

Supporting information

Changing the path of least resistance, or “three *exo*’s instead of one *endo*”: electronic effects in homoallylic ring expansion cascades of alkenyl isonitriles

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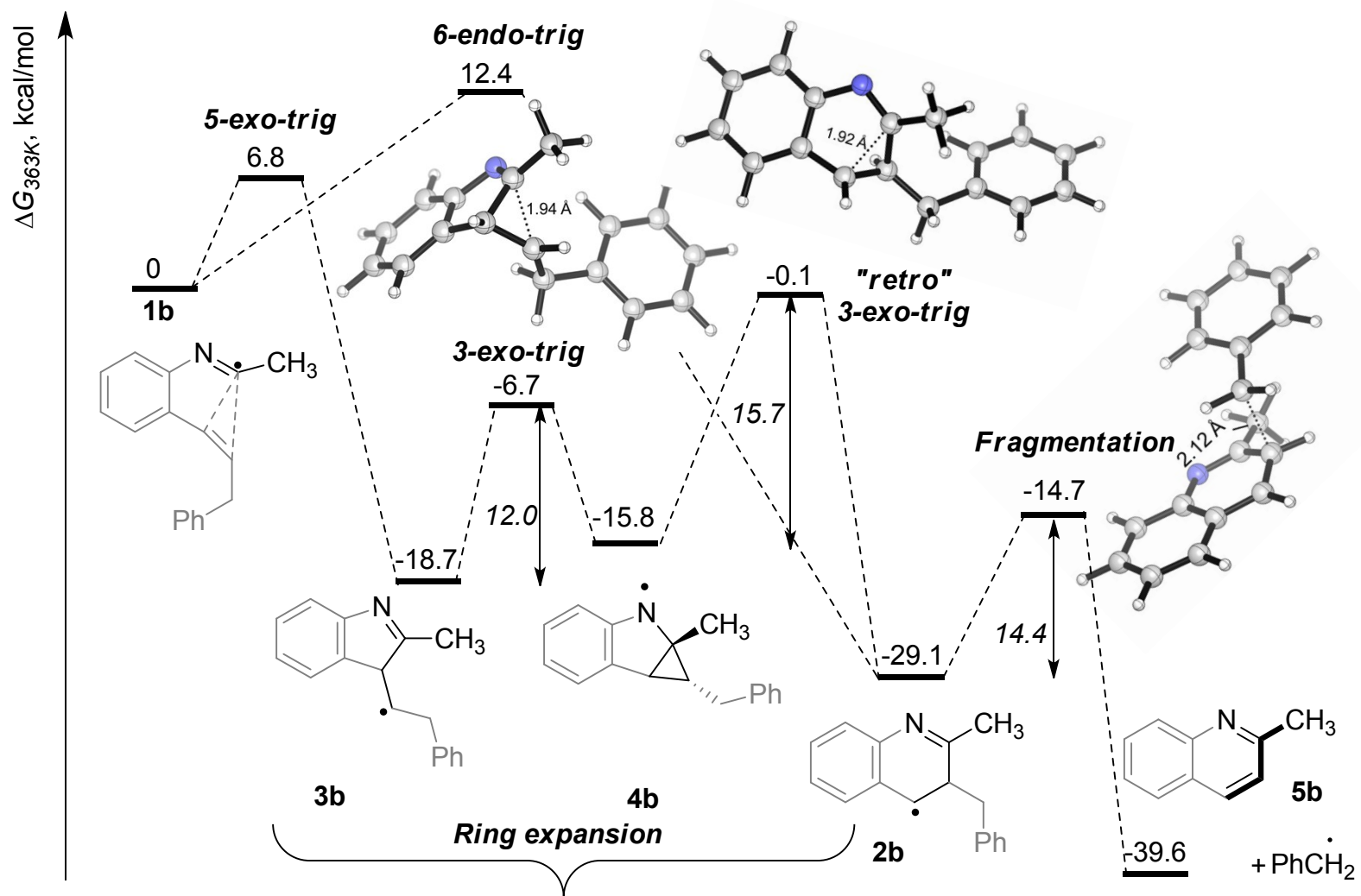
Computational Details

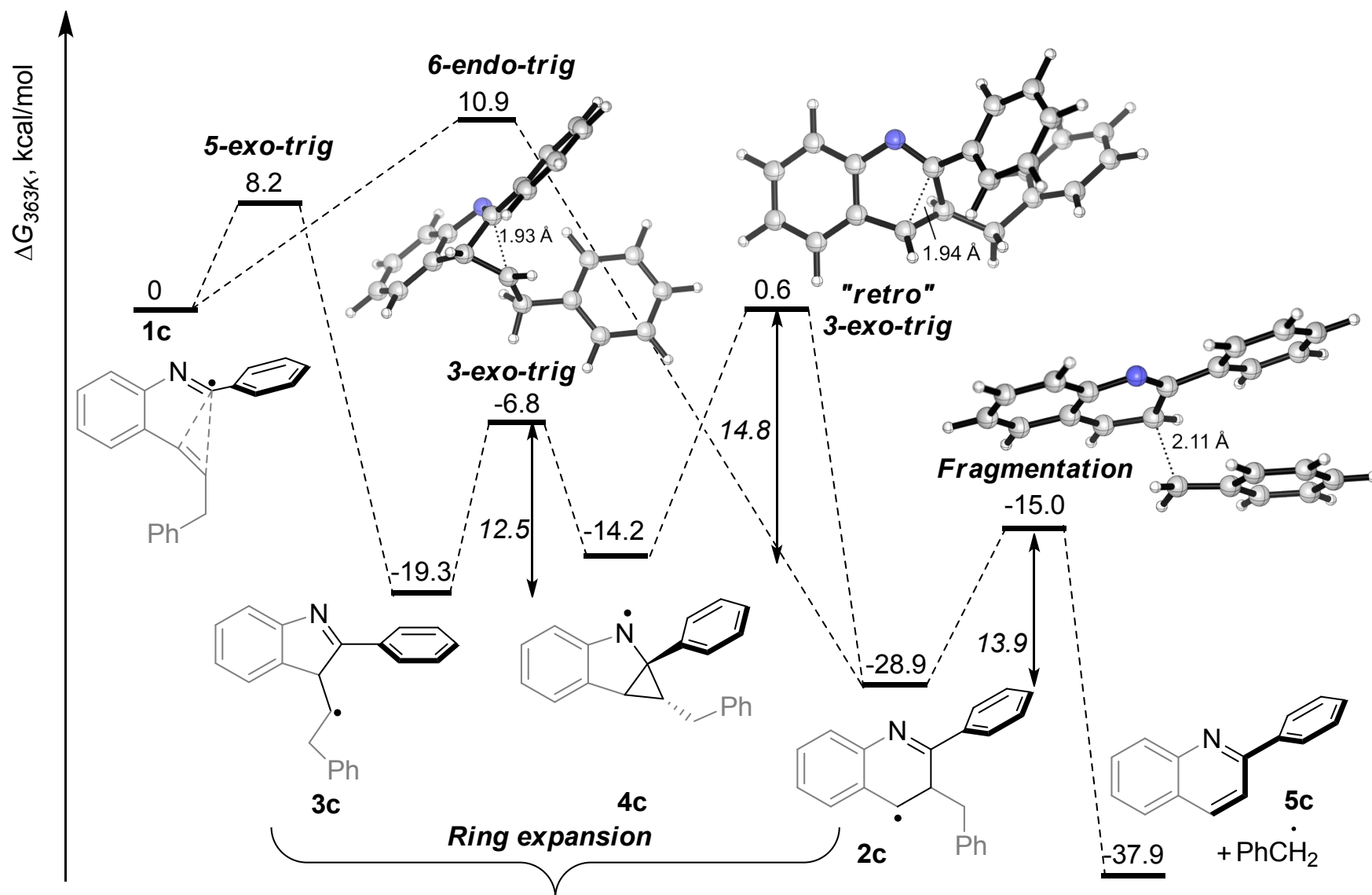
All calculations were carried with the Gaussian 09 software package,¹ using the M06-2X DFT functional² with the 6-311++G(d,p) basis set for all atoms except of Sn, for which we used the Def2-QZVP³ basis set. The implicit PCM⁴ solvation model was used to simulate the effects of toluene throughout the reaction pathways. We also performed Natural Bond Orbital⁵ (NBO) Analysis on key intermediates and transition states. The minimum energy pathway (MEP) was tracked using the intrinsic reaction coordinate (IRC) method to ensure that each TS structure correctly links two minima. Frequency calculations were carried for all structures to confirm them as either a minimum or a TS. Three-dimensional structures were produced with both CYLView 1.0.1⁶ and Chemcraft 1.8.⁷

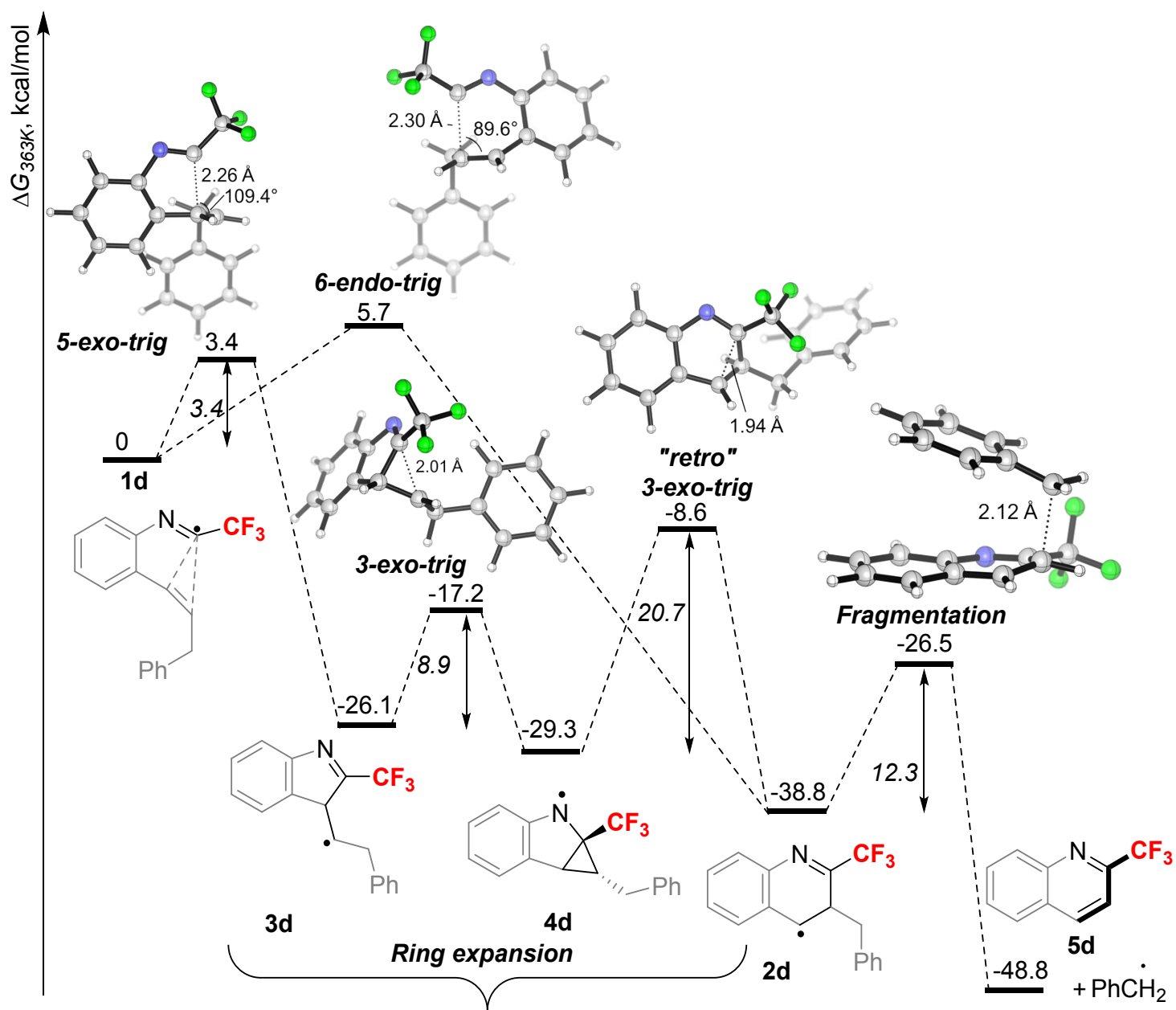
Full Potential Energy Surfaces

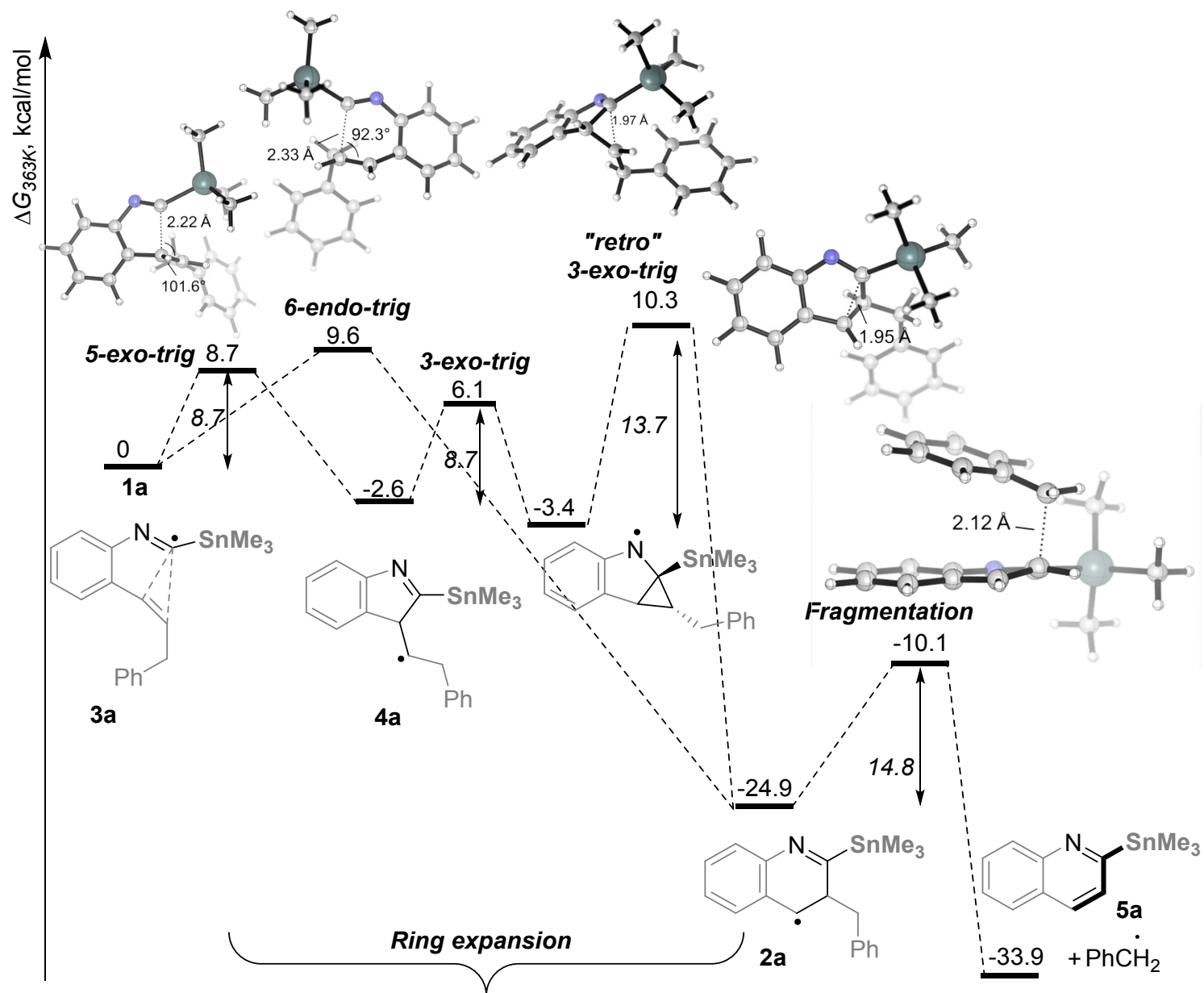
All four PES analyzed in the main article are available here.

Gibbs Free Energy diagram for full radical cascade initiated by the addition of the Me, Ph, CF₃, and SnMe₃ radicals, including HRE, direct 6-*endo* path and fragmentation:

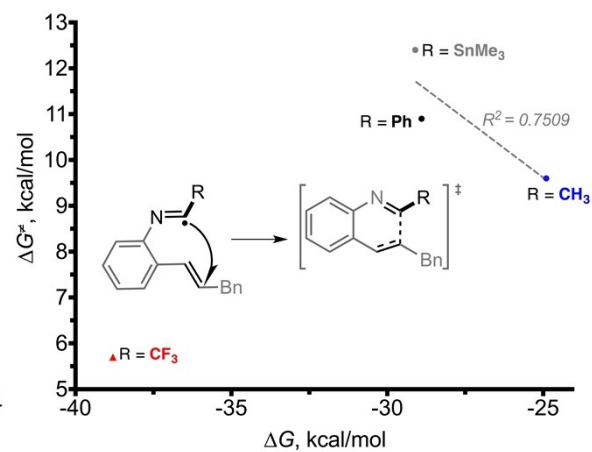
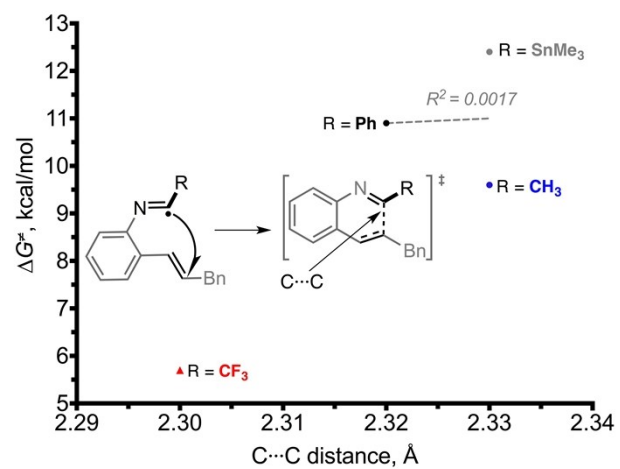
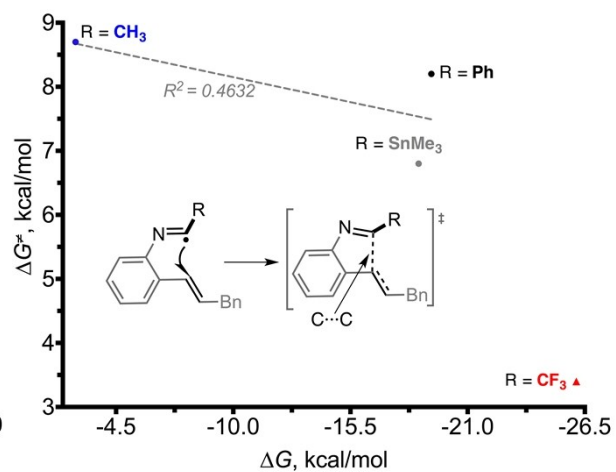
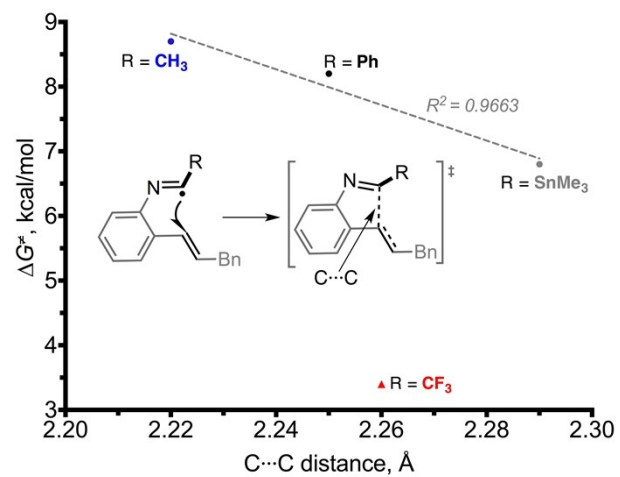


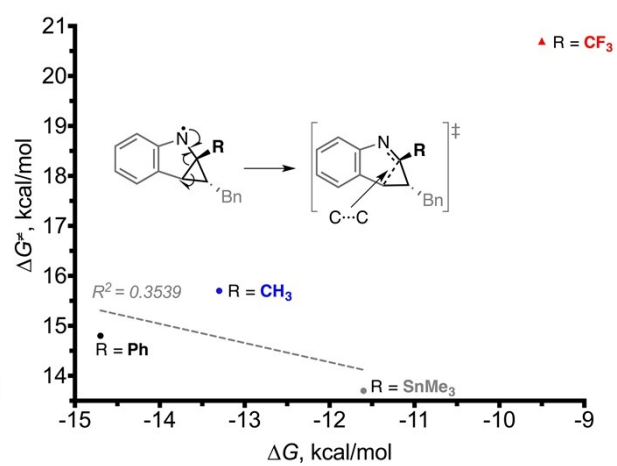
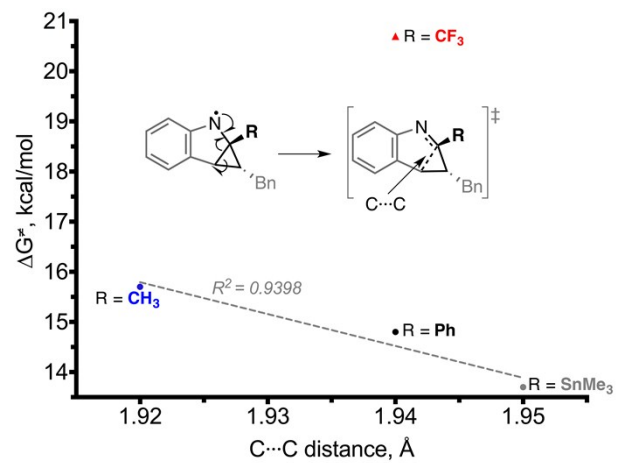
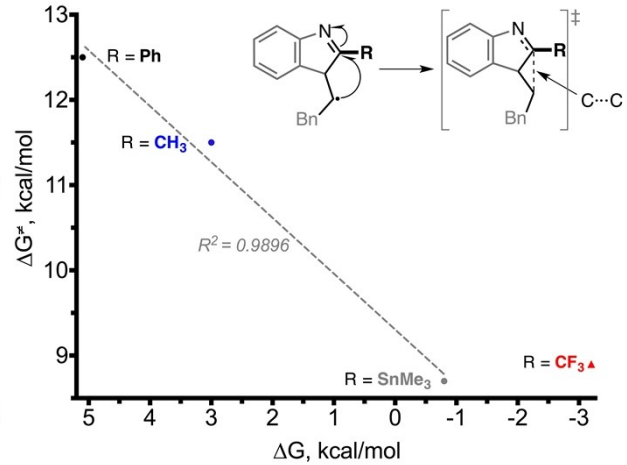
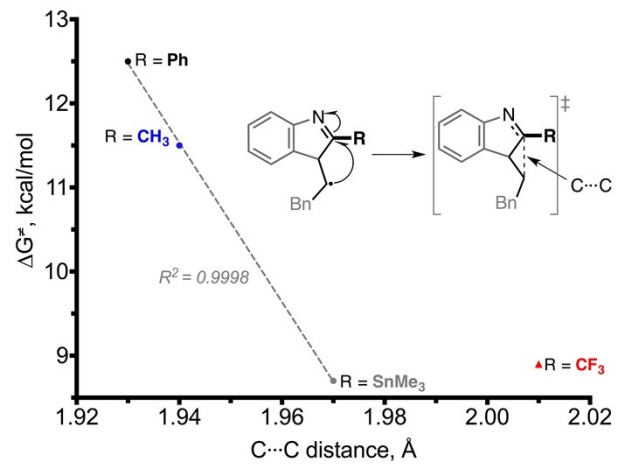






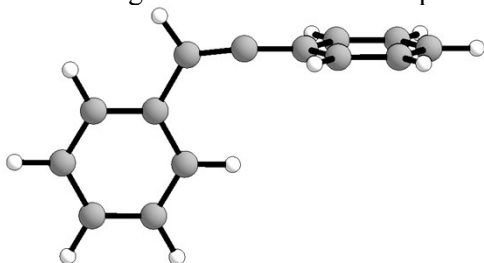
Correlations





Calculated Geometries

Calculated geometries with their respective energies (in hartree) and number of imaginary frequencies.



