catalysts

Supplementary Materials for Article:

Hydrocarbon Oxidation Depth: $H_2O_2/Cu_2Cl_4{\cdot}2DMG/CH_3CN$ System

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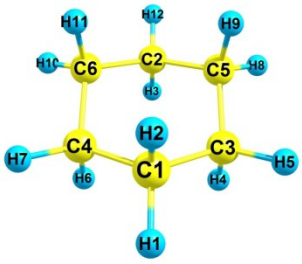
Orca – an ab initio, DFT, and semiempirical SCF-MO package – version 3.0.1 was used for all DFT calculations in the B3LYP/TZVPP level of theory.

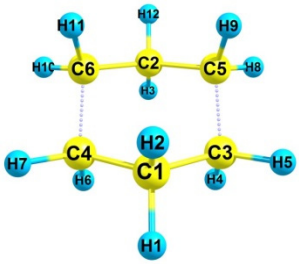
The ChemCraft 1.7 program was used to create input files, visualize and design the calculation results.

The XYZ coordinates of all atoms of all structures optimized by the DFT method are given below.

Table S1. The XYZ coordinates of all atoms of all structures optimized by the DFT method.

RH 2 (Cyclohexane)





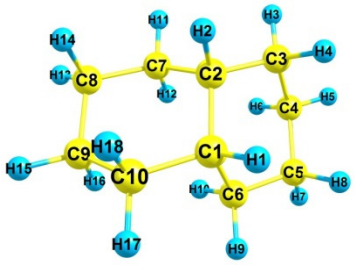
Molecule (Mol), E = -235.796416446930 Eh

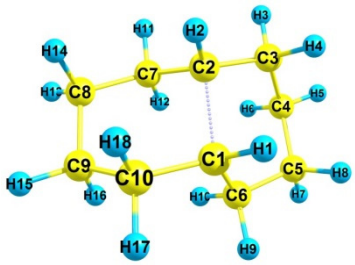
C	-0.000000000	-1.464185000	-0.227496000
C	0.000000000	1.464185000	0.227496000
C	-1.267536000	-0.731798000	0.227695000
C	1.267536000	-0.731798000	0.227695000
C	-1.267536000	0.731798000	-0.227695000
C	1.267536000	0.731798000	-0.227695000
H	-0.000000000	-2.490272000	0.148239000
H	-0.000000000	-1.535054000	-1.321176000
H	-0.000000000	1.535055000	1.321176000
H	-1.329542000	-0.767326000	1.321345000
H	-2.156484000	-1.244531000	-0.148615000
H	1.329542000	-0.767326000	1.321345000
H	2.156484000	-1.244531000	-0.148615000
H	-2.156484000	1.244531000	0.148616000
H	-1.329543000	0.767326000	-1.321345000
H	2.156484000	1.244531000	0.148616000
H	1.329543000	0.767326000	-1.321345000
H	0.000000000	2.490271000	-0.148241000

Radical Cation (RC(a)), E = -235.444603623664 Eh

C	1.363055000	0.394664000	-0.000000000
C	-1.363055000	-0.394664000	0.000000000
C	0.797425000	-0.173833000	-1.269382000
C	0.797425000	-0.173833000	1.269382000
C	-0.797425000	0.173833000	-1.269382000
C	-0.797425000	0.173833000	1.269382000
H	2.433529000	0.067029000	-0.000000000
H	1.365393000	1.485070000	-0.000000000
H	-1.365393000	-1.485070000	0.000000000
H	0.913623000	-1.254182000	-1.336093000
H	1.177950000	0.292699000	-2.178668000
H	0.913623000	-1.254182000	1.336093000
H	1.177950000	0.292699000	2.178668000
H	-1.177950000	-0.292699000	-2.178668000
H	-0.913623000	1.254182000	-1.336093000
H	-1.177950000	-0.292699000	2.178668000
H	-0.913623000	1.254182000	1.336093000
H	-2.433529000	-0.067029000	-0.000000000

RH *Cis*-3 (*Cis*-Decalin)





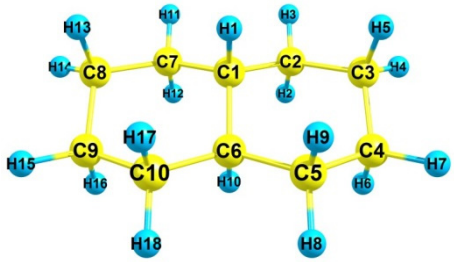
Molecule (Mol), E = -391.789367615470 Eh

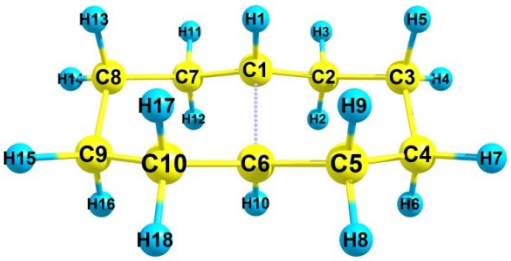
C	-0.125226000	0.763846000	-0.661116000
C	0.125226000	-0.763846000	-0.661116000
C	1.632264000	-1.072816000	-0.651165000
C	2.390741000	-0.356612000	0.471089000
C	2.137344000	1.153189000	0.436182000
C	0.639064000	1.470260000	0.471065000
H	0.281958000	1.154772000	-1.601581000
H	-0.281959000	-1.154772000	-1.601581000
H	1.786434000	-2.153858000	-0.583466000
H	2.056707000	-0.760591000	-1.611509000
H	3.460578000	-0.562471000	0.383612000
H	2.082440000	-0.753579000	1.442900000
H	2.646725000	1.643500000	1.269606000
H	2.572096000	1.569095000	-0.480126000
H	0.481890000	2.549800000	0.390008000
H	0.234905000	1.176266000	1.444000000
C	-0.639064000	-1.470259000	0.471065000
C	-2.137344000	-1.153190000	0.436182000
C	-2.390742000	0.356611000	0.471088000
C	-1.632264000	1.072816000	-0.651164000
H	-0.481889000	-2.549799000	0.390009000
H	-0.234904000	-1.176265000	1.444000000
H	-2.646724000	-1.643500000	1.269607000
H	-2.572096000	-1.569096000	-0.480126000
H	-3.460578000	0.562470000	0.383611000
H	-2.082442000	0.753579000	1.442900000
H	-1.786433000	2.153858000	-0.583465000
H	-2.056706000	0.760592000	-1.611509000

Radical Cation (RC(a)), E = -391.464651533436 Eh

C	-0.147810000	0.933809000	-0.653981000
C	0.147810000	-0.933809000	-0.653981000
C	1.644912000	-1.039979000	-0.666658000
C	2.386480000	-0.360225000	0.481679000
C	2.143573000	1.155380000	0.446096000
C	0.650250000	1.477039000	0.488803000
H	0.307294000	1.136290000	-1.623282000
H	-0.307294000	-1.136290000	-1.623281000
H	1.844184000	-2.125261000	-0.636096000
H	2.030816000	-0.697173000	-1.628233000
H	3.454289000	-0.560600000	0.390959000
H	2.074376000	-0.774782000	1.441764000
H	2.645269000	1.630169000	1.289421000
H	2.584419000	1.578550000	-0.460455000
H	0.533117000	2.571224000	0.398240000
H	0.212395000	1.211049000	1.451244000
C	-0.650250000	-1.477039000	0.488804000
C	-2.143573000	-1.155380000	0.446096000
C	-2.386479000	0.360225000	0.481679000
C	-1.644912000	1.039979000	-0.666658000
H	-0.533117000	-2.571224000	0.398240000
H	-0.212395000	-1.211049000	1.451244000
H	-2.645269000	-1.630169000	1.289421000
H	-2.584419000	-1.578550000	-0.460455000
H	-3.454289000	0.560600000	0.390959000
H	-2.074375000	0.774783000	1.441764000
H	-1.844184000	2.125261000	-0.636096000
H	-2.030816000	0.697173000	-1.628233000

RH *Trans*-3 (*Trans*-Decalin)





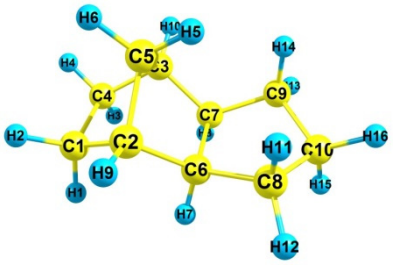
Molecule (Mol), E = -391.794723133146 Eh

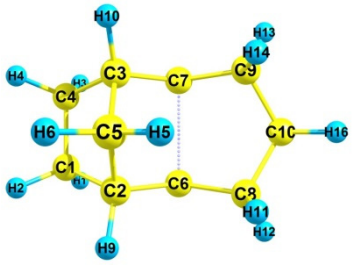
C	-0.751841000	0.170782000	0.000000000
C	-1.143282000	0.930756000	1.272893000
C	-0.745346000	0.175551000	2.544037000
C	0.745345000	-0.175549000	2.544038000
C	1.143282000	-0.930756000	1.272898000
C	0.751849000	-0.170782000	0.000000000
C	-1.143281000	0.930757000	-1.272893000
C	-0.745346000	0.175552000	-2.544037000
C	0.745344000	-0.175551000	-2.544039000
C	1.143282000	-0.930757000	-1.272897000
H	-1.299008000	-0.783099000	-0.000001000
H	-0.653740000	1.911818000	1.265545000
H	-2.219710000	1.125911000	1.270184000
H	-0.995139000	0.767119000	3.428552000
H	-1.333272000	-0.746396000	2.613675000
H	1.333272000	0.746397000	2.613677000
H	0.995136000	-0.767118000	3.428553000
H	2.219710000	-1.125915000	1.270193000
H	0.653736000	-1.911816000	1.265548000
H	1.299018000	0.783097000	0.000001000
H	-2.219709000	1.125913000	-1.270185000
H	-0.653738000	1.911818000	-1.265544000
H	-1.333273000	-0.746393000	-2.613676000
H	-0.995137000	0.767121000	-3.428552000
H	0.995133000	-0.767120000	-3.428554000
H	1.333272000	0.746394000	-2.613679000
H	0.653736000	-1.911817000	-1.265547000
H	2.219709000	-1.125916000	-1.270192000

