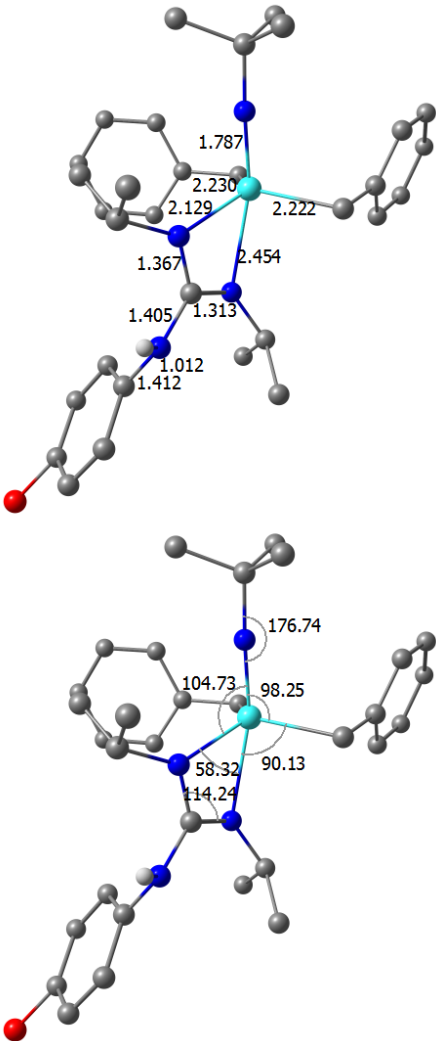
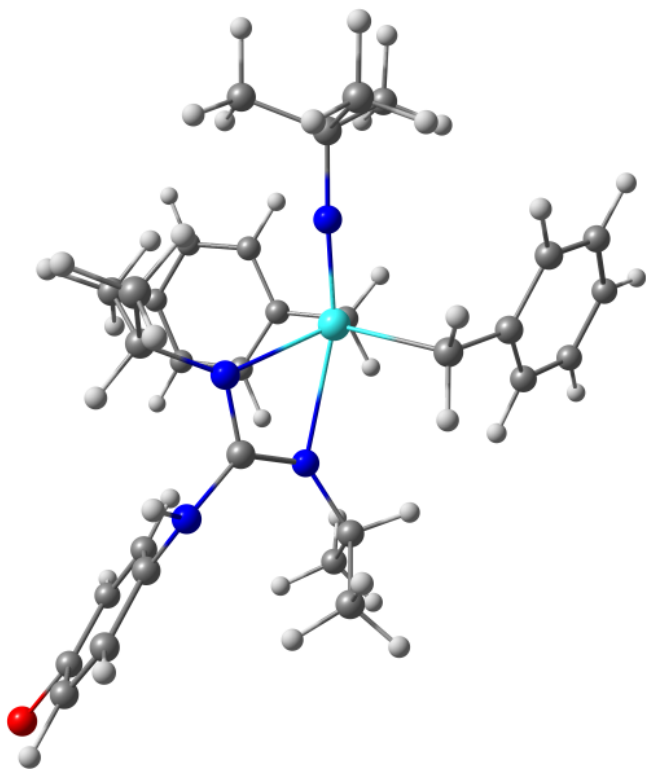


Nb	1.345062000	0.437473000	-0.419184000
Br	-6.640159000	0.833520000	0.170204000
N	-0.739434000	-0.792516000	-0.128554000
C	4.381453000	1.316692000	-1.107257000
N	1.088393000	-1.548557000	-1.195359000
N	-0.906923000	-2.870549000	-1.316293000
H	-0.375924000	-3.480277000	-1.925393000
C	-0.214106000	-1.767222000	-0.878396000
C	1.991418000	-2.575990000	-1.728678000
H	1.416580000	-3.487673000	-1.945391000
C	-1.899497000	-3.602781000	-0.502976000
H	-2.478558000	-2.857934000	0.043962000
C	2.611102000	-2.109843000	-3.052019000
H	1.832771000	-1.909727000	-3.797055000

H	3.288275000	-2.872803000	-3.453489000
H	3.177541000	-1.186405000	-2.900903000
C	-2.842592000	-4.359737000	-1.441075000
H	-3.357656000	-3.668876000	-2.115325000
H	-3.594891000	-4.908849000	-0.865379000
H	-2.292554000	-5.090635000	-2.049153000
C	3.049325000	-2.970497000	-0.688230000
H	3.668666000	-2.111098000	-0.419329000
H	3.702343000	-3.757563000	-1.084835000
H	2.575483000	-3.338684000	0.227174000
C	-1.209034000	-4.532466000	0.505904000
H	-0.620434000	-5.304217000	-0.007103000
H	-1.951153000	-5.039678000	1.133339000
H	-0.535681000	-3.967633000	1.159399000
N	3.032368000	0.875780000	-0.812756000
C	0.200844000	3.070937000	-0.647257000
C	1.176024000	4.087724000	-0.550462000
H	1.994591000	4.098223000	-1.265702000
C	0.323239000	1.972984000	-1.648166000
H	0.883869000	2.262617000	-2.539422000
H	-0.653012000	1.561890000	-1.933013000
C	1.094713000	5.078557000	0.424587000
H	1.853907000	5.855724000	0.466752000
C	-0.860450000	3.098233000	0.282292000
H	-1.637731000	2.341687000	0.221273000
C	0.039104000	5.081347000	1.342266000
H	-0.024120000	5.854922000	2.102682000
C	-0.938447000	4.088096000	1.262236000
H	-1.772352000	4.086639000	1.959689000
C	1.260872000	-1.585809000	2.751199000
H	0.189965000	-1.543949000	2.569959000
C	3.434248000	-0.554393000	2.671567000
H	4.065652000	0.299539000	2.438303000
C	1.450422000	0.744729000	1.790332000
H	2.018116000	1.654641000	2.007976000
H	0.409168000	0.892094000	2.102435000
C	2.050341000	-0.466194000	2.416391000
C	4.000830000	-1.700380000	3.226742000
H	5.070674000	-1.731713000	3.419658000
C	1.826197000	-2.734223000	3.306712000
H	1.187805000	-3.575923000	3.566405000
C	3.201229000	-2.801885000	3.545304000
H	3.641505000	-3.693318000	3.983959000
C	-4.803890000	0.306633000	0.064698000
C	-2.105930000	-0.480500000	-0.091725000
C	-2.683263000	-0.095236000	1.133564000
H	-2.066411000	-0.106468000	2.027328000
C	-2.922756000	-0.445258000	-1.241872000
H	-2.502059000	-0.723548000	-2.203163000
C	-4.019277000	0.294875000	1.216699000
H	-4.446598000	0.583925000	2.170988000

C	-4.260191000	-0.060569000	-1.165856000
H	-4.873356000	-0.036439000	-2.060594000
C	4.758831000	2.440295000	-0.116181000
H	4.050538000	3.271424000	-0.183157000
H	5.764970000	2.820096000	-0.332095000
H	4.745660000	2.066703000	0.912804000
C	5.375131000	0.146220000	-0.951720000
H	5.318470000	-0.276380000	0.056586000
H	6.400707000	0.494535000	-1.124357000
H	5.162504000	-0.650235000	-1.671636000
C	4.429832000	1.856051000	-2.553120000
H	4.149150000	1.075347000	-3.268212000
H	5.439729000	2.204259000	-2.801947000
H	3.736719000	2.694732000	-2.676881000

(1'a)
E(gas) = -4053.37407477

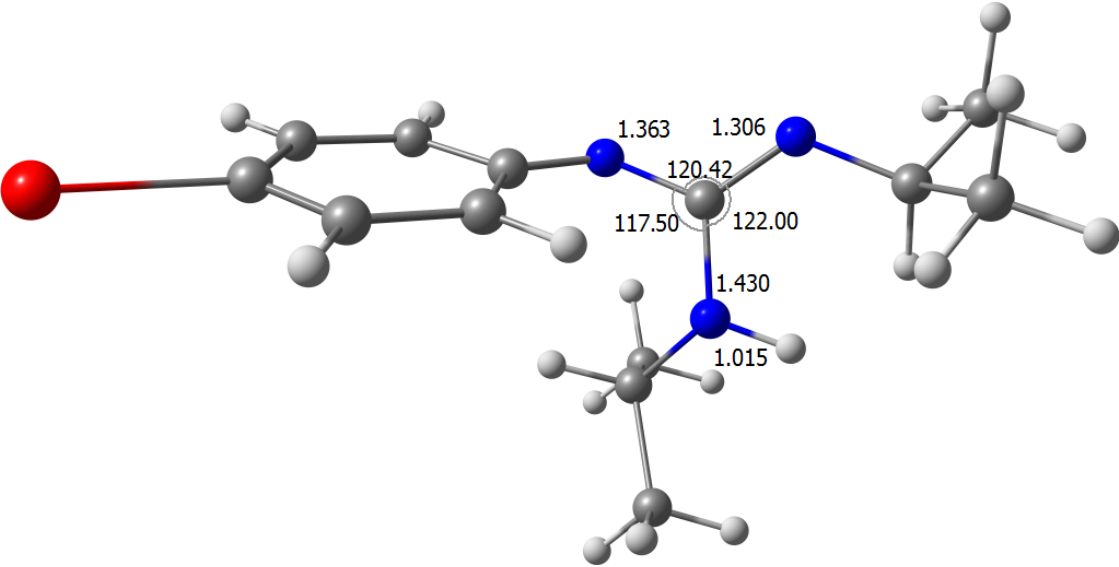


Nb	1.885240000	0.107057000	-0.340829000
Br	-7.583801000	0.130743000	0.517475000
N	-1.929758000	0.414056000	-1.803842000
C	4.317448000	-1.906256000	-1.045945000
N	0.185996000	-0.629064000	-1.391891000
N	-0.296298000	1.221808000	-0.205248000
H	-1.879568000	0.046783000	-2.745423000
C	-0.714906000	0.356936000	-1.099794000
C	-0.189328000	-1.894094000	-2.038516000
H	-1.256746000	-1.843920000	-2.291211000
C	-0.778320000	2.592022000	0.020232000
H	0.138947000	3.154253000	0.242550000
C	0.596457000	-2.088441000	-3.342423000
H	0.405356000	-1.267387000	-4.043801000
H	0.316830000	-3.030004000	-3.829424000
H	1.671663000	-2.109616000	-3.138966000
C	-1.426132000	3.310037000	-1.176771000
H	-0.819471000	3.198028000	-2.082310000
H	-1.496982000	4.380461000	-0.949493000

H	-2.434671000	2.948423000	-1.391482000
C	-0.020031000	-3.078467000	-1.076417000
H	1.023663000	-3.187180000	-0.770804000
H	-0.337672000	-4.010586000	-1.559651000
H	-0.620167000	-2.934829000	-0.172438000
C	-1.649903000	2.700865000	1.283081000
H	-2.625080000	2.225759000	1.144029000
H	-1.819997000	3.755331000	1.531569000
H	-1.153429000	2.227009000	2.136653000
N	3.198480000	-1.037026000	-0.741813000
C	3.686697000	2.459986000	-0.186974000
C	5.069478000	2.179914000	-0.211977000
H	5.474607000	1.613846000	-1.047040000
C	2.769501000	1.935814000	-1.241807000
H	3.287765000	1.727541000	-2.181457000
H	1.930177000	2.617769000	-1.431175000
C	5.919645000	2.628147000	0.795721000
H	6.982490000	2.405446000	0.740843000
C	3.202186000	3.215271000	0.900353000
H	2.145620000	3.470194000	0.940537000
C	5.414872000	3.366998000	1.870689000
H	6.078286000	3.716293000	2.657045000
C	4.051288000	3.660181000	1.914496000
H	3.645359000	4.244214000	2.736751000
C	-0.195756000	-1.165537000	2.616254000
H	-0.681932000	-0.194999000	2.556502000
C	1.782074000	-2.525633000	2.438322000
H	2.845638000	-2.622527000	2.234263000
C	1.961259000	-0.066444000	1.881215000
H	3.007299000	-0.114055000	2.200223000
H	1.518367000	0.867653000	2.251235000
C	1.180004000	-1.256189000	2.321313000
C	1.048001000	-3.647106000	2.819809000
H	1.545102000	-4.610320000	2.907957000
C	-0.932910000	-2.287753000	2.996929000
H	-1.990211000	-2.183061000	3.230434000
C	-0.317783000	-3.538219000	3.096727000
H	-0.890063000	-4.411215000	3.398626000
C	-5.812890000	0.225805000	-0.193899000
C	-3.218752000	0.365228000	-1.229112000
C	-4.323636000	0.713357000	-2.021330000
H	-4.166336000	1.051198000	-3.042479000
C	-3.434018000	-0.062267000	0.089575000
H	-2.592077000	-0.358220000	0.706845000
C	-5.618121000	0.636210000	-1.511647000
H	-6.466253000	0.904069000	-2.132142000
C	-4.726704000	-0.120781000	0.608127000
H	-4.887591000	-0.452711000	1.627974000
C	5.388477000	-1.722139000	0.052541000
H	5.700286000	-0.675411000	0.117597000
H	6.269426000	-2.339100000	-0.162984000

H	4.992222000	-2.018335000	1.029435000
C	3.863481000	-3.380758000	-1.076522000
H	3.402088000	-3.664462000	-0.125156000
H	4.723841000	-4.037713000	-1.252843000
H	3.136242000	-3.552745000	-1.876147000
C	4.901833000	-1.513809000	-2.420246000
H	4.146645000	-1.618174000	-3.206777000
H	5.754637000	-2.154965000	-2.674573000
H	5.243862000	-0.473751000	-2.413406000