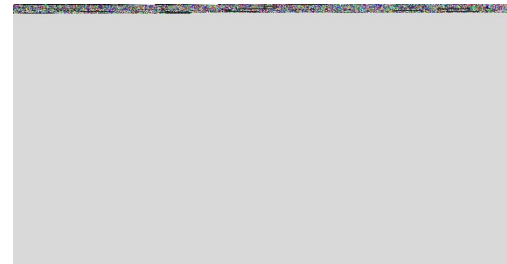
of imaginary frequencies: 0

E = -539.930678542

symmetry c1

C	4.176793000	1.089807000	0.000067000
C	2.903947000	1.659572000	0.000400000
C	1.775697000	0.851894000	0.000390000
C	1.902260000	-0.541306000	0.000056000
C	3.179760000	-1.104213000	-0.000277000
C	4.311189000	-0.293839000	-0.000274000
H	5.056266000	1.722809000	0.000057000
H	2.792896000	2.737665000	0.000668000
H	3.286252000	-2.184007000	-0.000567000
H	5.296721000	-0.744547000	-0.000543000
C	-0.526942000	-1.036230000	0.000088000
C	-1.784246000	-0.480023000	0.000050000
C	-2.457674000	-0.188593000	1.222932000
C	-2.457256000	-0.188077000	-1.222939000
C	-3.722709000	0.363423000	1.208743000
H	-1.957919000	-0.407059000	2.158714000
C	-3.722290000	0.363937000	-1.208963000
H	-1.957172000	-0.406114000	-2.158647000
C	-4.367223000	0.644273000	-0.000160000
H	-4.219645000	0.579474000	2.147411000
H	-4.218896000	0.580423000	-2.147702000
H	-5.360561000	1.075253000	-0.000228000
H	0.785408000	1.295580000	0.000620000

C	0.715789000	-1.431801000	-0.000034000
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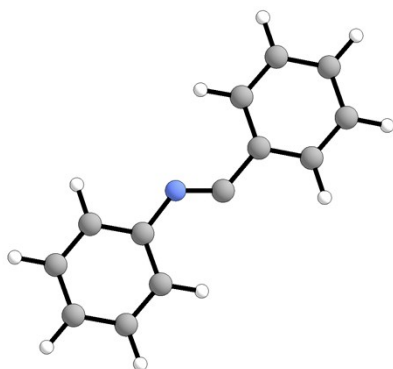


of imaginary frequencies: 0

E = -539.930678542

symmetry c1

C	4.176793000	1.089807000	0.000067000
C	2.903947000	1.659572000	0.000400000
C	1.775697000	0.851894000	0.000390000
C	1.902260000	-0.541306000	0.000056000
C	3.179760000	-1.104213000	-0.000277000
C	4.311189000	-0.293839000	-0.000274000
H	5.056266000	1.722809000	0.000057000
H	2.792896000	2.737665000	0.000668000
H	3.286252000	-2.184007000	-0.000567000
H	5.296721000	-0.744547000	-0.000543000
C	-0.526942000	-1.036230000	0.000088000
C	-1.784246000	-0.480023000	0.000050000
C	-2.457674000	-0.188593000	1.222932000
C	-2.457256000	-0.188077000	-1.222939000



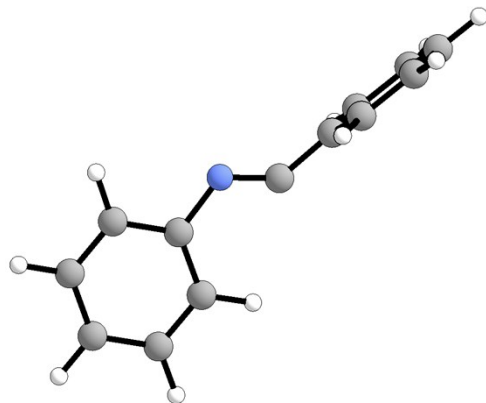
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E = -555.986673220

symmetry c1

C	4.629891000	0.207854000	-0.000041000
C	3.769050000	1.304683000	-0.000233000
C	2.393982000	1.118997000	-0.000206000
C	1.869537000	-0.177401000	0.000014000
C	2.728797000	-1.274590000	0.000194000
C	4.105703000	-1.080480000	0.000170000
H	5.702479000	0.359877000	-0.000071000
H	4.172663000	2.310471000	-0.000435000
H	2.302105000	-2.270394000	0.000350000
H	4.768359000	-1.937690000	0.000303000
N	0.481200000	-0.439274000	-0.000006000
C	-0.437980000	0.387262000	0.000166000
C	-1.884320000	0.180214000	0.000107000
C	-2.733625000	1.288281000	0.000241000
C	-2.425343000	-1.113002000	-0.000130000
C	-4.112500000	1.110391000	0.000131000
H	-2.302337000	2.282827000	0.000458000
C	-3.801292000	-1.285048000	-0.000228000
H	-1.754178000	-1.963649000	-0.000240000
C	-4.645794000	-0.174457000	-0.000105000
H	-4.769103000	1.971992000	0.000222000
H	-4.220090000	-2.284448000	-0.000447000
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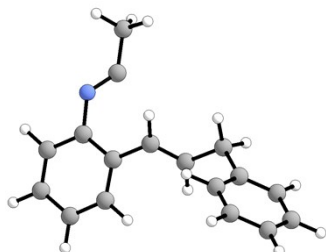
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E = -555.984615495

symmetry c1

C	4.608786000	0.262325000	0.228117000
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C	2.308429000	0.889598000	0.603998000
C	1.893616000	-0.192107000	-0.175832000
C	2.833867000	-1.038815000	-0.755432000
C	4.190786000	-0.812100000	-0.549710000
H	5.665532000	0.441042000	0.386498000
H	3.985667000	1.952288000	1.406151000
H	2.487159000	-1.867973000	-1.360388000
H	4.920381000	-1.475426000	-0.998685000
N	0.522545000	-0.477198000	-0.426507000
C	-0.440820000	0.081016000	0.094859000
C	-1.873938000	0.027503000	0.038348000
C	-2.586021000	-0.770143000	0.948757000
C	-2.574299000	0.833723000	-0.873703000
C	-3.972689000	-0.779344000	0.920828000
H	-2.043913000	-1.378357000	1.662815000
C	-3.961184000	0.814760000	-0.888248000
H	-2.023024000	1.458995000	-1.565755000
C	-4.665801000	0.011582000	0.006414000

H	-4.517045000	-1.405904000	1.617421000
H	-4.496313000	1.429050000	-1.602665000
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H	1.564024000	1.543921000	1.043449000



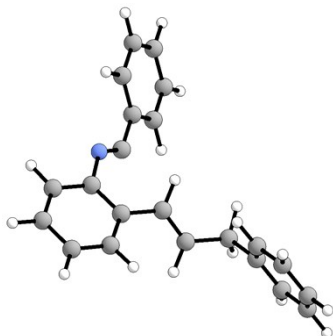
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E = -711.975503086

symmetry c1

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C	-3.034040000	-0.239922000	0.166750000
C	-4.039984000	-1.204686000	0.131228000
C	-3.737710000	-2.526512000	-0.158049000
H	-2.163830000	-3.932197000	-0.582714000
H	-0.373842000	-2.240994000	-0.434528000
H	-5.058450000	-0.889498000	0.323151000
H	-4.528675000	-3.265704000	-0.197219000
N	-3.429604000	1.082563000	0.460639000
C	-2.997550000	2.129825000	-0.024389000
C	-0.600857000	0.391344000	0.026810000
H	-0.709764000	1.181917000	0.765916000
C	0.497489000	0.364781000	-0.729378000
H	0.603969000	-0.398890000	-1.497539000
C	1.645944000	1.322461000	-0.588399000
H	1.398818000	2.078832000	0.163179000
H	1.811662000	1.846903000	-1.534490000
C	2.924534000	0.609259000	-0.192482000
C	2.970761000	-0.130928000	0.991142000
C	4.064958000	0.667064000	-0.990486000

C	4.133111000	-0.788964000	1.372076000
H	2.081713000	-0.191373000	1.611434000
C	5.231219000	0.004696000	-0.614744000
H	4.041940000	1.236856000	-1.913808000
C	5.268697000	-0.723554000	0.568176000
H	4.153892000	-1.356970000	2.294960000
H	6.109533000	0.058068000	-1.247670000
H	6.174814000	-1.239826000	0.862147000
C	-3.352729000	3.538523000	0.293873000
H	-2.455551000	4.082158000	0.595551000
H	-3.741366000	4.026298000	-0.601636000
H	-4.098312000	3.582657000	1.093167000



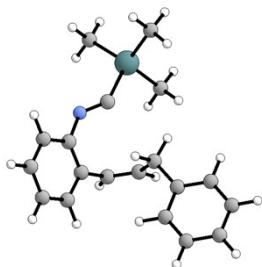
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E = -903.689822872

symmetry c1

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C	0.018503000	1.916515000	-0.121272000
C	1.383299000	2.239303000	0.013947000
C	1.798765000	3.571770000	0.035769000
C	0.879367000	4.599242000	-0.111489000
H	-1.203907000	5.092761000	-0.341662000
H	-1.948843000	2.742731000	-0.296818000
H	2.855589000	3.777059000	0.157039000
H	1.214722000	5.629334000	-0.105766000
N	2.381837000	1.259836000	0.163745000
C	2.439699000	0.131759000	-0.338606000

C	-0.458947000	0.522814000	-0.099228000
H	0.066319000	-0.167576000	0.556985000
C	-1.492899000	0.072427000	-0.812868000
H	-2.004995000	0.742786000	-1.500840000
C	-2.038772000	-1.323751000	-0.721290000
H	-1.400811000	-1.921433000	-0.062902000
H	-2.021693000	-1.796432000	-1.707930000
C	-3.463037000	-1.332004000	-0.198676000
C	-3.750402000	-0.777130000	1.050713000
C	-4.506083000	-1.878301000	-0.943999000
C	-5.048091000	-0.778849000	1.547727000
H	-2.945814000	-0.337556000	1.632175000
C	-5.809414000	-1.878710000	-0.451201000
H	-4.298422000	-2.309563000	-1.918038000
C	-6.083795000	-1.329954000	0.796101000
H	-5.252981000	-0.347597000	2.520931000
H	-6.608988000	-2.307835000	-1.044000000
H	-7.096747000	-1.329307000	1.180813000
C	3.411178000	-0.937475000	-0.108105000
C	3.408482000	-2.060396000	-0.937574000
C	4.331047000	-0.849623000	0.945556000
C	4.325572000	-3.084070000	-0.726211000
H	2.686393000	-2.118237000	-1.744179000
C	5.238951000	-1.876456000	1.156328000
H	4.318914000	0.027149000	1.582444000
C	5.238491000	-2.992749000	0.319787000
H	4.325988000	-3.952763000	-1.373505000
H	5.950157000	-1.809926000	1.971185000
H	5.951123000	-3.791956000	0.486669000



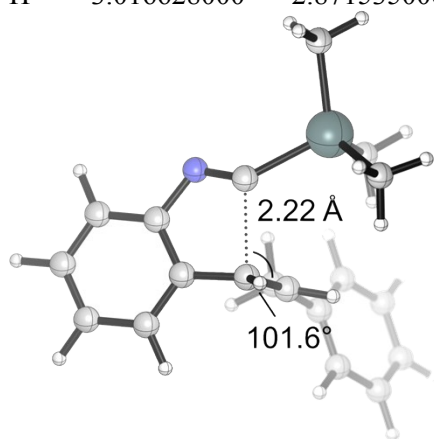
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E = -795.150618713

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C	2.226067000	3.054572000	0.701072000
C	1.131772000	2.183935000	0.688938000
C	0.056823000	2.491727000	-0.162997000
C	0.094392000	3.630180000	-0.970238000
C	1.207066000	4.457689000	-0.964537000
H	3.145271000	4.822183000	-0.098718000
H	3.053639000	2.833805000	1.367223000
H	-0.760653000	3.847881000	-1.599214000
H	1.232451000	5.329626000	-1.607314000
N	-1.126402000	1.718867000	-0.158430000
C	-1.279886000	0.514174000	-0.353653000
C	1.124522000	1.013294000	1.607879000
H	0.944207000	1.236089000	2.657376000
C	1.359405000	-0.249825000	1.254578000
H	1.361018000	-1.011038000	2.032201000
C	1.677740000	-0.733119000	-0.133660000
H	1.614506000	0.100328000	-0.838407000
H	0.925512000	-1.466055000	-0.441485000
C	3.053493000	-1.362916000	-0.195004000
C	4.189219000	-0.574212000	0.003764000
C	3.219021000	-2.725567000	-0.435144000
C	5.460251000	-1.133545000	-0.042545000
H	4.066026000	0.487961000	0.194263000
C	4.491401000	-3.291816000	-0.479659000

H	2.345109000	-3.349240000	-0.594063000
C	5.614976000	-2.497411000	-0.283901000
H	6.331960000	-0.507324000	0.109197000
H	4.602963000	-4.353260000	-0.669115000
H	6.605649000	-2.934987000	-0.320505000
Sn	-2.993654000	-0.769224000	-0.033356000
C	-4.676006000	0.356702000	0.636211000
H	-5.007617000	1.041053000	-0.145302000
H	-5.503031000	-0.307199000	0.893239000
H	-4.408942000	0.940429000	1.517794000
C	-3.353042000	-1.754725000	-1.884267000
H	-3.730717000	-1.051658000	-2.627566000
H	-2.426876000	-2.192021000	-2.259892000
H	-4.086959000	-2.551846000	-1.757058000
C	-2.266057000	-2.120588000	1.442346000
H	-1.375584000	-2.629586000	1.069315000
H	-1.997701000	-1.577622000	2.349647000
H	-3.016628000	-2.871535000	1.693027000



of imaginary frequencies: 1

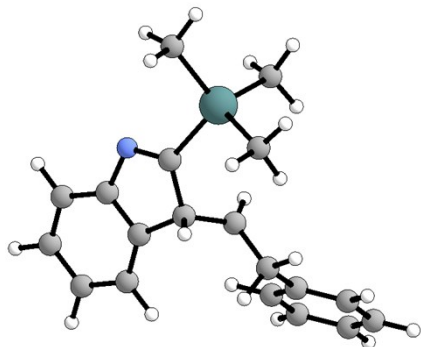
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symmetry c1

C	-0.208782000	4.960511000	0.235234000
C	-0.419137000	3.785132000	0.955669000
C	0.254539000	2.618446000	0.609324000

C	1.142479000	2.653553000	-0.477590000
C	1.349158000	3.815817000	-1.208071000
C	0.673181000	4.975910000	-0.841470000
H	-0.739768000	5.863227000	0.513126000
H	-1.114967000	3.772649000	1.787429000
H	2.034289000	3.800206000	-2.047052000
H	0.832340000	5.891269000	-1.398857000
N	1.783068000	1.426667000	-0.813964000
C	1.690449000	0.519196000	0.031481000
C	0.066214000	1.322027000	1.321554000
H	0.569157000	1.207323000	2.278588000
C	-0.965129000	0.477264000	1.023440000
H	-1.143352000	-0.383947000	1.662321000
C	-1.759211000	0.568912000	-0.251978000
H	-1.128041000	0.265088000	-1.100171000
H	-2.020241000	1.616732000	-0.444959000
C	-3.013263000	-0.272585000	-0.242450000
C	-3.937002000	-0.153409000	0.799462000
C	-3.280278000	-1.178365000	-1.268465000
C	-5.098489000	-0.917345000	0.812380000
H	-3.740794000	0.547859000	1.604888000
C	-4.441889000	-1.946683000	-1.259551000
H	-2.568913000	-1.285777000	-2.080986000
C	-5.354438000	-1.818679000	-0.218406000
H	-5.806135000	-0.809441000	1.626384000
H	-4.630650000	-2.647067000	-2.064966000
H	-6.258526000	-2.416117000	-0.208548000
Sn	1.972869000	-1.619623000	0.054847000
C	2.004587000	-2.091772000	2.128120000
H	1.087283000	-1.732321000	2.598038000
H	2.076443000	-3.168219000	2.289104000
H	2.853538000	-1.610188000	2.615375000
C	3.785124000	-2.138376000	-0.935209000
H	3.922579000	-3.220874000	-0.932751000
H	3.762616000	-1.791362000	-1.968647000
H	4.636538000	-1.678170000	-0.432861000

C	0.249484000	-2.430381000	-0.901243000
H	0.339635000	-3.513921000	-0.997920000
H	-0.645371000	-2.205577000	-0.317349000
H	0.131851000	-2.001926000	-1.898182000



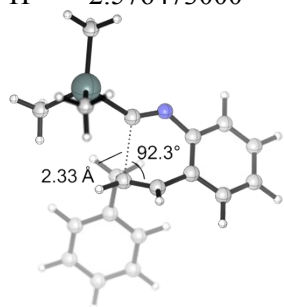
of imaginary frequencies: 0

E = -795.174606949

symmetry c1

C	-1.563714000	4.241887000	0.434506000
C	-1.494397000	2.909031000	0.847957000
C	-0.364280000	2.179092000	0.520603000
C	0.675229000	2.762129000	-0.210197000
C	0.617733000	4.085660000	-0.621375000
C	-0.520136000	4.820532000	-0.288654000
H	-2.437665000	4.834184000	0.679120000
H	-2.309200000	2.463295000	1.409408000
H	1.432798000	4.524297000	-1.184523000
H	-0.596704000	5.856427000	-0.597615000
N	1.727250000	1.834099000	-0.461593000
C	1.394195000	0.710387000	0.073307000
C	0.037158000	0.743652000	0.779658000
C	-0.917396000	-0.280017000	0.252471000
H	-0.952982000	-0.440881000	-0.819862000
C	-1.967253000	-0.900460000	1.118724000
H	-2.152374000	-0.246903000	1.981672000
H	-1.603608000	-1.846348000	1.545651000
C	-3.276728000	-1.162688000	0.405373000

C	-3.951927000	-2.371023000	0.572235000
C	-3.844358000	-0.185770000	-0.416495000
C	-5.170205000	-2.600754000	-0.061611000
H	-3.519697000	-3.140327000	1.203951000
C	-5.060695000	-0.411684000	-1.051513000
H	-3.325531000	0.757158000	-0.561727000
C	-5.728299000	-1.620964000	-0.875410000
H	-5.679534000	-3.547246000	0.078040000
H	-5.487217000	0.356178000	-1.686534000
H	-6.674854000	-1.798305000	-1.372139000
H	0.198238000	0.576968000	1.854636000
Sn	2.581538000	-1.080106000	-0.092668000
C	4.628165000	-0.522057000	-0.239822000
H	5.243167000	-1.379807000	-0.516164000
H	4.747011000	0.252490000	-0.998531000
H	4.986404000	-0.128447000	0.712248000
C	2.146564000	-2.202827000	1.671061000
H	2.424056000	-1.641855000	2.565125000
H	1.075715000	-2.414422000	1.713821000
H	2.683794000	-3.152333000	1.680081000
C	1.922270000	-2.145668000	-1.818445000
H	0.907712000	-2.517684000	-1.665053000
H	1.924785000	-1.494412000	-2.693558000
H	2.576473000	-2.996151000	-2.017715000



of imaginary frequencies: 1

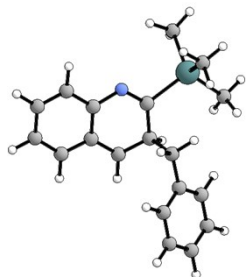
E = -795.140477535

symmetry c1

C	2.692349000	3.998954000	0.280390000
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C	2.420255000	2.868721000	1.032769000
C	1.353630000	2.015623000	0.710713000
C	0.495444000	2.399443000	-0.348520000
C	0.768791000	3.548921000	-1.097628000
C	1.875557000	4.327839000	-0.807087000
H	3.539191000	4.625903000	0.533239000
H	3.058995000	2.602639000	1.868871000
H	0.086246000	3.819599000	-1.894989000
H	2.090640000	5.206251000	-1.403679000
N	-0.737117000	1.746261000	-0.549855000
C	-1.063271000	0.596550000	-0.246517000
C	1.079204000	0.795960000	1.461129000
H	1.016462000	0.868874000	2.543282000
C	0.754885000	-0.372902000	0.844161000
H	0.441853000	-1.201690000	1.478824000
C	1.255562000	-0.798714000	-0.524266000
H	1.390705000	0.072029000	-1.168878000
H	0.523855000	-1.455615000	-1.000685000
C	2.575833000	-1.527619000	-0.380568000
C	3.758519000	-0.802839000	-0.215457000
C	2.634586000	-2.920096000	-0.375433000
C	4.973855000	-1.457192000	-0.056167000
H	3.716756000	0.282619000	-0.211865000
C	3.850711000	-3.580244000	-0.211936000
H	1.720678000	-3.492140000	-0.504973000
C	5.023108000	-2.850050000	-0.052858000
H	5.885332000	-0.882899000	0.064106000
H	3.881075000	-4.663716000	-0.212761000
H	5.970922000	-3.360554000	0.071140000
Sn	-2.878135000	-0.538873000	0.006258000
C	-4.468118000	0.207218000	-1.198693000
H	-4.222602000	0.104183000	-2.255951000
H	-5.384271000	-0.350574000	-0.997036000
H	-4.645602000	1.260893000	-0.982431000
C	-2.287991000	-2.507052000	-0.550893000
H	-1.442153000	-2.824737000	0.062578000

H	-3.103173000	-3.217414000	-0.405663000
H	-1.986369000	-2.536497000	-1.599204000
C	-3.270688000	-0.427696000	2.094967000
H	-2.368852000	-0.687753000	2.651523000
H	-3.571348000	0.582049000	2.375832000
H	-4.065120000	-1.120553000	2.376154000



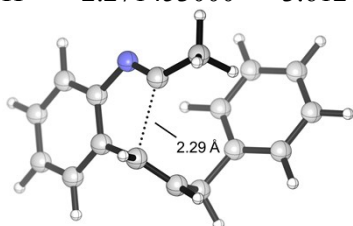
of imaginary frequencies: 0

E = -795.197753887

symmetry c1

C	-1.186723000	4.992512000	-0.199382000
C	-1.728732000	3.762818000	-0.506471000
C	-0.954189000	2.577610000	-0.394545000
C	0.405360000	2.700947000	0.019257000
C	0.932300000	3.951029000	0.322618000
C	0.147469000	5.094770000	0.223792000
H	-1.794009000	5.886199000	-0.283994000
H	-2.760344000	3.679824000	-0.832139000
H	1.970171000	4.005808000	0.630627000
H	0.567616000	6.063756000	0.463789000
N	1.261608000	1.584866000	0.092297000
C	0.804912000	0.406467000	-0.135842000
C	-1.467457000	1.306763000	-0.671720000
H	-2.490685000	1.197211000	-1.014999000
C	-0.648322000	0.086729000	-0.434702000
H	-0.677328000	-0.566441000	-1.320513000
C	-1.219447000	-0.772326000	0.737838000
H	-1.215845000	-0.162196000	1.644951000
H	-0.550333000	-1.622856000	0.907550000

C	-2.606540000	-1.278358000	0.441722000
C	-3.733161000	-0.649816000	0.971791000
C	-2.785514000	-2.365935000	-0.416043000
C	-5.012415000	-1.097875000	0.653548000
H	-3.604952000	0.196806000	1.638877000
C	-4.061194000	-2.816558000	-0.736521000
H	-1.914464000	-2.864796000	-0.831961000
C	-5.179617000	-2.181679000	-0.202194000
H	-5.877997000	-0.601055000	1.076186000
H	-4.183309000	-3.664121000	-1.400905000
H	-6.174544000	-2.532569000	-0.449196000
Sn	2.298197000	-1.156893000	-0.001825000
C	4.008636000	-0.477031000	-1.068693000
H	4.206318000	0.563066000	-0.805681000
H	4.886603000	-1.075517000	-0.820887000
H	3.838894000	-0.535330000	-2.144623000
C	2.740949000	-1.460434000	2.062365000
H	1.849782000	-1.788236000	2.600425000
H	3.518908000	-2.215282000	2.187930000
H	3.087893000	-0.526262000	2.506776000
C	1.474987000	-2.933547000	-0.869882000
H	0.838146000	-3.461301000	-0.157152000
H	0.879086000	-2.689867000	-1.752475000
H	2.271453000	-3.612744000	-1.179006000



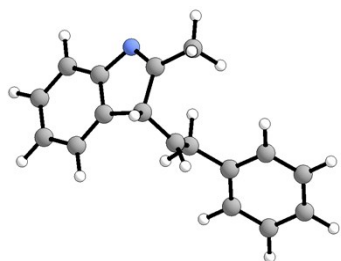
of imaginary frequencies: 1

E = -711.970475486

symmetry c1

C	3.820972000	0.774953000	-0.864216000
C	2.856723000	1.271298000	0.011221000
C	1.880792000	0.431682000	0.539958000

C	1.888541000	-0.924194000	0.171726000
C	2.849502000	-1.424645000	-0.697886000
C	3.818695000	-0.571155000	-1.214908000
H	4.572731000	1.441426000	-1.269909000
H	2.857844000	2.319702000	0.289856000
H	2.818315000	-2.474819000	-0.962245000
H	4.568244000	-0.956681000	-1.895807000
N	0.859081000	-1.765837000	0.665366000
C	0.013790000	-1.225329000	1.398726000
C	0.848225000	0.910138000	1.500662000
H	1.082843000	0.762759000	2.553448000
C	-0.140102000	1.787599000	1.189468000
H	-0.754396000	2.176598000	1.996587000
C	-0.617938000	2.058842000	-0.212974000
H	0.207236000	1.968165000	-0.922710000
H	-1.018426000	3.073011000	-0.287673000
C	-1.697631000	1.052201000	-0.562519000
C	-1.376263000	-0.116592000	-1.252848000
C	-3.009291000	1.231044000	-0.118643000
C	-2.342631000	-1.089458000	-1.489845000
H	-0.356748000	-0.270427000	-1.593560000
C	-3.979026000	0.262592000	-0.356478000
H	-3.270941000	2.136989000	0.419760000
C	-3.646440000	-0.903994000	-1.040599000
H	-2.073834000	-1.994471000	-2.022185000
H	-4.993738000	0.417804000	-0.008334000
H	-4.399911000	-1.660986000	-1.223910000
C	-1.253311000	-1.712001000	1.982419000
H	-1.273348000	-1.529962000	3.058446000
H	-2.076035000	-1.147784000	1.530122000
H	-1.391040000	-2.778359000	1.780979000