Radical Cation (RC(a)), E = -391.469260219338 Eh

C	-0.910824000	0.215089000	-0.000000000
C	-1.120398000	0.946050000	1.290295000
C	-0.747256000	0.171982000	2.550774000
C	0.747257000	-0.171982000	2.550774000
C	1.120398000	-0.946050000	1.290295000
C	0.910824000	-0.215089000	-0.000000000
C	-1.120398000	0.946050000	-1.290295000
C	-0.747256000	0.171982000	-2.550774000
C	0.747257000	-0.171982000	-2.550774000
C	1.120398000	-0.946050000	-1.290295000
H	-1.316400000	-0.797518000	-0.000000000
H	-0.639902000	1.926527000	1.262917000
H	-2.206513000	1.142816000	1.312814000
H	-0.990206000	0.765860000	3.432422000
H	-1.343226000	-0.741763000	2.612964000
H	1.343226000	0.741763000	2.612964000
H	0.990207000	-0.765859000	3.432422000
H	2.206513000	-1.142816000	1.312814000
H	0.639902000	-1.926527000	1.262917000
H	1.316400000	0.797518000	-0.000000000
H	-2.206513000	1.142816000	-1.312814000
H	-0.639902000	1.926527000	-1.262917000
H	-1.343226000	-0.741763000	-2.612965000
H	-0.990206000	0.765860000	-3.432422000
H	0.990206000	-0.765860000	-3.432422000
H	1.343226000	0.741763000	-2.612965000
H	0.639902000	-1.926527000	-1.262917000
H	2.206513000	-1.142816000	-1.312814000

RH *Exo*-4 (*Exo*-Tetrahydrodicyclopentadiene)





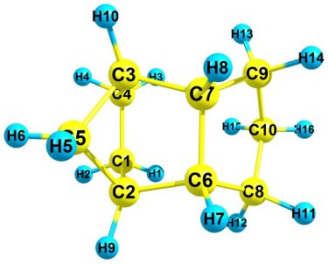
Molecule (Mol), E = -390.566031933795 Eh

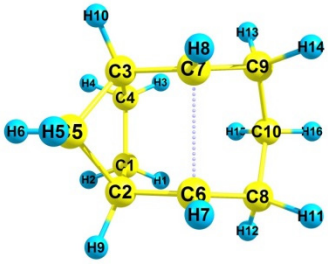
C	2.121071000	-0.454927000	-0.781073000
C	0.854529000	0.355807000	-1.132588000
C	0.854529000	0.355806000	1.132588000
C	2.121070000	-0.454930000	0.781073000
H	2.091002000	-1.461044000	-1.201243000
H	3.014794000	0.033322000	-1.173142000
H	2.090994000	-1.461049000	1.201239000
H	3.014793000	0.033313000	1.173148000
C	0.847150000	1.401146000	0.000001000
H	-0.032313000	2.045258000	0.000001000
H	1.734491000	2.037472000	0.000001000
C	-0.378629000	-0.506661000	-0.788019000
H	-0.258888000	-1.516922000	-1.184178000
C	-0.378631000	-0.506659000	0.788020000
H	-0.258891000	-1.516920000	1.184181000
H	0.849297000	0.746928000	-2.150062000
H	0.849299000	0.746926000	2.150063000
C	-1.753966000	0.053178000	-1.205926000
H	-1.686708000	1.130176000	-1.384549000
H	-2.122281000	-0.398601000	-2.127856000
C	-1.753968000	0.053179000	1.205925000
H	-2.122284000	-0.398602000	2.127853000
H	-1.686713000	1.130177000	1.384549000
C	-2.667020000	-0.212429000	-0.000002000
H	-2.987284000	-1.258278000	-0.000001000
H	-3.569629000	0.400775000	-0.000003000

Radical Cation (RC(a)), E = -390.240966496249 Eh

C	-2.108069000	0.584309000	-0.780257000
C	-0.912164000	-0.314516000	-1.160354000
C	-0.912164000	-0.314516000	1.160354000
C	-2.108069000	0.584309000	0.780257000
H	-2.020175000	1.585066000	-1.201184000
H	-3.029759000	0.155115000	-1.167994000
H	-2.020175000	1.585066000	1.201184000
H	-3.029759000	0.155115000	1.167994000
C	-0.884240000	-1.338362000	0.000000000
H	-0.023650000	-2.002398000	0.000000000
H	-1.784993000	-1.950563000	0.000000000
C	0.374209000	0.435567000	-1.126451000
H	0.330326000	1.517206000	-1.237729000
C	0.374209000	0.435566000	1.126451000
H	0.330326000	1.517206000	1.237730000
H	-1.009231000	-0.788800000	-2.144963000
H	-1.009231000	-0.788800000	2.144963000
C	1.716817000	-0.174266000	-1.260053000
H	1.655670000	-1.254127000	-1.391181000
H	2.210701000	0.248896000	-2.141015000
C	1.716817000	-0.174266000	1.260053000
H	2.210701000	0.248895000	2.141015000
H	1.655671000	-1.254127000	1.391181000
C	2.549864000	0.174958000	-0.000000000
H	2.790781000	1.238498000	0.000000000
H	3.488049000	-0.377465000	-0.000000000

RH *Endo*-4
(*Endo*-Tetrahydrodicyclopentadiene)





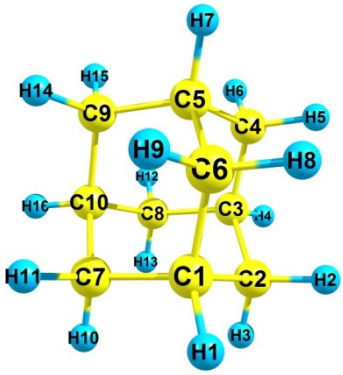
Molecule (Mol), E = -390.560161543720 Eh

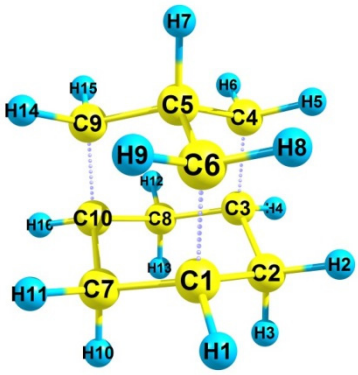
C	-1.171803000	1.152896000	-0.780429000
C	-0.973082000	-0.336996000	-1.130616000
C	-0.973079000	-0.336994000	1.130616000
C	-1.171802000	1.152897000	0.780425000
H	-0.403846000	1.795441000	-1.208516000
H	-2.128534000	1.502856000	-1.171829000
H	-0.403843000	1.795444000	1.208509000
H	-2.128532000	1.502860000	1.171826000
C	-1.776871000	-1.012728000	0.000001000
H	-1.691371000	-2.101192000	0.000002000
H	-2.835150000	-0.741275000	0.000002000
C	0.461020000	-0.814115000	-0.786339000
H	0.574336000	-1.828350000	-1.173037000
C	0.461019000	-0.814116000	0.786338000
H	0.574334000	-1.828352000	1.173035000
H	-1.274854000	-0.585661000	-2.148209000
H	-1.274850000	-0.585656000	2.148210000
C	1.666627000	0.043420000	-1.221871000
H	2.496416000	-0.616889000	-1.484751000
H	1.459711000	0.649306000	-2.106331000
C	1.666627000	0.043415000	1.221871000
H	1.459711000	0.649299000	2.106334000
H	2.496416000	-0.616894000	1.484750000
C	2.060606000	0.896326000	0.000002000
H	1.515179000	1.839983000	0.000004000
H	3.121816000	1.151002000	0.000002000

Radical Cation (RC(a)), E = -390.234485149963 Eh

C	-1.174069000	1.183195000	-0.781649000
C	-0.969611000	-0.297078000	-1.154421000
C	-0.969611000	-0.297079000	1.154420000
C	-1.174069000	1.183195000	0.781649000
H	-0.425416000	1.844701000	-1.211268000
H	-2.137659000	1.515256000	-1.163272000
H	-0.425415000	1.844701000	1.211269000
H	-2.137659000	1.515256000	1.163272000
C	-1.698079000	-1.029056000	-0.000000000
H	-1.560222000	-2.109865000	-0.000000000
H	-2.765418000	-0.811302000	-0.000000000
C	0.439388000	-0.785421000	-1.108449000
H	0.538672000	-1.861809000	-1.228950000
C	0.439389000	-0.785421000	1.108449000
H	0.538672000	-1.861809000	1.228949000
H	-1.370576000	-0.560563000	-2.142425000
H	-1.370576000	-0.560563000	2.142425000
C	1.681605000	0.013420000	-1.273621000
H	2.513426000	-0.653561000	-1.495654000
H	1.565013000	0.695671000	-2.122501000
C	1.681605000	0.013420000	1.273621000
H	1.565013000	0.695670000	2.122501000
H	2.513426000	-0.653561000	1.495653000
C	1.995125000	0.845103000	-0.000000000
H	1.415657000	1.762798000	-0.000000000
H	3.046296000	1.127695000	-0.000000000

RH 5 (Adamantane)





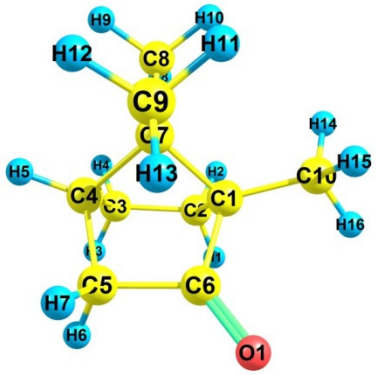
Molecule (Mol), E = -390.571017840896 Eh

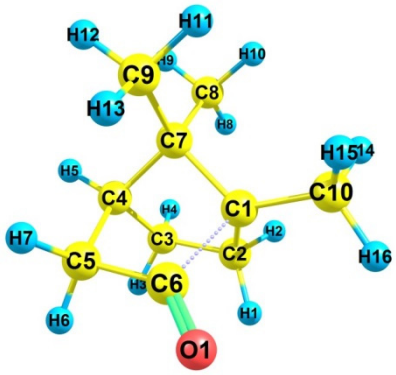
C	-0.727972000	-1.259927000	-0.506710000
C	-1.451791000	0.000000000	-1.019247000
C	-0.727972000	1.259929000	-0.506711000
C	0.725571000	1.257330000	-1.019047000
C	1.454746000	0.000000000	-0.507569000
C	0.725571000	-1.257331000	-1.019048000
H	-1.243659000	-2.153552000	-0.872337000
H	-1.475434000	-0.000000000	-2.114357000
H	-2.493031000	0.000000000	-0.678883000
H	-1.243658000	2.153554000	-0.872337000
H	0.738797000	1.280861000	-2.114076000
H	1.245596000	2.157894000	-0.674982000
H	2.486754000	0.000000000	-0.872347000
H	0.738798000	-1.280861000	-2.114077000
H	1.245597000	-2.157895000	-0.674983000
C	-0.725892000	-1.257495000	1.033675000
H	-1.753839000	-1.279623000	1.411274000
H	-0.228939000	-2.158524000	1.409479000
C	-0.725891000	1.257494000	1.033673000
H	-0.228939000	2.158523000	1.409478000
H	-1.753838000	1.279622000	1.411272000
C	1.451410000	-0.000000000	1.032790000
H	1.983851000	-0.879998000	1.409606000
H	1.983850000	0.879998000	1.409605000
C	-0.000113000	0.000000000	1.549819000
H	0.000426000	0.000001000	2.644328000