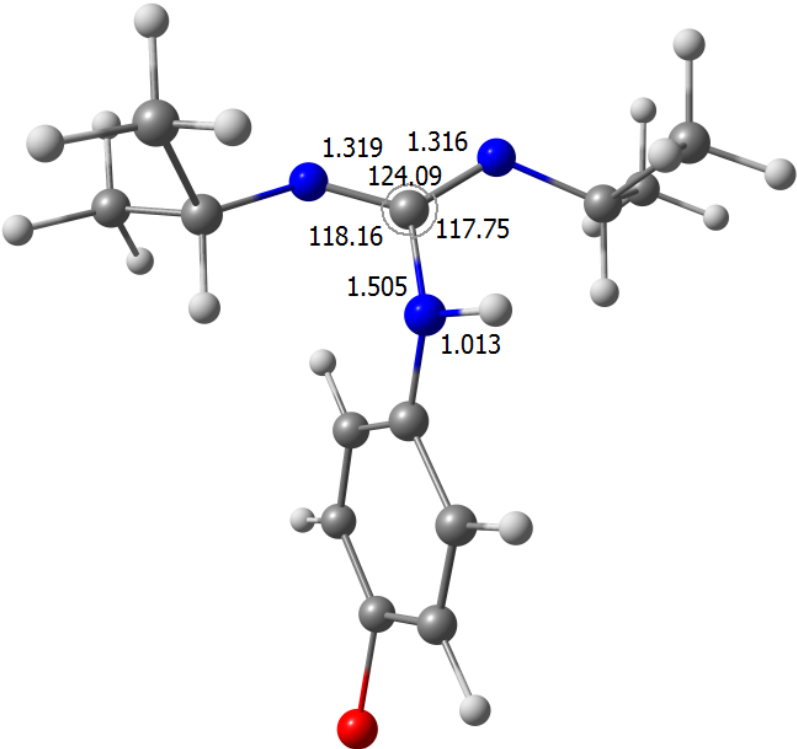
(3a)
E(gas)= -3242.50051774



C	-0.147746000	-0.349827000	0.804515000
C	-1.194580000	-0.222556000	1.778986000
H	-0.892348000	-0.145006000	2.820688000
C	-2.539109000	-0.206628000	1.442752000
H	-3.295480000	-0.108201000	2.217212000
C	-2.920930000	-0.318821000	0.101746000
C	-1.950087000	-0.448588000	-0.891906000
H	-2.249893000	-0.541685000	-1.932959000
C	-0.601110000	-0.463521000	-0.554986000
H	0.138637000	-0.568058000	-1.342948000
C	2.205660000	-0.313715000	0.410327000
C	1.676807000	2.096857000	-0.115519000
H	0.611308000	1.927381000	0.059640000
C	2.284422000	2.699118000	1.162612000
H	2.163440000	1.990422000	1.986917000
H	1.788321000	3.641526000	1.433305000
H	3.355809000	2.905712000	1.027539000
C	1.813026000	3.044950000	-1.312595000
H	1.345896000	2.610315000	-2.202964000
H	2.870299000	3.242221000	-1.544035000
H	1.336386000	4.010496000	-1.103983000
C	4.398870000	-1.029550000	-0.252677000
H	4.735742000	0.030601000	-0.323668000
C	4.268768000	-1.565658000	-1.694863000
H	3.502151000	-1.010807000	-2.247345000
H	3.958845000	-2.617302000	-1.664860000
H	5.216579000	-1.495872000	-2.248557000
C	5.513214000	-1.779741000	0.496407000
H	5.615529000	-1.383666000	1.512799000

H	6.482552000	-1.693183000	-0.015491000
H	5.252435000	-2.841591000	0.580609000
N	1.124631000	-0.400888000	1.235453000
N	3.168765000	-1.191876000	0.487583000
N	2.269424000	0.804874000	-0.478521000
H	3.196223000	0.929295000	-0.873607000
Br	-4.797583000	-0.292037000	-0.374248000

(3'a)
E(gas)= -3242.48091175



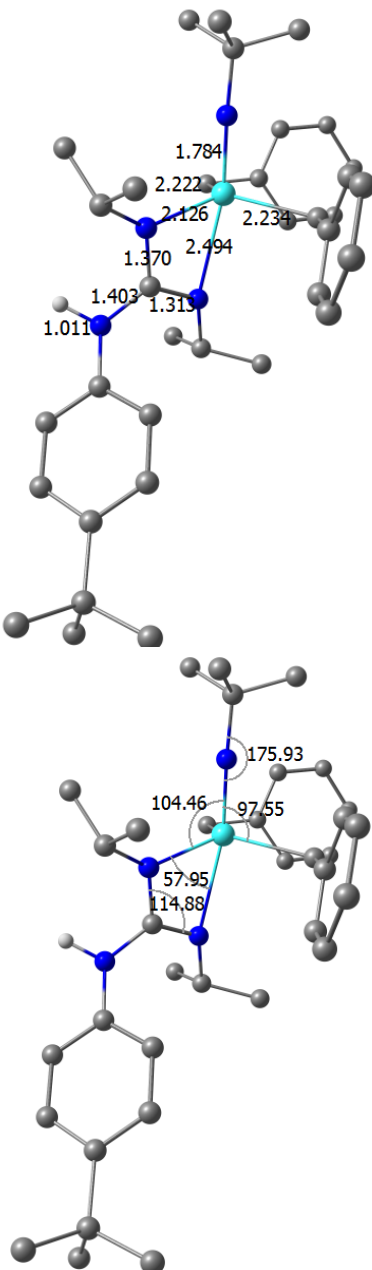
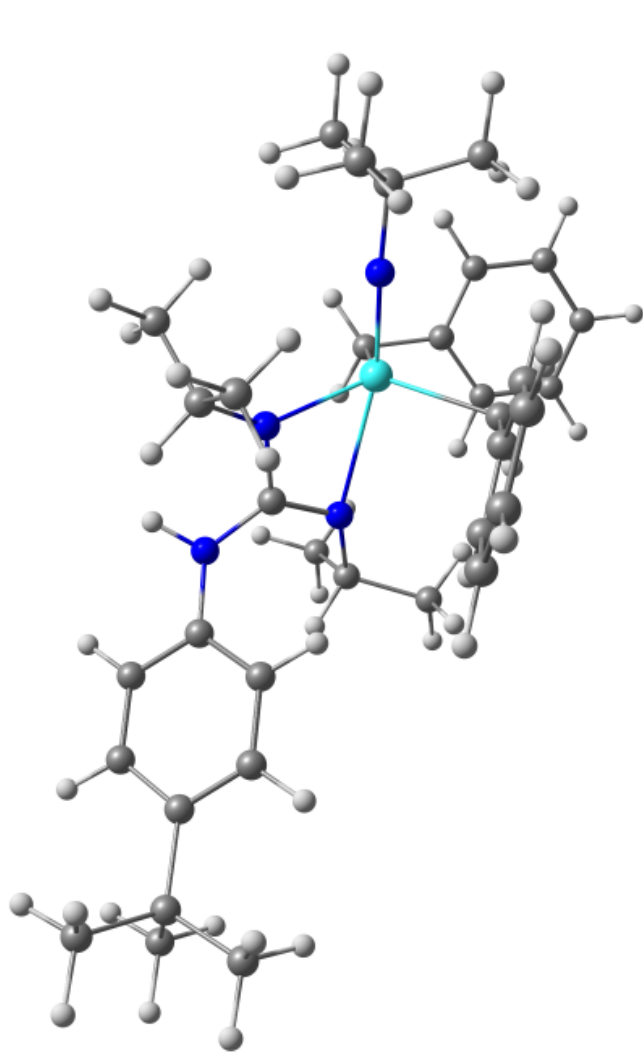
C	2.519726000	0.165284000	-0.201071000
C	2.963556000	-2.206945000	-0.274616000
H	1.907352000	-2.362652000	0.024277000
C	3.845943000	-2.750231000	0.873388000
H	3.655314000	-2.205320000	1.808110000
H	4.903395000	-2.599489000	0.622762000
H	3.677028000	-3.821217000	1.062958000
C	3.187695000	-3.053613000	-1.543332000
H	2.541056000	-2.693294000	-2.351013000
H	2.976618000	-4.120484000	-1.373877000
H	4.226632000	-2.949566000	-1.880437000
N	2.622727000	1.391432000	-0.676258000
N	3.292946000	-0.834866000	-0.566761000
N	1.460574000	-0.109255000	0.832093000
H	1.751515000	-0.772961000	1.539790000
H	0.229955000	0.921330000	-1.295439000
C	-0.446889000	0.458211000	-0.584519000
C	0.110692000	-0.138731000	0.573396000
C	-0.783346000	-0.759671000	1.480174000
H	-0.385555000	-1.234868000	2.375288000
H	-2.820386000	-1.253994000	1.969151000
C	-2.156471000	-0.773550000	1.256957000
C	-1.818899000	0.439724000	-0.808877000
C	-2.671742000	-0.170796000	0.111249000
H	-2.225207000	0.900523000	-1.704079000
C	2.116653000	2.517964000	0.075396000

H	1.141563000	2.333225000	0.565426000
C	1.914630000	3.693702000	-0.895637000
H	1.184058000	3.429854000	-1.669826000
H	2.860395000	3.924975000	-1.401805000
H	1.560762000	4.597557000	-0.378478000
C	3.098899000	2.927510000	1.196010000
H	3.207873000	2.111100000	1.919461000
H	2.760692000	3.824182000	1.739008000
H	4.088806000	3.129470000	0.767034000
Br	-4.575951000	-0.182363000	-0.200370000

H	-4.023837000	3.276121000	-0.189867000
C	0.226649000	-1.766920000	-0.889824000
C	-1.990727000	-2.592838000	-1.697144000
H	-1.416506000	-3.508771000	-1.897151000
C	-2.618155000	-2.151661000	-3.025662000
H	-3.185984000	-1.226860000	-2.887180000
H	-3.295833000	-2.922536000	-3.411151000
H	-1.843997000	-1.961831000	-3.777754000
C	-3.044165000	-2.967893000	-0.644878000
H	-2.565989000	-3.319686000	0.274679000
H	-3.699712000	-3.761648000	-1.023909000
H	-3.661608000	-2.103315000	-0.388780000
C	1.927797000	-3.593901000	-0.555977000
H	2.508371000	-2.848313000	-0.011694000
C	1.259861000	-4.537925000	0.454986000
H	0.589871000	-3.983946000	1.121152000
H	2.014785000	-5.042383000	1.069456000
H	0.671841000	-5.311824000	-0.055616000
C	2.863890000	-4.334967000	-1.513685000
H	2.311603000	-5.065128000	-2.120748000
H	3.628936000	-4.883040000	-0.953751000
H	3.362983000	-3.632927000	-2.188392000
C	-0.314893000	1.957402000	-1.670704000
H	0.654261000	1.537256000	-1.965866000
H	-0.886137000	2.245976000	-2.555581000
C	-0.171055000	3.060663000	-0.678752000
C	0.900077000	3.083175000	0.239799000
H	1.667879000	2.316969000	0.177848000
C	0.997178000	4.078713000	1.212322000
H	1.837193000	4.072196000	1.902502000
C	0.030673000	5.082474000	1.295846000
H	0.108896000	5.860017000	2.050918000
C	-1.034359000	5.083935000	0.389144000
H	-1.785911000	5.868427000	0.434268000
C	-1.135318000	4.087497000	-0.578342000
H	-1.961656000	4.101100000	-1.284669000
C	2.123730000	-0.479460000	-0.109656000
C	2.934489000	-0.412378000	-1.256879000
H	2.510522000	-0.666281000	-2.224149000
C	4.273661000	-0.026552000	-1.171471000
H	4.850709000	0.008934000	-2.089583000
C	4.870824000	0.320649000	0.048882000
C	4.049226000	0.261833000	1.188419000
H	4.456947000	0.521475000	2.162173000
C	2.713675000	-0.124821000	1.117622000
H	2.105809000	-0.157741000	2.017647000
C	6.343446000	0.749065000	0.176353000
C	7.089588000	-0.239438000	1.104436000
H	6.644706000	-0.272609000	2.104638000
H	8.140198000	0.056703000	1.215996000
H	7.064869000	-1.255744000	0.694234000

C	7.067134000	0.767103000	-1.183709000
H	8.109306000	1.076634000	-1.043952000
H	6.603838000	1.472744000	-1.882763000
H	7.077050000	-0.223320000	-1.653191000
C	6.420238000	2.171771000	0.780100000
H	5.960505000	2.217431000	1.772990000
H	5.904993000	2.896870000	0.139773000
H	7.465640000	2.489164000	0.881864000
C	-1.409185000	0.752951000	1.786827000
H	-0.363946000	0.900267000	2.084949000
H	-1.972760000	1.665915000	2.002774000
C	-2.004369000	-0.450845000	2.430413000
C	-3.385265000	-0.533876000	2.703077000
H	-4.017843000	0.319133000	2.469288000
C	-3.947461000	-1.673716000	3.275157000
H	-5.015068000	-1.701091000	3.480996000
C	-3.146456000	-2.774218000	3.593610000
H	-3.583306000	-3.660970000	4.045125000
C	-1.774322000	-2.711677000	3.337296000
H	-1.134606000	-3.552909000	3.595480000
C	-1.213332000	-1.569467000	2.765006000
H	-0.144894000	-1.531675000	2.569173000