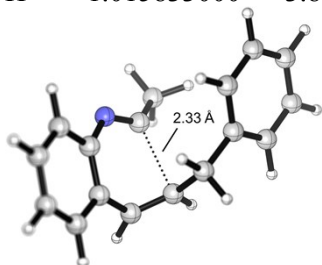
of imaginary frequencies: 0

E = -712.009896974

symmetry c1

C	-3.444149000	-2.196490000	0.366962000
C	-2.441507000	-1.497905000	1.045137000
C	-2.134660000	-0.217536000	0.621300000
C	-2.803471000	0.355280000	-0.464301000
C	-3.799263000	-0.329317000	-1.143302000
C	-4.112521000	-1.617451000	-0.710973000
H	-3.705787000	-3.199796000	0.681472000
H	-1.918881000	-1.952534000	1.880408000
H	-4.307385000	0.131618000	-1.981438000
H	-4.886085000	-2.178932000	-1.221605000
N	-2.328442000	1.662233000	-0.752274000
C	-1.401249000	1.922053000	0.092104000
C	-1.116817000	0.795926000	1.096222000
H	-1.362990000	1.156807000	2.101406000
C	0.303774000	0.324515000	1.057480000
H	0.882521000	0.264890000	1.970531000
C	0.842755000	-0.292853000	-0.193605000
H	0.493224000	0.284313000	-1.062330000
H	0.417979000	-1.297850000	-0.329083000
C	2.350648000	-0.375773000	-0.206086000
C	3.117374000	0.791758000	-0.191848000
C	3.006418000	-1.604661000	-0.214695000
C	4.505212000	0.732371000	-0.192085000
H	2.615742000	1.754641000	-0.182067000
C	4.397513000	-1.669883000	-0.212620000
H	2.422699000	-2.519343000	-0.225024000

C	5.150265000	-0.501756000	-0.202035000
H	5.085326000	1.647914000	-0.186406000
H	4.891832000	-2.634310000	-0.220342000
H	6.232630000	-0.550235000	-0.202701000
C	-0.632422000	3.199368000	0.103165000
H	-0.700292000	3.679639000	1.083151000
H	0.426992000	2.999104000	-0.083507000
H	-1.015833000	3.872569000	-0.661473000



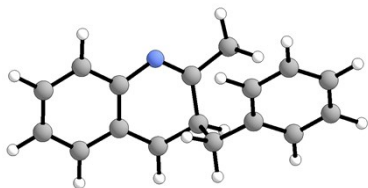
of imaginary frequencies: 1

E = -711.964157731

symmetry c1

C	-4.376992000	0.129093000	-0.887153000
C	-3.518252000	1.089781000	-0.372136000
C	-2.301433000	0.735002000	0.218764000
C	-1.994697000	-0.639647000	0.348467000
C	-2.868401000	-1.600974000	-0.163589000
C	-4.041223000	-1.221384000	-0.797653000
H	-5.304488000	0.430221000	-1.359171000
H	-3.768942000	2.142370000	-0.449181000
H	-2.612750000	-2.645791000	-0.032699000
H	-4.705931000	-1.976097000	-1.200612000
N	-0.899210000	-1.094799000	1.109242000
C	0.146229000	-0.473931000	1.347941000
C	-1.357403000	1.719757000	0.758176000
H	-1.699951000	2.369766000	1.558287000
C	-0.034824000	1.669745000	0.452407000
H	0.639258000	2.312185000	1.016792000
C	0.515770000	1.172692000	-0.871330000
H	0.591519000	2.051210000	-1.525593000

H	-0.198392000	0.493042000	-1.339583000
C	1.871337000	0.514223000	-0.775281000
C	2.981251000	1.230616000	-0.324545000
C	2.032958000	-0.832017000	-1.100747000
C	4.217941000	0.610652000	-0.178900000
H	2.876261000	2.283839000	-0.082271000
C	3.268938000	-1.456108000	-0.961641000
H	1.174055000	-1.400407000	-1.443400000
C	4.364320000	-0.737732000	-0.493007000
H	5.069116000	1.180685000	0.175339000
H	3.374394000	-2.505038000	-1.213082000
H	5.327001000	-1.221894000	-0.378917000
C	1.251910000	-0.790626000	2.288738000
H	1.292351000	-0.017779000	3.059962000
H	1.088772000	-1.764626000	2.759477000
H	2.207623000	-0.782946000	1.758886000



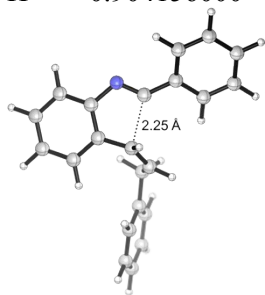
of imaginary frequencies: 0

E = -711.964157731

symmetry c1

C	4.612923000	-0.351927000	-0.780395000
C	3.655416000	-1.229101000	-0.319022000
C	2.407294000	-0.754416000	0.159472000
C	2.194819000	0.656592000	0.214932000
C	3.177394000	1.523306000	-0.254656000
C	4.371585000	1.030378000	-0.765153000
H	5.555421000	-0.730444000	-1.158257000
H	3.832940000	-2.299190000	-0.337955000
H	2.989123000	2.588348000	-0.187899000
H	5.126885000	1.715348000	-1.130772000
N	1.072184000	1.204973000	0.851505000

C	0.095872000	0.440449000	1.168782000
C	1.364193000	-1.595771000	0.564977000
H	1.493352000	-2.672401000	0.574460000
C	0.003850000	-1.012376000	0.737383000
H	-0.588608000	-1.569948000	1.470677000
C	-0.741803000	-1.115536000	-0.643131000
H	-0.775405000	-2.174314000	-0.915453000
H	-0.124581000	-0.603418000	-1.385961000
C	-2.129232000	-0.534164000	-0.629345000
C	-3.193769000	-1.249024000	-0.077818000
C	-2.362719000	0.754883000	-1.108249000
C	-4.461304000	-0.683714000	0.006638000
H	-3.025646000	-2.256197000	0.292023000
C	-3.629713000	1.323784000	-1.026934000
H	-1.539461000	1.320381000	-1.533381000
C	-4.681447000	0.607452000	-0.464879000
H	-5.278070000	-1.250423000	0.438427000
H	-3.794352000	2.327691000	-1.400530000
H	-5.668358000	1.049710000	-0.398256000
C	-1.001157000	0.986223000	2.034736000
H	-1.991829000	0.723154000	1.658919000
H	-0.905769000	0.547008000	3.034290000
H	-0.904156000	2.067664000	2.115093000



of imaginary frequencies: 1

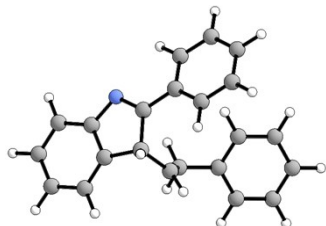
E = -903.680186170

symmetry c1

C	1.388895000	-3.672399000	0.155783000
C	1.258354000	-2.359877000	0.605771000

C	0.054520000	-1.678446000	0.451910000
C	-1.016333000	-2.336330000	-0.175892000
C	-0.895006000	-3.648016000	-0.619338000
C	0.313234000	-4.315825000	-0.450499000
H	2.331334000	-4.191633000	0.282040000
H	2.095749000	-1.861030000	1.081919000
H	-1.742206000	-4.122376000	-1.099844000
H	0.417590000	-5.336388000	-0.798819000
N	-2.213534000	-1.609322000	-0.368984000
C	-2.178611000	-0.403711000	-0.046207000
C	-0.160604000	-0.290307000	0.938965000
H	-0.731421000	-0.200428000	1.862693000
C	0.608172000	0.771219000	0.567885000
H	0.512026000	1.699151000	1.126074000
C	1.506858000	0.800824000	-0.630180000
H	1.124525000	1.540837000	-1.344642000
H	1.471880000	-0.166283000	-1.141976000
C	2.953235000	1.146395000	-0.324187000
C	3.529314000	0.862606000	0.914276000
C	3.750273000	1.733025000	-1.310177000
C	4.870511000	1.148480000	1.158905000
H	2.920759000	0.422084000	1.697194000
C	5.089359000	2.018837000	-1.070741000
H	3.313692000	1.965730000	-2.276486000
C	5.655731000	1.725394000	0.167171000
H	5.300152000	0.922599000	2.128220000
H	5.690638000	2.474380000	-1.849159000
H	6.698727000	1.949566000	0.357502000
C	-3.220761000	0.612098000	-0.024315000
C	-2.863483000	1.962853000	-0.009544000
C	-4.574023000	0.247866000	0.003933000
C	-3.848383000	2.943008000	0.017676000
H	-1.812676000	2.229517000	-0.024942000
C	-5.552045000	1.230952000	0.039212000
H	-4.836669000	-0.803523000	-0.002695000
C	-5.191211000	2.578065000	0.044492000

H	-3.569816000	3.990074000	0.022022000
H	-6.598583000	0.950300000	0.061848000
H	-5.958940000	3.342421000	0.072557000



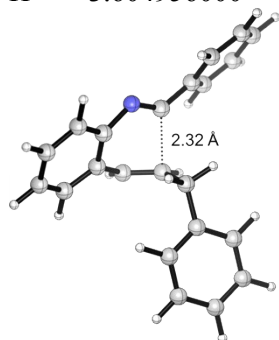
of imaginary frequencies: 0

E = -903.727525985

symmetry c1

C	-4.727996000	-1.565725000	0.243707000
C	-3.522320000	-1.446416000	0.939704000
C	-2.669454000	-0.413606000	0.595704000
C	-2.999582000	0.478367000	-0.429425000
C	-4.195390000	0.368796000	-1.125477000
C	-5.058062000	-0.668406000	-0.772527000
H	-5.415213000	-2.365072000	0.494139000
H	-3.264362000	-2.147292000	1.726515000
H	-4.439985000	1.068366000	-1.915598000
H	-5.999148000	-0.782331000	-1.297586000
N	-1.984546000	1.441722000	-0.635720000
C	-1.044877000	1.197044000	0.208539000
C	-1.312484000	-0.004156000	1.123418000
H	-1.397405000	0.343108000	2.159614000
C	-0.258778000	-1.064068000	1.021410000
H	0.118124000	-1.532348000	1.922535000
C	0.157819000	-1.613908000	-0.307883000
H	-0.156142000	-0.929894000	-1.104541000
H	-0.348849000	-2.568947000	-0.503239000
C	1.656913000	-1.823629000	-0.370997000
C	2.507138000	-0.748258000	-0.640257000
C	2.216650000	-3.073419000	-0.109617000
C	3.886530000	-0.920569000	-0.646921000
H	2.083190000	0.230850000	-0.843306000

C	3.598526000	-3.248918000	-0.113105000
H	1.565051000	-3.917147000	0.095520000
C	4.437062000	-2.172174000	-0.380489000
H	4.532062000	-0.076427000	-0.861701000
H	4.018441000	-4.227798000	0.088386000
H	5.512200000	-2.307645000	-0.385999000
C	0.214216000	1.957923000	0.241091000
C	1.091003000	1.852625000	1.324809000
C	0.568557000	2.757747000	-0.851346000
C	2.304437000	2.530789000	1.314665000
H	0.831432000	1.232994000	2.175327000
C	1.782919000	3.429162000	-0.861748000
H	-0.114606000	2.827727000	-1.689044000
C	2.655218000	3.314741000	0.219838000
H	2.979053000	2.440871000	2.157576000
H	2.054754000	4.038709000	-1.715484000
H	3.604956000	3.836559000	0.208360000



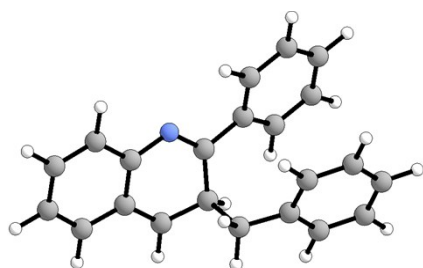
of imaginary frequencies: 1

E = -903.675991739

symmetry c1

C	2.297408000	3.886038000	0.194216000
C	2.064999000	2.749894000	0.953718000
C	0.919691000	1.967081000	0.761625000
C	-0.043554000	2.407991000	-0.176182000
C	0.190079000	3.565180000	-0.924943000
C	1.362044000	4.285818000	-0.762031000
H	3.202988000	4.461319000	0.344906000

H	2.790211000	2.430525000	1.694939000
H	-0.573767000	3.887884000	-1.622677000
H	1.538473000	5.172002000	-1.359711000
N	-1.313772000	1.808081000	-0.286289000
C	-1.600638000	0.647894000	0.045376000
C	0.665100000	0.758845000	1.545194000
H	0.676800000	0.845340000	2.627921000
C	0.253021000	-0.399168000	0.966651000
H	-0.043101000	-1.212989000	1.626575000
C	0.610528000	-0.844702000	-0.439180000
H	0.779457000	0.022257000	-1.081570000
H	-0.208922000	-1.427433000	-0.866605000
C	1.864167000	-1.694680000	-0.389924000
C	3.119616000	-1.088437000	-0.308282000
C	1.787375000	-3.086154000	-0.386196000
C	4.274117000	-1.858429000	-0.231606000
H	3.185111000	-0.004098000	-0.305281000
C	2.941946000	-3.861426000	-0.305571000
H	0.816374000	-3.567111000	-0.452830000
C	4.187907000	-3.249130000	-0.229021000
H	5.242729000	-1.375103000	-0.174562000
H	2.866824000	-4.942706000	-0.306943000
H	5.087918000	-3.849992000	-0.171183000
C	-2.832065000	-0.112196000	0.041262000
C	-3.653760000	-0.107574000	-1.096505000
C	-3.170726000	-0.917991000	1.136221000
C	-4.799251000	-0.891307000	-1.125037000
H	-3.382312000	0.512094000	-1.942920000
C	-4.328104000	-1.683184000	1.104213000
H	-2.528084000	-0.925701000	2.008948000
C	-5.141876000	-1.677695000	-0.026859000
H	-5.430511000	-0.885760000	-2.006010000
H	-4.593795000	-2.291222000	1.960915000
H	-6.038141000	-2.285878000	-0.052727000



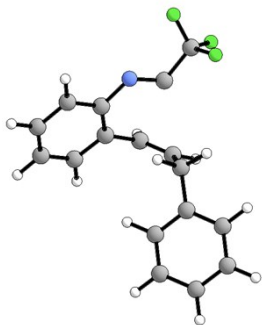
of imaginary frequencies: 0

E = -903.747203457

symmetry c1

C	-5.421468000	-0.402541000	0.154665000
C	-4.435074000	-1.111569000	-0.493419000
C	-3.089537000	-0.655117000	-0.485560000
C	-2.796501000	0.582292000	0.164566000
C	-3.814167000	1.284698000	0.809436000
C	-5.113464000	0.796352000	0.821041000
H	-6.440994000	-0.769647000	0.152370000
H	-4.666516000	-2.039970000	-1.004545000
H	-3.562948000	2.224310000	1.287443000
H	-5.894920000	1.347797000	1.329497000
N	-1.531921000	1.163967000	0.095899000
C	-0.543077000	0.516582000	-0.411134000
C	-2.036387000	-1.353834000	-1.074831000
H	-2.221156000	-2.282947000	-1.603128000
C	-0.627619000	-0.944814000	-0.816258000
H	-0.012526000	-1.136045000	-1.699551000
C	-0.050546000	-1.851303000	0.335542000
H	-0.285112000	-2.886231000	0.071300000
H	-0.597982000	-1.613631000	1.251624000
C	1.433291000	-1.699461000	0.540156000
C	2.327034000	-2.351897000	-0.310239000
C	1.942378000	-0.859164000	1.530454000
C	3.698240000	-2.151742000	-0.191009000
H	1.942949000	-3.017869000	-1.077865000
C	3.312189000	-0.651593000	1.651208000
H	1.256378000	-0.343270000	2.195149000

C	4.193853000	-1.294456000	0.787273000
H	4.379561000	-2.664728000	-0.860139000
H	3.690415000	0.017954000	2.415036000
H	5.261329000	-1.130930000	0.877995000
C	0.759857000	1.228648000	-0.507359000
C	1.761694000	0.836605000	-1.399703000
C	1.007042000	2.311378000	0.345676000
C	2.984421000	1.497894000	-1.426915000
H	1.604311000	0.009921000	-2.080000000
C	2.230060000	2.965023000	0.324351000
H	0.228381000	2.614671000	1.034098000
C	3.226900000	2.557109000	-0.559709000
H	3.751451000	1.174792000	-2.120949000
H	2.410778000	3.790670000	1.002873000
H	4.185350000	3.062850000	-0.571901000



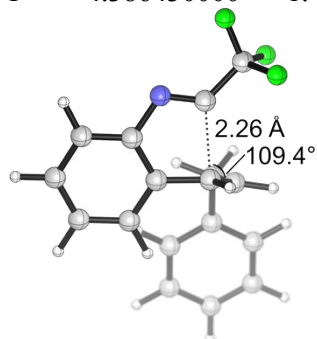
of imaginary frequencies: 0

E = -1009.70935770

symmetry c1

C	-0.092628000	3.962995000	0.012056000
C	0.229124000	2.893000000	0.837143000
C	-0.462513000	1.679399000	0.772328000
C	-1.529677000	1.590958000	-0.139292000
C	-1.872743000	2.673175000	-0.951808000
C	-1.144955000	3.850839000	-0.892555000
H	0.472987000	4.884536000	0.079209000
H	1.044314000	2.982775000	1.547016000
H	-2.714894000	2.566629000	-1.624511000

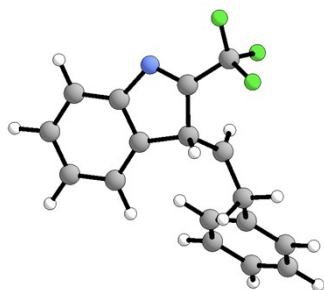
H	-1.407557000	4.681656000	-1.535594000
N	-2.356374000	0.453440000	-0.235723000
C	-2.122720000	-0.736983000	-0.082447000
C	-0.061592000	0.581769000	1.689967000
H	-0.260494000	0.752697000	2.744992000
C	0.575190000	-0.531212000	1.325601000
H	0.865525000	-1.235556000	2.101643000
C	0.996556000	-0.889529000	-0.073408000
H	0.572270000	-0.179700000	-0.788554000
H	0.606713000	-1.880526000	-0.324877000
C	2.506908000	-0.890488000	-0.191318000
C	3.197658000	0.322975000	-0.218463000
C	3.231939000	-2.079009000	-0.245598000
C	4.584252000	0.347586000	-0.305012000
H	2.635962000	1.251848000	-0.174142000
C	4.622720000	-2.058624000	-0.328078000
H	2.704843000	-3.027463000	-0.227383000
C	5.301604000	-0.845906000	-0.358541000
H	5.107673000	1.296339000	-0.332109000
H	5.173543000	-2.991069000	-0.371563000
H	6.382924000	-0.828449000	-0.426052000
C	-3.150608000	-1.840146000	-0.120055000
F	-3.193829000	-2.455555000	1.066351000
F	-2.813108000	-2.749548000	-1.040391000
F	-4.386430000	-1.420742000	-0.403864000



of imaginary frequencies: 1
E = -1009.70308064

symmetry c1

C	-0.574605000	3.415699000	0.392306000
C	-0.626108000	2.093049000	0.830053000
C	0.449593000	1.238617000	0.608152000
C	1.574047000	1.739782000	-0.065679000
C	1.633964000	3.055471000	-0.503891000
C	0.550971000	3.896500000	-0.270104000
H	-1.417416000	4.072363000	0.572865000
H	-1.503715000	1.719873000	1.346346000
H	2.519883000	3.399257000	-1.023644000
H	0.584729000	4.925234000	-0.607538000
N	2.648655000	0.845982000	-0.315910000
C	2.500839000	-0.310026000	0.106167000
C	0.454711000	-0.176423000	1.067336000
H	0.916121000	-0.367459000	2.034294000
C	-0.354763000	-1.132385000	0.540228000
H	-0.410205000	-2.094156000	1.042140000
C	-1.138527000	-0.984234000	-0.732271000
H	-0.930598000	-1.845256000	-1.376834000
H	-0.821107000	-0.086994000	-1.268052000
C	-2.629757000	-0.914323000	-0.460689000
C	-3.325364000	0.283248000	-0.620645000
C	-3.324929000	-2.043128000	-0.022358000
C	-4.689126000	0.354308000	-0.348139000
H	-2.793995000	1.165410000	-0.963990000
C	-4.685975000	-1.974844000	0.253706000
H	-2.797235000	-2.984417000	0.097411000
C	-5.372373000	-0.773984000	0.092687000
H	-5.217023000	1.291206000	-0.483680000
H	-5.213060000	-2.860428000	0.589487000
H	-6.433574000	-0.721026000	0.304841000
C	3.463816000	-1.446777000	-0.061585000
F	3.785739000	-1.961638000	1.132604000
F	4.602408000	-1.109325000	-0.673222000
F	2.893868000	-2.424458000	-0.779818000



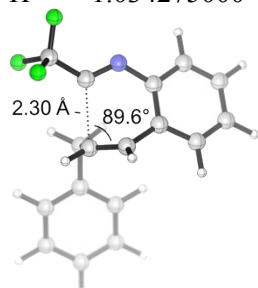
of imaginary frequencies: 0

E = -1009.74806166

symmetry c1

C	-0.615456000	3.648855000	-0.551852000
C	-0.231354000	2.355314000	-0.912698000
C	-1.037488000	1.303406000	-0.513672000
C	-2.198958000	1.538872000	0.227390000
C	-2.592460000	2.818088000	0.586921000
C	-1.777874000	3.875915000	0.186116000
H	-0.002023000	4.490741000	-0.850141000
H	0.673446000	2.187005000	-1.486863000
H	-3.498413000	2.978756000	1.158145000
H	-2.050341000	4.890448000	0.451133000
N	-2.875790000	0.326579000	0.539676000
C	-2.179167000	-0.610307000	0.031097000
C	-0.922062000	-0.195769000	-0.708190000
C	0.334234000	-0.807135000	-0.168072000
H	0.410827000	-0.965797000	0.901348000
C	1.535793000	-1.023398000	-1.028802000
H	1.423089000	-0.457290000	-1.962201000
H	1.599356000	-2.078276000	-1.331063000
C	2.840036000	-0.632158000	-0.362169000
C	3.968120000	-1.444711000	-0.468997000
C	2.941044000	0.563758000	0.352935000
C	5.173837000	-1.070101000	0.117475000
H	3.902138000	-2.380989000	-1.013735000
C	4.143982000	0.941709000	0.938866000
H	2.067673000	1.200307000	0.457429000

C	5.265731000	0.125765000	0.821841000
H	6.039567000	-1.716060000	0.028057000
H	4.204479000	1.872589000	1.490782000
H	6.202494000	0.417627000	1.281589000
C	-2.570113000	-2.054966000	0.192199000
F	-3.851134000	-2.208187000	0.508516000
F	-1.840194000	-2.647085000	1.151365000
F	-2.339177000	-2.730613000	-0.945855000
H	-1.034275000	-0.450974000	-1.770780000



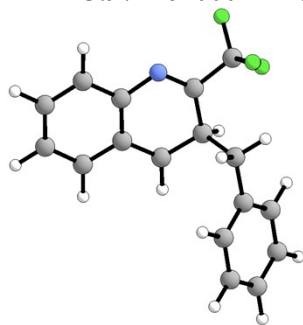
of imaginary frequencies: 1

E = -1009.70042623

symmetry c1

C	-0.365379000	4.046596000	0.169686000
C	0.037170000	2.954643000	0.926879000
C	-0.525259000	1.690128000	0.726682000
C	-1.566769000	1.567483000	-0.220415000
C	-1.985790000	2.672436000	-0.961253000
C	-1.369806000	3.902500000	-0.786780000
H	0.100386000	5.012186000	0.326585000
H	0.818944000	3.064700000	1.670633000
H	-2.799936000	2.545032000	-1.664352000
H	-1.686353000	4.753670000	-1.377138000
N	-2.302390000	0.370117000	-0.354356000
C	-1.879563000	-0.750832000	-0.048499000
C	-0.120222000	0.515323000	1.505357000
H	-0.234541000	0.559561000	2.584525000
C	0.213535000	-0.661484000	0.912461000
H	0.367793000	-1.522529000	1.559982000