Radical Cation (RC(a)), E = -390.241205996154 Eh

C	-0.770985000	-1.256376000	-0.489302000
C	-1.436221000	0.000563000	-1.035431000
C	-0.770085000	1.256468000	-0.488880000
C	0.750561000	1.262437000	-1.031090000
C	1.377515000	-0.000133000	-0.479633000
C	0.749833000	-1.262083000	-1.031457000
H	-1.229882000	-2.165523000	-0.884268000
H	-1.444447000	0.000721000	-2.127958000
H	-2.495177000	0.000807000	-0.734548000
H	-1.227766000	2.166119000	-0.884407000
H	0.726423000	1.280092000	-2.120627000
H	1.238853000	2.167312000	-0.669592000
H	2.438134000	-0.000717000	-0.854670000
H	0.725567000	-1.279272000	-2.121018000
H	1.237759000	-2.167441000	-0.670591000
C	-0.706936000	-1.266563000	1.032425000
H	-1.731019000	-1.326789000	1.430794000
H	-0.198146000	-2.160958000	1.399838000
C	-0.706401000	1.266568000	1.032851000
H	-0.197045000	2.160494000	1.400420000
H	-1.730539000	1.326695000	1.430920000
C	1.475944000	-0.000344000	1.030974000
H	1.975127000	-0.888174000	1.419207000
H	1.975050000	0.887376000	1.419506000
C	-0.045348000	-0.000435000	1.562268000
H	0.019229000	-0.000845000	2.652557000

RH 6 (Camphor)





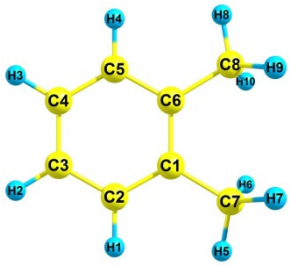
Molecule (Mol), E = -465.795123302806 Eh

C	-1.261031000	0.373042000	-0.025170000
C	-1.241867000	1.933851000	0.047156000
C	0.265316000	2.308301000	-0.037603000
C	0.956650000	0.928960000	-0.080911000
C	0.793724000	0.312160000	1.319374000
C	-0.697219000	-0.042380000	1.337417000
C	-0.025241000	0.076402000	-0.947457000
C	-0.171861000	0.583704000	-2.386215000
C	0.339311000	-1.414063000	-1.017376000
C	-2.605713000	-0.237127000	-0.356818000
O	-1.304773000	-0.538810000	2.251848000
H	-1.719487000	2.294081000	0.958910000
H	-1.810523000	2.342570000	-0.788391000
H	0.597768000	2.894873000	0.819117000
H	0.481188000	2.896955000	-0.928247000
H	1.984177000	0.951922000	-0.443867000
H	1.036187000	0.993956000	2.135812000
H	1.384141000	-0.592252000	1.470253000
H	-0.464290000	1.629283000	-2.454238000
H	0.776595000	0.472914000	-2.917620000
H	-0.916170000	-0.002778000	-2.927927000
H	-0.391101000	-1.957831000	-1.618899000
H	1.313901000	-1.545821000	-1.492638000
H	0.377142000	-1.900660000	-0.043537000
H	-2.978362000	0.123061000	-1.317375000
H	-2.552351000	-1.325926000	-0.395083000
H	-3.338677000	0.019924000	0.409069000

Radical Cation (RC(a)), E = -465.489025147050 Eh

C	-1.296490000	0.422406000	-0.137271000
C	-1.248056000	1.939130000	0.085706000
C	0.250265000	2.317075000	-0.023081000
C	0.948063000	0.941337000	-0.087668000
C	0.848587000	0.320047000	1.304434000
C	-0.623454000	-0.051175000	1.429273000
C	-0.015362000	0.069338000	-0.946070000
C	-0.172598000	0.572850000	-2.398933000
C	0.326436000	-1.424851000	-1.000812000
C	-2.612934000	-0.236783000	-0.388089000
O	-1.306822000	-0.505412000	2.254400000
H	-1.726721000	2.247746000	1.016188000
H	-1.852945000	2.390566000	-0.707157000
H	0.594253000	2.910792000	0.822010000
H	0.445273000	2.900622000	-0.919337000
H	1.973122000	0.975299000	-0.450926000
H	1.101050000	0.979310000	2.137278000
H	1.400845000	-0.613153000	1.431348000
H	-0.466298000	1.616604000	-2.472604000
H	0.786702000	0.456471000	-2.906296000
H	-0.903381000	-0.027581000	-2.938402000
H	-0.392351000	-1.959566000	-1.620686000
H	1.309685000	-1.565533000	-1.450233000
H	0.337354000	-1.918981000	-0.028951000
H	-2.958304000	0.062723000	-1.382804000
H	-2.546674000	-1.323551000	-0.376712000
H	-3.371810000	0.082583000	0.324975000

RH 7 (*o*-Xylene)



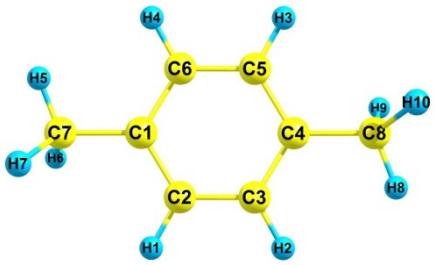
Molecule (Mol), E = -310.790774450045 Eh

C	0.703501000	-0.000004000	0.532968000
C	1.378513000	0.000001000	-0.687174000
C	0.693852000	0.000000000	-1.897556000
C	-0.693854000	-0.000002000	-1.897552000
C	-1.378510000	-0.000002000	-0.687171000
C	-0.703496000	-0.000005000	0.532965000
H	2.462535000	0.000005000	-0.687973000
H	1.243192000	0.000003000	-2.830258000
H	-1.243198000	-0.000002000	-2.830251000
H	-2.462532000	0.000000000	-0.687965000
C	1.477575000	-0.000002000	1.825393000
H	2.551020000	0.000003000	1.638464000
H	1.244226000	0.876801000	2.435613000
H	1.244234000	-0.876809000	2.435610000
C	-1.477575000	0.000002000	1.825387000
H	-2.551019000	0.000004000	1.638455000
H	-1.244234000	-0.876802000	2.435609000
H	-1.244229000	0.876808000	2.435604000

Radical Cation (RC(a)), E = -310.486706493782 Eh

C	0.736066000	0.000000000	0.533846000
C	1.414879000	0.000000000	-0.688962000
C	0.717014000	0.000000000	-1.874622000
C	-0.717014000	-0.000000000	-1.874622000
C	-1.414879000	-0.000000000	-0.688961000
C	-0.736067000	0.000000000	0.533846000
H	2.496411000	0.000001000	-0.694702000
H	1.243534000	0.000000000	-2.819981000
H	-1.243534000	-0.000000000	-2.819980000
H	-2.496411000	-0.000000000	-0.694702000
C	1.482942000	0.000000000	1.813024000
H	2.557859000	0.000000000	1.653758000
H	1.217198000	0.871822000	2.421361000
H	1.217198000	-0.871822000	2.421360000
C	-1.482942000	0.000000000	1.813025000
H	-2.557860000	0.000000000	1.653759000
H	-1.217199000	-0.871822000	2.421361000
H	-1.217199000	0.871823000	2.421361000

RH 8 (*p*-Xylene)



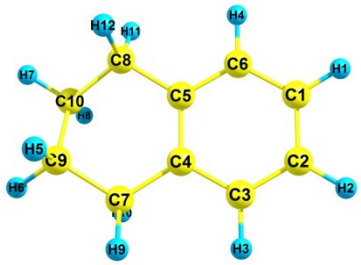
Molecule (Mol), E = -310.791222286329 Eh

C	-1.372240000	0.356611000	0.000000000
C	-0.372698000	1.329893000	0.000000000
C	0.972467000	0.979994000	0.000001000
C	1.372238000	-0.356610000	0.000000000
C	0.372699000	-1.329896000	0.000001000
C	-0.972463000	-0.979991000	0.000001000
H	-0.648625000	2.378478000	0.000001000
H	1.724660000	1.760204000	0.000002000
H	0.648625000	-2.378480000	0.000002000
H	-1.724656000	-1.760203000	0.000002000
C	-2.829140000	0.742273000	-0.000001000
H	-3.472588000	-0.137239000	0.000003000
H	-3.081801000	1.340515000	0.878753000
H	-3.081801000	1.340508000	-0.878760000
C	2.829138000	-0.742273000	-0.000001000
H	3.472588000	0.137238000	0.000004000
H	3.081799000	-1.340517000	0.878753000
H	3.081798000	-1.340507000	-0.878761000

Radical Cation (RC(a)), E = -310.492657788520 Eh

C	-1.370692000	0.337300000	0.000000000
C	-0.360588000	1.355004000	0.000000000
C	0.963089000	1.027608000	0.000000000
C	1.370692000	-0.337301000	0.000000000
C	0.360588000	-1.355004000	0.000000000
C	-0.963089000	-1.027608000	0.000000000
H	-0.667739000	2.393011000	0.000000000
H	1.719545000	1.800813000	0.000000000
H	0.667739000	-2.393012000	0.000001000
H	-1.719545000	-1.800813000	0.000001000
C	-2.797871000	0.717394000	-0.000000000
H	-3.466772000	-0.138550000	0.000004000
H	-3.018365000	1.349480000	0.869496000
H	-3.018366000	1.349471000	-0.869503000
C	2.797871000	-0.717394000	-0.000000000
H	3.466772000	0.138550000	0.000005000
H	3.018365000	-1.349481000	0.869495000
H	3.018366000	-1.349471000	-0.869503000

RH 9 (Tetralin)