(1'b)
E(gas) = -1639.82963265

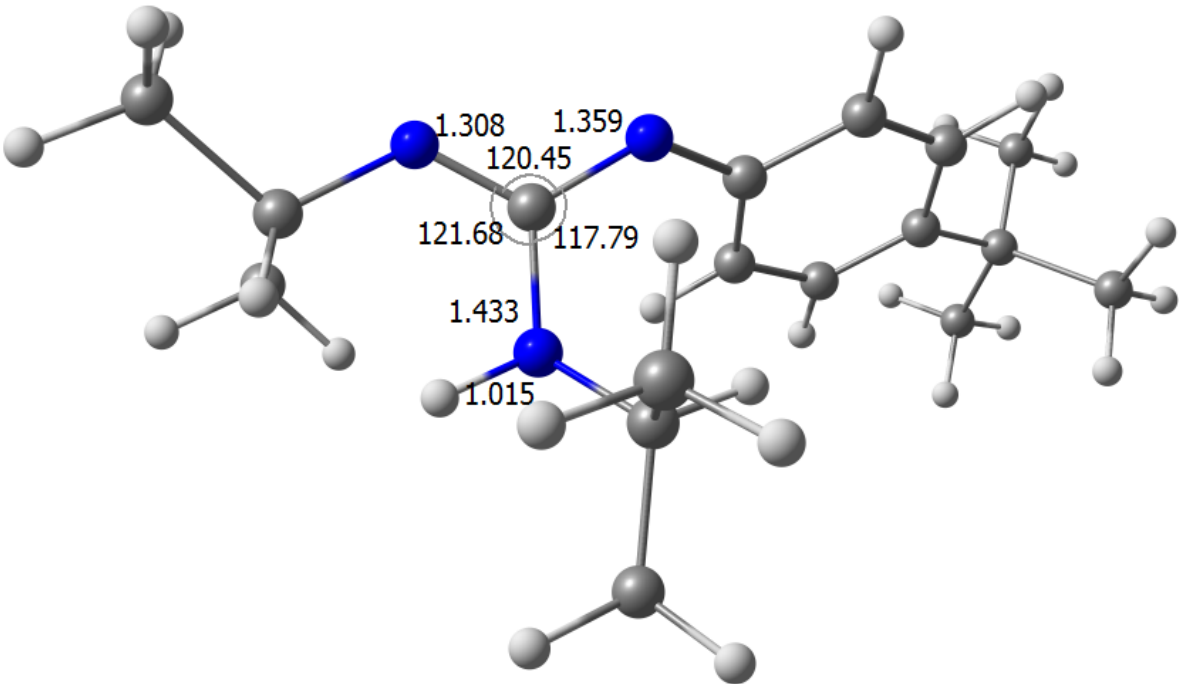


Nb	-1.829852000	0.080341000	-0.377079000
N	-3.107504000	-1.123758000	-0.696310000
N	-0.145766000	-0.632982000	-1.460186000
N	2.020601000	0.339320000	-1.800616000
N	0.407165000	1.171745000	-0.214938000
H	1.984885000	-0.046383000	-2.734542000
C	-4.211668000	-2.039565000	-0.907654000
C	-3.714587000	-3.500270000	-0.884431000
H	-3.020477000	-3.693213000	-1.708226000
H	-4.561771000	-4.189390000	-0.985954000
H	-3.200563000	-3.719722000	0.056580000
C	-4.863445000	-1.733507000	-2.273906000
H	-5.234830000	-0.704035000	-2.304636000

H	-5.707143000	-2.409807000	-2.457447000
H	-4.140049000	-1.857885000	-3.086663000
C	-5.246237000	-1.831430000	0.221250000
H	-4.810176000	-2.074632000	1.195413000
H	-6.118120000	-2.478235000	0.064421000
H	-5.582852000	-0.790851000	0.252308000
C	0.793812000	0.304956000	-1.121723000
C	0.198885000	-1.902159000	-2.118263000
H	1.236700000	-1.838910000	-2.470764000
C	-0.692083000	-2.135107000	-3.344422000
H	-1.744830000	-2.176964000	-3.050224000
H	-0.431973000	-3.078653000	-3.838445000
H	-0.578610000	-1.321718000	-4.070613000
C	0.146544000	-3.072792000	-1.125167000
H	0.826868000	-2.898965000	-0.285206000
H	0.437354000	-4.008501000	-1.618544000
H	-0.861495000	-3.194165000	-0.720065000
C	1.141073000	2.422166000	0.020131000
H	2.219864000	2.242784000	-0.049304000
C	0.793191000	3.493969000	-1.027789000
H	0.987993000	3.126064000	-2.040713000
H	1.401676000	4.392966000	-0.870749000
H	-0.260737000	3.786502000	-0.965341000
C	0.860743000	2.919807000	1.442040000
H	-0.209595000	3.095215000	1.596055000
H	1.392193000	3.859473000	1.632379000
H	1.189724000	2.186845000	2.186212000
C	-2.795480000	1.809215000	-1.384527000
H	-1.980409000	2.483156000	-1.674869000
H	-3.347161000	1.499582000	-2.275786000
C	-3.680331000	2.413359000	-0.345411000
C	-3.181293000	3.321001000	0.610792000
H	-2.142601000	3.634616000	0.550448000
C	-3.997415000	3.842898000	1.615151000
H	-3.581376000	4.544140000	2.334375000
C	-5.342049000	3.477243000	1.691990000
H	-5.979681000	3.885695000	2.471170000
C	-5.862407000	2.589289000	0.745144000
H	-6.912254000	2.308682000	0.782410000
C	-5.044650000	2.065059000	-0.252909000
H	-5.462201000	1.382576000	-0.988789000
C	3.310174000	0.317365000	-1.219340000
C	3.527804000	0.056927000	0.137463000
H	2.683375000	-0.136879000	0.791338000
C	4.827251000	0.031493000	0.649010000
H	4.947042000	-0.172422000	1.707407000
C	5.952031000	0.242162000	-0.158863000
C	5.709792000	0.487842000	-1.522071000
H	6.544014000	0.658300000	-2.197201000
C	4.422918000	0.533934000	-2.046038000
H	4.273851000	0.745943000	-3.102563000

C	7.394450000	0.213523000	0.376712000
C	8.068335000	1.582791000	0.119328000
H	8.097669000	1.828911000	-0.947537000
H	9.101531000	1.575736000	0.487846000
H	7.529263000	2.387224000	0.632739000
C	7.449465000	-0.070904000	1.889772000
H	8.492341000	-0.080540000	2.226216000
H	7.014276000	-1.045872000	2.137667000
H	6.922990000	0.696585000	2.468600000
C	8.194104000	-0.894004000	-0.350482000
H	8.225578000	-0.729789000	-1.432892000
H	7.746929000	-1.879218000	-0.175076000
H	9.228981000	-0.920237000	0.012605000
C	-1.902582000	0.000942000	1.854119000
H	-1.455044000	0.944218000	2.190140000
H	-2.952053000	-0.027575000	2.165539000
C	-1.135268000	-1.178058000	2.345549000
C	-1.753501000	-2.432877000	2.523770000
H	-2.819545000	-2.523052000	2.331962000
C	-1.033330000	-3.546965000	2.950262000
H	-1.544112000	-4.497571000	3.085628000
C	0.336095000	-3.446192000	3.212111000
H	0.898349000	-4.313462000	3.547679000
C	0.967501000	-2.210539000	3.052638000
H	2.028553000	-2.110878000	3.270568000
C	0.243349000	-1.095480000	2.628525000
H	0.742995000	-0.136524000	2.522486000

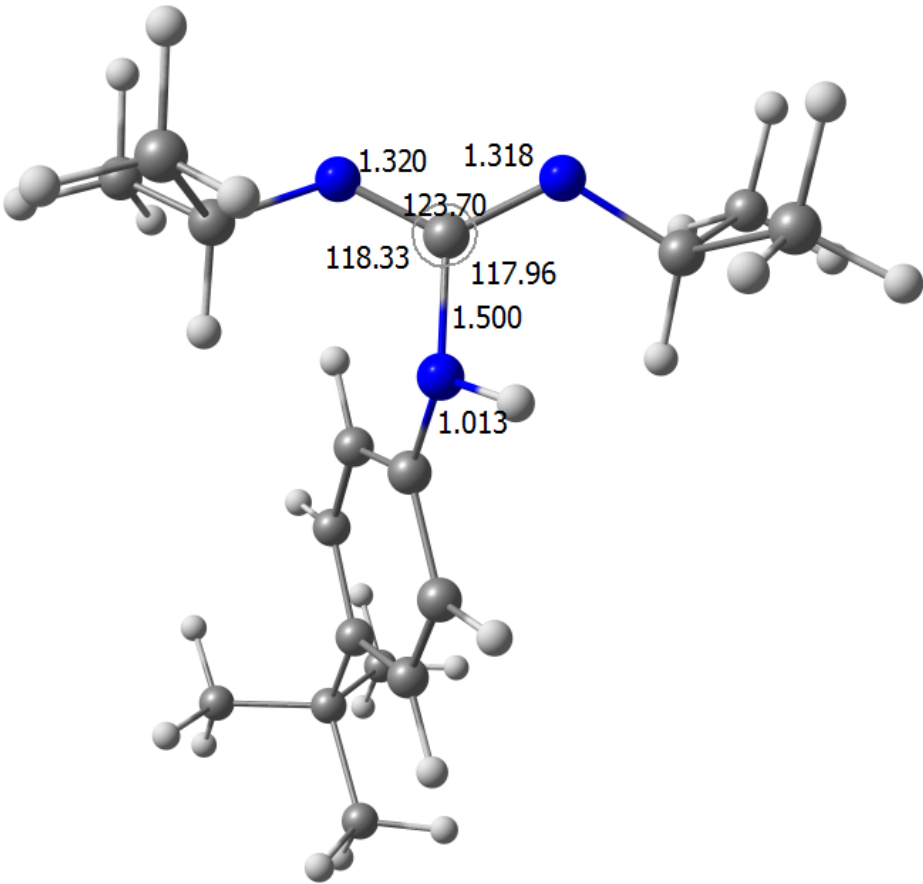
(3b)
E(gas)= -828.939055043



C	0.181128000	-0.392436000	-0.769513000
C	1.232722000	-0.284595000	-1.737552000
H	0.936593000	-0.234995000	-2.783459000
C	2.571420000	-0.254874000	-1.386209000
H	3.307769000	-0.172088000	-2.186933000
C	3.008904000	-0.329267000	-0.045126000
C	1.990164000	-0.435958000	0.916852000
H	2.247909000	-0.503371000	1.972291000
C	0.637648000	-0.465888000	0.586072000
H	-0.100431000	-0.553665000	1.378430000
C	4.507497000	-0.294772000	0.291036000
C	5.235527000	-1.475527000	-0.397891000
H	6.315691000	-1.455663000	-0.188984000
H	5.102983000	-1.445804000	-1.484793000
H	4.834678000	-2.432670000	-0.044057000
C	4.771527000	-0.401253000	1.805511000
H	5.851360000	-0.375346000	2.004724000
H	4.376914000	-1.337360000	2.217325000
H	4.309762000	0.428121000	2.353790000
C	5.134135000	1.032059000	-0.204896000
H	6.213560000	1.068559000	0.005777000
H	4.659477000	1.888897000	0.287848000
H	4.998212000	1.156965000	-1.284697000
C	-2.179637000	-0.340416000	-0.400992000
C	-1.624768000	2.072848000	0.079522000
H	-0.559194000	1.887206000	-0.077791000
C	-2.209825000	2.649368000	-1.221081000
H	-2.088259000	1.917151000	-2.024478000

H	-1.698589000	3.578132000	-1.510880000
H	-3.280160000	2.872808000	-1.104433000
C	-1.765178000	3.053284000	1.249909000
H	-1.312361000	2.637193000	2.156459000
H	-2.823185000	3.266132000	1.464204000
H	-1.277334000	4.009101000	1.022125000
C	-4.402421000	-0.988821000	0.238856000
H	-4.718091000	0.080022000	0.279358000
C	-4.311516000	-1.492360000	1.696414000
H	-3.541887000	-0.941917000	2.249175000
H	-4.025145000	-2.551198000	1.696990000
H	-5.267133000	-1.387881000	2.231597000
C	-5.521398000	-1.732225000	-0.510914000
H	-5.596211000	-1.359797000	-1.538612000
H	-6.497726000	-1.611221000	-0.019211000
H	-5.283475000	-2.801528000	-0.564099000
N	-1.092653000	-0.469550000	-1.206296000
N	-3.165260000	-1.197253000	-0.475236000
N	-2.235586000	0.797420000	0.468314000
H	-3.166813000	0.944881000	0.844869000

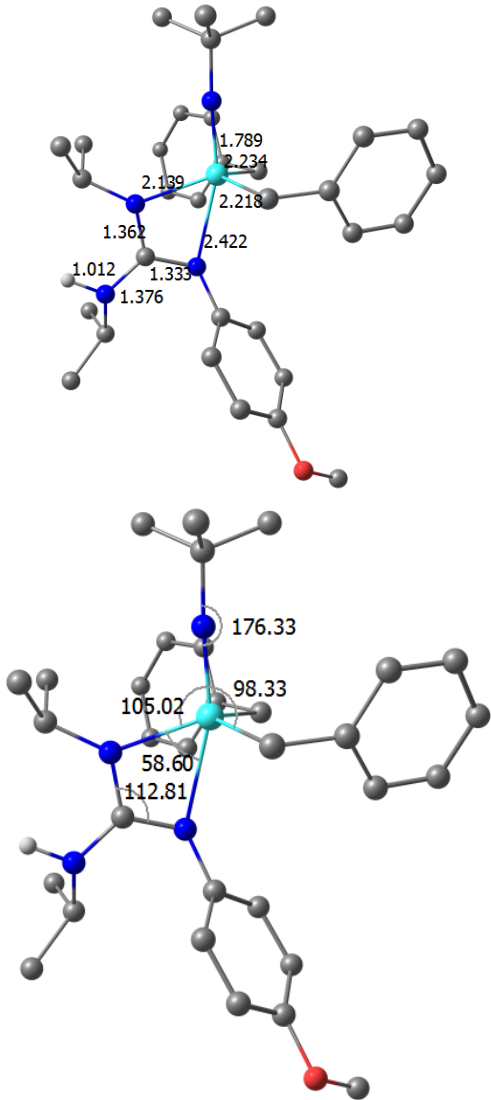
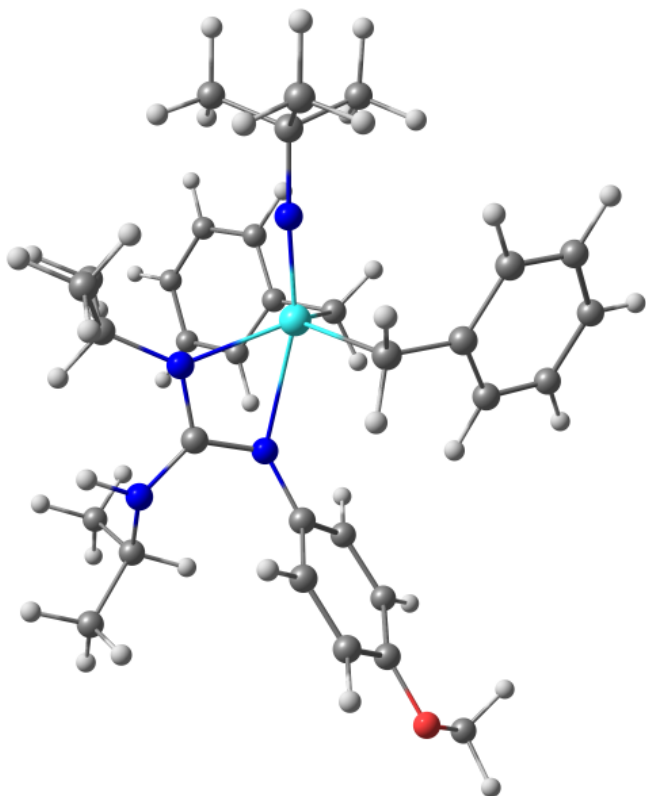
(3'b)
E(gas)= -828.922596635