C	0.817907000	-0.794342000	-0.472568000
H	0.475952000	0.017947000	-1.117754000
H	0.506898000	-1.738133000	-0.924978000
C	2.328602000	-0.752845000	-0.361390000
C	2.985791000	0.474843000	-0.258313000
C	3.080518000	-1.925659000	-0.324504000
C	4.368104000	0.528883000	-0.126470000
H	2.403791000	1.391768000	-0.282620000
C	4.466108000	-1.875354000	-0.189270000
H	2.579561000	-2.885039000	-0.407848000
C	5.112562000	-0.648415000	-0.090289000
H	4.866701000	1.488529000	-0.053124000
H	5.039037000	-2.795059000	-0.165572000
H	6.190595000	-0.607749000	0.011682000
C	-2.708925000	-2.005853000	-0.018238000
F	-2.739223000	-2.499513000	1.226710000
F	-2.161026000	-2.942363000	-0.806328000
F	-3.971262000	-1.836348000	-0.417937000



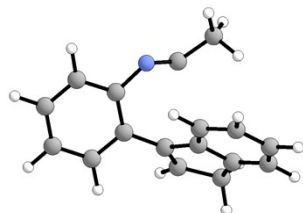
of imaginary frequencies: 0

E = -1009.77665909

symmetry c1

C	-2.767946000	3.516575000	0.199434000
C	-1.533261000	2.976848000	0.485480000
C	-1.312203000	1.577598000	0.379229000
C	-2.411331000	0.756564000	-0.011391000
C	-3.651170000	1.319406000	-0.293044000
C	-3.834894000	2.692889000	-0.196401000

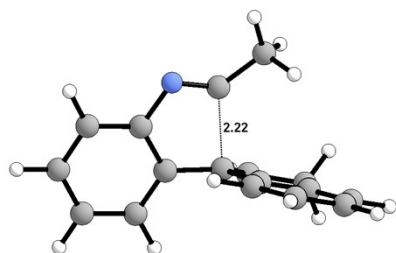
H	-2.919196000	4.586486000	0.281182000
H	-0.708508000	3.611865000	0.789888000
H	-4.460497000	0.660115000	-0.583378000
H	-4.801669000	3.127654000	-0.417162000
N	-2.283611000	-0.634526000	-0.090804000
C	-1.151824000	-1.168405000	0.130401000
C	-0.076536000	0.984064000	0.641429000
H	0.761236000	1.592855000	0.960565000
C	0.152796000	-0.474904000	0.438231000
H	0.575440000	-0.917778000	1.351174000
C	1.198566000	-0.747945000	-0.695536000
H	0.775815000	-0.407582000	-1.644206000
H	1.365416000	-1.825209000	-0.769231000
C	2.502077000	-0.044283000	-0.419350000
C	2.825182000	1.143418000	-1.075201000
C	3.386318000	-0.546525000	0.537671000
C	4.007171000	1.817916000	-0.782679000
H	2.142980000	1.543039000	-1.818871000
C	4.567543000	0.125392000	0.833873000
H	3.149051000	-1.474052000	1.050542000
C	4.880092000	1.311383000	0.174757000
H	4.245689000	2.737990000	-1.303327000
H	5.246829000	-0.278673000	1.575469000
H	5.800959000	1.834527000	0.403380000
C	-1.113867000	-2.682627000	0.000609000
F	-0.169768000	-3.211692000	0.800760000
F	-0.803517000	-3.050726000	-1.256333000
F	-2.269888000	-3.259109000	0.308298000



of imaginary frequencies: 0
E = -710.792157808

symmetry c1

C	3.700532000	-1.279829000	-0.627525000
C	2.379465000	-1.583344000	-0.321608000
C	1.461680000	-0.587587000	0.025300000
C	1.911173000	0.746904000	0.057554000
C	3.230475000	1.051646000	-0.276718000
C	4.126496000	0.044905000	-0.607128000
H	4.388949000	-2.072685000	-0.893768000
H	2.033410000	-2.610078000	-0.361954000
H	3.536921000	2.090774000	-0.257524000
H	5.151632000	0.294459000	-0.853920000
N	1.062929000	1.826627000	0.387702000
C	0.140188000	1.807753000	1.208076000
C	0.068154000	-0.963452000	0.342389000
C	-0.318030000	-1.874941000	1.253952000
H	0.351346000	-2.425786000	1.902395000
C	-1.816860000	-1.998757000	1.307126000
H	-2.204261000	-1.739637000	2.298894000
H	-2.157096000	-3.017359000	1.090358000
C	-2.264536000	-1.021654000	0.252168000
C	-3.538651000	-0.690252000	-0.183442000
C	-1.136024000	-0.421269000	-0.323683000
C	-3.675388000	0.245501000	-1.209558000
H	-4.415248000	-1.150418000	0.259934000
C	-1.269072000	0.500452000	-1.358092000
C	-2.550364000	0.829466000	-1.793990000
H	-4.663795000	0.517474000	-1.560979000
H	-0.395180000	0.960254000	-1.806802000
H	-2.676353000	1.548679000	-2.594943000
C	-0.916408000	2.809132000	1.488546000
H	-0.715233000	3.749432000	0.966517000
H	-1.866787000	2.395165000	1.136978000
H	-1.005784000	2.985299000	2.560700000



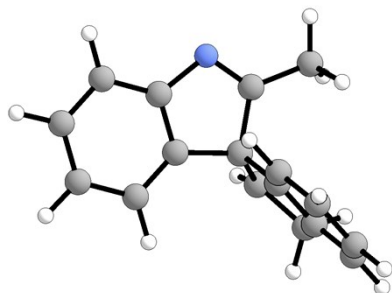
of imaginary frequencies: 1

E = -710.780950619

symmetry c1

C	3.446341000	-1.678438000	-0.059963000
C	2.131758000	-1.597982000	0.398142000
C	1.433367000	-0.398741000	0.313863000
C	2.074926000	0.724560000	-0.231366000
C	3.381706000	0.649841000	-0.693749000
C	4.066857000	-0.558914000	-0.605689000
H	3.983100000	-2.617137000	0.007690000
H	1.641208000	-2.469852000	0.816591000
H	3.847093000	1.536454000	-1.107008000
H	5.088189000	-0.624909000	-0.961438000
N	1.344326000	1.943812000	-0.272974000
C	0.216880000	1.895599000	0.250762000
C	0.025434000	-0.254860000	0.763112000
C	-0.430641000	-0.443556000	2.046181000
H	0.198367000	-0.457715000	2.926287000
C	-1.931032000	-0.545275000	2.085271000
H	-2.387629000	0.302867000	2.612902000
H	-2.274406000	-1.450449000	2.598903000
C	-2.299040000	-0.548239000	0.621598000
C	-3.538661000	-0.658505000	0.009047000
C	-1.140590000	-0.408294000	-0.151374000
C	-3.605763000	-0.636495000	-1.384853000
H	-4.442775000	-0.765334000	0.599104000
C	-1.200071000	-0.387531000	-1.539511000
C	-2.446902000	-0.505711000	-2.150718000
H	-4.566577000	-0.727000000	-1.877974000

H	-0.295764000	-0.275543000	-2.129322000
H	-2.518330000	-0.494955000	-3.232090000
C	-0.881146000	2.872320000	0.389709000
H	-0.631167000	3.820069000	-0.095097000
H	-1.786320000	2.453996000	-0.059381000
H	-1.085805000	3.044153000	1.448880000



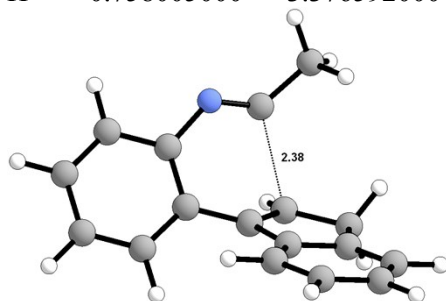
of imaginary frequencies: 0

E = -710.821087213

symmetry c1

C	2.990941000	-1.911124000	0.676615000
C	1.700282000	-1.438799000	0.930032000
C	1.325429000	-0.234222000	0.365253000
C	2.209127000	0.491540000	-0.437015000
C	3.490637000	0.030946000	-0.696126000
C	3.870939000	-1.184657000	-0.125477000
H	3.312901000	-2.852481000	1.106019000
H	1.011450000	-2.003134000	1.550336000
H	4.167123000	0.602696000	-1.319890000
H	4.866708000	-1.571770000	-0.307643000
N	1.624912000	1.698889000	-0.910856000
C	0.433342000	1.754476000	-0.442760000
C	0.032526000	0.544592000	0.426897000
C	-0.449487000	0.920667000	1.801394000
H	0.181787000	1.421626000	2.521741000
C	-1.883646000	0.547145000	2.028577000
H	-2.521673000	1.424283000	2.204221000
H	-2.012856000	-0.103222000	2.903168000
C	-2.250384000	-0.158358000	0.743137000

C	-3.457121000	-0.751731000	0.388457000
C	-1.179370000	-0.173005000	-0.147538000
C	-3.573370000	-1.354026000	-0.862046000
H	-4.296952000	-0.748399000	1.074867000
C	-1.287572000	-0.772323000	-1.396160000
C	-2.496467000	-1.364752000	-1.749421000
H	-4.508544000	-1.820412000	-1.149170000
H	-0.443018000	-0.779023000	-2.078219000
H	-2.602842000	-1.838207000	-2.718373000
C	-0.515792000	2.873890000	-0.696856000
H	-0.078326000	3.591392000	-1.388688000
H	-1.452208000	2.486281000	-1.108396000
H	-0.758005000	3.376592000	0.244234000



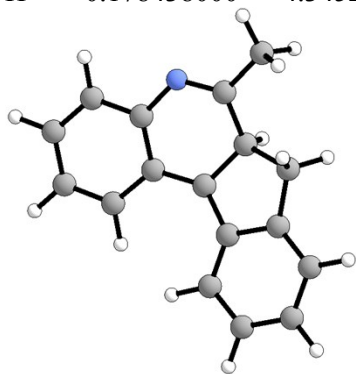
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E = -710.781746639

symmetry c1

C	2.971676000	-2.236476000	0.423883000
C	1.675012000	-1.816620000	0.686418000
C	1.263287000	-0.512688000	0.392345000
C	2.177231000	0.359822000	-0.239122000
C	3.476059000	-0.074457000	-0.511045000
C	3.878891000	-1.355313000	-0.164043000
H	3.276339000	-3.244204000	0.679380000
H	0.966736000	-2.491328000	1.155860000
H	4.152741000	0.609173000	-1.009986000
H	4.893531000	-1.674769000	-0.369879000
N	1.788513000	1.618640000	-0.740546000
C	0.879888000	2.337879000	-0.299703000

C	-0.091968000	-0.040109000	0.679704000
C	-0.377001000	1.131979000	1.320297000
H	0.301924000	1.654435000	1.979133000
C	-1.862963000	1.395936000	1.305283000
H	-2.111684000	2.368975000	0.868587000
H	-2.268799000	1.393105000	2.322679000
C	-2.395552000	0.247246000	0.485920000
C	-3.684974000	-0.032077000	0.066837000
C	-1.329853000	-0.600784000	0.134276000
C	-3.910609000	-1.177540000	-0.700177000
H	-4.509378000	0.622610000	0.328720000
C	-1.551558000	-1.735220000	-0.643718000
C	-2.853417000	-2.017741000	-1.050500000
H	-4.915288000	-1.414284000	-1.029937000
H	-0.727484000	-2.379092000	-0.930769000
H	-3.048709000	-2.897767000	-1.652332000
C	0.266348000	3.554153000	-0.892394000
H	0.851838000	3.906927000	-1.746358000
H	-0.742786000	3.302559000	-1.230574000
H	0.178438000	4.345239000	-0.146254000



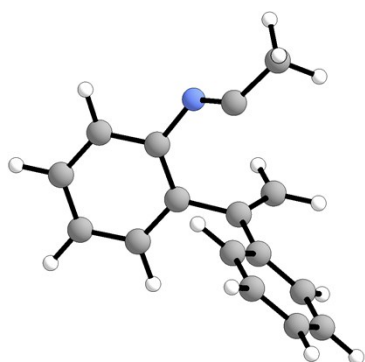
of imaginary frequencies: 0

E = -710.847898165

symmetry c1

C	2.681601000	-2.593341000	0.039889000
C	1.401152000	-2.082188000	0.147459000
C	1.165273000	-0.689631000	0.115649000

C	2.287825000	0.173556000	-0.062767000
C	3.567369000	-0.364218000	-0.178240000
C	3.773978000	-1.736209000	-0.119049000
H	2.835738000	-3.664954000	0.084528000
H	0.575613000	-2.762982000	0.295317000
H	4.391625000	0.323131000	-0.327470000
H	4.775663000	-2.139271000	-0.205428000
N	2.173770000	1.569239000	-0.210607000
C	1.055171000	2.144783000	0.015797000
C	-0.106900000	-0.069833000	0.228140000
C	-0.158240000	1.405401000	0.517184000
H	-0.149653000	1.534671000	1.616687000
C	-1.544580000	1.856975000	0.013291000
H	-1.471469000	2.231130000	-1.014442000
H	-1.995509000	2.640025000	0.624354000
C	-2.328079000	0.567978000	0.014211000
C	-3.694845000	0.405165000	-0.112560000
C	-1.456688000	-0.547384000	0.084897000
C	-4.223932000	-0.885336000	-0.179141000
H	-4.347771000	1.269641000	-0.166758000
C	-2.001328000	-1.840475000	-0.007601000
C	-3.376094000	-1.992785000	-0.134085000
H	-5.293810000	-1.028688000	-0.272124000
H	-1.377801000	-2.722255000	0.023982000
H	-3.795801000	-2.990111000	-0.195009000
C	0.944854000	3.631825000	-0.132044000
H	1.916644000	4.056587000	-0.375300000
H	0.229561000	3.889476000	-0.918002000
H	0.571366000	4.073221000	0.797732000



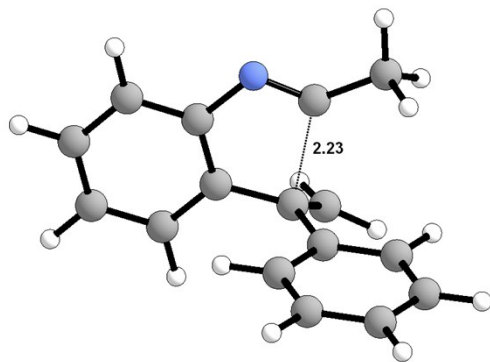
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E = -672.675469121

symmetry c1

C	2.282685000	-2.570827000	-0.037270000
C	1.146265000	-1.952463000	0.467714000
C	1.012902000	-0.561834000	0.471306000
C	2.051176000	0.207833000	-0.076921000
C	3.202035000	-0.412239000	-0.565815000
C	3.316350000	-1.794530000	-0.554737000
H	2.363920000	-3.650915000	-0.021108000
H	0.338770000	-2.550327000	0.877316000
H	3.993057000	0.212578000	-0.962827000
H	4.210202000	-2.263985000	-0.947730000
N	1.998876000	1.620849000	-0.138675000
C	1.008417000	2.281848000	-0.462167000
C	-0.214968000	0.041722000	1.073772000
C	-0.137724000	0.738584000	2.210270000
H	0.813913000	0.883081000	2.708674000
C	-2.706641000	-0.294344000	1.068345000
C	-3.908192000	-0.472824000	0.393403000
C	-1.501861000	-0.187434000	0.365434000
C	-3.925519000	-0.554681000	-0.996404000
H	-4.831865000	-0.560279000	0.953658000
C	-1.528599000	-0.290820000	-1.029523000
C	-2.731189000	-0.465244000	-1.704919000
H	-4.862376000	-0.698332000	-1.521566000

H	-0.599277000	-0.222367000	-1.584745000
H	-2.734750000	-0.533764000	-2.786490000
C	0.784193000	3.747353000	-0.475700000
H	1.694927000	4.286416000	-0.198752000
H	0.448799000	4.065214000	-1.463697000
H	-0.013101000	3.984761000	0.232302000
H	-2.697677000	-0.259046000	2.151776000
H	-1.012659000	1.200428000	2.653188000



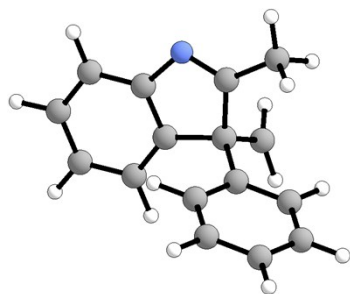
of imaginary frequencies: 1

E = -672.667238280

symmetry c1

C	3.238747000	-1.576203000	0.454521000
C	2.005550000	-1.235616000	1.009941000
C	1.287284000	-0.154548000	0.512585000
C	1.830764000	0.591379000	-0.543394000
C	3.058661000	0.260620000	-1.099758000
C	3.761263000	-0.831487000	-0.598119000
H	3.789706000	-2.422778000	0.846515000
H	1.592023000	-1.815440000	1.828056000
H	3.450895000	0.863426000	-1.909868000
H	4.720601000	-1.096705000	-1.026295000
N	1.094515000	1.715793000	-1.002706000
C	0.018836000	1.921776000	-0.417211000
C	-0.046463000	0.249790000	1.058090000
C	-0.100704000	0.743112000	2.332515000
H	0.806119000	1.052214000	2.837098000

C	-2.543342000	0.166512000	0.708419000
C	-3.675883000	-0.371946000	0.113178000
C	-1.267971000	-0.325458000	0.403565000
C	-3.559538000	-1.412408000	-0.806525000
H	-4.653087000	0.025382000	0.362584000
C	-1.162273000	-1.363611000	-0.525939000
C	-2.298591000	-1.902033000	-1.123963000
H	-4.443557000	-1.831302000	-1.272134000
H	-0.185730000	-1.757845000	-0.782251000
H	-2.193065000	-2.708871000	-1.839904000
C	-1.034653000	2.944959000	-0.562283000
H	-0.707715000	3.745428000	-1.231245000
H	-1.936789000	2.476733000	-0.963354000
H	-1.281525000	3.359617000	0.417763000
H	-2.650457000	0.991903000	1.403406000
H	-1.039143000	0.878666000	2.854847000



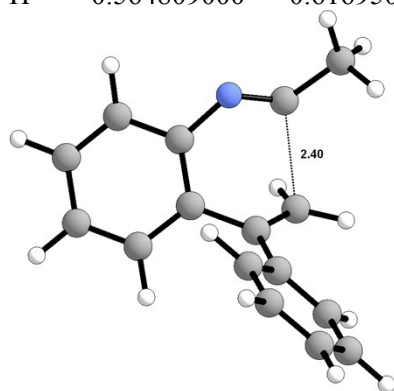
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E = -672.705880598

symmetry c1

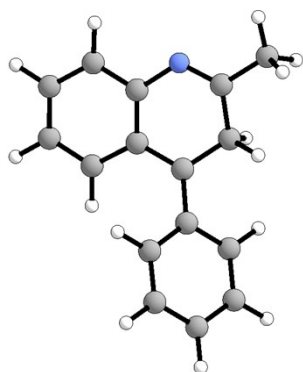
C	2.942809000	-1.823048000	0.648554000
C	1.688078000	-1.338523000	1.026363000
C	1.231967000	-0.175651000	0.431627000
C	2.006329000	0.498381000	-0.514809000
C	3.253890000	0.027295000	-0.894084000
C	3.713481000	-1.147224000	-0.297758000
H	3.322707000	-2.734442000	1.094775000
H	1.087043000	-1.865153000	1.760160000
H	3.842895000	0.559481000	-1.631144000

H	4.684074000	-1.541988000	-0.574210000
N	1.355585000	1.663791000	-1.001492000
C	0.227372000	1.749852000	-0.400741000
C	-0.045959000	0.621091000	0.618484000
C	-0.091113000	1.185678000	2.006611000
H	0.616121000	1.959657000	2.277309000
C	-2.546456000	0.212398000	0.790919000
C	-3.714980000	-0.424815000	0.382694000
C	-1.316342000	-0.127684000	0.226589000
C	-3.669372000	-1.407109000	-0.600050000
H	-4.661071000	-0.150247000	0.834529000
C	-1.280656000	-1.110388000	-0.765449000
C	-2.447715000	-1.745197000	-1.174976000
H	-4.578126000	-1.904901000	-0.916960000
H	-0.332929000	-1.382098000	-1.217607000
H	-2.400448000	-2.507647000	-1.943762000
C	-0.760560000	2.838204000	-0.640151000
H	-0.354453000	3.563732000	-1.342603000
H	-1.687862000	2.419521000	-1.041331000
H	-1.011109000	3.335235000	0.301686000
H	-2.595771000	0.985804000	1.549801000
H	-0.564809000	0.616950000	2.796852000



of imaginary frequencies: 1
 E = -672.668843344
 symmetry c1

C	2.094173000	-2.686447000	0.407739000
C	0.985532000	-1.918030000	0.730241000
C	0.952455000	-0.543763000	0.469613000
C	2.049133000	0.040947000	-0.197352000
C	3.155542000	-0.743186000	-0.538285000
C	3.190203000	-2.090706000	-0.218308000
H	2.106123000	-3.744570000	0.639841000
H	0.127224000	-2.373132000	1.213615000
H	3.975330000	-0.271041000	-1.066879000
H	4.060341000	-2.683092000	-0.475450000
N	2.023757000	1.369168000	-0.669888000
C	1.440810000	2.330258000	-0.151047000
C	-0.209299000	0.287375000	0.848657000
C	0.025747000	1.419420000	1.557207000
H	0.952037000	1.547854000	2.101457000
C	-2.712294000	0.329908000	0.971351000
C	-3.961238000	0.038178000	0.439289000
C	-1.539828000	-0.050559000	0.303362000
C	-4.066535000	-0.648546000	-0.768131000
H	-4.855791000	0.333881000	0.975196000
C	-1.660238000	-0.750952000	-0.904441000
C	-2.911069000	-1.043282000	-1.435484000
H	-5.041480000	-0.880764000	-1.180049000
H	-0.764383000	-1.055275000	-1.434062000
H	-2.982944000	-1.578675000	-2.375110000
C	1.208552000	3.699432000	-0.678079000
H	0.134706000	3.848052000	-0.810742000
H	1.559437000	4.444312000	0.037840000
H	1.715912000	3.836377000	-1.637610000
H	-0.763047000	2.137781000	1.754759000
H	-2.639638000	0.833835000	1.928428000



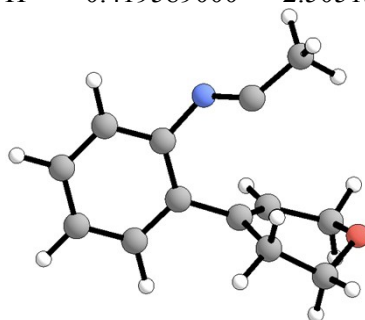
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E = -672.740151953

symmetry c1

C	-1.664581000	-2.887191000	-0.361173000
C	-0.623961000	-1.977327000	-0.364283000
C	-0.851560000	-0.599576000	-0.131633000
C	-2.196299000	-0.179893000	0.079624000
C	-3.228431000	-1.113570000	0.095028000
C	-2.974701000	-2.461639000	-0.122158000
H	-1.461358000	-3.933232000	-0.558341000
H	0.379009000	-2.315115000	-0.592324000
H	-4.233194000	-0.752286000	0.279909000
H	-3.788861000	-3.175996000	-0.114204000
N	-2.546760000	1.161353000	0.320035000
C	-1.671919000	2.070839000	0.133475000
C	0.173992000	0.391957000	-0.152016000
C	-0.263321000	1.810935000	-0.346485000
H	-0.232475000	2.093490000	-1.414889000
C	2.536179000	0.935874000	-0.690286000
C	3.898994000	0.696107000	-0.579526000
C	1.597113000	0.107695000	-0.047087000
C	4.366151000	-0.364289000	0.191951000
H	4.599849000	1.339845000	-1.098198000
C	2.089983000	-0.949567000	0.741977000
C	3.452780000	-1.179419000	0.857890000

H	5.429972000	-0.547795000	0.282578000
H	1.394150000	-1.565754000	1.298334000
H	3.805693000	-1.991228000	1.483264000
C	-2.032123000	3.505937000	0.370264000
H	-3.093437000	3.597895000	0.592261000
H	-1.449302000	3.904425000	1.206117000
H	-1.784576000	4.107955000	-0.509373000
H	2.192490000	1.761920000	-1.302503000
H	0.419589000	2.505155000	0.153755000