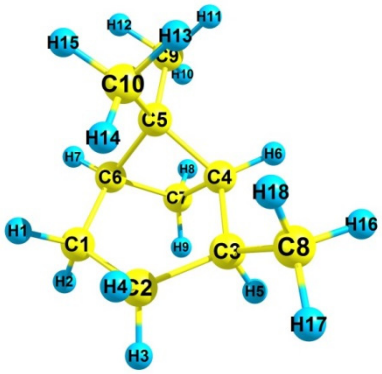
Molecule (Mol), E = -388.186775526325 Eh

C	-0.684626000	-0.125081000	2.523289000
C	0.684628000	0.125081000	2.523290000
C	1.355442000	0.249459000	1.315966000
C	0.688803000	0.128413000	0.093224000
C	-0.688805000	-0.128419000	0.093225000
C	-1.355446000	-0.249459000	1.315967000
H	-1.223183000	-0.222263000	3.457278000
H	1.223188000	0.222267000	3.457278000
H	2.421990000	0.445161000	1.314160000
C	1.461509000	0.306290000	-1.199011000
C	-1.461508000	-0.306292000	-1.199013000
H	-2.421995000	-0.445158000	1.314165000
C	0.727295000	-0.233859000	-2.426901000
C	-0.727294000	0.233860000	-2.426901000
H	0.754355000	-1.328490000	-2.422354000
H	1.238463000	0.089516000	-3.336335000
H	-1.238462000	-0.089512000	-3.336335000
H	-0.754354000	1.328491000	-2.422351000
H	2.442285000	-0.165519000	-1.103613000
H	1.656855000	1.375039000	-1.344698000
H	-2.442284000	0.165516000	-1.103614000
H	-1.656855000	-1.375041000	-1.344703000

Radical Cation (RC(a)), E = -387.887710689243 Eh

C	0.716028000	0.039859000	-2.499773000
C	-0.716028000	-0.039859000	-2.499773000
C	-1.413363000	-0.073475000	-1.316821000
C	-0.732260000	-0.019106000	-0.093521000
C	0.732260000	0.019106000	-0.093521000
C	1.413363000	0.073475000	-1.316821000
H	1.240823000	0.063965000	-3.445689000
H	-1.240823000	-0.063965000	-3.445689000
H	-2.494102000	-0.120753000	-1.320639000
C	-1.480490000	0.059968000	1.188571000
C	1.480490000	-0.059968000	1.188571000
H	2.494102000	0.120753000	-1.320639000
C	-0.681437000	-0.341781000	2.432803000
C	0.681437000	0.341781000	2.432803000
H	-0.557590000	-1.428030000	2.455076000
H	-1.250730000	-0.072363000	3.321414000
H	1.250730000	0.072363000	3.321414000
H	0.557590000	1.428030000	2.455076000
H	-2.423432000	-0.484653000	1.097643000
H	-1.781511000	1.117131000	1.295063000
H	2.423432000	0.484653000	1.097643000
H	1.781511000	-1.117131000	1.295063000

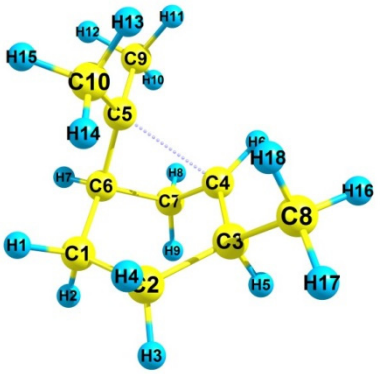
RH *Cis*-10 (*Cis*-Pinane)



Molecule (Mol), E = -391.740816783849 Eh

C	-1.926576000	-0.514662000	0.886159000
C	-0.871471000	-1.184255000	-0.042861000
C	-0.094788000	-0.210396000	-0.981509000
C	-0.314977000	1.254573000	-0.568948000
C	-0.343838000	1.508131000	0.984467000
C	-1.827082000	1.013419000	0.896936000
C	-1.845120000	1.511778000	-0.569068000
H	-1.819311000	-0.905659000	1.900781000
H	-2.935918000	-0.782870000	0.563547000
H	-1.350408000	-1.957329000	-0.645885000
H	-0.146355000	-1.714085000	0.575915000
C	1.380445000	-0.598705000	-1.116754000
H	-0.530048000	-0.293564000	-1.983438000
H	0.316694000	1.921783000	-1.161124000
C	-0.261685000	3.008760000	1.296741000
C	0.624340000	0.796740000	1.929356000
H	-2.539516000	1.450796000	1.600625000
H	-2.115182000	2.559769000	-0.671160000
H	-2.436696000	0.929278000	-1.277752000
H	-0.917936000	3.614238000	0.674419000
H	0.758897000	3.371783000	1.150441000
H	-0.530450000	3.195101000	2.339722000
H	1.646143000	1.151218000	1.770925000
H	0.631268000	-0.284447000	1.825452000
H	0.363915000	1.024661000	2.967061000
H	1.888832000	0.045665000	-1.837584000
H	1.479700000	-1.628700000	-1.467165000
H	1.911077000	-0.521139000	-0.167154000

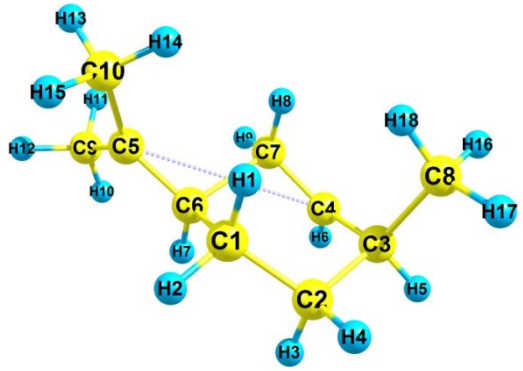
Closed form



Radical Cation (RC(a)), E = -391.439831739236 Eh

C	-1.868740000	-0.499934000	0.877705000
C	-0.844117000	-1.201254000	-0.056321000
C	-0.097219000	-0.273427000	-1.075595000
C	-0.402125000	1.159333000	-0.882582000
C	-0.402811000	1.577741000	1.276622000
C	-1.765088000	1.025829000	0.878147000
C	-1.822636000	1.508582000	-0.601986000
H	-1.757482000	-0.884925000	1.892464000
H	-2.885427000	-0.748085000	0.572753000
H	-1.338518000	-2.004276000	-0.598910000
H	-0.075567000	-1.690983000	0.540155000
C	1.387848000	-0.605696000	-1.227549000
H	-0.573806000	-0.448280000	-2.060220000
H	0.305206000	1.907070000	-1.228707000
C	-0.236406000	3.058141000	1.355852000
C	0.567277000	0.800103000	2.089975000
H	-2.553171000	1.479200000	1.492333000
H	-2.042598000	2.565339000	-0.709491000
H	-2.540146000	0.932458000	-1.187095000
H	-0.902331000	3.622665000	0.710749000
H	0.795411000	3.362685000	1.178385000
H	-0.463931000	3.352334000	2.389962000
H	1.575703000	1.205912000	2.021029000
H	0.578970000	-0.264967000	1.891006000
H	0.257655000	0.921339000	3.140349000
H	1.853481000	0.002759000	-2.003412000
H	1.513174000	-1.650802000	-1.507878000
H	1.931344000	-0.446976000	-0.295596000

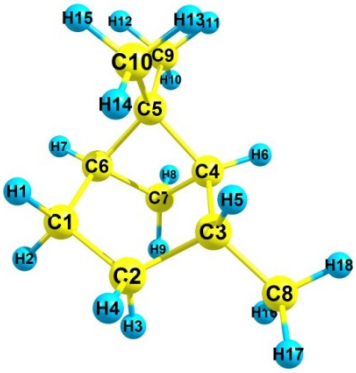
Opened form



Radical Cation (RC(a)), E = -391.456331969359 E_h

C	-2.012450000	-0.539515000	0.920197000
C	-1.626773000	-0.957240000	-0.498725000
C	-0.244544000	-0.368265000	-0.957561000
C	-0.343315000	1.086670000	-0.697447000
C	-2.273919000	1.581013000	2.360172000
C	-2.109361000	0.971146000	1.080092000
C	-0.444906000	1.600508000	0.617252000
H	-1.321850000	-0.963087000	1.649451000
H	-2.996394000	-0.957759000	1.151260000
H	-2.402377000	-0.637119000	-1.197892000
H	-1.568158000	-2.044084000	-0.568965000
C	0.941597000	-1.068425000	-0.274487000
H	-0.168477000	-0.530596000	-2.033014000
H	-0.608212000	1.743195000	-1.520038000
C	-2.889544000	2.924105000	2.476580000
C	-1.784320000	0.931949000	3.601962000
H	-2.742838000	1.430207000	0.324886000
H	0.169166000	1.125253000	1.373820000
H	-0.479706000	2.679570000	0.708794000
H	-3.259918000	3.314111000	1.531418000
H	-2.178115000	3.636981000	2.909381000
H	-3.719641000	2.882253000	3.191406000
H	-1.632041000	1.649713000	4.406085000
H	-0.868382000	0.358876000	3.449499000
H	-2.537034000	0.210141000	3.946849000
H	1.887155000	-0.634580000	-0.597884000
H	0.946412000	-2.122761000	-0.549947000
H	0.900404000	-1.011484000	0.813480000

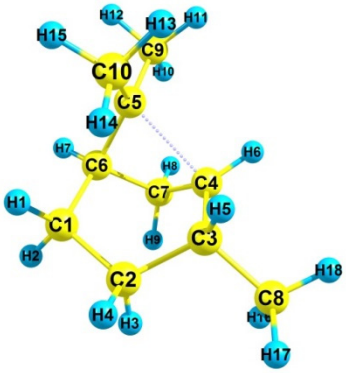
RH *Trans*-10 (*Trans*-Pinane)



Molecule (Mol), E = -391.744786580034 Eh

C	-1.760333000	-0.586480000	0.920805000
C	-1.090348000	-1.141561000	-0.362983000
C	-0.078363000	-0.173495000	-1.037236000
C	-0.411657000	1.282059000	-0.666289000
C	-0.313628000	1.520843000	0.881147000
C	-1.770916000	0.945678000	0.925915000
C	-1.950083000	1.454818000	-0.529789000
H	-1.260660000	-0.955132000	1.818784000
H	-2.787177000	-0.957055000	0.974265000
H	-1.875301000	-1.354501000	-1.091017000
H	-0.611663000	-2.101932000	-0.160947000
C	-0.052247000	-0.382414000	-2.553052000
H	0.926640000	-0.388658000	-0.664629000
H	0.130789000	1.984006000	-1.304882000
C	-0.274538000	3.013695000	1.227392000
C	0.786375000	0.823556000	1.678118000
H	-2.433513000	1.340432000	1.699956000
H	-2.265766000	2.493323000	-0.583467000
H	-2.588831000	0.869711000	-1.191814000
H	-1.040666000	3.591563000	0.712877000
H	0.695440000	3.442391000	0.962235000
H	-0.416243000	3.159760000	2.301423000
H	1.764877000	1.238722000	1.421274000
H	0.836174000	-0.250941000	1.513999000
H	0.639002000	0.985471000	2.749662000
H	-1.005964000	-0.099182000	-3.006387000
H	0.134176000	-1.429214000	-2.803589000
H	0.731058000	0.216810000	-3.021659000