C	-2.491669000	0.169000000	0.193806000
C	-2.948646000	-2.199909000	0.266081000
H	-1.893593000	-2.360551000	-0.034411000
C	-3.834988000	-2.737500000	-0.882227000
H	-3.641905000	-2.192041000	-1.816071000
H	-4.891429000	-2.580935000	-0.630394000
H	-3.672624000	-3.809373000	-1.074081000
C	-3.175677000	-3.049414000	1.532812000
H	-2.525981000	-2.694428000	2.340480000
H	-2.970929000	-4.117362000	1.360748000
H	-4.213621000	-2.940302000	1.871730000
N	-2.595115000	1.395023000	0.671495000
N	-3.271382000	-0.827662000	0.562269000
N	-1.440065000	-0.105719000	-0.840017000
H	-1.734078000	-0.778080000	-1.538249000
H	-0.177371000	0.910619000	1.286907000
C	0.487609000	0.443325000	0.567635000
C	-0.085467000	-0.145459000	-0.584643000
C	0.803405000	-0.767953000	-1.488674000
H	0.401566000	-1.240553000	-2.384265000
H	2.802914000	-1.281814000	-2.003312000
C	2.178225000	-0.787350000	-1.264298000
C	1.860566000	0.408413000	0.772629000

C	2.755651000	-0.199003000	-0.129340000
H	2.245193000	0.876274000	1.677688000
C	4.268312000	-0.192569000	0.148454000
C	4.782729000	1.265845000	0.216808000
H	5.860728000	1.294193000	0.430643000
H	4.269718000	1.834961000	0.999213000
H	4.608811000	1.782631000	-0.734346000
C	5.067435000	-0.924917000	-0.946684000
H	6.139302000	-0.895985000	-0.712340000
H	4.928289000	-0.458352000	-1.928840000
H	4.771602000	-1.977463000	-1.027185000
C	4.561202000	-0.892910000	1.497263000
H	5.638028000	-0.886560000	1.717926000
H	4.222441000	-1.935232000	1.473230000
H	4.046278000	-0.397785000	2.327150000
C	-2.074925000	2.519742000	-0.072481000
H	-1.095535000	2.331598000	-0.551998000
C	-1.877318000	3.692321000	0.903732000
H	-1.155964000	3.422171000	1.684404000
H	-2.827139000	3.926435000	1.401211000
H	-1.514095000	4.596484000	0.393063000
C	-3.042636000	2.937987000	-1.202824000
H	-3.146684000	2.123806000	-1.929377000
H	-2.694404000	3.834794000	-1.739802000
H	-4.036426000	3.143462000	-0.784258000

(1c)
E(gas) = -1597.10861888

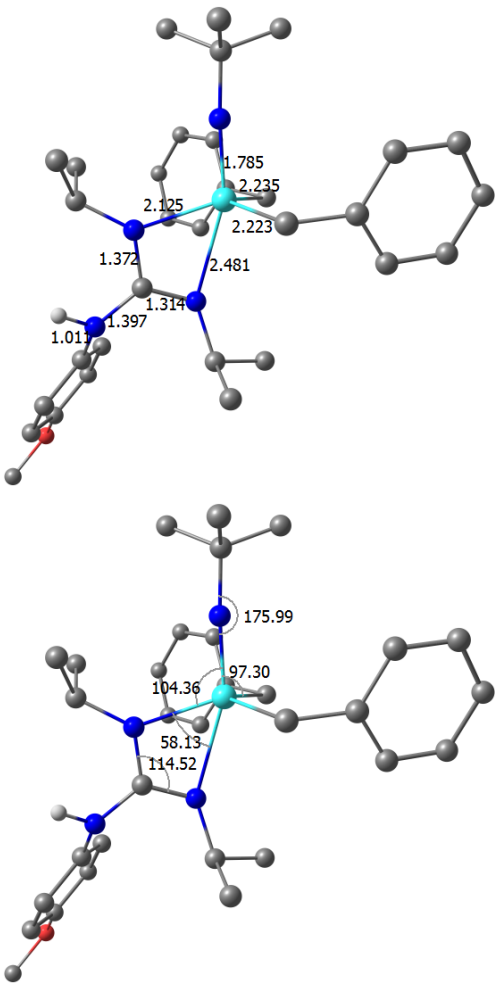
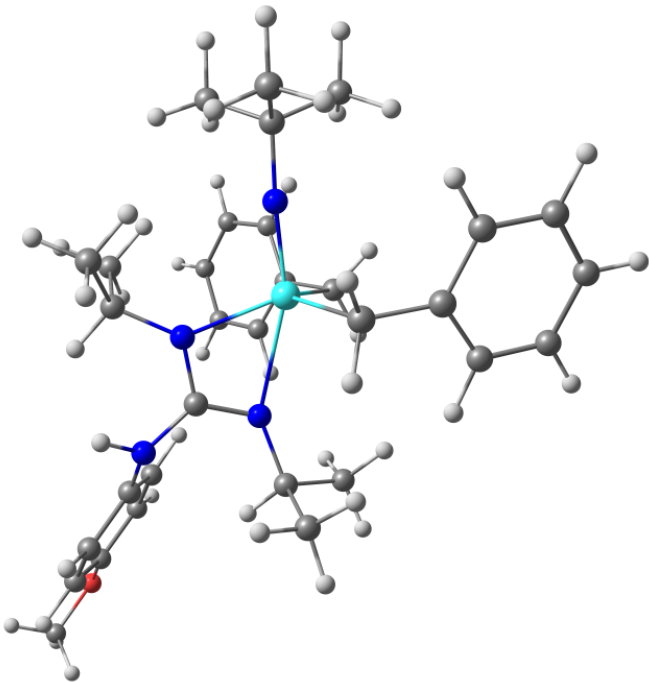


Nb	1.001573000	0.360988000	-0.408403000
O	-6.425640000	1.382980000	-0.103094000
N	2.734894000	0.629523000	-0.762159000
N	0.574667000	-1.589016000	-1.176259000
N	-1.193796000	-0.634165000	-0.175171000
N	-1.551325000	-2.679453000	-1.382923000
H	-1.067890000	-3.332751000	-1.986749000
C	4.125257000	0.936983000	-1.030261000
C	5.002379000	-0.317531000	-0.835333000
H	4.881370000	-0.719146000	0.175889000
H	6.060065000	-0.068224000	-0.984320000
H	4.734558000	-1.100731000	-1.551421000
C	4.257886000	1.447246000	-2.481579000
H	3.920059000	0.685337000	-3.192390000
H	5.301719000	1.694153000	-2.711049000
H	3.650115000	2.345467000	-2.633020000
C	4.581151000	2.035772000	-0.044075000
H	3.947960000	2.923403000	-0.133521000

H	5.620678000	2.324071000	-0.243109000
H	4.515313000	1.676797000	0.988230000
C	-0.758527000	-1.661307000	-0.905075000
C	1.380677000	-2.712329000	-1.667264000
H	0.721377000	-3.570316000	-1.861904000
C	2.059784000	-2.349230000	-2.994563000
H	1.314580000	-2.084878000	-3.753400000
H	2.654617000	-3.190357000	-3.369916000
H	2.722154000	-1.488623000	-2.859761000
C	2.385312000	-3.175302000	-0.602360000
H	3.078877000	-2.369844000	-0.348545000
H	2.966369000	-4.030371000	-0.969294000
H	1.869323000	-3.472882000	0.315841000
C	-2.631478000	-3.316046000	-0.602185000
H	-3.129953000	-2.523995000	-0.041932000
C	-2.065540000	-4.344151000	0.388843000
H	-1.561613000	-5.164517000	-0.138807000
H	-2.869380000	-4.780041000	0.993680000
H	-1.341858000	-3.877152000	1.065394000
C	-3.640319000	-3.938354000	-1.570991000
H	-4.064059000	-3.176496000	-2.232101000
H	-4.458364000	-4.413505000	-1.019358000
H	-3.166499000	-4.710901000	-2.191616000
C	0.162035000	1.985143000	-1.663564000
H	0.748297000	2.181294000	-2.564253000
H	-0.855499000	1.678588000	-1.935333000
C	0.166215000	3.127498000	-0.705957000
C	1.233556000	4.051210000	-0.671836000
H	2.034934000	3.953374000	-1.400058000
C	1.266211000	5.087866000	0.257070000
H	2.095681000	5.790917000	0.250239000
C	0.235204000	5.231377000	1.191313000
H	0.260482000	6.040338000	1.916412000
C	-0.831750000	4.331636000	1.173300000
H	-1.646635000	4.439025000	1.885075000
C	-0.868409000	3.296109000	0.238460000
H	-1.714828000	2.614158000	0.226060000
C	-2.528674000	-0.183562000	-0.158416000
C	-3.320500000	-0.064771000	-1.322207000
H	-2.915666000	-0.387980000	-2.276479000
C	-4.607584000	0.454236000	-1.265690000
H	-5.212307000	0.546094000	-2.163097000
C	-5.150774000	0.887920000	-0.046953000
C	-4.377299000	0.792711000	1.114400000
H	-4.763109000	1.122803000	2.072543000
C	-3.084823000	0.261910000	1.049588000
H	-2.489092000	0.190945000	1.955223000
C	-7.009406000	1.853854000	1.098016000
H	-7.097038000	1.055231000	1.847669000
H	-8.007742000	2.205939000	0.830562000
H	-6.436010000	2.686249000	1.528727000

C	1.080927000	0.669117000	1.803069000
H	1.732353000	1.518567000	2.031076000
H	0.051742000	0.922436000	2.086085000
C	1.538240000	-0.590269000	2.453030000
C	2.900137000	-0.819662000	2.737148000
H	3.622063000	-0.039617000	2.507272000
C	3.332740000	-2.012011000	3.314892000
H	4.389624000	-2.152869000	3.529503000
C	2.416345000	-3.020295000	3.627274000
H	2.752355000	-3.948021000	4.082740000
C	1.060727000	-2.811851000	3.360124000
H	0.332775000	-3.579463000	3.613971000
C	0.629492000	-1.617111000	2.782585000
H	-0.427484000	-1.465897000	2.579267000

(1'c)
E(gas) = -1597.09678503

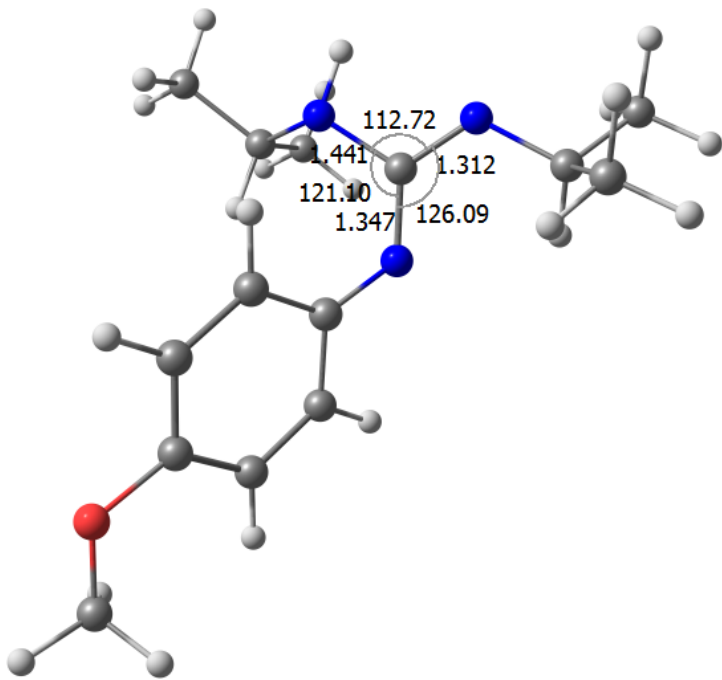


Nb	1.408706000	0.084851000	-0.382639000
O	-7.501043000	0.217963000	0.853590000
N	2.695901000	-1.094979000	-0.755388000
N	-0.292330000	-0.643360000	-1.427935000
N	-2.493546000	0.277059000	-1.651187000
N	-0.830867000	1.121654000	-0.123949000
H	-2.505322000	-0.155941000	-2.564503000
C	3.805539000	-1.993959000	-1.006702000
C	3.329598000	-3.461791000	-0.987888000
H	2.845945000	-3.700372000	-0.035449000
H	4.183203000	-4.137341000	-1.122118000
H	2.615141000	-3.654800000	-1.794009000
C	4.417616000	-1.663814000	-2.385825000
H	3.674196000	-1.785262000	-3.180764000
H	5.262892000	-2.328856000	-2.600858000
H	4.777923000	-0.630293000	-2.413458000
C	4.866930000	-1.785771000	0.097084000
H	5.192306000	-0.741780000	0.130980000
H	5.741936000	-2.420497000	-0.089201000
H	4.459054000	-2.044335000	1.079442000
C	-1.241372000	0.264110000	-1.031593000