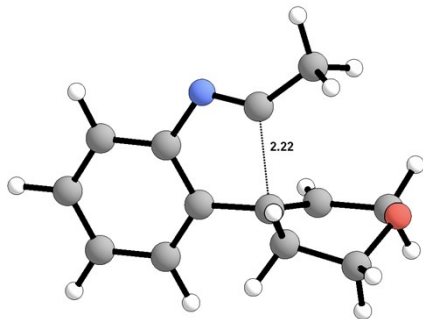
of imaginary frequencies: 0

E = -633.585596416

symmetry c1

C	-3.102131000	-1.656101000	0.022743000
C	-1.713896000	-1.716706000	-0.001882000
C	-0.932848000	-0.560772000	-0.068892000
C	-1.588043000	0.682801000	-0.093626000
C	-2.981719000	0.743075000	-0.089374000
C	-3.737561000	-0.418574000	-0.020825000
H	-3.683547000	-2.569192000	0.066288000
H	-1.213825000	-2.679679000	0.018553000
H	-3.454509000	1.716993000	-0.132998000
H	-4.819205000	-0.357919000	-0.007978000
N	-0.885014000	1.908548000	-0.168087000
C	0.165183000	2.169753000	0.424928000
C	0.551514000	-0.678126000	-0.108132000
C	1.245827000	-0.459156000	-1.223985000
H	0.736513000	-0.212469000	-2.151325000

C	2.748796000	-0.492455000	-1.252405000
H	3.132638000	0.396844000	-1.758393000
H	3.100560000	-1.370264000	-1.816935000
C	1.055946000	3.352576000	0.343671000
H	0.657213000	4.098757000	-0.349996000
H	1.180978000	3.793697000	1.333655000
H	2.041788000	3.023712000	0.006708000
C	1.256387000	-1.058671000	1.171874000
H	1.213383000	-0.213340000	1.868303000
H	0.732045000	-1.893333000	1.649388000
O	3.317705000	-0.490726000	0.040798000
C	2.699542000	-1.448343000	0.883775000
H	2.733996000	-2.435325000	0.400938000
H	3.293448000	-1.488309000	1.796787000



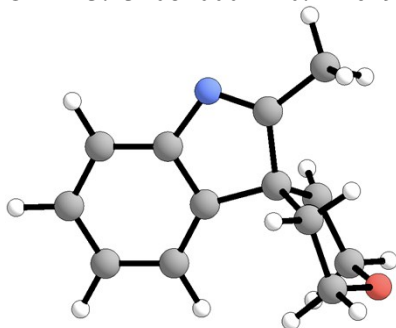
of imaginary frequencies: 1

E = -633.575337030

symmetry c1

C	3.171024000	-1.505843000	0.071634000
C	1.778696000	-1.585358000	0.088154000
C	1.008309000	-0.429111000	0.043753000
C	1.654630000	0.815362000	-0.015942000
C	3.040489000	0.901541000	-0.028447000
C	3.798464000	-0.265599000	0.011522000
H	3.762873000	-2.412721000	0.108246000
H	1.287130000	-2.551483000	0.139717000
H	3.507818000	1.878094000	-0.069872000
H	4.880229000	-0.205338000	-0.001033000

N	0.844252000	1.983041000	-0.034376000
C	-0.379473000	1.765968000	-0.128356000
C	-0.485655000	-0.447364000	0.045982000
C	-1.164987000	-0.618546000	1.215951000
H	-0.639689000	-0.587516000	2.165316000
C	-2.663200000	-0.683158000	1.246117000
H	-3.066636000	0.082480000	1.916016000
H	-3.002304000	-1.659489000	1.629175000
C	-1.555833000	2.659898000	-0.088014000
H	-2.160097000	2.409172000	0.787402000
H	-1.251897000	3.709215000	-0.036841000
H	-2.182696000	2.493493000	-0.966355000
C	-1.182076000	-0.779267000	-1.270681000
H	-1.167656000	0.076855000	-1.949148000
H	-0.622798000	-1.583179000	-1.761406000
C	-2.611389000	-1.246664000	-1.013687000
H	-3.222635000	-1.171002000	-1.912873000
H	-2.612731000	-2.293831000	-0.680501000
O	-3.234084000	-0.444649000	-0.024391000



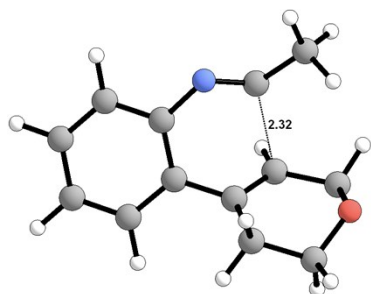
of imaginary frequencies: 0

E = -633.619320324

symmetry c1

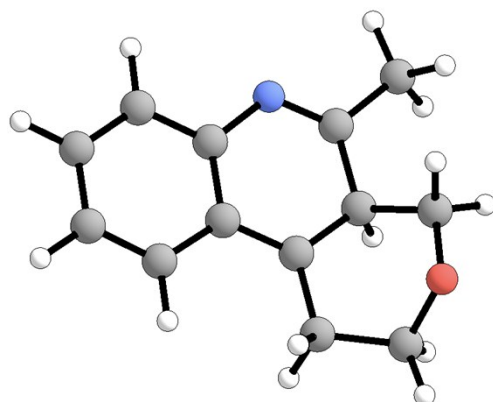
C	-2.540043000	-1.893288000	-0.017563000
C	-1.170356000	-1.612537000	-0.027586000
C	-0.766690000	-0.286985000	-0.002773000
C	-1.719496000	0.738699000	0.003974000
C	-3.079335000	0.470311000	0.012516000

C	-3.480461000	-0.865561000	0.005660000
H	-2.873794000	-2.924027000	-0.032066000
H	-0.456136000	-2.426634000	-0.062133000
H	-3.797796000	1.281018000	0.020316000
H	-4.536776000	-1.107580000	0.011805000
N	-1.118401000	2.024075000	-0.011463000
C	0.151639000	1.848010000	-0.023454000
C	0.596976000	0.382855000	-0.008075000
C	1.386100000	0.032711000	-1.238345000
H	1.024102000	0.381970000	-2.199247000
C	2.278804000	-1.162603000	-1.202900000
H	3.010425000	-1.123793000	-2.011644000
H	1.687650000	-2.087809000	-1.341249000
C	1.132468000	2.971596000	-0.038428000
H	0.624790000	3.905176000	-0.274138000
H	1.610162000	3.071605000	0.940695000
H	1.923549000	2.780724000	-0.768311000
C	1.435713000	0.083601000	1.257015000
H	2.194799000	0.862755000	1.371757000
H	0.791707000	0.096156000	2.139870000
C	2.158726000	-1.250993000	1.138004000
H	1.444387000	-2.083424000	1.077396000
H	2.797493000	-1.417619000	2.005803000
O	3.009998000	-1.263994000	0.006638000



of imaginary frequencies: 1
 E = -633.577994518
 symmetry c1

C	3.317179000	-1.347439000	0.155662000
C	1.950687000	-1.587326000	0.186524000
C	1.026700000	-0.539387000	0.117771000
C	1.513635000	0.776028000	-0.063253000
C	2.890536000	1.007856000	-0.110998000
C	3.787343000	-0.040839000	0.020841000
H	4.014483000	-2.172410000	0.238089000
H	1.580879000	-2.600802000	0.302673000
H	3.235902000	2.023108000	-0.266984000
H	4.852693000	0.155047000	-0.002459000
N	0.652753000	1.853663000	-0.352401000
C	-0.518995000	1.964741000	0.042704000
C	-0.424893000	-0.765790000	0.174718000
C	-1.175702000	-0.025436000	1.027732000
H	-0.718830000	0.432074000	1.898919000
C	-2.678214000	-0.090826000	1.007544000
H	-3.107130000	0.906474000	1.128615000
H	-3.035460000	-0.708659000	1.845925000
C	-1.578105000	2.911875000	-0.391471000
H	-1.177550000	3.646521000	-1.096082000
H	-2.374778000	2.340732000	-0.876623000
H	-2.014075000	3.422089000	0.469143000
C	-1.080528000	-1.621191000	-0.877543000
H	-0.974660000	-1.140836000	-1.858509000
H	-0.570852000	-2.588371000	-0.948377000
C	-2.553108000	-1.831190000	-0.549139000
H	-2.656266000	-2.531162000	0.291727000
H	-3.099303000	-2.231013000	-1.403274000
O	-3.172942000	-0.599360000	-0.212816000



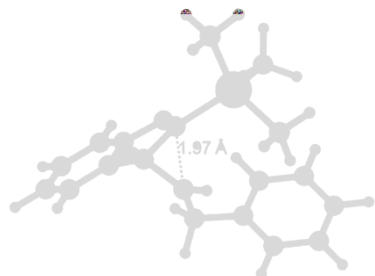
of imaginary frequencies: 0

E = -633.640023765

symmetry c1

C	3.249973000	-1.362988000	-0.099174000
C	1.899797000	-1.600797000	0.064218000
C	0.971218000	-0.528250000	0.113506000
C	1.477210000	0.800807000	-0.013547000
C	2.840500000	1.015077000	-0.179861000
C	3.730498000	-0.053070000	-0.222914000
H	3.941830000	-2.196551000	-0.131395000
H	1.539951000	-2.618155000	0.163702000
H	3.185398000	2.037974000	-0.275523000
H	4.790409000	0.128420000	-0.351740000
N	0.642142000	1.929245000	0.014126000
C	-0.615672000	1.787435000	0.189727000
C	-0.408597000	-0.715291000	0.279943000
C	-1.315959000	0.463194000	0.388338000
H	-1.743625000	0.489289000	1.406690000
C	-2.520113000	0.316052000	-0.590478000
H	-2.261379000	0.749521000	-1.559535000
H	-3.389734000	0.849202000	-0.186052000
C	-1.488591000	3.008148000	0.227160000
H	-0.873200000	3.905208000	0.207170000
H	-2.167931000	3.023464000	-0.630836000
H	-2.109649000	3.004857000	1.128207000

C	-1.065003000	-2.059526000	0.385653000
H	-0.701045000	-2.717323000	-0.410948000
H	-0.821616000	-2.548708000	1.339123000
O	-2.858050000	-1.035929000	-0.841341000
C	-2.578176000	-1.898746000	0.247509000
H	-3.025468000	-1.505835000	1.170004000
H	-3.057045000	-2.850913000	0.022496000



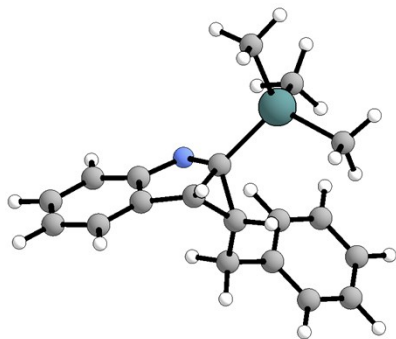
of imaginary frequencies: 1

E = -795.169316935

symmetry c1

C	-5.148660000	0.638303000	-0.239969000
C	-4.139955000	0.342079000	-1.157526000
C	-2.901998000	-0.045036000	-0.670564000
C	-2.660842000	-0.128217000	0.712500000
C	-3.665153000	0.182935000	1.630282000
C	-4.908663000	0.559678000	1.135851000
H	-6.128189000	0.935240000	-0.595138000
H	-4.326243000	0.414441000	-2.223273000
H	-3.471308000	0.122430000	2.694460000
H	-5.708991000	0.796238000	1.827498000
N	-1.353353000	-0.523091000	1.000774000
C	-0.733573000	-0.766864000	-0.155418000
C	-1.614950000	-0.379854000	-1.339739000
C	-0.623422000	0.738584000	-1.416800000
H	0.227273000	0.586299000	-2.072120000
C	-0.705378000	2.060350000	-0.722643000
H	-1.434139000	2.025055000	0.090053000
H	-1.054418000	2.824826000	-1.429186000

C	0.663505000	2.432532000	-0.193647000
C	1.097373000	1.927090000	1.034560000
C	1.542000000	3.198866000	-0.957861000
C	2.388792000	2.180667000	1.484403000
H	0.417191000	1.322275000	1.627974000
C	2.836436000	3.451879000	-0.510364000
H	1.211942000	3.596371000	-1.912771000
C	3.264155000	2.939761000	0.710391000
H	2.712903000	1.785142000	2.440454000
H	3.509267000	4.048484000	-1.115583000
H	4.270880000	3.135341000	1.060408000
H	-1.629955000	-1.021060000	-2.218635000
Sn	1.244072000	-1.619755000	-0.034123000
C	1.078177000	-3.664985000	-0.629569000
H	2.045013000	-4.165390000	-0.549844000
H	0.363728000	-4.189105000	0.007010000
H	0.737618000	-3.740001000	-1.663829000
C	1.824446000	-1.437786000	2.005465000
H	1.994598000	-2.420459000	2.447870000
H	2.738749000	-0.848994000	2.089644000
H	1.023800000	-0.940433000	2.555050000
C	2.606795000	-0.613910000	-1.332395000
H	2.305821000	-0.706392000	-2.377987000
H	2.668677000	0.446190000	-1.074438000
H	3.601141000	-1.053544000	-1.228610000



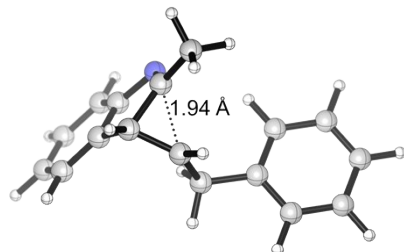
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E = -795.183876008

symmetry c1

C	-4.986030000	1.162174000	-0.203873000
C	-4.034230000	0.740662000	-1.135678000
C	-2.790315000	0.343271000	-0.677207000
C	-2.490273000	0.365920000	0.715065000
C	-3.452081000	0.815574000	1.643744000
C	-4.692154000	1.201714000	1.168577000
H	-5.967083000	1.470956000	-0.544809000
H	-4.269204000	0.729837000	-2.193943000
H	-3.211592000	0.839171000	2.699854000
H	-5.452665000	1.540016000	1.862447000
N	-1.228077000	-0.031407000	0.998700000
C	-0.608356000	-0.418342000	-0.227732000
C	-1.580838000	-0.131464000	-1.374506000
C	-0.331895000	0.718682000	-1.222822000
H	0.434792000	0.474021000	-1.954654000
C	-0.287274000	2.169150000	-0.797727000
H	-1.040615000	2.372564000	-0.033575000
H	-0.512785000	2.805866000	-1.657917000
C	1.095307000	2.483624000	-0.270156000
C	1.532971000	1.908393000	0.927318000
C	1.975532000	3.291332000	-0.988307000
C	2.822573000	2.141303000	1.392027000
H	0.851068000	1.278045000	1.491834000
C	3.268216000	3.525620000	-0.524290000
H	1.647011000	3.740971000	-1.920135000
C	3.695981000	2.949100000	0.666372000
H	3.147088000	1.693692000	2.325003000
H	3.939171000	4.157285000	-1.095200000
H	4.700901000	3.129212000	1.029846000
H	-1.659770000	-0.751530000	-2.259970000
Sn	0.881320000	-1.953175000	-0.013129000
C	-0.046456000	-3.870721000	-0.127870000
H	0.692638000	-4.662971000	0.004005000
H	-0.804802000	-3.972974000	0.649862000

H	-0.527452000	-4.006582000	-1.097970000
C	1.813532000	-1.635950000	1.875306000
H	2.214820000	-2.567940000	2.276525000
H	2.628192000	-0.917792000	1.771153000
H	1.079849000	-1.235262000	2.576580000
C	2.272343000	-1.663191000	-1.605755000
H	2.724701000	-0.672555000	-1.514376000
H	3.068124000	-2.408824000	-1.561993000
H	1.788860000	-1.737694000	-2.581934000



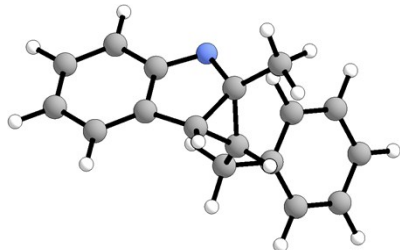
of imaginary frequencies: 1

E = -711.998474361

symmetry c1

C	3.876869000	-1.583225000	-0.192615000
C	3.170635000	-0.806719000	-1.113081000
C	2.272621000	0.129665000	-0.629803000
C	2.056651000	0.283570000	0.754461000
C	2.750198000	-0.505681000	1.672348000
C	3.663454000	-1.432473000	1.181047000
H	4.596405000	-2.312095000	-0.546041000
H	3.327977000	-0.935848000	-2.178176000
H	2.576910000	-0.387269000	2.735131000
H	4.222351000	-2.050096000	1.874544000
N	1.108350000	1.261635000	1.043536000
C	0.710248000	1.772971000	-0.115546000
C	1.314349000	1.050725000	-1.301980000
C	-0.088659000	0.521008000	-1.362427000
H	-0.800247000	1.092584000	-1.947187000
C	-0.552419000	-0.786858000	-0.808419000
H	0.117983000	-1.123865000	-0.013139000

H	-0.497648000	-1.550076000	-1.596718000
C	-1.967592000	-0.693046000	-0.281902000
C	-2.216226000	0.007750000	0.901363000
C	-3.036996000	-1.269642000	-0.963324000
C	-3.510817000	0.121594000	1.394143000
H	-1.382431000	0.458699000	1.432760000
C	-4.336284000	-1.153466000	-0.472908000
H	-2.853018000	-1.817255000	-1.882218000
C	-4.575687000	-0.458376000	0.706955000
H	-3.690872000	0.660174000	2.317456000
H	-5.158742000	-1.610157000	-1.011419000
H	-5.584659000	-0.369926000	1.092261000
C	-0.095607000	3.035062000	-0.178522000
H	1.632443000	1.629462000	-2.166658000
H	-0.991339000	2.954738000	0.440460000
H	-0.391683000	3.272544000	-1.200347000
H	0.509686000	3.859783000	0.205805000



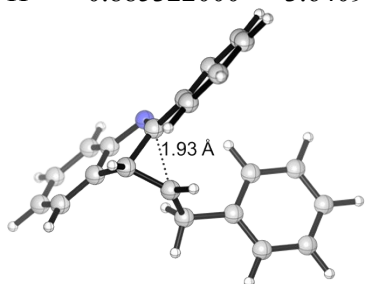
of imaginary frequencies: 0

E = -712.014390834

symmetry c1

C	4.001072000	-1.469470000	-0.323860000
C	3.308253000	-0.590433000	-1.164438000
C	2.312078000	0.195512000	-0.620364000
C	1.989397000	0.100294000	0.768649000
C	2.683386000	-0.806173000	1.600275000
C	3.686485000	-1.575337000	1.040050000
H	4.793462000	-2.084640000	-0.733468000
H	3.554879000	-0.531488000	-2.218303000
H	2.428795000	-0.873939000	2.651064000

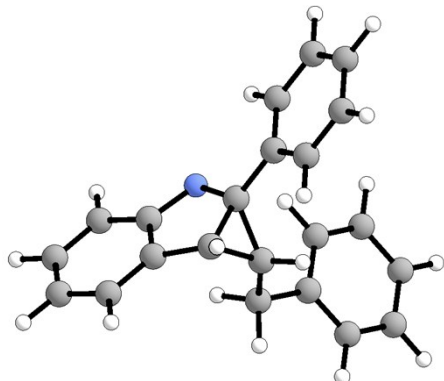
H	4.242173000	-2.269933000	1.658523000
N	0.989980000	0.918340000	1.149117000
C	0.564729000	1.641989000	-0.013053000
C	1.386477000	1.183963000	-1.209722000
C	-0.090184000	0.814301000	-1.115306000
H	-0.723432000	1.423991000	-1.754398000
C	-0.603614000	-0.597427000	-0.938832000
H	0.050281000	-1.166409000	-0.273335000
H	-0.585296000	-1.102569000	-1.908939000
C	-2.012407000	-0.597780000	-0.389214000
C	-2.260348000	-0.106398000	0.895884000
C	-3.084665000	-1.063373000	-1.148355000
C	-3.552322000	-0.088721000	1.408456000
H	-1.428400000	0.257095000	1.492070000
C	-4.380849000	-1.044951000	-0.637469000
H	-2.905088000	-1.447205000	-2.147668000
C	-4.617890000	-0.557710000	0.642623000
H	-3.729047000	0.290648000	2.408520000
H	-5.203438000	-1.411498000	-1.240772000
H	-5.624942000	-0.542837000	1.042523000
C	0.097768000	3.053547000	0.224569000
H	1.701909000	1.855234000	-1.998695000
H	-0.778030000	3.052055000	0.877528000
H	-0.173200000	3.531169000	-0.718517000
H	0.885322000	3.640949000	0.700685000



of imaginary frequencies: 1
 E = -903.710467836
 symmetry c1

C	-4.798450000	0.399189000	-0.232708000
C	-3.801797000	-0.007680000	-1.121803000
C	-2.588247000	-0.420231000	-0.600445000
C	-2.351276000	-0.413156000	0.789005000
C	-3.343614000	0.011282000	1.675443000
C	-4.565650000	0.409127000	1.146554000
H	-5.762574000	0.713728000	-0.613693000
H	-3.980836000	-0.001741000	-2.191068000
H	-3.155213000	0.020318000	2.742106000
H	-5.355425000	0.733313000	1.814234000
N	-1.076612000	-0.851637000	1.117714000
C	-0.467374000	-1.177837000	-0.023086000
C	-1.309178000	-0.838454000	-1.239887000
H	-1.334150000	-1.524871000	-2.082878000
C	-0.285463000	0.251327000	-1.312315000
H	0.618160000	0.033544000	-1.869601000
C	-0.453168000	1.645460000	-0.803676000
H	-1.193019000	1.672799000	0.001406000
H	-0.859002000	2.271471000	-1.610175000
C	0.859292000	2.219107000	-0.316359000
C	1.473280000	1.662542000	0.808485000
C	1.482493000	3.278612000	-0.971584000
C	2.687613000	2.157929000	1.267286000
H	0.987141000	0.839748000	1.324443000
C	2.700361000	3.777762000	-0.512587000
H	1.013334000	3.719147000	-1.845490000
C	3.305518000	3.217993000	0.606652000
H	3.152811000	1.717908000	2.141800000
H	3.174290000	4.603386000	-1.030972000
H	4.252866000	3.604347000	0.964094000
C	0.808985000	-1.921981000	-0.032329000
C	1.316320000	-2.489879000	-1.204628000
C	1.517444000	-2.086003000	1.162021000
C	2.512695000	-3.196829000	-1.185974000
H	0.776494000	-2.386476000	-2.139840000
C	2.714245000	-2.790246000	1.176967000

H	1.111681000	-1.661368000	2.072233000
C	3.217966000	-3.347078000	0.004077000
H	2.892445000	-3.633219000	-2.102298000
H	3.254660000	-2.908148000	2.108923000
H	4.150645000	-3.898175000	0.018129000



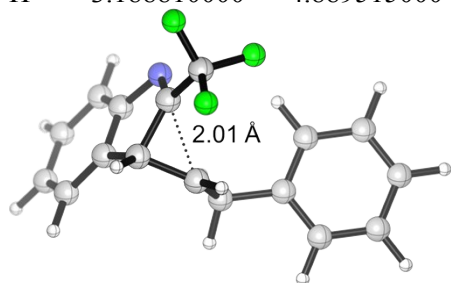
of imaginary frequencies: 0

E = -903.723173674

symmetry c1

C	4.736001000	-0.731244000	-0.187149000
C	3.793285000	-0.252299000	-1.105344000
C	2.559425000	0.146001000	-0.633431000
C	2.250341000	0.060734000	0.758281000
C	3.203143000	-0.445400000	1.669694000
C	4.438042000	-0.829473000	1.180771000
H	5.713816000	-1.037659000	-0.539136000
H	4.034157000	-0.197793000	-2.160626000
H	2.957402000	-0.512409000	2.722517000
H	5.190749000	-1.210976000	1.860208000
N	1.007755000	0.476316000	1.065269000
C	0.379923000	0.878621000	-0.154594000
C	1.346949000	0.649184000	-1.313922000
H	1.412512000	1.327241000	-2.155922000
C	0.128273000	-0.240341000	-1.181561000
H	-0.678711000	0.022681000	-1.859423000
C	0.176234000	-1.714430000	-0.849135000

H	0.956393000	-1.920830000	-0.112466000
H	0.444544000	-2.266202000	-1.755020000
C	-1.157698000	-2.204644000	-0.332051000
C	-1.709888000	-1.652176000	0.827392000
C	-1.863715000	-3.202142000	-1.002605000
C	-2.939174000	-2.093936000	1.303201000
H	-1.167739000	-0.875047000	1.358056000
C	-3.095389000	-3.646750000	-0.527429000
H	-1.445544000	-3.637070000	-1.904742000
C	-3.636537000	-3.092873000	0.627083000
H	-3.355254000	-1.657646000	2.204026000
H	-3.630125000	-4.424610000	-1.060427000
H	-4.595087000	-3.435718000	0.998720000
C	-0.600100000	2.000456000	-0.075469000
C	-1.068723000	2.631088000	-1.230759000
C	-1.073136000	2.429800000	1.165757000
C	-1.994871000	3.663947000	-1.148257000
H	-0.707555000	2.321612000	-2.206224000
C	-2.002379000	3.462489000	1.245907000
H	-0.703126000	1.951510000	2.063731000
C	-2.467680000	4.083535000	0.092034000
H	-2.345080000	4.143591000	-2.054848000
H	-2.360789000	3.784714000	2.216828000
H	-3.188810000	4.889515000	0.157367000