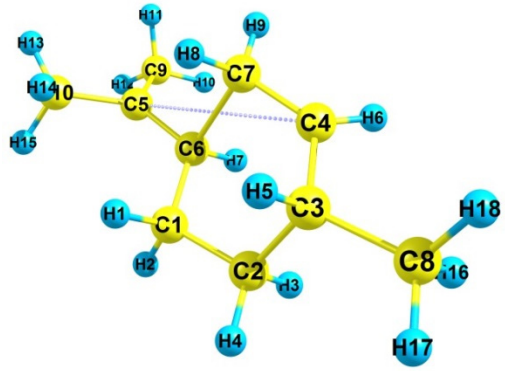
Closed form



Radical Cation (RC(a)), E = -391.443377526896 Eh

C	-1.864972000	-0.513645000	1.107425000
C	-1.250003000	-1.218498000	-0.134821000
C	-0.225781000	-0.360491000	-0.910487000
C	-0.578938000	1.079301000	-0.848000000
C	-0.397361000	1.588839000	1.206719000
C	-1.793791000	1.010832000	0.994693000
C	-1.989435000	1.416536000	-0.505969000
H	-1.387388000	-0.843936000	2.029074000
H	-2.912706000	-0.801108000	1.193302000
H	-2.058371000	-1.476741000	-0.819606000
H	-0.792648000	-2.164983000	0.149241000
C	-0.160257000	-0.768272000	-2.413450000
H	0.787600000	-0.499001000	-0.525373000
H	0.084855000	1.807241000	-1.305255000
C	-0.259033000	3.074691000	1.244904000
C	0.686572000	0.839817000	1.895362000
H	-2.515037000	1.511302000	1.651951000
H	-2.240118000	2.461981000	-0.647166000
H	-2.736208000	0.796344000	-1.001825000
H	-1.012806000	3.608503000	0.673585000
H	0.735070000	3.402265000	0.940150000
H	-0.372682000	3.381728000	2.293642000
H	1.666310000	1.272796000	1.695793000
H	0.704549000	-0.225659000	1.690051000
H	0.511372000	0.949206000	2.976427000
H	-1.116564000	-0.607953000	-2.912010000
H	0.079585000	-1.830024000	-2.468394000
H	0.612398000	-0.214659000	-2.944175000

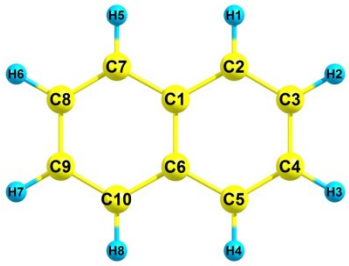
Opened form



Radical Cation (RC(a)), E = -391.459874400365 Eh

C	-2.088731000	-0.546248000	0.909587000
C	-1.733932000	-0.982430000	-0.510042000
C	-0.335495000	-0.438870000	-0.973179000
C	-0.399585000	1.016698000	-0.743489000
C	-2.251164000	1.573308000	2.360856000
C	-2.124440000	0.969246000	1.070178000
C	-0.482700000	1.541665000	0.572390000
H	-1.396016000	-0.993663000	1.624473000
H	-3.082423000	-0.928312000	1.159410000
H	-2.498309000	-0.644160000	-1.214344000
H	-1.704947000	-2.070855000	-0.572631000
C	-0.019628000	-0.834974000	-2.414539000
H	0.404034000	-0.876642000	-0.293132000
H	-0.654165000	1.663302000	-1.578465000
C	-2.839404000	2.925416000	2.500494000
C	-1.737790000	0.908904000	3.583926000
H	-2.771303000	1.446213000	0.337305000
H	0.149766000	1.055869000	1.309458000
H	-0.480649000	2.622369000	0.656788000
H	-3.236334000	3.323849000	1.569794000
H	-2.099469000	3.624698000	2.907759000
H	-3.642416000	2.897761000	3.246343000
H	-1.562483000	1.617192000	4.391657000
H	-0.829179000	0.331831000	3.403183000
H	-2.485987000	0.186986000	3.938476000
H	-0.753811000	-0.420354000	-3.107742000
H	-0.030827000	-1.919319000	-2.522882000
H	0.966372000	-0.480132000	-2.713381000

RH 11 (Naphthalene)



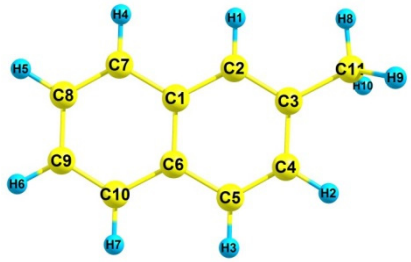
Molecule (Mol), E = -385.786100633399 Eh

C	-0.714256000	0.000000000	-0.005342000
C	-1.397446000	0.000000000	1.235974000
C	-0.706061000	0.000001000	2.419855000
C	0.706057000	-0.000000000	2.419855000
C	1.397448000	-0.000000000	1.235972000
C	0.714258000	0.000000000	-0.005336000
C	-1.397600000	-0.000000000	-1.246558000
C	-0.706033000	-0.000001000	-2.430371000
C	0.706031000	-0.000000000	-2.430367000
C	1.397601000	0.000000000	-1.246557000
H	-2.481102000	0.000000000	1.234777000
H	-1.241066000	0.000001000	3.360802000
H	1.241065000	-0.000001000	3.360800000
H	2.481103000	-0.000001000	1.234773000
H	-2.481241000	-0.000000000	-1.245367000
H	-1.240827000	-0.000001000	-3.371444000
H	1.240829000	0.000001000	-3.371440000
H	2.481242000	0.000001000	-1.245373000

Radical Cation (RC(a)), E = -385.500788851354 Eh

C	-0.713717000	0.000000000	-0.000011000
C	-1.396878000	0.000000000	1.231795000
C	-0.693107000	-0.000000000	2.442965000
C	0.693107000	0.000000000	2.442965000
C	1.396878000	0.000000000	1.231795000
C	0.713717000	0.000000000	-0.000011000
C	-1.396876000	0.000000000	-1.231819000
C	-0.693108000	-0.000000000	-2.442990000
C	0.693108000	-0.000000000	-2.442990000
C	1.396876000	0.000000000	-1.231819000
H	-2.479883000	-0.000000000	1.239034000
H	-1.236952000	-0.000000000	3.377570000
H	1.236952000	-0.000000000	3.377570000
H	2.479883000	0.000000000	1.239034000
H	-2.479881000	0.000000000	-1.239057000
H	-1.236950000	-0.000000000	-3.377596000
H	1.236950000	-0.000000000	-3.377596000
H	2.479881000	-0.000000000	-1.239057000

RH 12 (2-Methylnaphthalene)



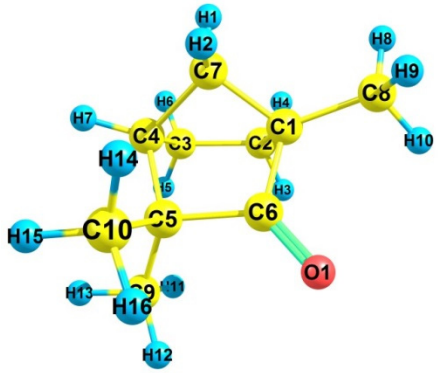
Molecule (Mol), E = -425.089647255078 Eh

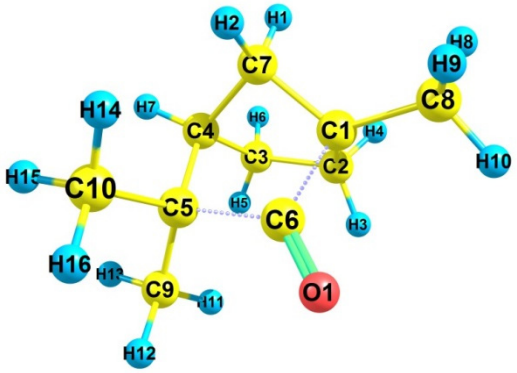
C	-0.714806000	0.000009000	-0.005948000
C	-1.400636000	-0.000000000	1.234613000
C	-0.731615000	0.000003000	2.434305000
C	0.687916000	0.000010000	2.417302000
C	1.385563000	0.000010000	1.239806000
C	0.711808000	0.000002000	-0.006900000
C	-1.396244000	0.000011000	-1.247725000
C	-0.702843000	0.000005000	-2.431310000
C	0.708752000	-0.000009000	-2.430964000
C	1.398162000	-0.000010000	-1.245077000
H	-2.484889000	-0.000005000	1.223275000
H	1.224089000	0.000013000	3.359138000
H	2.469009000	0.000011000	1.248098000
H	-2.479638000	0.000014000	-1.248690000
H	-1.237380000	0.000007000	-3.372571000
H	1.244674000	-0.000016000	-3.371302000
H	2.481576000	-0.000020000	-1.241357000
C	-1.462412000	-0.000006000	3.750202000
H	-2.542432000	-0.000014000	3.606232000
H	-1.202404000	-0.878341000	4.346295000
H	-1.202419000	0.878332000	4.346298000

Radical Cation (RC(a)), E = -424.810540387290 Eh

C	-0.714060000	0.000000000	-0.007400000
C	-1.396387000	0.000001000	1.218614000
C	-0.713053000	0.000001000	2.456553000
C	0.685093000	0.000000000	2.437397000
C	1.386461000	-0.000000000	1.240331000
C	0.711763000	-0.000000000	-0.005845000
C	-1.399746000	0.000000000	-1.243979000
C	-0.696818000	0.000000000	-2.449881000
C	0.690134000	-0.000000000	-2.443178000
C	1.394209000	-0.000000000	-1.227947000
H	-2.479649000	0.000001000	1.217957000
H	1.229921000	-0.000000000	3.372431000
H	2.469284000	-0.000001000	1.252355000
H	-2.482394000	0.000001000	-1.249500000
H	-1.236373000	0.000000000	-3.386715000
H	1.237782000	-0.000001000	-3.375663000
H	2.476839000	-0.000001000	-1.236177000
C	-1.465529000	0.000001000	3.747876000
H	-2.542345000	-0.000001000	3.595847000
H	-1.200649000	-0.875945000	4.345323000
H	-1.200653000	0.875950000	4.345320000