C	-0.627638000	-1.909511000	-2.095597000
H	-1.673867000	-1.864635000	-2.426497000
C	0.238727000	-2.106706000	-3.345441000
H	0.093978000	-1.282823000	-4.053857000
H	-0.016754000	-3.046109000	-3.849800000
H	1.298434000	-2.135123000	-3.076344000
C	-0.532517000	-3.093632000	-1.121644000
H	0.484283000	-3.196941000	-0.734047000
H	-0.809821000	-4.028751000	-1.623862000
H	-1.203031000	-2.947739000	-0.268485000
C	-1.571424000	2.356215000	0.166674000
H	-2.648612000	2.154824000	0.178469000
C	-1.325282000	3.434872000	-0.903063000
H	-0.275131000	3.746824000	-0.918939000
H	-1.937349000	4.322193000	-0.699762000
H	-1.587519000	3.063251000	-1.899269000
C	-1.196980000	2.861278000	1.564002000
H	-1.455869000	2.123613000	2.330725000
H	-1.731804000	3.790519000	1.792342000
H	-0.122077000	3.058151000	1.638985000
C	2.316449000	1.841561000	-1.399142000
H	2.843571000	1.542451000	-2.308860000
H	1.481685000	2.502673000	-1.662234000
C	3.225912000	2.461919000	-0.390871000
C	4.591709000	2.113690000	-0.325304000
H	4.990977000	1.418448000	-1.059289000
C	5.434052000	2.653860000	0.643532000
H	6.484096000	2.371918000	0.660366000
C	4.938084000	3.559220000	1.586772000
H	5.594706000	3.979906000	2.343368000
C	3.592722000	3.926875000	1.534650000
H	3.195233000	4.642687000	2.250041000
C	2.752022000	3.388901000	0.559535000
H	1.713898000	3.707136000	0.516193000
C	-3.757371000	0.291362000	-1.001254000
C	-3.915957000	-0.089478000	0.341585000
H	-3.048699000	-0.388750000	0.921995000
C	-5.175428000	-0.088482000	0.926641000
H	-5.305612000	-0.377284000	1.964926000
C	-6.311369000	0.264463000	0.183242000
C	-6.162236000	0.628713000	-1.159416000
H	-7.018092000	0.907855000	-1.763204000
C	-4.889885000	0.651500000	-1.736202000
H	-4.779318000	0.958256000	-2.773435000
C	-8.679814000	0.564890000	0.147691000
H	-8.646520000	1.602535000	-0.211440000
H	-9.499667000	0.457599000	0.860386000
H	-8.852712000	-0.104863000	-0.705784000
C	1.558534000	-0.025513000	1.844241000
H	2.618258000	-0.049430000	2.119038000
H	1.114245000	0.907948000	2.210479000

C	0.819179000	-1.219491000	2.342437000
C	1.456478000	-2.468698000	2.490305000
H	2.518480000	-2.544332000	2.271215000
C	0.760866000	-3.596584000	2.921818000
H	1.286605000	-4.542234000	3.032492000
C	-0.602252000	-3.515984000	3.220393000
H	-1.145124000	-4.393853000	3.560255000
C	-1.251883000	-2.286018000	3.092834000
H	-2.307532000	-2.201341000	3.341474000
C	-0.552460000	-1.157412000	2.663018000
H	-1.066622000	-0.203829000	2.581887000

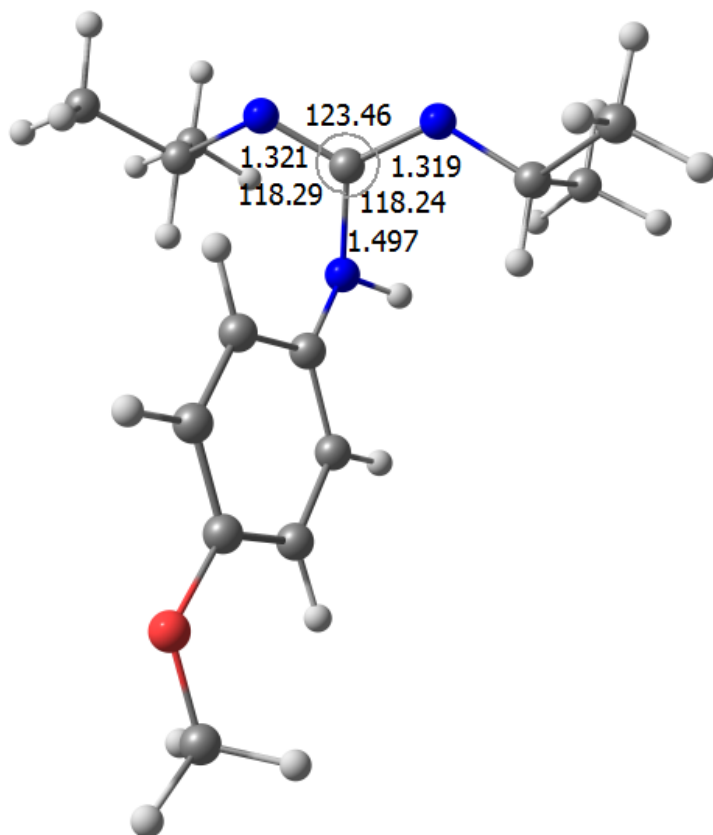
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N	-1.552801000	1.408922000	-0.704959000
H	-2.474709000	1.713352000	-1.016053000
C	-1.755650000	0.096164000	-0.147411000
C	-3.258711000	-1.693017000	0.132273000
H	-2.654152000	-1.957570000	1.015814000
C	-4.745773000	-1.805422000	0.501500000
H	-4.992570000	-1.104247000	1.307985000
H	-5.010010000	-2.821273000	0.830410000
H	-5.373773000	-1.547458000	-0.362055000
C	-2.895423000	-2.697319000	-0.978434000
H	-3.442602000	-2.458770000	-1.900830000
H	-3.135201000	-3.733162000	-0.692675000
H	-1.822900000	-2.638406000	-1.189141000
C	-0.927125000	2.431894000	0.140764000
H	0.075700000	2.071515000	0.389687000
C	-1.685212000	2.684050000	1.457126000
H	-2.698861000	3.060133000	1.260047000
H	-1.164418000	3.421853000	2.083930000
H	-1.770550000	1.749794000	2.020243000
C	-0.777843000	3.718566000	-0.679075000
H	-0.207610000	3.524234000	-1.593687000
H	-0.264237000	4.499482000	-0.103699000
H	-1.762087000	4.113884000	-0.970313000
C	0.565842000	-0.432306000	0.215803000
C	1.148405000	0.010523000	-1.015233000
H	0.488377000	0.357876000	-1.803510000

C	2.523084000	0.010816000	-1.223119000
H	2.937421000	0.349512000	-2.171351000
C	3.408215000	-0.426032000	-0.231289000
C	2.881192000	-0.870344000	0.986173000
H	3.532215000	-1.221153000	1.782827000
C	1.502052000	-0.870584000	1.194874000
H	1.098406000	-1.227489000	2.139606000
C	5.663004000	-0.825639000	0.434188000
H	5.601975000	-0.226456000	1.357627000
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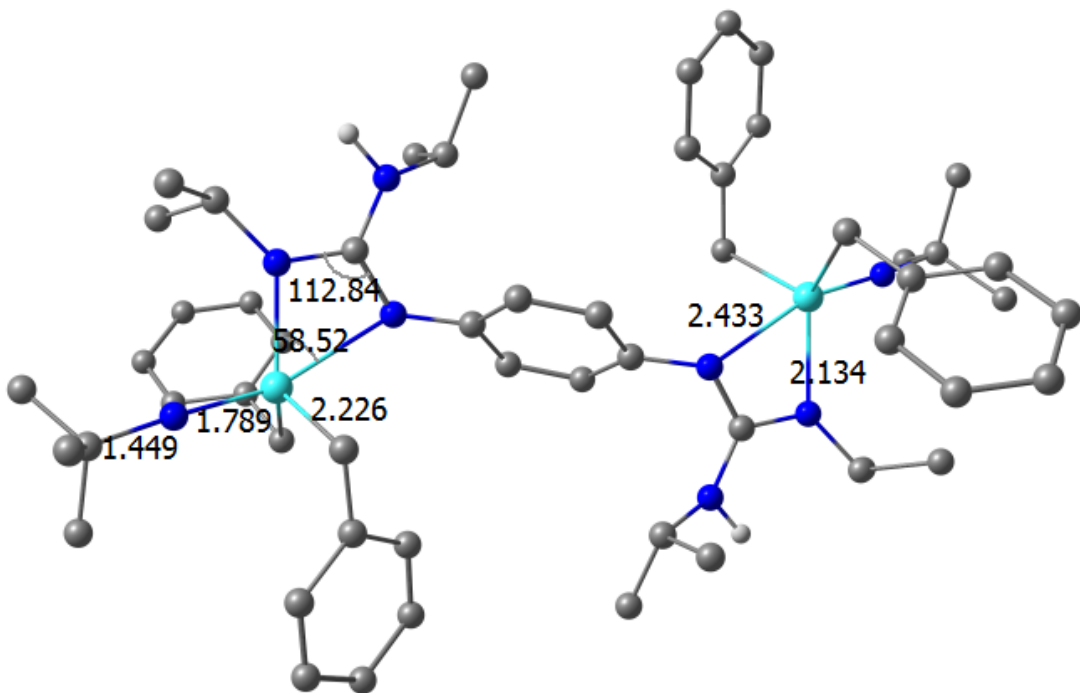
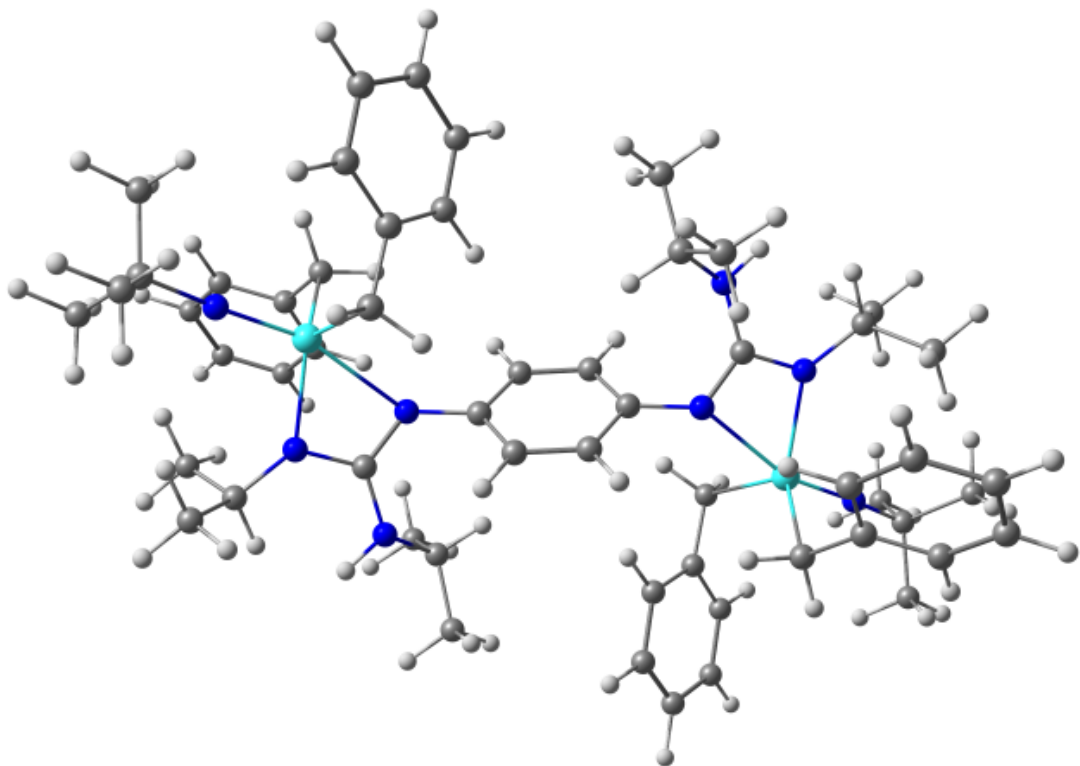
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N	-0.800807000	-0.116469000	0.813314000
N	-2.092660000	1.363832000	-0.601043000
H	-1.020648000	-0.834900000	1.492736000
C	-1.923130000	0.135874000	-0.144768000
C	-2.321709000	-2.243431000	-0.224722000
H	-1.246054000	-2.379705000	0.008593000
C	-3.121792000	-2.824741000	0.965062000
H	-2.889310000	-2.287576000	1.894658000
H	-2.917660000	-3.894221000	1.129078000
H	-4.195389000	-2.695809000	0.778490000
C	-2.601603000	-3.079243000	-1.490232000
H	-3.660883000	-2.994250000	-1.763702000
H	-2.357559000	-4.143679000	-1.349850000
H	-2.012312000	-2.693055000	-2.329287000
C	-1.561240000	2.495160000	0.125028000
H	-0.547291000	2.333530000	0.538314000
C	-2.466198000	2.867120000	1.321353000
H	-3.491100000	3.045393000	0.970834000
H	-2.112456000	3.767795000	1.848346000
H	-2.495984000	2.040055000	2.039984000
C	-1.463838000	3.685972000	-0.844525000
H	-0.784623000	3.450712000	-1.672929000