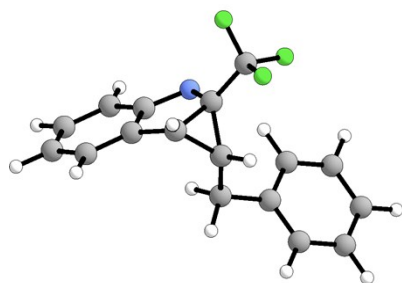
of imaginary frequencies: 1

E = -1009.73923858

symmetry c1

C	3.897207000	-2.165023000	-0.263191000
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C	3.142651000	-1.401109000	-1.154790000
C	2.301473000	-0.433001000	-0.634012000
C	2.198095000	-0.236960000	0.755818000
C	2.939710000	-1.008376000	1.647184000
C	3.793133000	-1.969860000	1.117297000
H	4.572589000	-2.920884000	-0.645442000
H	3.218160000	-1.564633000	-2.223641000
H	2.848584000	-0.851756000	2.714886000
H	4.390497000	-2.579771000	1.784666000
N	1.285907000	0.772722000	1.085745000
C	0.834085000	1.236063000	-0.053545000
C	1.313826000	0.488682000	-1.273460000
C	-0.090916000	-0.043119000	-1.302072000
H	-0.817879000	0.524474000	-1.870268000
C	-0.524887000	-1.327888000	-0.679207000
H	0.126324000	-1.586020000	0.161219000
H	-0.397637000	-2.133651000	-1.415892000
C	-1.962146000	-1.269541000	-0.215062000
C	-2.274188000	-0.585389000	0.961234000
C	-2.988234000	-1.858874000	-0.950029000
C	-3.590974000	-0.496426000	1.396530000
H	-1.476568000	-0.118741000	1.532091000
C	-4.309131000	-1.769511000	-0.516723000
H	-2.753395000	-2.395401000	-1.863795000
C	-4.612429000	-1.088752000	0.657333000
H	-3.821134000	0.035657000	2.312139000
H	-5.099100000	-2.234707000	-1.094866000
H	-5.639189000	-1.020185000	0.996813000
C	0.020453000	2.499654000	-0.075212000
F	0.743950000	3.530393000	0.382358000
F	-0.363892000	2.815954000	-1.323225000
F	-1.078638000	2.426373000	0.680344000
H	1.608238000	1.058662000	-2.151979000



of imaginary frequencies: 0

E = -1009.76206969

symmetry c1

C	4.002259000	-2.064529000	-0.258294000
C	3.303217000	-1.242296000	-1.150825000
C	2.311679000	-0.426226000	-0.649664000
C	2.000503000	-0.430308000	0.746535000
C	2.701757000	-1.279889000	1.631618000
C	3.699553000	-2.082198000	1.112866000
H	4.792238000	-2.704142000	-0.633155000
H	3.542959000	-1.250191000	-2.207543000
H	2.455392000	-1.277802000	2.686271000
H	4.262383000	-2.734715000	1.769209000
N	1.007156000	0.409461000	1.087352000
C	0.571647000	1.027507000	-0.122438000
C	1.378659000	0.520723000	-1.303367000
C	-0.096257000	0.169031000	-1.187709000
H	-0.723336000	0.752168000	-1.855247000
C	-0.625140000	-1.219502000	-0.906117000
H	0.027890000	-1.746425000	-0.206707000
H	-0.611843000	-1.785335000	-1.841597000
C	-2.032671000	-1.167135000	-0.356744000
C	-2.269079000	-0.627052000	0.910120000
C	-3.113332000	-1.633962000	-1.103038000
C	-3.560892000	-0.562708000	1.419274000
H	-1.433022000	-0.258624000	1.497018000
C	-4.408547000	-1.569919000	-0.594835000
H	-2.941696000	-2.055049000	-2.088649000

C	-4.635005000	-1.034387000	0.668038000
H	-3.729611000	-0.142819000	2.404228000
H	-5.238763000	-1.938047000	-1.186433000
H	-5.641752000	-0.982836000	1.065596000
C	0.146334000	2.454800000	0.023951000
F	-0.175536000	2.993681000	-1.164714000
F	-0.919509000	2.583314000	0.822511000
F	1.122742000	3.212052000	0.544924000
H	1.691672000	1.164476000	-2.115162000



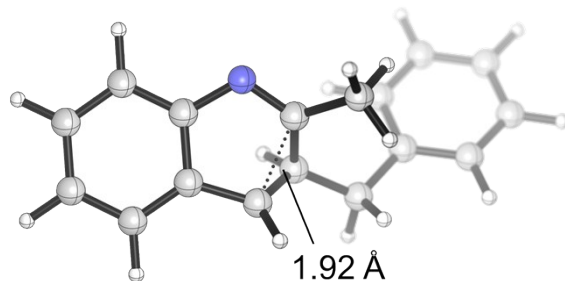
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E = -795.157463771

symmetry c1

C	-0.284763000	4.918696000	0.514384000
C	-0.735348000	3.674709000	0.968453000
C	-0.149840000	2.517950000	0.477719000
C	0.918515000	2.603602000	-0.451061000
C	1.361349000	3.846280000	-0.899593000
C	0.744397000	5.000161000	-0.421310000
H	-0.740965000	5.824599000	0.895085000
H	-1.547472000	3.614735000	1.684584000
H	2.193462000	3.897183000	-1.591888000
H	1.084775000	5.970458000	-0.762973000
N	1.556141000	1.398882000	-0.723352000
C	0.863830000	0.322832000	-0.375057000
C	-0.525364000	1.128550000	0.738562000
H	-0.685749000	0.717421000	1.729592000
C	-0.687505000	0.317333000	-0.458012000

H	-1.013299000	0.874973000	-1.340670000
C	-1.341262000	-1.038263000	-0.328929000
H	-0.943693000	-1.548680000	0.557644000
H	-1.066420000	-1.653752000	-1.191934000
C	-2.852983000	-0.998499000	-0.216803000
C	-3.577492000	0.190905000	-0.146087000
C	-3.552043000	-2.208681000	-0.180622000
C	-4.967795000	0.169510000	-0.041145000
H	-3.063829000	1.145555000	-0.171017000
C	-4.936220000	-2.232984000	-0.073805000
H	-2.999312000	-3.141681000	-0.238303000
C	-5.651194000	-1.039033000	-0.003364000
H	-5.514135000	1.104181000	0.010647000
H	-5.458821000	-3.182094000	-0.046861000
H	-6.731480000	-1.053750000	0.078659000
Sn	2.041837000	-1.433419000	0.081453000
C	1.728570000	-1.905757000	2.142078000
H	0.687290000	-2.171315000	2.335058000
H	2.355284000	-2.748816000	2.439078000
H	1.986045000	-1.047456000	2.765021000
C	1.448963000	-3.088739000	-1.135344000
H	0.568521000	-3.579998000	-0.717314000
H	1.215625000	-2.758821000	-2.148988000
H	2.256739000	-3.820827000	-1.191659000
C	4.059693000	-0.882747000	-0.284911000
H	4.734797000	-1.701509000	-0.030900000
H	4.195320000	-0.627206000	-1.336225000
H	4.321442000	-0.009372000	0.313264000



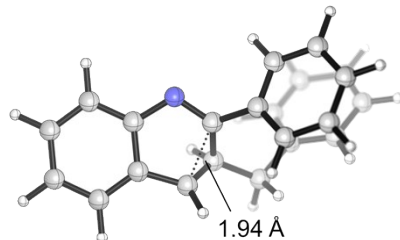
of imaginary frequencies: 1

E = -711.984775003

symmetry c1

C	4.737421000	-0.274790000	0.864480000
C	3.671393000	-1.156744000	0.648477000
C	2.517701000	-0.689127000	0.045339000
C	2.429006000	0.662903000	-0.370626000
C	3.491966000	1.534468000	-0.151741000
C	4.639763000	1.058840000	0.480291000
H	5.644366000	-0.636950000	1.333293000
H	3.746548000	-2.191553000	0.963317000
H	3.419892000	2.557846000	-0.499910000
H	5.472593000	1.730108000	0.652633000
N	1.308842000	0.968651000	-1.128602000
C	0.335870000	0.079141000	-1.021733000
C	1.248060000	-1.389631000	-0.187377000
H	1.160410000	-2.365567000	-0.650624000
C	0.080263000	-0.661043000	0.309709000
H	0.310915000	-0.012913000	1.157640000
C	-1.232129000	-1.404751000	0.457857000
H	-1.189500000	-1.950880000	1.407436000
H	-1.320861000	-2.166102000	-0.322053000
C	-2.468345000	-0.530000000	0.441776000
C	-2.444552000	0.786063000	0.904138000
C	-3.673548000	-1.045523000	-0.036910000
C	-3.597733000	1.565030000	0.890019000
H	-1.519654000	1.220144000	1.266960000
C	-4.828371000	-0.270979000	-0.050887000
H	-3.705515000	-2.064972000	-0.408810000
C	-4.793771000	1.039740000	0.413465000
H	-3.558056000	2.587051000	1.248260000
H	-5.753404000	-0.689394000	-0.430440000
H	-5.690311000	1.647999000	0.399777000
C	-0.676606000	-0.022818000	-2.132840000
H	-1.044655000	-1.042847000	-2.249810000
H	-1.538608000	0.616615000	-1.922642000

H -0.214369000 0.296184000 -3.065439000



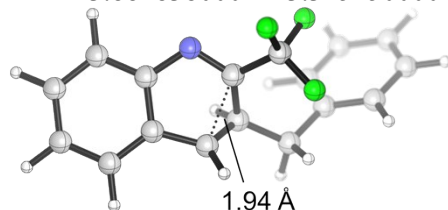
of imaginary frequencies: 1

E = -903.699210066

symmetry c1

C	-5.347551000	-0.396238000	0.254826000
C	-4.279554000	-0.264228000	1.149730000
C	-3.009735000	-0.014434000	0.657943000
C	-2.803018000	0.139666000	-0.736764000
C	-3.871422000	0.008032000	-1.620840000
C	-5.139593000	-0.275327000	-1.116615000
H	-6.342656000	-0.592062000	0.635638000
H	-4.443675000	-0.372998000	2.215971000
H	-3.705559000	0.152305000	-2.681879000
H	-5.975228000	-0.378154000	-1.798501000
N	-1.540554000	0.585953000	-1.099705000
C	-0.637857000	0.440635000	-0.145943000
C	-1.743371000	0.048517000	1.394743000
H	-1.596951000	0.610194000	2.310397000
C	-0.688067000	-0.777355000	0.816282000
H	-1.067144000	-1.643144000	0.268610000
C	0.556106000	-1.089578000	1.631456000
H	0.307263000	-1.936868000	2.279572000
H	0.800355000	-0.252662000	2.288961000
C	1.761158000	-1.427740000	0.780534000
C	1.669530000	-2.369108000	-0.246348000
C	2.981528000	-0.788070000	0.993758000
C	2.768415000	-2.653292000	-1.050280000
H	0.731513000	-2.883910000	-0.427143000
C	4.083670000	-1.070443000	0.193174000

H	3.061956000	-0.040851000	1.776712000
C	3.979293000	-2.001184000	-0.835421000
H	2.677814000	-3.384488000	-1.845338000
H	5.020638000	-0.553641000	0.366464000
H	4.834373000	-2.219162000	-1.464473000
C	0.590490000	1.279970000	-0.171291000
C	0.975238000	2.056402000	0.920633000
C	1.390163000	1.265470000	-1.316858000
C	2.156910000	2.790748000	0.879650000
H	0.342934000	2.100611000	1.800917000
C	2.569406000	1.997645000	-1.355450000
H	1.086403000	0.663480000	-2.165439000
C	2.960973000	2.756406000	-0.254561000
H	2.443545000	3.395259000	1.732545000
H	3.189194000	1.970199000	-2.244207000
H	3.882838000	3.325250000	-0.285022000



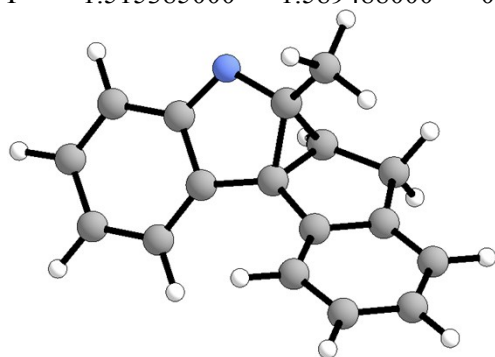
of imaginary frequencies: 1

E = -1009.72893076

symmetry c1

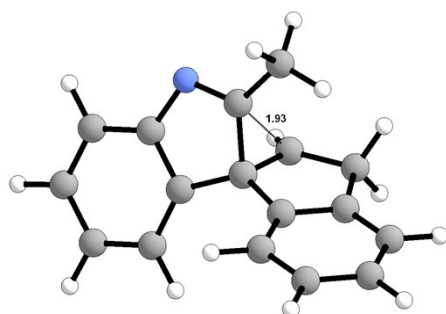
C	-4.926669000	-1.085763000	0.276624000
C	-3.857138000	-0.896587000	1.158974000
C	-2.674573000	-0.357813000	0.680805000
C	-2.573222000	0.040082000	-0.675871000
C	-3.643928000	-0.144156000	-1.546735000
C	-4.813454000	-0.727659000	-1.064151000
H	-5.852240000	-1.511569000	0.644755000
H	-3.947404000	-1.187335000	2.199218000
H	-3.560489000	0.190937000	-2.573507000
H	-5.651974000	-0.876746000	-1.733426000
N	-1.440414000	0.778384000	-0.982836000

C	-0.471897000	0.638727000	-0.102583000
C	-1.407917000	-0.176960000	1.392525000
H	-1.315027000	0.269648000	2.376226000
C	-0.235807000	-0.673549000	0.664158000
H	-0.474290000	-1.501529000	-0.007256000
C	1.047778000	-0.918442000	1.446410000
H	0.910058000	-1.883376000	1.946413000
H	1.165058000	-0.172390000	2.232741000
C	2.295026000	-0.967681000	0.592299000
C	2.352155000	-1.778184000	-0.543304000
C	3.411785000	-0.203547000	0.926438000
C	3.496190000	-1.815376000	-1.332057000
H	1.497373000	-2.387807000	-0.818637000
C	4.560485000	-0.241110000	0.141718000
H	3.377479000	0.437250000	1.801076000
C	4.604272000	-1.043818000	-0.992675000
H	3.521862000	-2.445853000	-2.213262000
H	5.418033000	0.363323000	0.413705000
H	5.495011000	-1.068426000	-1.609269000
C	0.533035000	1.769908000	-0.068296000
F	1.110068000	1.889539000	1.140550000
F	-0.034039000	2.945058000	-0.345946000
F	1.515385000	1.589488000	-0.961784000



of imaginary frequencies: 0
 E = -710.820272456
 symmetry c1

C	3.192887000	-1.982087000	0.409509000
C	1.816995000	-1.727660000	0.446737000
C	1.377611000	-0.457366000	0.133119000
C	2.304014000	0.576303000	-0.217097000
C	3.691295000	0.306087000	-0.225528000
C	4.114061000	-0.973552000	0.082300000
H	3.557133000	-2.975733000	0.642179000
H	1.116623000	-2.510078000	0.716506000
H	4.389164000	1.093340000	-0.483540000
H	5.171726000	-1.208245000	0.069437000
N	1.724582000	1.752335000	-0.515921000
C	0.304348000	1.585197000	-0.380631000
C	0.045340000	0.159735000	0.116264000
C	-0.147726000	1.373955000	1.047627000
H	0.582241000	1.556075000	1.827564000
C	-1.634951000	1.466473000	1.366805000
H	-2.065456000	2.425183000	1.059409000
H	-1.798558000	1.370401000	2.443125000
C	-2.259548000	0.304370000	0.617403000
C	-3.597338000	-0.053320000	0.540111000
C	-1.289906000	-0.452176000	-0.051966000
C	-3.956181000	-1.189414000	-0.187648000
H	-4.356086000	0.531596000	1.049057000
C	-1.642899000	-1.580148000	-0.782067000
C	-2.986738000	-1.948224000	-0.839286000
H	-4.997230000	-1.485391000	-0.242883000
H	-0.886761000	-2.157176000	-1.303223000
H	-3.279622000	-2.827052000	-1.401849000
C	-0.541347000	2.323072000	-1.383282000
H	-0.227638000	2.063609000	-2.395705000
H	-1.596624000	2.069469000	-1.275301000
H	-0.420498000	3.400192000	-1.247558000



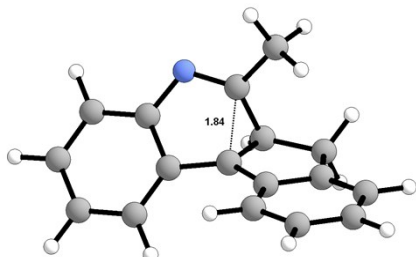
of imaginary frequencies: 1

E = -710.801413667

symmetry c1

C	3.167434000	-1.960617000	0.510382000
C	1.801316000	-1.677611000	0.548410000
C	1.384443000	-0.426109000	0.129385000
C	2.303565000	0.548685000	-0.308194000
C	3.670589000	0.268077000	-0.324083000
C	4.085394000	-0.995118000	0.083626000
H	3.522488000	-2.937242000	0.816694000
H	1.087354000	-2.419056000	0.890565000
H	4.377844000	1.017877000	-0.657653000
H	5.141308000	-1.239635000	0.067592000
N	1.687558000	1.731214000	-0.707371000
C	0.378177000	1.565960000	-0.554210000
C	0.054563000	0.235046000	0.110953000
C	-0.167222000	1.182057000	1.261898000
H	0.638501000	1.493445000	1.910998000
C	-1.631442000	1.263852000	1.590964000
H	-2.060974000	2.256617000	1.401949000
H	-1.799608000	1.053963000	2.653378000
C	-2.245654000	0.202362000	0.698650000
C	-3.572425000	-0.197177000	0.613847000
C	-1.279135000	-0.397490000	-0.114001000
C	-3.915459000	-1.214288000	-0.276021000
H	-4.330826000	0.264960000	1.236448000
C	-1.615961000	-1.406565000	-1.005800000

C	-2.945945000	-1.816605000	-1.076399000
H	-4.945724000	-1.543505000	-0.343455000
H	-0.857785000	-1.864253000	-1.631737000
H	-3.229841000	-2.608095000	-1.759727000
C	-0.607648000	2.515381000	-1.161467000
H	-0.526173000	2.452563000	-2.249210000
H	-1.634353000	2.273954000	-0.887817000
H	-0.382648000	3.540873000	-0.864065000



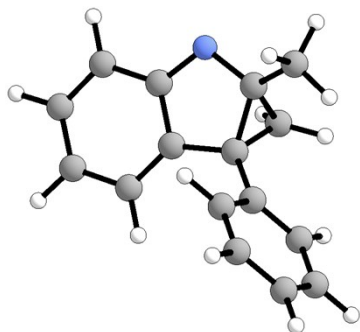
of imaginary frequencies: 1

E = -710.805651093

symmetry c1

C	3.318351000	-1.904213000	0.406833000
C	1.933409000	-1.707495000	0.503771000
C	1.410636000	-0.472357000	0.174676000
C	2.254314000	0.578448000	-0.262945000
C	3.630429000	0.378122000	-0.348347000
C	4.153243000	-0.867923000	-0.001978000
H	3.739824000	-2.871323000	0.652986000
H	1.285720000	-2.508985000	0.841735000
H	4.268852000	1.180053000	-0.699305000
H	5.221412000	-1.036463000	-0.070327000
N	1.584682000	1.705055000	-0.705290000
C	0.295782000	1.728008000	-0.339703000
C	0.036058000	0.024576000	0.301582000
C	-0.139157000	1.276104000	1.066657000
H	0.578655000	1.518074000	1.847006000
C	-1.630144000	1.389686000	1.387034000
H	-2.059355000	2.360816000	1.128304000
H	-1.777263000	1.248383000	2.461664000

C	-2.258806000	0.249665000	0.612033000
C	-3.597035000	-0.063840000	0.440368000
C	-1.264179000	-0.550692000	0.020263000
C	-3.935969000	-1.195736000	-0.304932000
H	-4.372144000	0.550945000	0.884895000
C	-1.601045000	-1.675120000	-0.733801000
C	-2.946860000	-1.993921000	-0.881924000
H	-4.979070000	-1.457567000	-0.436910000
H	-0.828255000	-2.279424000	-1.195422000
H	-3.232007000	-2.865834000	-1.458867000
C	-0.683464000	2.498199000	-1.179532000
H	-0.248488000	2.677595000	-2.160989000
H	-1.616430000	1.941844000	-1.304666000
H	-0.927605000	3.457444000	-0.713396000



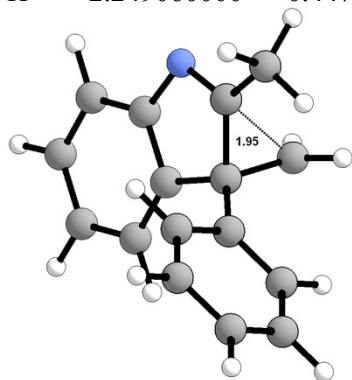
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E = -672.712690860

symmetry c1

C	2.654556000	-2.240322000	0.305458000
C	1.377062000	-1.718316000	0.543606000
C	1.158010000	-0.381439000	0.285990000
C	2.202453000	0.448690000	-0.219057000
C	3.490015000	-0.087480000	-0.436529000
C	3.695598000	-1.430051000	-0.172622000
H	2.844943000	-3.290194000	0.494611000
H	0.579471000	-2.352378000	0.914564000
H	4.280215000	0.549301000	-0.815369000
H	4.672104000	-1.868422000	-0.340976000

N	1.819106000	1.719336000	-0.457350000
C	0.443366000	1.824913000	-0.069608000
C	-0.048538000	0.470508000	0.447972000
C	0.185732000	1.619672000	1.411082000
H	1.039734000	1.561639000	2.075007000
C	-2.436696000	-0.005083000	1.117418000
C	-3.697475000	-0.521077000	0.826702000
C	-1.408820000	-0.074878000	0.178195000
C	-3.942148000	-1.116516000	-0.405345000
H	-4.486757000	-0.459990000	1.567017000
C	-1.662689000	-0.680019000	-1.057301000
C	-2.918705000	-1.196207000	-1.347997000
H	-4.922996000	-1.517985000	-0.630953000
H	-0.863657000	-0.741594000	-1.789547000
H	-3.101448000	-1.659012000	-2.310922000
C	-0.415522000	2.776139000	-0.855876000
H	-0.418412000	2.500188000	-1.912653000
H	-1.443611000	2.751754000	-0.490269000
H	-0.030670000	3.793631000	-0.763389000
H	-0.690804000	2.118604000	1.807223000
H	-2.249060000	0.447897000	2.084569000



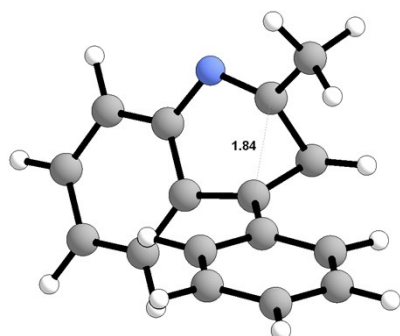
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E = -672.692672621

symmetry c1

C	2.703526000	-2.216555000	0.217323000
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C	1.433069000	-1.721815000	0.517790000
C	1.176992000	-0.387929000	0.257047000
C	2.160773000	0.453998000	-0.290840000
C	3.433889000	-0.036941000	-0.574213000
C	3.688594000	-1.380570000	-0.316634000
H	2.929451000	-3.260547000	0.398891000
H	0.667155000	-2.367449000	0.933775000
H	4.190815000	0.615202000	-0.992984000
H	4.667313000	-1.790029000	-0.538441000
N	1.694080000	1.751181000	-0.508942000
C	0.432263000	1.780871000	-0.112519000
C	-0.031786000	0.465258000	0.500856000
C	0.134588000	1.265871000	1.747183000
H	1.076090000	1.247376000	2.276961000
C	-2.328303000	-0.368155000	1.148362000
C	-3.575852000	-0.883294000	0.801925000
C	-1.391188000	-0.074204000	0.161456000
C	-3.892546000	-1.104658000	-0.533014000
H	-4.298929000	-1.108876000	1.577026000
C	-1.712476000	-0.304715000	-1.178334000
C	-2.956313000	-0.814985000	-1.524493000
H	-4.864129000	-1.501028000	-0.803199000
H	-0.977384000	-0.082045000	-1.946058000
H	-3.197855000	-0.987519000	-2.566719000
C	-0.473169000	2.934630000	-0.416271000
H	-0.640539000	2.975328000	-1.495619000
H	-1.441178000	2.821523000	0.072364000
H	-0.016850000	3.876102000	-0.108068000
H	-2.080722000	-0.197131000	2.190619000
H	-0.684177000	1.859986000	2.130303000