RH 13 (Fenchone)





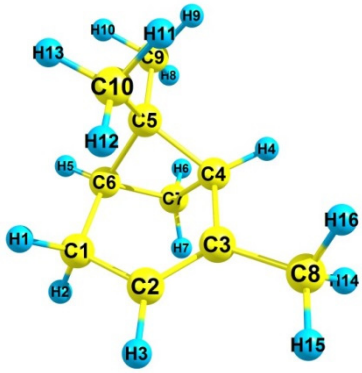
Molecule (Mol), E = -465.797429387663 Eh

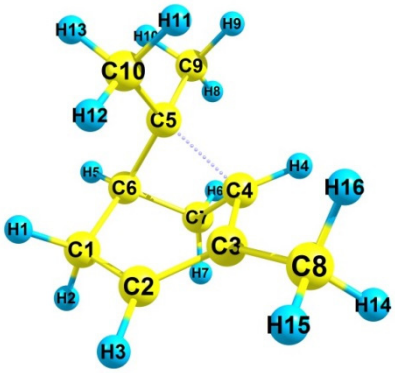
C	-1.240667000	0.390124000	0.020951000
C	-1.233808000	1.954052000	0.010623000
C	0.269820000	2.328219000	-0.129271000
C	0.974998000	0.957130000	-0.058763000
C	0.843588000	0.344301000	1.367555000
C	-0.668053000	0.021403000	1.390819000
C	-0.015470000	0.099127000	-0.875312000
H	-0.153383000	0.469911000	-1.892639000
H	0.236515000	-0.959383000	-0.928419000
C	-2.569978000	-0.254959000	-0.306125000
O	-1.277038000	-0.429833000	2.328762000
H	-1.698059000	2.367355000	0.906810000
H	-1.817466000	2.303020000	-0.842911000
H	0.607674000	3.028479000	0.631631000
H	0.464979000	2.792636000	-1.096681000
H	2.003055000	0.971461000	-0.420758000
H	-2.930144000	0.070145000	-1.284271000
H	-2.489001000	-1.343143000	-0.316692000
H	-3.321104000	0.007344000	0.440136000
C	1.225606000	1.259978000	2.536791000
H	0.635844000	2.175201000	2.568569000
H	1.064796000	0.737664000	3.479994000
H	2.280334000	1.538121000	2.477393000
C	1.648858000	-0.963011000	1.497274000
H	1.450130000	-1.664602000	0.687959000
H	2.718079000	-0.740594000	1.493727000
H	1.406305000	-1.461066000	2.436294000

Radical Cation (RC(a)), E = -465.496018891036 Eh

C	-1.255349000	0.406149000	-0.047310000
C	-1.240458000	1.958251000	0.041452000
C	0.254026000	2.341284000	-0.108731000
C	0.969162000	0.973276000	-0.050467000
C	0.908310000	0.365030000	1.370087000
C	-0.688281000	0.033572000	1.432905000
C	0.007621000	0.096180000	-0.862518000
H	-0.128591000	0.453231000	-1.885553000
H	0.258877000	-0.960639000	-0.909191000
C	-2.563306000	-0.279876000	-0.341028000
O	-1.301501000	-0.361417000	2.343653000
H	-1.715884000	2.338288000	0.945364000
H	-1.846382000	2.315261000	-0.794862000
H	0.592236000	3.044451000	0.646933000
H	0.438987000	2.802932000	-1.076900000
H	1.998927000	1.000314000	-0.406286000
H	-2.863457000	-0.010309000	-1.357160000
H	-2.477212000	-1.365002000	-0.298445000
H	-3.353647000	0.038963000	0.337035000
C	1.260471000	1.272186000	2.542609000
H	0.633632000	2.158534000	2.611826000
H	1.205305000	0.734929000	3.487173000
H	2.291526000	1.609214000	2.403654000
C	1.605085000	-0.997428000	1.497246000
H	1.331328000	-1.709045000	0.721946000
H	2.678798000	-0.811774000	1.410268000
H	1.416188000	-1.447474000	2.469744000

RH 14 (*α*-Pinene)





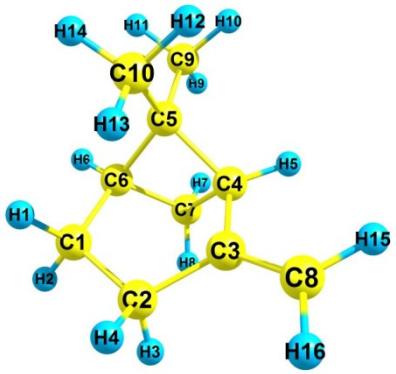
Molecule (Mol), E = -390.527843271624 Eh

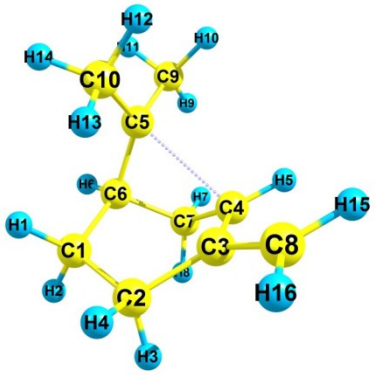
C	-1.838652000	-0.530431000	0.801471000
C	-0.865729000	-1.019863000	-0.245015000
C	-0.109807000	-0.144707000	-0.910798000
C	-0.322681000	1.323989000	-0.588632000
C	-0.348634000	1.548796000	0.973956000
C	-1.819279000	1.004009000	0.875513000
C	-1.860163000	1.568626000	-0.569707000
H	-1.595576000	-0.965887000	1.777877000
H	-2.852882000	-0.875529000	0.570020000
H	-0.786918000	-2.086290000	-0.427729000
C	0.906486000	-0.516094000	-1.946236000
H	0.309949000	1.982584000	-1.185778000
C	-0.305359000	3.035358000	1.343285000
C	0.657868000	0.813120000	1.851967000
H	-2.542661000	1.381471000	1.601612000
H	-2.133079000	2.619732000	-0.607756000
H	-2.446842000	1.017332000	-1.303555000
H	-0.989866000	3.647735000	0.759577000
H	0.701649000	3.434429000	1.196625000
H	-0.559370000	3.170484000	2.397996000
H	1.658270000	1.233773000	1.717655000
H	0.714561000	-0.250865000	1.634831000
H	0.397720000	0.932197000	2.907647000
H	0.680113000	-0.045641000	-2.908264000
H	0.953660000	-1.595054000	-2.096904000
H	1.903670000	-0.167089000	-1.659159000

Radical Cation (RC(a)), E = -390.241999967480 Eh

C	-1.876955000	-0.523098000	0.770125000
C	-0.945964000	-0.985723000	-0.286612000
C	-0.141099000	-0.057942000	-0.960179000
C	-0.452303000	1.335945000	-0.736428000
C	-0.374291000	1.520087000	1.003968000
C	-1.841903000	1.000392000	0.902640000
C	-1.964040000	1.585028000	-0.516404000
H	-1.646733000	-1.048389000	1.705264000
H	-2.893337000	-0.863513000	0.520730000
H	-0.846260000	-2.045317000	-0.492525000
C	1.017881000	-0.472465000	-1.789172000
H	0.150925000	2.046180000	-1.293701000
C	-0.241969000	3.004139000	1.291000000
C	0.676665000	0.749618000	1.775886000
H	-2.526914000	1.355844000	1.671938000
H	-2.194928000	2.643834000	-0.530516000
H	-2.628866000	1.070947000	-1.208395000
H	-0.935591000	3.633094000	0.740820000
H	0.773154000	3.351394000	1.097489000
H	-0.436226000	3.157777000	2.357646000
H	1.678540000	1.102206000	1.525397000
H	0.652294000	-0.328037000	1.628964000
H	0.533637000	0.941890000	2.842763000
H	0.843547000	-0.183597000	-2.832090000
H	1.209283000	-1.542104000	-1.746530000
H	1.917899000	0.067995000	-1.481581000

RH 15 (*β*-Pinene)





Molecule (Mol), E = -390.523793840712 Eh

C	-1.699245000	-0.711897000	0.996792000
C	-0.937386000	-1.223603000	-0.255343000
C	0.016619000	-0.196511000	-0.847135000
C	-0.333499000	1.224837000	-0.507931000
C	-0.289912000	1.422904000	1.059469000
C	-1.736115000	0.819639000	1.040424000
C	-1.880957000	1.364687000	-0.404987000
H	-1.242518000	-1.095929000	1.910788000
H	-2.720239000	-1.099605000	0.980608000
H	-1.670922000	-1.468654000	-1.027764000
H	-0.409939000	-2.154075000	-0.042098000
C	1.058202000	-0.528094000	-1.605777000
H	0.221838000	1.940453000	-1.115630000
C	-0.287248000	2.905076000	1.444701000
C	0.803596000	0.715287000	1.852649000
H	-2.430556000	1.180330000	1.802756000
H	-2.206950000	2.400328000	-0.441356000
H	-2.485497000	0.787259000	-1.104189000
H	-1.052990000	3.483416000	0.930179000
H	0.680229000	3.358710000	1.215321000
H	-0.456006000	3.016765000	2.519030000
H	1.772766000	1.182894000	1.660876000
H	0.904623000	-0.339232000	1.604875000
H	0.609130000	0.794150000	2.926020000
H	1.695062000	0.226390000	-2.050461000
H	1.305942000	-1.562349000	-1.812824000

Radical Cation (RC(a)), E = -390.236902273183 Eh

C	-1.663399000	-0.700019000	0.969828000
C	-0.930508000	-1.231841000	-0.299980000
C	-0.058401000	-0.191114000	-0.964273000
C	-0.539883000	1.133594000	-0.950973000
C	-0.316692000	1.446615000	1.334281000
C	-1.673994000	0.830231000	1.030805000
C	-1.913756000	1.381624000	-0.394840000
H	-1.216492000	-1.115580000	1.871862000
H	-2.695409000	-1.047096000	0.958270000
H	-1.682916000	-1.537032000	-1.031784000
H	-0.353437000	-2.126912000	-0.074484000
C	1.130429000	-0.494226000	-1.575696000
H	0.002820000	1.905592000	-1.484118000
C	-0.215744000	2.923674000	1.465797000
C	0.784607000	0.676714000	1.957582000
H	-2.412743000	1.182290000	1.760729000
H	-2.181991000	2.432814000	-0.411815000
H	-2.694611000	0.831129000	-0.925871000
H	-0.999136000	3.477985000	0.959134000
H	0.763076000	3.296708000	1.163872000
H	-0.301585000	3.148184000	2.539419000
H	1.739950000	1.193365000	1.879970000
H	0.883659000	-0.342328000	1.596747000
H	0.547656000	0.605555000	3.031127000
H	1.713020000	0.268871000	-2.075139000
H	1.513510000	-1.505621000	-1.601458000