H	-1.098929000	4.595465000	-0.344482000
H	-2.450161000	3.894286000	-1.278547000
C	0.537589000	-0.114694000	0.451096000
C	1.000035000	0.515695000	-0.729741000
H	0.265065000	0.976718000	-1.381712000
C	2.351010000	0.527875000	-1.049483000
H	2.695900000	1.012059000	-1.959786000
C	3.300023000	-0.079983000	-0.217911000
C	2.866100000	-0.714561000	0.947588000
H	3.567640000	-1.204939000	1.615579000
C	1.505570000	-0.730465000	1.269571000
H	1.185646000	-1.232034000	2.181785000
C	5.589935000	-0.612219000	0.179845000
H	5.619824000	-0.173930000	1.189994000
H	6.555736000	-0.446311000	-0.307067000
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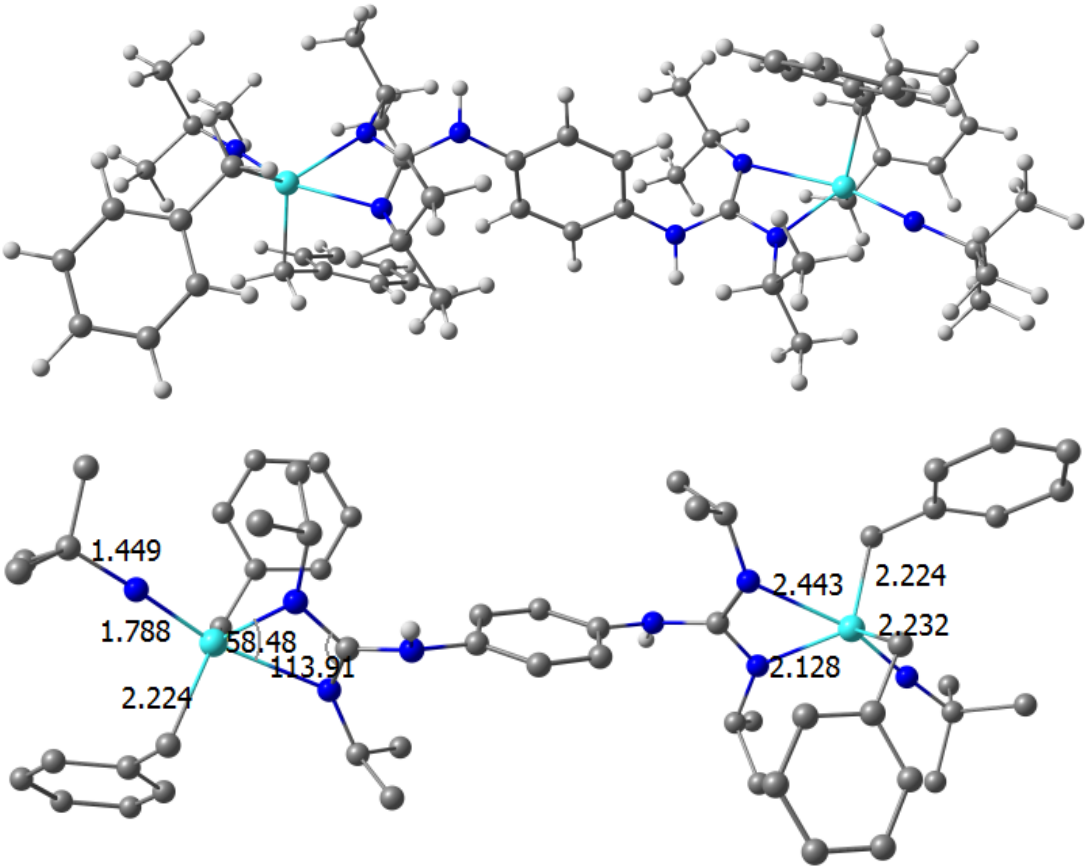
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N	-4.516686000	1.682849000	1.125924000
N	-2.697887000	0.870996000	0.084537000
N	-2.473003000	2.902162000	1.354085000
H	-3.004666000	3.513462000	1.960375000
C	-7.760706000	-1.201600000	1.358432000

C	-8.789342000	-0.053172000	1.295245000
H	-8.517920000	0.757517000	1.978697000
H	-9.783259000	-0.419240000	1.579981000
H	-8.849709000	0.356012000	0.281539000
C	-7.647090000	-1.719777000	2.808309000
H	-6.928743000	-2.543770000	2.869552000
H	-8.618459000	-2.082187000	3.166427000
H	-7.308726000	-0.922826000	3.479366000
C	-8.217492000	-2.345847000	0.425736000
H	-8.322530000	-1.983552000	-0.602229000
H	-9.186418000	-2.743404000	0.752047000
H	-7.486608000	-3.159787000	0.424348000
C	-3.192349000	1.846291000	0.850855000
C	-5.382189000	2.739844000	1.662229000
H	-4.804391000	3.673511000	1.722401000
C	-5.854321000	2.389243000	3.080476000
H	-6.419535000	1.451842000	3.068490000
H	-6.499130000	3.178684000	3.484469000
H	-5.001621000	2.258812000	3.756898000
C	-6.551576000	3.027332000	0.710821000
H	-6.185018000	3.318034000	-0.278269000
H	-7.172366000	3.840227000	1.107032000
H	-7.180561000	2.142879000	0.587648000
C	-1.394343000	3.605416000	0.628416000
H	-0.671877000	2.853488000	0.305827000
C	-3.708799000	-1.899717000	1.456659000
H	-2.680481000	-1.537938000	1.573862000
H	-4.136977000	-2.130744000	2.435210000
C	-3.795418000	-3.043261000	0.505422000
C	-2.979358000	-3.099921000	-0.644224000
H	-2.230122000	-2.326987000	-0.801206000
C	-3.110818000	-4.132438000	-1.575407000
H	-2.473274000	-4.144271000	-2.455845000
C	-4.050569000	-5.145753000	-1.380607000
H	-4.149592000	-5.951167000	-2.103272000
C	-4.858322000	-5.116880000	-0.238819000
H	-5.584425000	-5.907729000	-0.066533000
C	-4.736390000	-4.080582000	0.682961000
H	-5.366292000	-4.070377000	1.569097000
C	-1.344303000	0.485316000	0.065251000
C	-0.544980000	0.381133000	1.221979000
H	-0.959737000	0.671858000	2.182988000
C	-0.766442000	0.086767000	-1.154343000
H	-1.362639000	0.162934000	-2.060021000
C	-5.091605000	-0.531399000	-1.820224000
H	-4.072431000	-0.649551000	-2.210914000
H	-5.653527000	-1.450840000	-2.012972000
C	-5.757895000	0.672485000	-2.391535000
C	-7.158099000	0.740971000	-2.535512000
H	-7.757897000	-0.120314000	-2.250584000
C	-7.781219000	1.879107000	-3.044299000

H	-8.863404000	1.897216000	-3.150996000
C	-7.023239000	2.990056000	-3.425920000
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C	-5.632823000	2.941064000	-3.296448000
H	-5.027828000	3.791975000	-3.601423000
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H	-3.928149000	1.769886000	-2.693965000
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N	2.697679000	-0.870546000	-0.085352000
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H	3.004023000	-3.512718000	-1.961737000
C	3.192012000	-1.845826000	-0.851788000
C	5.382031000	-2.739628000	-1.662615000
H	4.803718000	-3.672843000	-1.724668000
C	5.856688000	-2.388092000	-3.079777000
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H	6.501394000	-3.177763000	-3.483482000
H	5.005142000	-2.256270000	-3.757377000
C	6.549669000	-3.028709000	-0.709507000
H	6.181282000	-3.320656000	0.278539000
H	7.171028000	-3.841189000	-1.105681000
H	7.178579000	-2.144534000	-0.583938000
C	1.393213000	-3.604450000	-0.630190000
H	0.669372000	-2.852664000	-0.310331000
C	1.925576000	-4.340068000	0.607377000
H	1.102299000	-4.813615000	1.154531000
H	2.639775000	-5.122877000	0.321819000
H	2.431225000	-3.644867000	1.285342000
C	0.703781000	-4.552858000	-1.613184000
H	0.332624000	-4.006868000	-2.486830000
H	1.395291000	-5.332467000	-1.961875000
H	-0.144501000	-5.048733000	-1.132447000
C	1.344198000	-0.484536000	-0.066148000
C	0.544916000	-0.380232000	-1.222890000
H	0.959669000	-0.670946000	-2.183907000
C	0.766366000	-0.085882000	1.153433000
H	1.362559000	-0.162060000	2.059112000
Nb	4.813027000	0.294709000	-0.379870000
N	6.461291000	0.740982000	-0.912069000
C	7.762220000	1.199720000	-1.356208000
C	8.790344000	0.050990000	-1.290203000
H	8.519655000	-0.760362000	-1.973155000
H	9.784808000	0.416395000	-1.573883000
H	8.849047000	-0.357103000	-0.275960000
C	7.650857000	1.716255000	-2.806849000
H	6.932714000	2.540276000	-2.870086000
H	8.622815000	2.078124000	-3.163911000
H	7.313405000	0.918599000	-3.477528000
C	8.218082000	2.344897000	-0.424202000
H	8.321557000	1.983767000	0.604332000
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H	7.487470000	3.159081000	-0.424781000
C	3.710013000	1.900038000	-1.457304000
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H	4.138349000	2.130416000	-2.435946000
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H	2.231290000	2.328932000	0.800187000
C	3.112551000	4.134456000	1.573593000
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C	4.052651000	5.147365000	1.378359000
H	4.151877000	5.953109000	2.100628000
C	4.860464000	5.117675000	0.236637000
H	5.586827000	5.908211000	0.064006000
C	4.738263000	4.080960000	-0.684644000
H	5.368226000	4.070110000	-1.570733000
C	5.090740000	0.531385000	1.820233000
H	4.071459000	0.650249000	2.210432000
H	5.653175000	1.450475000	2.013152000
C	5.756000000	-0.672855000	2.392009000
C	7.156051000	-0.742002000	2.537166000
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C	7.778218000	-1.880475000	3.046370000
H	8.860305000	-1.899097000	3.153965000
C	7.019398000	-2.991086000	3.427298000
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C	5.629110000	-2.941419000	3.296704000
H	5.023463000	-3.792055000	3.601151000
C	5.008476000	-1.800352000	2.787560000
H	3.925492000	-1.769391000	2.692876000
C	-1.928475000	4.343660000	-0.606839000
H	-1.105911000	4.817808000	-1.154547000
H	-2.641754000	5.126347000	-0.318649000
H	-2.435693000	3.649998000	-1.285227000
C	-0.702134000	4.551432000	1.611754000
H	0.145307000	5.047871000	1.130110000
H	-0.329328000	4.003418000	2.483414000
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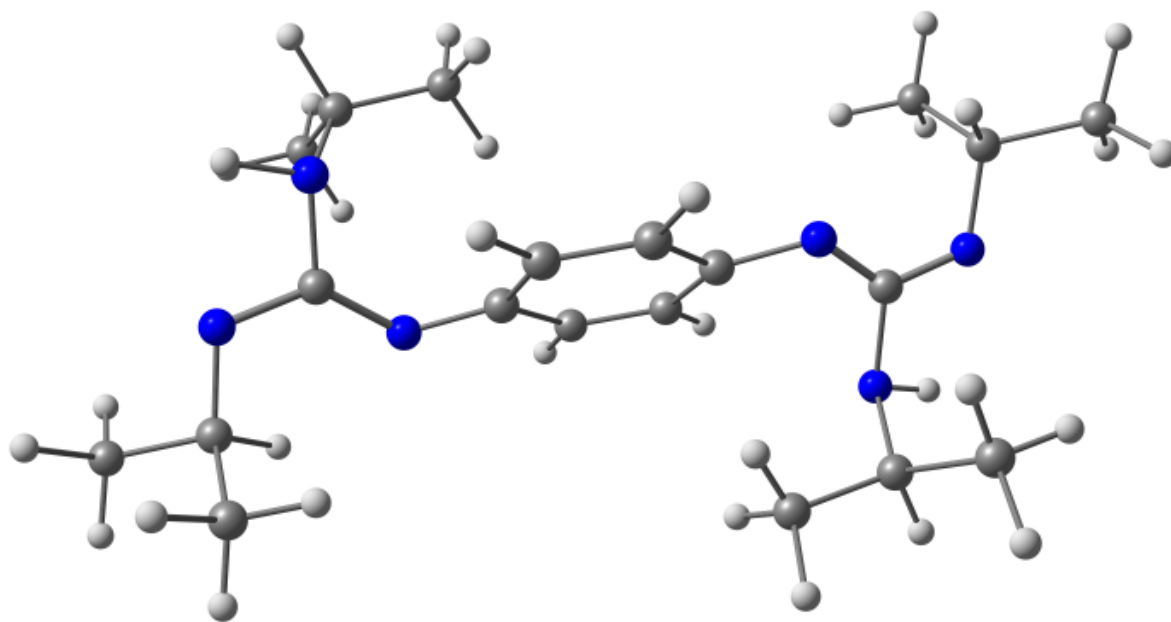
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N	2.459708000	-0.208858000	-1.383886000
N	4.209041000	-1.080663000	0.050597000
H	2.421878000	0.193991000	-2.311373000
C	8.880488000	1.739458000	-1.331291000
C	8.519315000	3.239520000	-1.340596000
H	7.722588000	3.449389000	-2.061082000
H	9.394941000	3.838837000	-1.618108000
H	8.181184000	3.560576000	-0.350136000
C	9.292324000	1.293103000	-2.750813000
H	9.558183000	0.231106000	-2.760098000
H	10.158000000	1.868721000	-3.100492000
H	8.469888000	1.444403000	-3.458332000
C	10.045963000	1.500206000	-0.345393000
H	9.776030000	1.842538000	0.659264000
H	10.939805000	2.048587000	-0.667021000
H	10.289558000	0.435421000	-0.285872000
C	3.741165000	-0.211591000	-0.818071000
C	4.300821000	1.987200000	-1.862996000
H	3.211614000	2.002725000	-2.003337000
C	4.956219000	2.112819000	-3.244902000
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H	4.681221000	3.060952000	-3.721747000
H	4.646993000	1.292473000	-3.903457000
C	4.642090000	3.173514000	-0.950117000
H	4.133659000	3.081623000	0.014699000
H	4.332772000	4.116407000	-1.417696000
H	5.717110000	3.220706000	-0.758448000
C	3.685382000	-2.419007000	0.357178000
H	4.590743000	-3.021274000	0.516084000
C	7.091550000	-2.004385000	-1.269679000
H	6.198281000	-2.639795000	-1.327633000
H	7.492680000	-1.849646000	-2.274901000
C	8.109268000	-2.559425000	-0.329351000
C	7.730522000	-3.234558000	0.848731000
H	6.674329000	-3.401706000	1.048269000
C	8.680622000	-3.709336000	1.754032000
H	8.354179000	-4.229311000	2.651294000
C	10.041864000	-3.528409000	1.506244000
H	10.783259000	-3.901848000	2.207227000
C	10.440903000	-2.871091000	0.337858000
H	11.498533000	-2.736747000	0.124160000
C	9.490973000	-2.392270000	-0.560783000
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C	1.177513000	0.387573000	0.640882000
H	2.085349000	0.711448000	1.139866000
C	0.050747000	-0.505733000	-1.296174000
H	0.089977000	-0.916587000	-2.301818000
C	6.732503000	0.113887000	1.862658000
H	6.276267000	-0.782283000	2.303705000
H	7.807462000	0.103687000	2.068337000
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C	6.763557000	2.586300000	2.394360000
H	7.810454000	2.610281000	2.101147000
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H	6.701268000	4.686884000	2.849200000
C	4.795389000	3.741364000	3.207871000
H	4.308129000	4.653227000	3.542356000
C	4.094068000	2.533347000	3.177138000
H	3.054639000	2.501217000	3.496697000
C	4.722750000	1.361530000	2.754319000
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C	-4.302278000	-1.990180000	1.860842000
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C	-4.954139000	-2.111749000	3.244817000
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H	-5.725406000	-3.220217000	0.761455000
C	-3.680831000	2.413735000	-0.362369000
H	-4.585435000	3.017155000	-0.521295000
C	-2.918603000	2.449927000	-1.698095000
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H	-1.963736000	1.920747000	-1.633226000
H	-3.514305000	1.990158000	-2.493986000
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C	-1.239179000	0.113119000	0.659636000
C	-1.175574000	-0.394790000	-0.644947000
H	-2.083442000	-0.718599000	-1.143923000
C	-0.048794000	0.498482000	1.292104000
H	-0.088027000	0.909384000	2.297728000
Nb	-6.412908000	0.104072000	0.335013000
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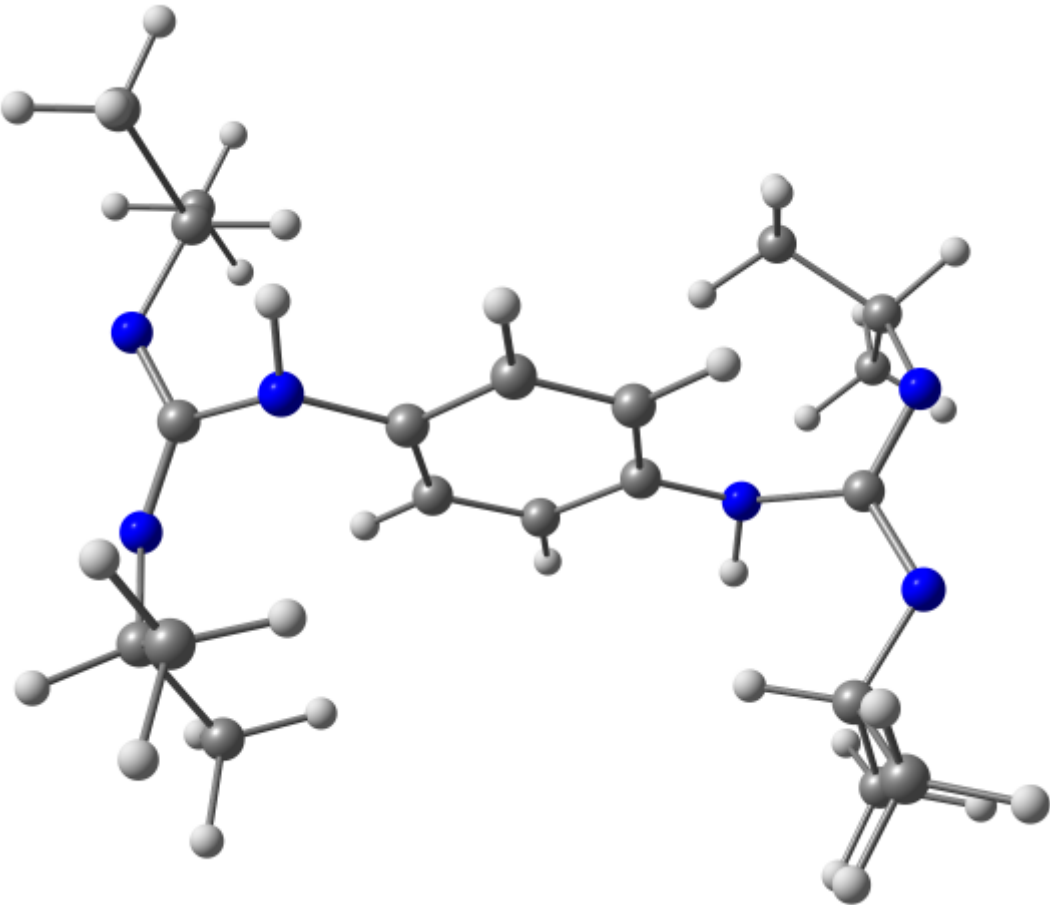
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C	5.294151000	-1.480308000	0.272288000
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C	6.802956000	-1.605400000	0.543386000
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H	7.059308000	-2.554725000	1.039864000
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C	4.797143000	-2.666003000	-0.580912000
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C	-3.507305000	-2.746209000	0.365950000
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C	-2.044573000	-3.134542000	0.114734000
H	-1.990224000	-4.160075000	-0.282117000
H	-1.563870000	-2.458938000	-0.597071000
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H	-1.463589000	-0.132446000	1.992704000
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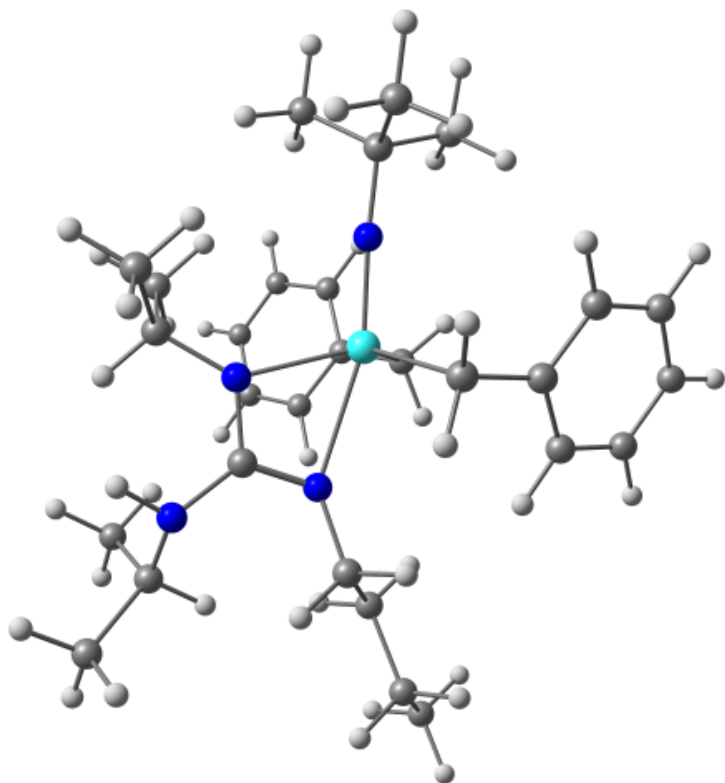