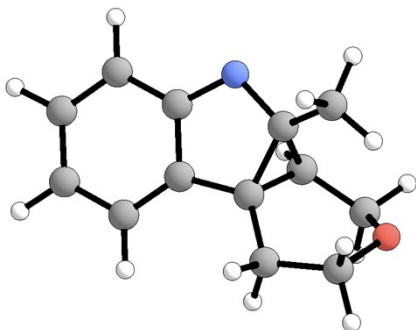
of imaginary frequencies: 1

E = -672.699222485

symmetry c1

C	2.857086000	-2.091836000	0.436776000
C	1.554587000	-1.650128000	0.704076000
C	1.192535000	-0.368573000	0.335459000
C	2.120893000	0.483570000	-0.305879000
C	3.416006000	0.040083000	-0.569498000
C	3.776660000	-1.250045000	-0.184558000
H	3.148278000	-3.097699000	0.714500000
H	0.840680000	-2.304926000	1.192184000
H	4.113490000	0.693285000	-1.080145000
H	4.779356000	-1.608004000	-0.386095000
N	1.590416000	1.689663000	-0.729288000
C	0.421993000	1.955264000	-0.134804000
C	-0.081868000	0.348043000	0.596324000
C	0.161400000	1.597753000	1.331386000
H	1.039776000	1.618165000	1.971827000
C	-2.572619000	0.295808000	0.848575000
C	-3.812010000	-0.218325000	0.490114000
C	-1.395534000	-0.193606000	0.260303000
C	-3.904660000	-1.233738000	-0.457507000
H	-4.708785000	0.169910000	0.958562000
C	-1.504330000	-1.219266000	-0.694976000
C	-2.743940000	-1.732582000	-1.045830000
H	-4.872375000	-1.634404000	-0.734396000

H	-0.605238000	-1.601629000	-1.164323000
H	-2.808069000	-2.522081000	-1.785464000
C	-0.557325000	2.886487000	-0.788537000
H	-0.366130000	2.937276000	-1.859401000
H	-1.581057000	2.537418000	-0.627958000
H	-0.474338000	3.889794000	-0.360858000
H	-2.519669000	1.069479000	1.605167000
H	-0.692078000	2.132320000	1.732878000



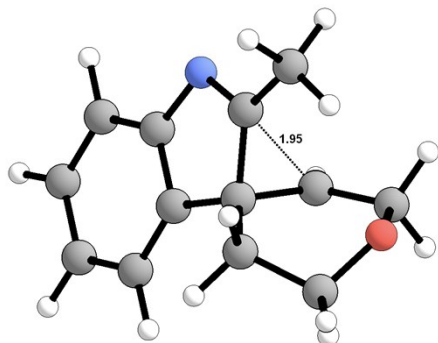
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E = -633.610337021

symmetry c1

C	3.302477000	-1.317608000	0.007133000
C	1.925652000	-1.558645000	-0.074708000
C	1.069820000	-0.475746000	-0.080520000
C	1.574415000	0.857260000	-0.008675000
C	2.965068000	1.083367000	0.093813000
C	3.810029000	-0.011604000	0.096075000
H	3.991052000	-2.154194000	0.002939000
H	1.548430000	-2.573625000	-0.134442000
H	3.341925000	2.097359000	0.152645000
H	4.881448000	0.135833000	0.160703000
N	0.616150000	1.798928000	-0.052204000
C	-0.656765000	1.131987000	-0.160356000
C	-0.400807000	-0.376059000	-0.125368000
C	-0.989305000	0.329642000	1.089992000
H	-0.340200000	0.485199000	1.947013000

C	-2.394092000	-0.110038000	1.435967000
H	-2.905042000	0.651115000	2.029202000
H	-2.322896000	-1.019768000	2.050471000
C	-1.670203000	1.909457000	-0.968094000
H	-1.364939000	1.939306000	-2.016476000
H	-2.671261000	1.494686000	-0.890077000
H	-1.687635000	2.935341000	-0.594403000
C	-2.736083000	-1.148895000	-0.747011000
H	-3.326365000	-2.069563000	-0.775998000
H	-2.937275000	-0.593743000	-1.667515000
O	-3.226599000	-0.334342000	0.316106000
C	-1.248959000	-1.495958000	-0.677495000
H	-0.914571000	-1.778755000	-1.679242000
H	-1.100406000	-2.369915000	-0.032764000



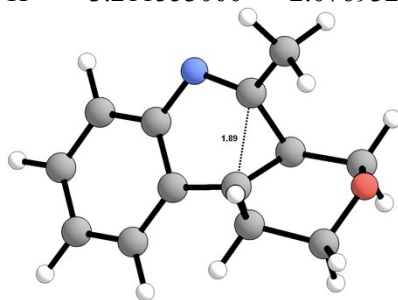
of imaginary frequencies: 1

E = -633.602610389

symmetry c1

C	3.170200000	-1.446139000	0.074765000
C	1.789499000	-1.566710000	-0.094505000
C	1.032716000	-0.409204000	-0.142420000
C	1.627676000	0.859377000	-0.012775000
C	3.004950000	0.977486000	0.172392000
C	3.764205000	-0.187721000	0.209643000
H	3.788291000	-2.335639000	0.101252000
H	1.329154000	-2.544887000	-0.190145000
H	3.460901000	1.955054000	0.273832000

H	4.837997000	-0.120682000	0.341256000
N	0.702323000	1.896429000	-0.106447000
C	-0.485724000	1.339461000	-0.301282000
C	-0.439624000	-0.178666000	-0.250755000
C	-1.022196000	0.094618000	1.106286000
H	-0.349325000	0.257344000	1.938248000
C	-2.483802000	-0.071045000	1.367752000
H	-2.962563000	0.875020000	1.645724000
H	-2.605461000	-0.759095000	2.220292000
C	-1.680503000	2.157418000	-0.683825000
H	-1.519348000	2.564070000	-1.685541000
H	-2.594379000	1.564535000	-0.695311000
H	-1.800278000	2.998679000	0.001112000
C	-1.307691000	-1.039113000	-1.172943000
H	-1.666676000	-0.438237000	-2.012010000
H	-0.703530000	-1.850824000	-1.585285000
O	-3.197192000	-0.566884000	0.250551000
C	-2.498682000	-1.608310000	-0.412749000
H	-2.168109000	-2.357048000	0.320496000
H	-3.211553000	-2.076932000	-1.090704000



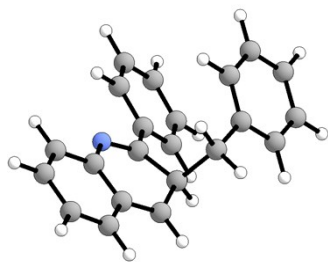
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E = -633.600628033

symmetry c1

C	3.311923000	-1.326185000	0.080489000
C	1.936584000	-1.561614000	-0.042756000
C	1.068242000	-0.485634000	-0.073439000
C	1.564735000	0.839256000	-0.010717000
C	2.933022000	1.066937000	0.112817000

C	3.799167000	-0.025070000	0.169852000
H	3.998520000	-2.163680000	0.105032000
H	1.560054000	-2.577589000	-0.097691000
H	3.306425000	2.083877000	0.137278000
H	4.865571000	0.143377000	0.262612000
N	0.614140000	1.822257000	-0.239341000
C	-0.634107000	1.383080000	-0.109249000
C	-0.402106000	-0.491810000	-0.102691000
C	-0.999499000	0.331631000	0.956011000
H	-0.398216000	0.441892000	1.859866000
C	-2.473263000	0.100665000	1.249423000
H	-2.983476000	1.035191000	1.487286000
H	-2.540771000	-0.560707000	2.123911000
C	-1.747568000	2.114235000	-0.806458000
H	-2.257098000	2.793273000	-0.115853000
H	-1.334389000	2.696257000	-1.628575000
H	-2.494823000	1.416768000	-1.188902000
O	-3.177387000	-0.477785000	0.167957000
C	-1.247456000	-1.367038000	-0.979483000
H	-1.440796000	-0.879004000	-1.941715000
H	-0.700703000	-2.289462000	-1.200216000
C	-2.571728000	-1.675420000	-0.287196000
H	-2.408667000	-2.352213000	0.562771000
H	-3.279194000	-2.139699000	-0.973695000



of imaginary frequencies: 0

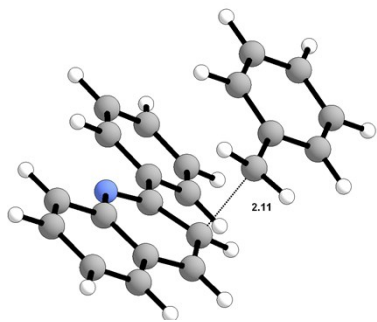
E = -903.747203454

symmetry c1

C	-3.089490000	-0.655017000	-0.485657000
C	-2.796364000	0.582309000	0.164594000

N	-1.531747000	1.163934000	0.095917000
C	-0.543015000	0.516510000	-0.411256000
C	-2.036398000	-1.353766000	-1.075026000
H	-2.221277000	-2.282889000	-1.603268000
C	-0.627603000	-0.944863000	-0.816410000
H	-0.012439000	-1.136104000	-1.699650000
C	-0.050672000	-1.851348000	0.335453000
H	-0.285223000	-2.886283000	0.071220000
H	-0.598230000	-1.613711000	1.251475000
C	1.433120000	-1.699504000	0.540223000
C	2.326902000	-2.351893000	-0.310173000
C	1.942141000	-0.859191000	1.530531000
C	3.698100000	-2.151768000	-0.190851000
H	1.942850000	-3.017857000	-1.077824000
C	3.311941000	-0.651538000	1.651282000
H	1.256102000	-0.343292000	2.195181000
C	4.193652000	-1.294426000	0.787414000
H	4.379460000	-2.664767000	-0.859932000
H	3.690122000	0.018058000	2.415089000
H	5.261120000	-1.130873000	0.878176000
C	0.759951000	1.228553000	-0.507483000
C	1.761824000	0.836541000	-1.399800000
C	1.007061000	2.311255000	0.345600000
C	2.984521000	1.497892000	-1.426942000
H	1.604492000	0.009853000	-2.080107000
C	2.230067000	2.964920000	0.324376000
H	0.228357000	2.614506000	1.033995000
C	3.226933000	2.557073000	-0.559679000
H	3.751588000	1.174878000	-2.120975000
H	2.410749000	3.790546000	1.002934000
H	4.185371000	3.062842000	-0.571827000
C	-3.813959000	1.284701000	0.809575000
C	-4.435040000	-1.111391000	-0.493494000
C	-5.113288000	0.796429000	0.821186000
H	-5.894693000	1.347867000	1.329728000
C	-5.421382000	-0.402376000	0.154700000

H	-6.440926000	-0.769431000	0.152412000
H	-3.562662000	2.224249000	1.287669000
H	-4.666549000	-2.039736000	-1.004694000



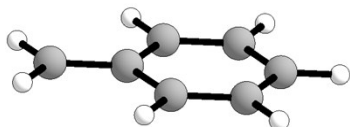
of imaginary frequencies: 1

E = -903.722653878

symmetry c1

C	-3.088326000	-0.553064000	-0.576101000
C	-2.744197000	0.594046000	0.193788000
N	-1.491214000	1.148865000	0.154849000
C	-0.542788000	0.557883000	-0.517765000
C	-2.063930000	-1.169537000	-1.315949000
H	-2.286502000	-2.037260000	-1.927908000
C	-0.740257000	-0.741570000	-1.146034000
H	0.008914000	-1.108588000	-1.834921000
C	-0.045510000	-2.021682000	0.386645000
H	-0.338665000	-2.941044000	-0.109149000
H	-0.730252000	-1.674769000	1.154613000
C	1.367140000	-1.800142000	0.588072000
C	2.321346000	-2.462068000	-0.207016000
C	1.823682000	-0.856977000	1.528193000
C	3.674005000	-2.187640000	-0.069957000
H	1.985364000	-3.194729000	-0.934708000
C	3.176002000	-0.584452000	1.661960000
H	1.097886000	-0.329794000	2.139369000
C	4.107825000	-1.245522000	0.862208000
H	4.395304000	-2.708394000	-0.689316000
H	3.508468000	0.151603000	2.385003000

H	5.164406000	-1.028423000	0.964922000
C	0.783102000	1.231900000	-0.563256000
C	1.800877000	0.817968000	-1.427858000
C	1.037563000	2.300496000	0.306077000
C	3.044495000	1.439482000	-1.409280000
H	1.642822000	0.002638000	-2.121450000
C	2.278494000	2.918928000	0.325060000
H	0.248387000	2.622921000	0.972857000
C	3.290891000	2.487446000	-0.529893000
H	3.823112000	1.096759000	-2.080609000
H	2.460580000	3.736996000	1.012452000
H	4.262975000	2.966268000	-0.510083000
C	-3.735857000	1.224316000	0.974516000
C	-5.023234000	0.739902000	0.992215000
C	-5.373446000	-0.387057000	0.214008000
H	-6.393269000	-0.752807000	0.230130000
C	-4.429718000	-1.016830000	-0.557422000
H	-4.690717000	-1.884812000	-1.153785000
H	-3.451117000	2.098263000	1.548630000
H	-5.778143000	1.228165000	1.596745000



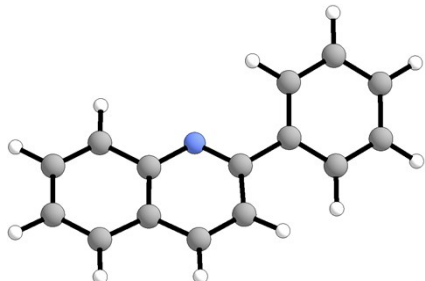
of imaginary frequencies: 0

E = -270.852270302

symmetry c1

C	-1.832372000	0.000010000	-0.000076000
C	-1.130176000	1.207180000	-0.000026000
C	0.252048000	1.212612000	0.000078000
C	0.986745000	-0.000003000	0.000131000
C	0.252031000	-1.212620000	0.000064000
C	-1.130187000	-1.207174000	-0.000027000
H	-2.915361000	0.000016000	-0.000153000
H	-1.671825000	2.145898000	-0.000065000
H	0.794084000	2.152060000	0.000114000
H	0.794033000	-2.152090000	0.000096000

H	-1.671848000	-2.145885000	-0.000063000
C	2.396345000	-0.000004000	0.000201000
H	2.952153000	0.928019000	-0.001077000
H	2.952158000	-0.928025000	-0.000920000



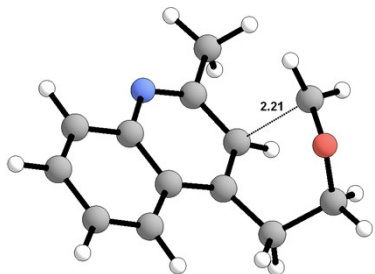
of imaginary frequencies: 0

E = -632.880211774

symmetry c1

C	-4.485117000	-0.173678000	0.044171000
C	-3.682601000	0.925066000	-0.118704000
C	-2.272714000	0.788658000	-0.103498000
C	-1.695234000	-0.494467000	0.079596000
C	-2.549874000	-1.614604000	0.245899000
C	-3.910517000	-1.455127000	0.228122000
H	-5.563167000	-0.067013000	0.033229000
H	-4.112151000	1.911176000	-0.260834000
H	-2.090555000	-2.585802000	0.386530000
H	-4.558192000	-2.314496000	0.355641000
N	-0.349888000	-0.694829000	0.106363000
C	0.449856000	0.337540000	-0.040863000
C	-1.385464000	1.879578000	-0.272864000
H	-1.788077000	2.874333000	-0.434086000
C	-0.038640000	1.662143000	-0.244240000
H	0.656672000	2.476126000	-0.400872000
C	1.913932000	0.073059000	-0.010582000
C	2.820892000	1.048310000	0.411574000
C	2.398740000	-1.177861000	-0.402896000
C	4.185396000	0.779745000	0.437634000
H	2.464105000	2.014382000	0.749651000

C	3.761795000	-1.442209000	-0.385027000
H	1.692092000	-1.932810000	-0.724377000
C	4.660071000	-0.464220000	0.035205000
H	4.876556000	1.541257000	0.779180000
H	4.125351000	-2.412889000	-0.701398000
H	5.723460000	-0.672049000	0.051620000



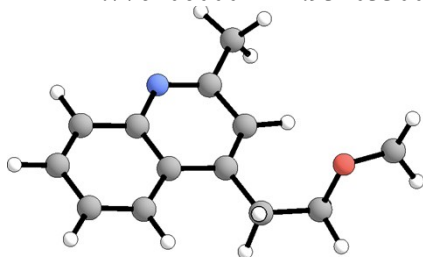
of imaginary frequencies: 1

E = -633.603816360

symmetry c1

C	-3.094247000	-1.413546000	0.080152000
C	-1.779165000	-1.575288000	-0.282905000
C	-0.885239000	-0.471839000	-0.311222000
C	-1.397078000	0.811856000	0.038554000
C	-2.750175000	0.947941000	0.408567000
C	-3.588510000	-0.142054000	0.434150000
H	-3.756833000	-2.271063000	0.093017000
H	-1.427961000	-2.560480000	-0.560840000
H	-3.100163000	1.939918000	0.668929000
H	-4.626622000	-0.026021000	0.721255000
N	-0.629751000	1.955097000	0.020596000
C	0.620148000	1.858357000	-0.320013000
C	0.481939000	-0.562199000	-0.686489000
C	1.254254000	0.597724000	-0.619894000
H	2.209435000	0.634806000	-1.135273000
C	2.416221000	0.066370000	1.181158000
H	1.954145000	0.558701000	2.029880000
H	3.402734000	0.410584000	0.865851000
C	1.463886000	3.099824000	-0.347698000

H	0.860710000	3.969189000	-0.093493000
H	2.286972000	3.011519000	0.368747000
H	1.907683000	3.242318000	-1.336691000
C	1.206791000	-1.862515000	-0.916227000
H	0.577537000	-2.709479000	-0.648354000
H	1.486444000	-1.984101000	-1.969368000
O	2.241932000	-1.283467000	1.203836000
C	2.484713000	-1.904589000	-0.054473000
H	3.321267000	-1.400061000	-0.550459000
H	2.776206000	-2.934033000	0.149988000



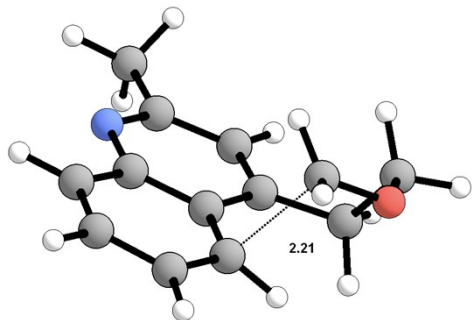
of imaginary frequencies: 0

E = -633.626179532

symmetry c1

C	-3.035059000	-1.905347000	0.120969000
C	-1.673415000	-1.809539000	-0.022485000
C	-1.035974000	-0.544362000	-0.064280000
C	-1.830609000	0.625008000	0.046112000
C	-3.233917000	0.498288000	0.191274000
C	-3.823925000	-0.738875000	0.227563000
H	-3.508701000	-2.879252000	0.154535000
H	-1.080756000	-2.713235000	-0.098801000
H	-3.813724000	1.410064000	0.271605000
H	-4.898322000	-0.826105000	0.339629000
N	-1.305861000	1.887048000	0.020797000
C	-0.009979000	2.012120000	-0.108377000
C	0.379073000	-0.381090000	-0.212977000
C	0.868463000	0.895092000	-0.226179000
H	1.931545000	1.089761000	-0.308205000
C	4.499145000	-0.238923000	0.521823000

H	4.924368000	0.095718000	1.456310000
H	5.124646000	-0.571877000	-0.299648000
C	0.572707000	3.398115000	-0.132784000
H	-0.215874000	4.135891000	0.001831000
H	1.316383000	3.515018000	0.659386000
H	1.077540000	3.582716000	-1.084655000
C	1.258073000	-1.600696000	-0.357263000
H	1.146044000	-2.235223000	0.528319000
H	0.906416000	-2.192532000	-1.208894000
O	3.261155000	-0.765856000	0.637545000
C	2.730246000	-1.316598000	-0.562571000
H	2.886455000	-0.610436000	-1.386213000
H	3.266810000	-2.242158000	-0.796085000



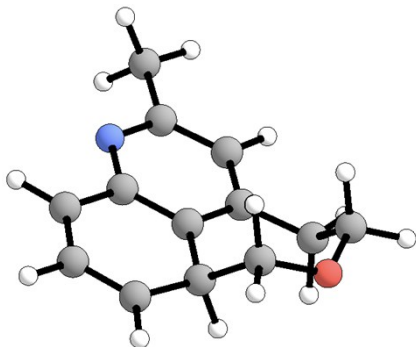
of imaginary frequencies: 1

E = -633.609604774

symmetry c1

C	-1.537937000	2.292824000	-0.502007000
C	-1.372011000	0.909845000	-0.624126000
C	-0.063000000	0.345134000	-0.409731000
C	0.991136000	1.179555000	0.036236000
C	0.747160000	2.564134000	0.244651000
C	-0.493868000	3.097397000	-0.024870000
H	-2.491593000	2.740432000	-0.755418000
H	-2.087594000	0.352127000	-1.217618000
H	1.570799000	3.176223000	0.590294000
H	-0.660193000	4.161028000	0.105238000
N	2.250260000	0.712738000	0.278094000

C	2.488661000	-0.565881000	0.101333000
C	0.200003000	-1.043673000	-0.536605000
C	1.479059000	-1.480644000	-0.294407000
H	1.726796000	-2.533262000	-0.385631000
C	-2.440537000	-0.105852000	1.028653000
H	-3.269787000	0.566267000	1.215194000
H	-1.647025000	-0.161357000	1.773401000
C	3.888420000	-1.064002000	0.337418000
H	3.886866000	-1.937852000	0.992811000
H	4.347807000	-1.363481000	-0.608658000
H	4.490598000	-0.275999000	0.785771000
C	-0.898185000	-2.032816000	-0.844872000
H	-1.485624000	-1.722399000	-1.713554000
H	-0.438565000	-2.991787000	-1.096731000
O	-2.851120000	-1.283237000	0.489061000
C	-1.853662000	-2.285577000	0.328842000
H	-1.288792000	-2.389331000	1.263447000
H	-2.407982000	-3.206545000	0.149218000



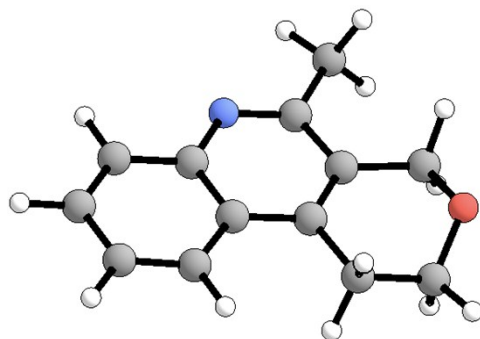
of imaginary frequencies: 0

E = -633.649578820

symmetry c1

C	1.696635000	2.164631000	0.331359000
C	1.517834000	0.680096000	0.408130000
C	0.076471000	0.240870000	0.258872000
C	-0.946740000	1.172442000	-0.024493000
C	-0.636403000	2.570443000	-0.138405000

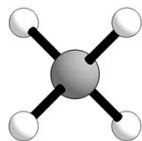
C	0.673904000	3.027325000	0.056470000
H	2.700350000	2.544245000	0.489161000
H	1.895420000	0.337347000	1.384578000
H	-1.450284000	3.248267000	-0.358864000
H	0.876440000	4.090924000	-0.003644000
N	-2.238447000	0.819985000	-0.192802000
C	-2.569703000	-0.459431000	-0.075950000
C	-0.283433000	-1.103751000	0.378633000
C	-1.621614000	-1.446762000	0.211778000
H	-1.932882000	-2.481669000	0.300042000
C	2.454788000	0.009797000	-0.632539000
H	3.384129000	0.579541000	-0.684212000
H	1.974574000	0.034705000	-1.620483000
C	-4.022428000	-0.803311000	-0.263145000
H	-4.375048000	-0.422444000	-1.223214000
H	-4.187431000	-1.880072000	-0.225321000
H	-4.620035000	-0.328460000	0.518005000
C	0.742248000	-2.173344000	0.657328000
H	1.231944000	-1.990325000	1.620251000
H	0.234685000	-3.137939000	0.732432000
O	2.841842000	-1.302923000	-0.297929000
C	1.831277000	-2.283737000	-0.413712000
H	1.380223000	-2.242399000	-1.414851000
H	2.345293000	-3.239837000	-0.306789000



of imaginary frequencies: 0
 E = -633.098679483

symmetry c1

C	3.236447000	-1.403687000	-0.052660000
C	1.879872000	-1.611677000	-0.051119000
C	0.981658000	-0.516050000	-0.012878000
C	1.507283000	0.799246000	0.020320000
C	2.911251000	0.986730000	0.024737000
C	3.757737000	-0.091162000	-0.011196000
H	3.913331000	-2.249056000	-0.086567000
H	1.491790000	-2.622428000	-0.089227000
H	3.282856000	2.004134000	0.054253000
H	4.830720000	0.059859000	-0.009932000
N	0.713058000	1.909374000	0.050536000
C	-0.585682000	1.750828000	0.027716000
C	-0.437859000	-0.665440000	-0.012199000
C	-1.213431000	0.464827000	-0.018320000
C	-2.721131000	0.372245000	-0.062826000
H	-3.121543000	1.057403000	-0.812490000
H	-3.141315000	0.665800000	0.912385000
C	-1.435035000	2.993022000	0.042136000
H	-0.802143000	3.858935000	0.224304000
H	-1.942126000	3.124745000	-0.918393000
H	-2.206283000	2.940671000	0.815035000
C	-1.082721000	-2.028726000	-0.000336000
H	-0.974487000	-2.494350000	-0.985614000
H	-0.578376000	-2.676258000	0.722124000
O	-3.180675000	-0.913063000	-0.413925000
C	-2.556121000	-1.917496000	0.363462000
H	-2.666366000	-1.678833000	1.430510000
H	-3.085672000	-2.847698000	0.160242000