16 (Water)



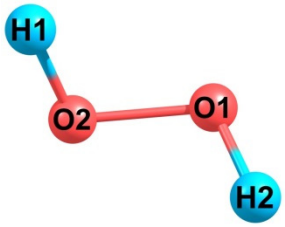
Molecule (Mol), E = -76.429588867406 Eh

O	0.000000000	0.000000000	-0.059793000
H	0.000000000	0.761905000	0.525880000
H	0.000000000	-0.761905000	0.525880000

Radical Cation (RC(a)), E = -75.969951537539 Eh

O	0.000000000	0.000000000	-0.054917000
H	0.000000000	0.822474000	0.523442000
H	0.000000000	-0.822474000	0.523442000

17 (Hydrogen peroxide)



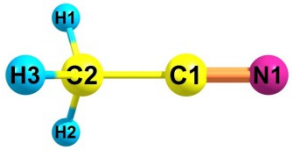
Molecule (Mol), E = -151.553995970550 Eh

O	0.148628000	-0.709939000	0.040044000
O	-0.148628000	0.709939000	0.040044000
H	-0.967971000	0.720003000	-0.471235000
H	0.967971000	-0.720003000	-0.471235000

Radical Cation (RC(a)), E = -151.172707685586 Eh

O	0.089297000	-0.648222000	-0.215588000
O	-0.089297000	0.648222000	-0.215588000
H	-1.078191000	0.764802000	-0.215603000
H	1.078191000	-0.764802000	-0.215603000

18 (Acetonitrile)



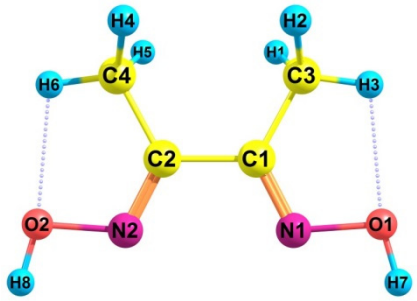
Molecule (Mol), E = -132.730425658549 Eh

C	-0.000015000	-0.000000000	0.130696000
N	0.000027000	0.000000000	1.280395000
C	-0.000034000	0.000000000	-1.324785000
H	-0.511456000	-0.885941000	-1.700816000
H	-0.511456000	0.885941000	-1.700816000
H	1.022933000	-0.000000000	-1.700778000

Radical Cation (RC(a)), E = -132.293392421907 Eh

C	0.018198000	0.000002000	0.086569000
N	-0.031525000	-0.000008000	1.288342000
C	0.057407000	0.000013000	-1.310130000
H	-0.556333000	-0.856037000	-1.680838000
H	-0.556345000	0.856039000	-1.680854000
H	1.068598000	-0.000009000	-1.719192000

Cis-19 (*Cis*-Dimethylglyoxime)



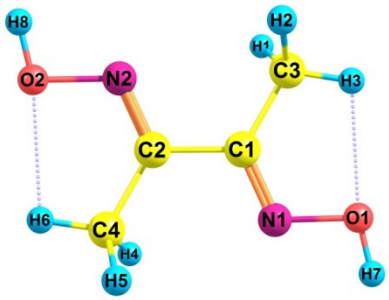
Molecule (Mol), E = -417.022028262935 Eh

N	-1.333538000	0.000029000	0.911094000
N	1.333538000	-0.000033000	0.911093000
C	-0.748624000	-0.000003000	-0.226178000
C	0.748624000	-0.000004000	-0.226179000
C	-1.465466000	-0.000036000	-1.549343000
C	1.465465000	0.000036000	-1.549344000
H	-1.192655000	0.877760000	-2.138105000
H	-1.192663000	-0.877868000	-2.138056000
H	-2.539869000	-0.000028000	-1.404900000
H	1.192660000	-0.877760000	-2.138107000
H	1.192660000	0.877868000	-2.138055000
H	2.539869000	0.000033000	-1.404900000
O	-2.730182000	0.000024000	0.813369000
O	2.730182000	-0.000022000	0.813368000
H	-2.995648000	0.000053000	1.737717000
H	2.995646000	-0.000048000	1.737717000

Radical Cation (RC(a)), E = -416.725628407721 Eh

N	-1.275338000	-0.000000000	0.921674000
N	1.275338000	0.000000000	0.921674000
C	-0.720716000	-0.000000000	-0.290641000
C	0.720716000	-0.000000000	-0.290641000
C	-1.484538000	0.000000000	-1.567797000
C	1.484538000	-0.000000000	-1.567797000
H	-1.218239000	0.876424000	-2.164139000
H	-1.218239000	-0.876424000	-2.164139000
H	-2.555536000	-0.000000000	-1.402495000
H	1.218239000	-0.876424000	-2.164139000
H	1.218239000	0.876424000	-2.164139000
H	2.555536000	-0.000000000	-1.402495000
O	-2.597644000	-0.000000000	0.872873000
O	2.597644000	0.000000000	0.872873000
H	-2.891050000	-0.000000000	1.800259000
H	2.891050000	0.000000000	1.800259000

Trans-19 (*Trans*-Dimethylglyoxime)



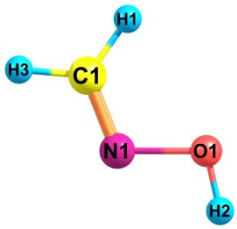
Molecule (Mol), E = -417.034738983103 Eh

N	1.281121000	-1.153931000	-0.000003000
N	-1.281119000	1.153928000	-0.000002000
C	0.069322000	-0.737227000	-0.000002000
C	-0.069319000	0.737227000	-0.000001000
C	-1.153627000	-1.606484000	0.000002000
C	1.153627000	1.606487000	0.000002000
H	-1.767217000	-1.387399000	0.874000000
H	-1.767221000	-1.387400000	-0.873994000
H	-0.883022000	-2.656700000	0.000002000
H	1.767218000	1.387403000	0.874000000
H	1.767221000	1.387404000	-0.873994000
H	0.883021000	2.656702000	0.000002000
O	1.389679000	-2.547416000	-0.000002000
O	-1.389682000	2.547413000	-0.000002000
H	2.342195000	-2.680229000	-0.000003000
H	-2.342198000	2.680222000	-0.000004000

Radical Cation (RC(a)), E = -416.728471544019 Eh

N	1.292594000	-1.153543000	-0.000000000
N	-1.292594000	1.153543000	-0.000000000
C	0.030947000	-0.717318000	0.000000000
C	-0.030947000	0.717318000	0.000000000
C	-1.171096000	-1.602431000	0.000000000
C	1.171096000	1.602431000	0.000000000
H	-1.787589000	-1.397337000	0.875595000
H	-1.787589000	-1.397337000	-0.875595000
H	-0.890512000	-2.649481000	0.000000000
H	1.787589000	1.397337000	0.875595000
H	1.787589000	1.397337000	-0.875595000
H	0.890512000	2.649481000	0.000000000
O	1.382679000	-2.471533000	-0.000000000
O	-1.382679000	2.471533000	-0.000000000
H	2.335204000	-2.670770000	-0.000000000
H	-2.335204000	2.670770000	-0.000000000

20 (Formaldehyde oxime)



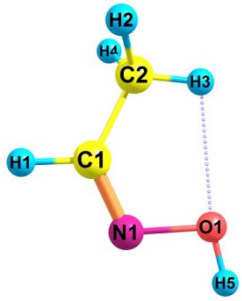
Molecule (Mol), E = -169.802678736992 Eh

C	-1.172803000	-0.208808000	0.000000000
H	-1.136398000	-1.295684000	0.000000000
N	-0.134073000	0.513413000	-0.000000000
O	1.033149000	-0.257525000	-0.000000000
H	1.730985000	0.404905000	0.000000000
H	-2.122521000	0.308844000	0.000000000

Radical Cation (RC(a)), E = -169.435077031170 Eh

C	-1.217476000	-0.251490000	-0.000001000
H	-1.331003000	-1.342376000	-0.000021000
N	-0.082929000	0.256153000	0.000021000
O	1.131970000	-0.174711000	0.000046000
H	1.777814000	0.564897000	-0.000045000
H	-2.080038000	0.412670000	-0.000000000

21 (Acetaldehyde oxime)



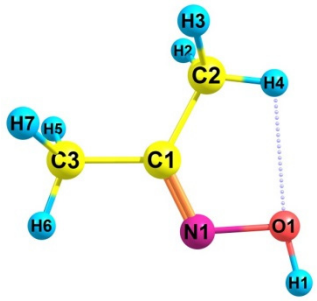
Molecule (Mol), E = -209.110507501338 Eh

C	-0.800568000	0.375289000	0.000000000
H	-1.580710000	1.130955000	0.000001000
N	0.368748000	0.871682000	0.000000000
C	-1.203459000	-1.063980000	0.000000000
H	-1.818943000	-1.278143000	-0.877279000
H	-0.342946000	-1.725752000	0.000001000
H	-1.818945000	-1.278143000	0.877278000
O	1.378216000	-0.110645000	-0.000000000
H	2.179635000	0.420270000	-0.000001000

Radical Cation (RC(a)), E = -208.763348867177 Eh

C	-0.814702000	0.327956000	-0.000000000
H	-1.582878000	1.096413000	-0.000000000
N	0.421871000	0.876202000	0.000000000
C	-1.177840000	-1.071989000	-0.000000000
H	-1.848561000	-1.247002000	-0.858297000
H	-0.350932000	-1.772755000	-0.000000000
H	-1.848561000	-1.247002000	0.858297000
O	1.351457000	-0.045924000	0.000000000
H	2.211174000	0.425633000	-0.000000000

22 (Acetone oxime)



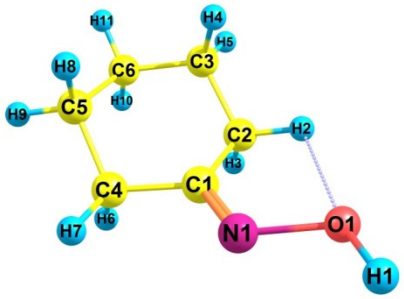
Molecule (Mol), E = -248.417877328829 Eh