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C	3.868882000	0.323143000	-0.126445000
C	4.321772000	-2.041590000	0.064087000
H	3.243474000	-2.167008000	0.286697000
C	5.101405000	-2.507897000	1.318037000
H	6.178001000	-2.376497000	1.144593000
H	4.910289000	-3.563109000	1.572143000
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H	4.058910000	-2.687565000	-1.994351000
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C	0.399288000	-0.330602000	1.321847000
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N	-2.727587000	-0.341391000	-0.746132000

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C	-3.840996000	-0.343083000	0.255369000
C	-3.875597000	2.072513000	0.179114000
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H	-4.923075000	3.106076000	1.781602000
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C	-2.587349000	-3.379031000	0.262666000
H	-2.590106000	-4.438539000	-0.044461000
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H	-4.523681000	-3.903431000	-1.658111000
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H	1.702793000	2.978525000	-1.282260000
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C	3.093878000	2.995656000	1.136905000
H	3.052266000	4.076893000	1.349935000
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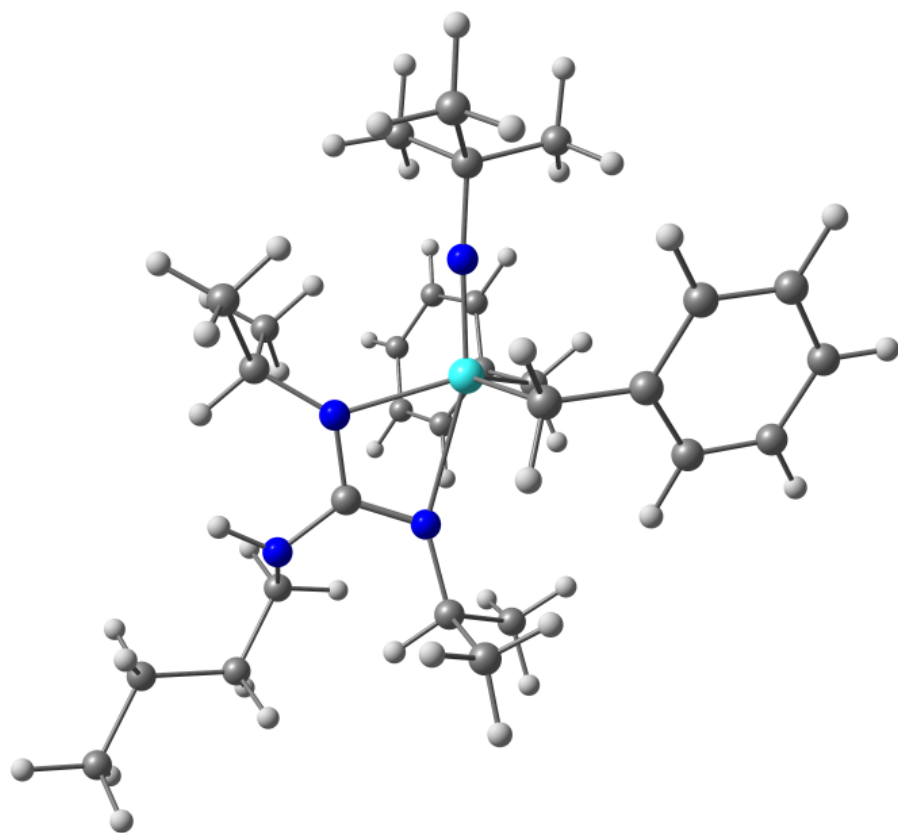
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H	-2.896493000	-1.761896000	-2.324839000
C	-1.785305000	-0.543008000	-1.172623000
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H	-1.768378000	-3.084569000	-1.674187000
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H	-0.341228000	-4.686822000	-0.471439000
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C	-4.431458000	-2.002709000	-0.061783000
H	-4.421508000	-2.975467000	-0.570355000

H	-5.381410000	-1.919615000	0.479501000
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C	3.853618000	3.668229000	0.133522000
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H	0.129476000	1.322102000	1.832929000
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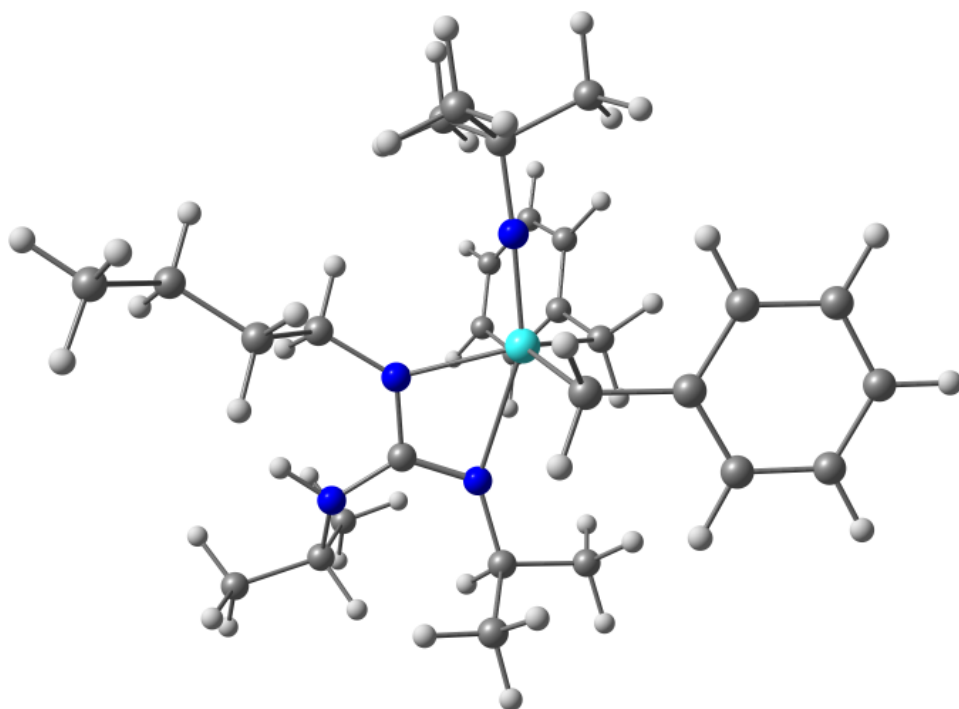
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C	1.529875000	1.747114000	-1.834696000
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H	6.168972000	-0.767558000	1.090401000
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H	0.323569000	3.104478000	-0.633488000
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H	-5.621290000	-3.481573000	1.866171000
C	-3.492088000	-3.483843000	1.506776000
H	-3.255597000	-4.034045000	2.414246000
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H	1.360050000	0.384897000	2.691467000
C	-1.217895000	2.568399000	2.395201000
H	-2.263979000	2.607814000	2.101527000
C	-1.199960000	0.111565000	1.787464000
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C	0.752360000	3.688372000	3.251407000
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H	3.081614000	-2.394524000	0.522806000
C	1.701076000	-2.749876000	2.121908000
H	2.191475000	-3.670421000	2.460174000
H	2.054858000	-1.924372000	2.749657000
H	0.623566000	-2.857689000	2.291572000
C	1.581867000	-3.697262000	-0.222427000
H	1.788888000	-3.506310000	-1.281003000
H	2.139897000	-4.592258000	0.079663000
H	0.514411000	-3.916497000	-0.117383000
C	6.383808000	-0.404790000	-1.030081000