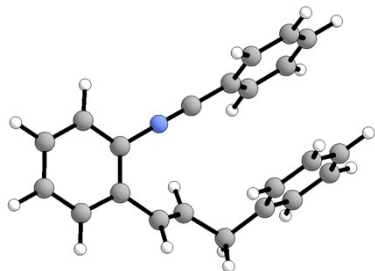


of imaginary frequencies: 0

E = -40.4969544741

symmetry td

C	0.000000000	0.000000000	0.000000000
H	0.628926000	0.628926000	0.628926000
H	-0.628926000	-0.628926000	0.628926000
H	-0.628926000	0.628926000	-0.628926000
H	0.628926000	-0.628926000	-0.628926000



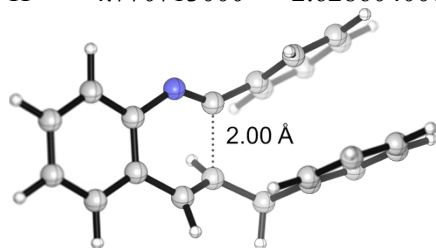
of imaginary frequencies: 0

E = -903.534997691

symmetry c1

C	5.452190000	-0.153575000	0.123921000
C	4.513364000	0.858452000	0.272439000
C	3.145305000	0.608251000	0.142954000
C	2.779017000	-0.725185000	-0.103353000
C	3.705703000	-1.757259000	-0.258172000
C	5.053054000	-1.461389000	-0.148958000
H	6.505910000	0.077560000	0.220106000
H	4.836137000	1.872244000	0.478513000
H	3.360395000	-2.765483000	-0.448144000
H	5.787776000	-2.247043000	-0.267204000
N	1.427711000	-1.065973000	-0.142767000
C	0.312275000	-1.338536000	-0.147245000
C	2.160429000	1.694791000	0.286859000
H	2.329642000	2.388914000	1.106619000
C	1.128065000	1.881017000	-0.536008000
H	1.001362000	1.225654000	-1.397154000
C	0.067979000	2.923582000	-0.346989000
H	-0.054891000	3.505722000	-1.263536000
H	0.365779000	3.613138000	0.447634000
C	-1.254341000	2.267311000	0.012937000

C	-2.390284000	2.441929000	-0.776701000
C	-1.351231000	1.485543000	1.166866000
C	-3.603333000	1.863685000	-0.410767000
H	-2.332256000	3.051577000	-1.672528000
C	-2.561111000	0.907772000	1.536081000
H	-0.470760000	1.342093000	1.787194000
C	-3.692646000	1.099353000	0.748160000
H	-4.480796000	2.020271000	-1.027683000
H	-2.622862000	0.314810000	2.441731000
H	-4.637640000	0.653568000	1.036015000
C	-1.060281000	-1.677454000	-0.188967000
C	-1.581063000	-2.533305000	0.792372000
C	-1.858263000	-1.147641000	-1.212854000
C	-2.922798000	-2.868210000	0.730592000
H	-0.941547000	-2.920985000	1.575236000
C	-3.195740000	-1.501226000	-1.255487000
H	-1.436723000	-0.469615000	-1.944396000
C	-3.722321000	-2.358049000	-0.291048000
H	-3.345470000	-3.530997000	1.474587000
H	-3.831141000	-1.100154000	-2.034547000
H	-4.770713000	-2.628604000	-0.332869000



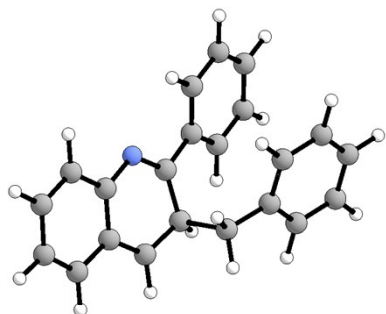
of imaginary frequencies: 1

E = -903.500766314

symmetry c1

C	5.317747000	-0.513574000	-0.116623000
C	4.225108000	-1.071446000	0.529644000
C	2.961569000	-0.473524000	0.440436000
C	2.824307000	0.676523000	-0.375481000
C	3.906040000	1.202340000	-1.065291000

C	5.158115000	0.616971000	-0.915783000
H	6.293675000	-0.970694000	-0.013431000
H	4.344553000	-1.959717000	1.138951000
H	3.754820000	2.060616000	-1.707034000
H	6.008789000	1.035419000	-1.438873000
N	1.556202000	1.231521000	-0.565686000
C	0.497750000	0.955384000	-0.051025000
C	1.789413000	-1.093747000	0.999177000
H	1.777304000	-2.182771000	1.020835000
C	0.672595000	-0.408166000	1.406166000
H	0.870472000	0.562533000	1.880284000
C	-0.594044000	-1.124893000	1.829108000
H	-1.128953000	-0.520982000	2.562922000
H	-0.295557000	-2.046791000	2.340417000
C	-1.538190000	-1.472456000	0.690563000
C	-2.899085000	-1.201523000	0.816957000
C	-1.074140000	-2.059556000	-0.486825000
C	-3.779735000	-1.497160000	-0.218727000
H	-3.272771000	-0.742737000	1.726581000
C	-1.951766000	-2.353953000	-1.525185000
H	-0.020645000	-2.291483000	-0.608782000
C	-3.307960000	-2.068757000	-1.395467000
H	-4.834131000	-1.272749000	-0.106950000
H	-1.576429000	-2.810385000	-2.433562000
H	-3.991936000	-2.296660000	-2.204073000
C	-0.877538000	1.415026000	-0.022531000
C	-1.630023000	1.267951000	-1.191747000
C	-1.428121000	1.974650000	1.132186000
C	-2.947597000	1.701658000	-1.197937000
H	-1.188831000	0.809514000	-2.068110000
C	-2.744722000	2.408974000	1.106264000
H	-0.835444000	2.078838000	2.034432000
C	-3.503239000	2.266968000	-0.053823000
H	-3.542382000	1.588179000	-2.095638000
H	-3.179884000	2.855837000	1.991282000
H	-4.534975000	2.597248000	-0.063779000



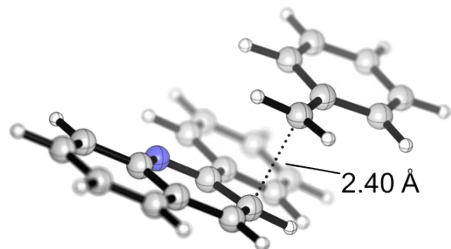
of imaginary frequencies: 0

E = -903.548402102

symmetry c1

C	-5.403479000	-0.427731000	0.139505000
C	-4.423923000	-1.140090000	-0.477830000
C	-3.075351000	-0.649275000	-0.469628000
C	-2.765505000	0.616557000	0.157319000
C	-3.805645000	1.314522000	0.796144000
C	-5.081074000	0.799428000	0.785533000
H	-6.425250000	-0.783417000	0.151199000
H	-4.631168000	-2.082881000	-0.971043000
H	-3.577983000	2.258610000	1.273706000
H	-5.874929000	1.349380000	1.278437000
N	-1.530739000	1.186095000	0.113827000
C	-0.533258000	0.539781000	-0.428051000
C	-2.031574000	-1.355078000	-0.995528000
H	-2.197452000	-2.329376000	-1.448952000
C	-0.654392000	-0.891526000	-0.839915000
H	-0.048646000	-1.145209000	-1.710459000
C	-0.063761000	-1.826638000	0.353277000
H	-0.304417000	-2.854395000	0.079306000
H	-0.612903000	-1.569574000	1.260455000
C	1.414508000	-1.657660000	0.530601000
C	2.303266000	-2.329133000	-0.310829000
C	1.916684000	-0.809591000	1.518249000
C	3.674000000	-2.146795000	-0.174175000
H	1.921147000	-3.000948000	-1.074150000

C	3.287426000	-0.623305000	1.654424000
H	1.230794000	-0.287098000	2.177546000
C	4.166950000	-1.287822000	0.804974000
H	4.357226000	-2.677007000	-0.826624000
H	3.667811000	0.041143000	2.420941000
H	5.235537000	-1.142778000	0.910104000
C	0.757283000	1.221157000	-0.526210000
C	1.018913000	2.306064000	0.327019000
C	1.753680000	0.792036000	-1.415526000
C	2.259305000	2.919639000	0.313239000
H	0.245679000	2.632572000	1.010325000
C	2.990695000	1.417555000	-1.432566000
H	1.571590000	-0.016418000	-2.111608000
C	3.248971000	2.472386000	-0.561588000
H	2.461611000	3.743915000	0.985886000
H	3.753933000	1.081206000	-2.123138000
H	4.220277000	2.952717000	-0.569356000



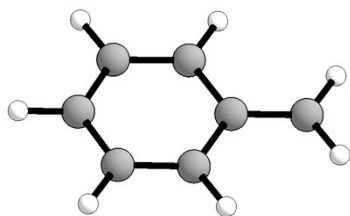
of imaginary frequencies: 1

E = -903.534644410

symmetry c1

C	-5.318937000	0.334360000	-0.293001000
C	-4.414365000	0.983234000	0.499070000
C	-3.076270000	0.510454000	0.581459000
C	-2.683898000	-0.644737000	-0.159981000
C	-3.647061000	-1.292711000	-0.973690000
C	-4.927703000	-0.811383000	-1.034981000
H	-6.340260000	0.687977000	-0.358225000
H	-4.697883000	1.857802000	1.073958000
H	-3.340352000	-2.170933000	-1.528178000

H	-5.661282000	-1.313018000	-1.654676000
N	-1.429114000	-1.159172000	-0.105868000
C	-0.517124000	-0.579877000	0.644821000
C	-2.094438000	1.126366000	1.368407000
H	-2.344868000	2.003954000	1.956326000
C	-0.800225000	0.631829000	1.364489000
H	-0.066537000	1.065562000	2.029366000
C	-0.102870000	2.033789000	-0.451387000
H	-0.401678000	2.908980000	0.113875000
H	-0.852563000	1.573531000	-1.087642000
C	1.250600000	1.743689000	-0.626007000
C	2.238686000	2.455338000	0.107966000
C	1.648377000	0.721552000	-1.528533000
C	3.570107000	2.160973000	-0.070460000
H	1.928052000	3.229815000	0.801432000
C	2.987624000	0.438581000	-1.702551000
H	0.888242000	0.180314000	-2.082136000
C	3.939347000	1.151250000	-0.971150000
H	4.331646000	2.700172000	0.477970000
H	3.299189000	-0.337287000	-2.389711000
H	4.990659000	0.921956000	-1.104802000
C	0.840310000	-1.170081000	0.653616000
C	1.857379000	-0.684211000	1.485826000
C	1.137669000	-2.218395000	-0.232807000
C	3.143052000	-1.203805000	1.406003000
H	1.664078000	0.094691000	2.212230000
C	2.418495000	-2.741350000	-0.302239000
H	0.347738000	-2.603645000	-0.864346000
C	3.430309000	-2.226229000	0.507286000
H	3.919273000	-0.814670000	2.054044000
H	2.632779000	-3.550016000	-0.990595000
H	4.433193000	-2.632794000	0.449248000

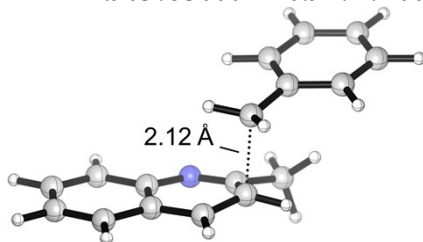


of imaginary frequencies: 0

E = -270.632285509

symmetry c1

C	1.790240000	0.000000000	0.000000000
C	1.115982000	-1.232127000	0.000000000
C	-0.254304000	-1.242414000	0.000000000
C	-0.975026000	0.000000000	0.000000000
C	-0.254304000	1.242414000	0.000000000
C	1.115982000	1.232127000	-0.000001000
H	2.874897000	0.000000000	-0.000001000
H	1.679376000	-2.155439000	0.000000000
H	-0.809353000	-2.173844000	0.000001000
H	-0.809353000	2.173844000	0.000000000
H	1.679376000	2.155438000	-0.000001000
C	-2.339809000	0.000000000	0.000001000
H	-2.903753000	-0.927472000	0.000000000
H	-2.903753000	0.927472000	0.000001000



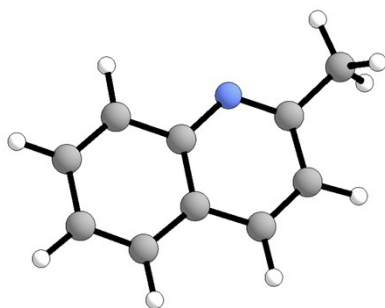
of imaginary frequencies: 1

E = -712.006728327

symmetry c1

C	4.545089000	-0.148461000	-0.846618000
C	3.665018000	-1.111806000	-0.419621000
C	2.416843000	-0.748531000	0.145854000

C	2.103284000	0.631442000	0.293567000
C	3.023765000	1.598430000	-0.151374000
C	4.219658000	1.218123000	-0.718659000
H	5.492958000	-0.436282000	-1.285638000
H	3.905311000	-2.165040000	-0.520707000
H	2.761490000	2.641587000	-0.021365000
H	4.920890000	1.970056000	-1.060460000
N	0.955248000	1.063547000	0.927154000
C	0.069567000	0.184368000	1.280216000
C	1.450061000	-1.688781000	0.559107000
H	1.654191000	-2.750734000	0.473475000
C	0.183405000	-1.225964000	0.932554000
H	-0.526575000	-1.906506000	1.391623000
C	-0.824135000	-1.197633000	-0.927494000
H	-0.833048000	-2.273624000	-1.066199000
H	-0.038876000	-0.670691000	-1.460429000
C	-2.097232000	-0.530212000	-0.791945000
C	-3.249225000	-1.234436000	-0.395088000
C	-2.196542000	0.861754000	-0.973509000
C	-4.447911000	-0.571530000	-0.180787000
H	-3.189528000	-2.309121000	-0.254044000
C	-3.398209000	1.519975000	-0.760690000
H	-1.312264000	1.419127000	-1.265671000
C	-4.528390000	0.809518000	-0.358950000
H	-5.325700000	-1.129921000	0.123585000
H	-3.455781000	2.592807000	-0.903718000
H	-5.465498000	1.325964000	-0.189909000
C	-1.113181000	0.635594000	2.086749000
H	-2.032223000	0.138076000	1.769692000
H	-0.943286000	0.383512000	3.138935000
H	-1.229990000	1.714861000	2.000882000

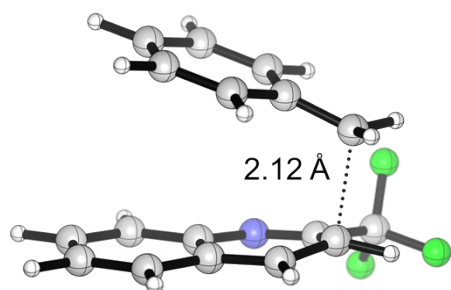


of imaginary frequencies: 0

E = -441.167426124

symmetry c1

C	2.922232000	0.296214000	-0.000001000
C	1.912037000	1.222292000	0.000000000
C	0.558865000	0.804706000	0.000000000
C	0.255331000	-0.580300000	0.000001000
C	1.318974000	-1.516076000	0.000001000
C	2.620157000	-1.086148000	-0.000002000
H	3.956495000	0.619119000	-0.000003000
H	2.132517000	2.284666000	0.000001000
H	1.062825000	-2.568743000	0.000000000
H	3.429051000	-1.807217000	-0.000004000
N	-1.024276000	-1.054665000	0.000004000
C	-2.012521000	-0.195650000	0.000004000
C	-0.534360000	1.708091000	0.000000000
H	-0.344275000	2.776621000	-0.000002000
C	-1.805779000	1.216234000	0.000001000
H	-2.665190000	1.876834000	-0.000002000
C	-3.416296000	-0.735492000	-0.000003000
H	-3.961825000	-0.389202000	0.881636000
H	-3.961736000	-0.389393000	-0.881772000
H	-3.389772000	-1.823258000	0.000112000



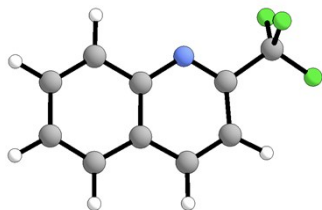
of imaginary frequencies: 1

E = -1009.75539066

symmetry c1

C	-3.263192000	1.979768000	-0.046591000
C	-2.355883000	1.842020000	-1.066305000
C	-1.026404000	1.425998000	-0.793573000
C	-0.643664000	1.213693000	0.562894000
C	-1.590925000	1.366115000	1.590362000
C	-2.884674000	1.731019000	1.291385000
H	-4.281219000	2.279997000	-0.265843000
H	-2.646171000	2.021018000	-2.096104000
H	-1.269522000	1.187875000	2.609676000
H	-3.615005000	1.840214000	2.083897000
N	0.654535000	0.903060000	0.904351000
C	1.490599000	0.673872000	-0.050406000
C	-0.076387000	1.182741000	-1.800045000
H	-0.332389000	1.351124000	-2.840232000
C	1.159771000	0.610332000	-1.454274000
H	1.970850000	0.609277000	-2.171348000
C	0.897559000	-1.480539000	-1.647862000
H	1.888488000	-1.810405000	-1.350035000
H	0.724512000	-1.460076000	-2.718926000
C	-0.215258000	-1.824521000	-0.794805000
C	-0.012610000	-2.207904000	0.544306000
C	-1.538097000	-1.672075000	-1.251082000
C	-1.089692000	-2.411202000	1.393391000
H	0.999648000	-2.328007000	0.913223000
C	-2.612423000	-1.868208000	-0.397192000

H	-1.710480000	-1.376951000	-2.281470000
C	-2.392185000	-2.230939000	0.930919000
H	-0.914655000	-2.699322000	2.423368000
H	-3.623707000	-1.731404000	-0.762234000
H	-3.231261000	-2.376453000	1.600948000
C	2.903994000	0.346259000	0.388549000
F	3.316333000	1.117138000	1.391868000
F	3.776689000	0.493878000	-0.622806000
F	3.013198000	-0.931781000	0.800559000



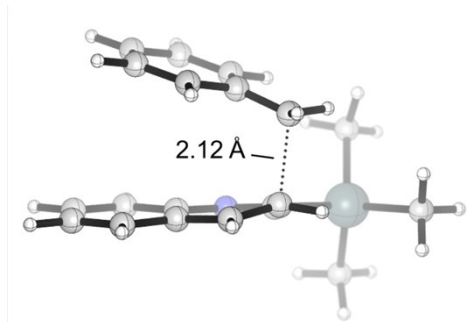
of imaginary frequencies: 0

E = -738.911012228

symmetry c1

C	3.870895000	0.034922000	0.005869000
C	2.991355000	1.083225000	0.005005000
C	1.593180000	0.841661000	-0.000604000
C	1.120437000	-0.498779000	-0.005111000
C	2.054566000	-1.566567000	-0.004377000
C	3.396993000	-1.301553000	0.000960000
H	4.938012000	0.221191000	0.010189000
H	3.346224000	2.107905000	0.008510000
H	1.668656000	-2.578613000	-0.008278000
H	4.109410000	-2.117768000	0.001436000
N	-0.205930000	-0.794738000	-0.010060000
C	-1.050562000	0.200251000	-0.012878000
C	0.633433000	1.879437000	-0.002595000
H	0.963910000	2.912543000	0.000221000
C	-0.699785000	1.568234000	-0.009108000
H	-1.465689000	2.331249000	-0.012889000
C	-2.507559000	-0.216379000	-0.000230000
F	-3.325951000	0.839961000	-0.124510000

F	-2.829779000	-0.832225000	1.144898000
F	-2.792796000	-1.058854000	-0.997094000



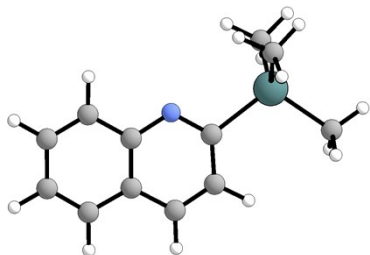
of imaginary frequencies: 1

E = -795.175170799

symmetry c1

C	-4.157997000	-2.052099000	-0.169535000
C	-3.351021000	-1.915512000	0.933410000
C	-2.012398000	-1.467729000	0.795621000
C	-1.503028000	-1.219810000	-0.510655000
C	-2.348246000	-1.370636000	-1.622820000
C	-3.658413000	-1.767653000	-1.457965000
H	-5.185027000	-2.378059000	-0.052924000
H	-3.733378000	-2.118668000	1.928590000
H	-1.937081000	-1.163901000	-2.604243000
H	-4.306709000	-1.872007000	-2.319872000
N	-0.180460000	-0.870421000	-0.727329000
C	0.579838000	-0.612891000	0.298852000
C	-1.165102000	-1.223759000	1.894393000
H	-1.513450000	-1.426825000	2.902082000
C	0.072546000	-0.606955000	1.664026000
H	0.800361000	-0.564745000	2.469007000
C	-0.278978000	1.480323000	1.830484000
H	0.728066000	1.841156000	1.635579000
H	-0.557088000	1.453341000	2.879024000
C	-1.304456000	1.802432000	0.867963000
C	-0.970421000	2.205058000	-0.438127000
C	-2.664647000	1.612562000	1.176390000

C	-1.953339000	2.400148000	-1.396042000
H	0.073263000	2.348601000	-0.695012000
C	-3.645228000	1.797658000	0.213737000
H	-2.939008000	1.294965000	2.177421000
C	-3.293808000	2.187474000	-1.077883000
H	-1.674955000	2.705484000	-2.398080000
H	-4.686224000	1.630551000	0.465237000
H	-4.060360000	2.325026000	-1.831496000
Sn	2.626243000	-0.128247000	-0.174782000
C	2.688163000	1.704820000	-1.268897000
H	1.969618000	1.675583000	-2.089971000
H	2.456028000	2.557507000	-0.627890000
H	3.684662000	1.854837000	-1.688613000
C	3.666981000	0.089147000	1.680747000
H	3.635693000	-0.838811000	2.254832000
H	4.713191000	0.346727000	1.507235000
H	3.219644000	0.882150000	2.284136000
C	3.407175000	-1.716794000	-1.356360000
H	2.739721000	-1.902560000	-2.199121000
H	4.396942000	-1.467549000	-1.741641000
H	3.481432000	-2.632211000	-0.767894000



of imaginary frequencies: 0

E = -524.330768096

symmetry c1

C	5.021514000	-0.126699000	-0.001581000
C	4.221107000	0.984667000	0.000459000
C	2.809340000	0.851174000	0.003015000
C	2.231482000	-0.444981000	0.004357000
C	3.084755000	-1.578515000	0.002393000

C	4.445315000	-1.421235000	-0.000852000
H	6.099789000	-0.020986000	-0.004041000
H	4.651552000	1.980553000	-0.000345000
H	2.623282000	-2.558871000	0.002707000
H	5.091438000	-2.291298000	-0.003021000
N	0.881485000	-0.645002000	0.005822000
C	0.079236000	0.404261000	0.004166000
C	1.928379000	1.959786000	0.003042000
H	2.337591000	2.965457000	0.002103000
C	0.578639000	1.739151000	0.002611000
H	-0.118913000	2.569835000	0.000415000
Sn	-2.016786000	-0.100314000	-0.001447000
C	-2.352750000	-1.396260000	-1.658363000
H	-1.651716000	-2.231065000	-1.612875000
H	-3.369138000	-1.792672000	-1.643088000
H	-2.199370000	-0.867846000	-2.600194000
C	-2.453931000	-1.102873000	1.827808000
H	-2.387306000	-0.414755000	2.671576000
H	-3.458062000	-1.529244000	1.805454000
H	-1.736238000	-1.910122000	1.981922000
C	-3.129602000	1.715607000	-0.177434000
H	-2.924873000	2.377095000	0.666624000
H	-2.868873000	2.240229000	-1.098374000
H	-4.201150000	1.509932000	-0.194975000

References and Notes

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