C	-1.237870000	0.273198000	-2.033096000
N	-2.140793000	-0.247308000	-1.299743000
O	-3.325373000	-0.548291000	-2.007507000
H	-3.880697000	-0.922667000	-1.318204000
C	-1.354944000	0.562839000	-3.500802000
H	-1.200357000	1.629489000	-3.682420000
H	-0.570543000	0.033165000	-4.047345000
H	-2.321952000	0.272275000	-3.897852000
C	0.050608000	0.619956000	-1.345508000
H	0.259272000	1.689225000	-1.437595000
H	0.005477000	0.358023000	-0.290719000
H	0.887578000	0.090109000	-1.808164000

Radical Cation (RC(a)), E = -248.094069626012 Eh

C	-1.207244000	0.285276000	-2.075848000
N	-2.140186000	-0.328753000	-1.413457000
O	-3.409358000	-0.269579000	-1.720704000
H	-3.830369000	-1.084635000	-1.380914000
C	-1.340191000	0.551412000	-3.533602000
H	-1.237100000	1.634319000	-3.672734000
H	-0.506684000	0.091051000	-4.068881000
H	-2.285464000	0.212631000	-3.944753000
C	0.035130000	0.611224000	-1.333605000
H	0.271819000	1.667283000	-1.489356000
H	-0.046393000	0.397313000	-0.272024000
H	0.866446000	0.042471000	-1.763077000

23 (Cyclohexanone oxime)



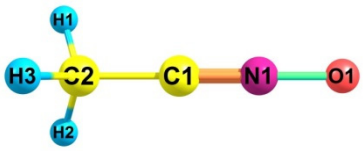
Molecule (Mol), E = -365.112887996007 Eh

C	0.028960000	2.237937000	-3.319879000
N	0.120527000	1.143495000	-2.674694000
O	0.115943000	1.326050000	-1.271974000
H	0.179532000	0.421697000	-0.953057000
C	-0.108463000	3.618793000	-2.736578000
H	-0.205981000	3.569278000	-1.655649000
H	0.813192000	4.171006000	-2.955832000
C	-1.298492000	4.363417000	-3.370778000
H	-2.228734000	3.898875000	-3.029555000
H	-1.313065000	5.394710000	-3.011864000
C	0.028603000	2.142340000	-4.822293000
H	0.953677000	2.596408000	-5.197670000
H	0.035554000	1.093865000	-5.118376000
C	-1.169597000	2.893525000	-5.425794000
H	-2.090883000	2.360570000	-5.170546000
H	-1.095115000	2.887707000	-6.515447000
C	-1.249870000	4.329541000	-4.900719000
H	-0.375745000	4.891446000	-5.248939000
H	-2.126807000	4.833234000	-5.314069000

Radical Cation (RC(a)), E = -364.799893373906 Eh

C	0.035198000	2.285432000	-3.330607000
N	-0.038949000	1.189174000	-2.627585000
O	0.385490000	1.167247000	-1.382002000
H	-0.033380000	0.395347000	-0.955859000
C	-0.109123000	3.641038000	-2.733420000
H	-0.186242000	3.591229000	-1.650269000
H	0.812546000	4.176359000	-2.998791000
C	-1.309066000	4.390728000	-3.376502000
H	-2.235331000	3.953397000	-2.997327000
H	-1.280241000	5.423433000	-3.031068000
C	0.066742000	2.147821000	-4.807478000
H	0.969780000	2.655681000	-5.162285000
H	0.113188000	1.103435000	-5.106806000
C	-1.174901000	2.882901000	-5.405949000
H	-2.075272000	2.321937000	-5.147076000
H	-1.072962000	2.843823000	-6.490814000
C	-1.266417000	4.318694000	-4.903425000
H	-0.420480000	4.899844000	-5.280879000
H	-2.167344000	4.786374000	-5.305571000

24 (Acetonitrile N-oxide)



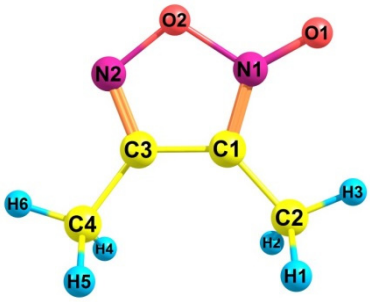
Molecule (Mol), E = -207.879576709614 Eh

C	-0.000062000	0.000000000	0.162139000
N	0.000021000	0.000000000	1.318098000
C	-0.000042000	-0.000000000	-1.294703000
H	-0.510457000	-0.884233000	-1.679803000
H	-0.510457000	0.884233000	-1.679803000
H	1.020962000	0.000000000	-1.679718000
O	0.000114000	-0.000000000	2.528082000

Radical Cation (RC(a)), E = -207.525434053952 Eh

C	-0.015044000	-0.000000000	0.135387000
N	0.001859000	-0.000000000	1.304321000
C	-0.026280000	-0.000000000	-1.293468000
H	-0.502107000	-0.907934000	-1.673804000
H	-0.502107000	0.907934000	-1.673803000
H	1.024800000	0.000000000	-1.628381000
O	0.018959000	0.000000000	2.504039000

25 (Dimethyl-Furoxane (Farazane) N-oxide)



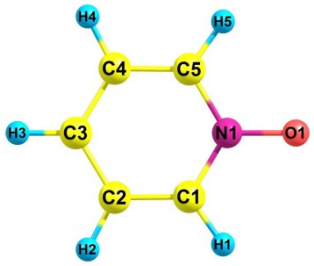
Molecule (Mol), E = -415.802311396769 Eh

C	1.614490000	-0.213885000	-0.071978000
N	2.115386000	-0.165052000	1.155094000
C	2.484317000	-0.385705000	-1.264789000
H	2.209501000	-1.279603000	-1.828039000
H	2.403811000	0.469333000	-1.939078000
H	3.522163000	-0.480293000	-0.950929000
O	3.237160000	-0.232118000	1.626357000
C	0.206042000	-0.073437000	0.057391000
N	-0.140246000	0.055500000	1.308221000
C	-0.806177000	-0.064541000	-1.034734000
H	-0.614861000	0.747181000	-1.739041000
H	-0.784644000	-1.000356000	-1.596459000
H	-1.800250000	0.066223000	-0.612374000
O	0.999914000	0.007884000	2.056950000

Radical Cation (RC(a)), E = -415.480874509974 Eh

C	0.090779000	0.699883000	0.000000000
N	1.069998000	-0.255177000	-0.000000000
C	0.414792000	2.137800000	-0.000000000
H	-0.026833000	2.615148000	-0.879378000
H	-0.026834000	2.615148000	0.879378000
H	1.489264000	2.305090000	0.000000000
O	2.263823000	-0.226460000	-0.000000000
C	-1.125672000	0.008818000	0.000000000
N	-0.895579000	-1.315753000	0.000000000
C	-2.505841000	0.547726000	0.000000000
H	-2.675147000	1.169170000	0.881705000
H	-2.675147000	1.169170000	-0.881705000
H	-3.222990000	-0.269702000	-0.000000000
O	0.383529000	-1.569647000	-0.000000000

26 (Pyridine N-oxide)



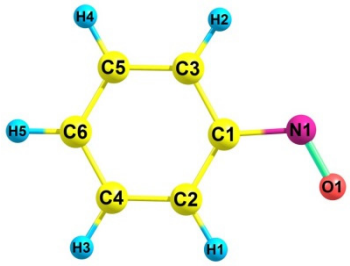
Molecule (Mol), E = -323.394811420757 Eh

C	1.175593000	0.000000000	0.254069000
C	1.189722000	-0.000000000	-1.123811000
C	0.000000000	-0.000000000	-1.843523000
C	-1.189722000	0.000000000	-1.123811000
C	-1.175593000	-0.000000000	0.254069000
N	-0.000000000	0.000000000	0.954099000
H	2.054678000	0.000000000	0.878085000
H	2.147366000	-0.000000000	-1.626299000
H	0.000000000	-0.000000000	-2.923832000
H	-2.147365000	0.000000000	-1.626300000
H	-2.054679000	-0.000000000	0.878085000
O	0.000000000	-0.000000000	2.226491000

Radical Cation (RC(a)), E = -323.096133440060 Eh

C	1.206540000	-0.000000000	0.250898000
C	1.216172000	-0.000000000	-1.116656000
C	-0.000000000	0.000000000	-1.813088000
C	-1.216172000	0.000000000	-1.116656000
C	-1.206540000	-0.000000000	0.250898000
N	0.000000000	0.000000000	0.915101000
H	2.073926000	-0.000000000	0.894588000
H	2.161363000	0.000000000	-1.640558000
H	0.000000000	0.000000000	-2.895455000
H	-2.161363000	0.000000000	-1.640558000
H	-2.073926000	-0.000000000	0.894587000
O	0.000000000	0.000000000	2.194219000

27 (Nitrosobenzene)



Molecule (Mol), E = -361.475462562199 Eh

C	0.476949000	-0.234873000	-0.000000000
C	0.044818000	1.093676000	-0.000001000
C	-0.434407000	-1.288217000	0.000000000
H	0.780445000	1.886027000	-0.000001000
H	-0.054613000	-2.301584000	0.000001000
C	-1.313344000	1.357670000	0.000001000
C	-1.796551000	-1.015922000	-0.000000000
H	-1.667120000	2.380429000	0.000001000
H	-2.513886000	-1.825611000	-0.000001000
C	-2.232581000	0.304917000	-0.000001000
H	-3.293282000	0.520757000	0.000000000
N	1.862613000	-0.624174000	0.000000000
O	2.661502000	0.285501000	0.000000000

Radical Cation (RC(a)), E = -361.183887006740 Eh

C	0.466993000	-0.212248000	0.000000000
C	0.032963000	1.142854000	0.000000000
C	-0.435350000	-1.305205000	-0.000000000
H	0.756799000	1.946396000	0.000000000
H	-0.049593000	-2.315523000	-0.000000000
C	-1.318036000	1.376038000	-0.000000000
C	-1.784255000	-1.034358000	-0.000000000
H	-1.692408000	2.390398000	-0.000000000
H	-2.502608000	-1.841593000	0.000000000
C	-2.219915000	0.295735000	0.000000000
H	-3.282640000	0.502290000	0.000000000
N	1.785323000	-0.519434000	0.000000000
O	2.763271000	0.113246000	-0.000000000