H	6.550019000	0.679337000	-0.943529000
H	5.802197000	-0.560638000	-1.948942000
C	7.733583000	-1.118034000	-1.164755000
H	8.290971000	-0.756449000	-2.036069000
H	8.357499000	-0.954891000	-0.277493000
H	7.598438000	-2.200260000	-1.280471000
H	4.445038000	0.921182000	0.540731000

(4c)

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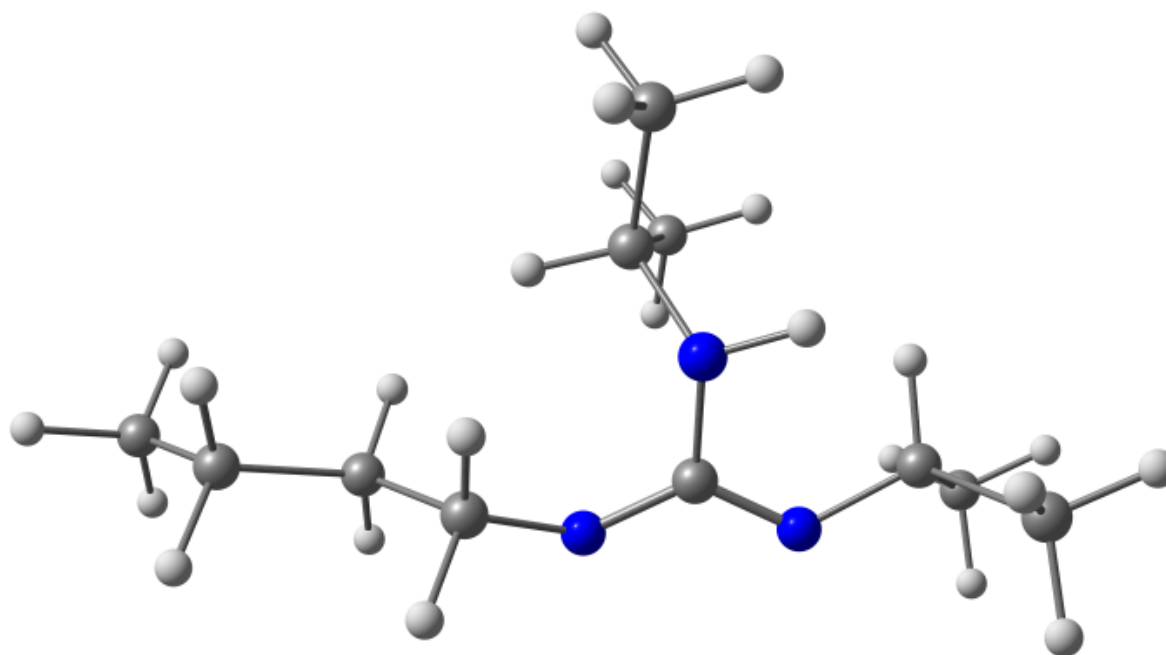
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C	-1.524695000	3.191376000	-0.284447000
N	1.470574000	0.387491000	-0.388524000
N	3.303850000	-1.117141000	-0.428681000
H	3.816939000	-0.266140000	-0.616510000
C	1.951988000	-0.896186000	-0.260777000
C	2.323042000	1.561523000	-0.483157000
H	3.199597000	1.463017000	0.180459000
C	4.146474000	-2.135281000	0.225518000
H	3.808557000	-3.122090000	-0.102552000
C	2.783239000	1.896376000	-1.914579000
H	3.331509000	1.045484000	-2.345399000
H	1.889017000	2.024679000	-2.538858000
N	-1.159433000	1.791003000	-0.314005000
C	-2.762889000	-1.124548000	-1.947103000
C	-3.883087000	-0.292791000	-1.735904000
H	-3.767579000	0.780765000	-1.856932000
C	-1.424426000	-0.548627000	-2.268761000
H	-1.483276000	0.295056000	-2.961288000
H	-0.740819000	-1.306193000	-2.673169000
C	-5.123961000	-0.821415000	-1.385864000
H	-5.968994000	-0.153808000	-1.235814000
C	-2.954212000	-2.513670000	-1.798439000
H	-2.120237000	-3.183830000	-1.991455000
C	-5.287188000	-2.200958000	-1.231146000
H	-6.254679000	-2.612817000	-0.957393000
C	-4.194876000	-3.044249000	-1.445303000

H	-4.310395000	-4.120928000	-1.346858000
C	0.075549000	-0.541021000	3.368921000
H	0.526616000	-1.421420000	2.917562000
C	-1.650188000	1.133862000	3.408010000
H	-2.558761000	1.563690000	2.992198000
C	-1.676151000	-0.578472000	1.545826000
H	-2.733914000	-0.314069000	1.433077000
H	-1.582860000	-1.670904000	1.532570000
C	-1.084847000	0.004002000	2.782964000
C	-1.082273000	1.696100000	4.550127000
H	-1.550565000	2.562241000	5.012326000
C	0.647436000	0.021589000	4.510419000
H	1.540159000	-0.427441000	4.940369000
C	0.075305000	1.146431000	5.108554000
H	0.516673000	1.581380000	6.001362000
C	-3.029469000	3.304899000	0.045711000
H	-3.632644000	2.789397000	-0.708363000
H	-3.337996000	4.357008000	0.073186000
H	-3.244626000	2.855421000	1.020041000
C	-0.707791000	3.928578000	0.798710000
H	-0.848341000	3.457119000	1.775841000
H	-1.020650000	4.977952000	0.865361000
H	0.361483000	3.910696000	0.562755000
C	-1.248969000	3.812292000	-1.671017000
H	-0.186613000	3.731966000	-1.926016000
H	-1.527250000	4.873368000	-1.683119000
H	-1.824877000	3.295532000	-2.446317000
C	1.148235000	-3.221049000	-0.117021000
H	2.012439000	-3.547769000	0.478210000
C	-0.071270000	-3.911217000	0.504439000
H	0.039368000	-5.000702000	0.451301000
H	-0.183251000	-3.631074000	1.556873000
H	-0.993296000	-3.635817000	-0.017668000
C	1.370867000	-3.692090000	-1.566053000
H	2.246210000	-3.207908000	-2.012850000
H	1.521804000	-4.778076000	-1.605671000
H	0.500856000	-3.446864000	-2.186156000
C	3.654306000	3.157800000	-1.980473000
H	4.542803000	3.023676000	-1.346133000
H	3.099628000	4.002766000	-1.548222000
C	4.093724000	3.511558000	-3.405302000
H	4.710360000	4.417434000	-3.420157000
H	3.226666000	3.686815000	-4.053606000
H	4.681477000	2.700272000	-3.852344000
H	1.752826000	2.407483000	-0.091462000
C	4.069520000	-2.061190000	1.756684000
H	4.660003000	-2.865253000	2.211375000
H	4.461030000	-1.102391000	2.117486000
H	3.035817000	-2.155008000	2.103616000
C	5.579682000	-1.947086000	-0.282133000
H	5.978110000	-0.968309000	0.017395000

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H	5.623371000	-2.019550000	-1.373998000

(5)

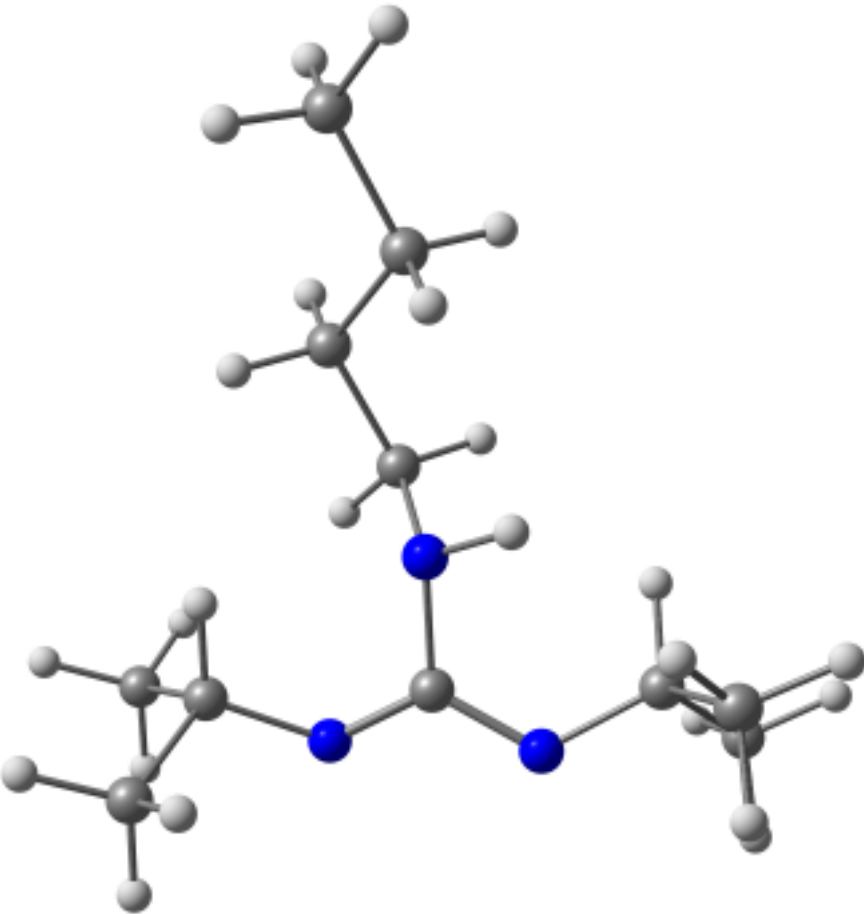
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N	-0.670368000	0.691388000	-0.739843000
H	-1.616255000	1.006822000	-0.937352000
C	-0.703550000	-0.669172000	-0.177703000
C	-3.107025000	-0.520757000	0.112368000
H	-3.015207000	0.576429000	0.293442000
C	0.010744000	1.730442000	0.042618000
H	1.072422000	1.466514000	0.083451000
C	-3.853487000	-0.680104000	-1.236966000
H	-3.265370000	-0.250188000	-2.057866000
H	-4.845709000	-0.200142000	-1.235534000
H	-3.979521000	-1.748574000	-1.453463000
C	-0.106993000	3.066276000	-0.703032000
H	0.280682000	2.970136000	-1.723513000
H	0.445819000	3.863908000	-0.189125000
H	-1.157801000	3.384160000	-0.769996000
C	-3.993174000	-1.059078000	1.254698000
H	-4.142293000	-2.138496000	1.125777000
H	-4.978150000	-0.567515000	1.290897000
H	-3.490233000	-0.910131000	2.217053000
C	-0.485486000	1.853631000	1.496106000
H	-1.534715000	2.177780000	1.527074000
H	0.112555000	2.582371000	2.063383000
H	-0.412524000	0.881054000	1.992056000
C	1.631228000	-0.943278000	-0.680527000
H	1.914486000	-1.747519000	-1.399620000
H	1.557281000	-0.029870000	-1.304055000
C	2.837477000	-0.791136000	0.271976000
H	2.645487000	0.038454000	0.969942000

H	2.890471000	-1.697826000	0.891802000
C	4.177170000	-0.566169000	-0.440191000
H	4.120406000	0.350330000	-1.047080000
H	4.349100000	-1.386646000	-1.153333000
C	5.374807000	-0.467008000	0.512721000
H	6.319541000	-0.308513000	-0.025823000
H	5.250827000	0.365275000	1.218215000
H	5.480247000	-1.383551000	1.107905000

(5')
E(gas)= -597.857904302



N	-0.758386000	1.872499000	-0.225425000
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N	0.159624000	-0.327304000	0.149957000
H	-0.170540000	-1.224447000	0.487785000
C	-0.993951000	0.583883000	-0.031966000
C	-2.495924000	-1.306271000	-0.084895000
H	-1.674739000	-1.904634000	-0.544420000
C	1.019984000	-0.527211000	-1.013694000
H	0.997491000	0.397289000	-1.597625000
C	-2.769124000	-1.925044000	1.309129000
H	-1.883567000	-1.841015000	1.952535000
H	-3.056690000	-2.987596000	1.256791000
H	-3.576944000	-1.365632000	1.797902000
C	2.473451000	-0.855633000	-0.635241000
H	2.876402000	-0.024459000	-0.040473000
H	3.078749000	-0.917400000	-1.555074000
C	-3.728293000	-1.518907000	-0.988951000
H	-4.583715000	-0.967353000	-0.578984000
H	-4.004765000	-2.581105000	-1.082667000
H	-3.528763000	-1.118010000	-1.989229000
C	0.484866000	2.476591000	0.176476000
H	1.287032000	1.751643000	0.411414000

C	1.003164000	3.398770000	-0.946664000
H	1.914384000	3.944205000	-0.655226000
H	1.223078000	2.820506000	-1.853204000
H	0.226947000	4.129784000	-1.207827000
C	0.266781000	3.309623000	1.462775000
H	-0.057669000	2.653632000	2.279016000
H	1.178405000	3.840260000	1.785007000
H	-0.529165000	4.046754000	1.294945000
C	2.627586000	-2.159682000	0.156492000
H	2.197379000	-2.991644000	-0.422390000
H	2.034897000	-2.081487000	1.077067000
C	4.081591000	-2.487833000	0.514590000
H	4.159317000	-3.419457000	1.090247000
H	4.698291000	-2.601477000	-0.387169000
H	4.528009000	-1.686253000	1.116991000
H	0.643292000	-1.325596000	-1.685673000