Strain and stereoelectronics in cycloalkyne click chemistry

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Table of Contents

Computational Details

All calculations were carried with the Gaussian 16 software package.[1] Ring strain energies were calculated using the M06-2X[2] DFT functional with the 6-311+G(d,p) basis set for all atoms, unless otherwise noted. Energies of activation for the click reactions were calculated using the M06-2X DFT functional with the 6-311+G(d,p) basis set for all atoms with Grimme's D3 version for empirical dispersion[3] was also included, unless otherwise noted. Frequency calculations were carried out for all structures to confirm them as either a minimum or a TS. Three-dimensional structures were produced with UCSF Chimera.[4] NBO 3.1 was used to obtain 2nd order perturbation energies.[5]

n,m-MOBO	$\Delta E^{\ddagger}$ (kcal/mol)	ΔE_{rxn} (kcal/mol)
3,4-MOBO (1,4)	10.4	-81.7
3,4-MOBO (1,5)	9.2	-82.3
4,5-MOBO (1,4)	9.7	-83.5
4,5-MOBO (1,5)	9.9	-83.7
5,6-MOBO	8.9	-79.9

Table S1. Activation energies and reaction energies for the click reaction of the n,m-MOBOs with methylazide.

	$\Delta E^{\ddagger}$ (kcal/mol)	ΔE_{rxn} (kcal/mol)
DIBC	10.1	-76.1
S-DIBO (1,4)	8.3	-74.9
S-DIBO (1,5)	10.2	-75.4
R-DIBO (1,4)	7.7	-81.2
R-DIBO (1,5)	9.5	-80.6
DIBAC (1,4)	7.6	-72.9
DIBAC (1,5)	9.2	-69.5
DIBAC-Me (1,4)	6.9	-76.4
DIBAC-Me (1,5)	8.1	-76.3
DIBONE (1,4)	6.8	-81.7
DIBONE (1,5)	8.2	-80.0
ODIBO (1,4)	6.2	-80.1
ODIBO (1,5)	7.6	-80.6
BARAC (1,4)	5.9	-74.8
BARAC (1,5)	7.1	-70.9

Table S2. Activation energies and reaction energies for the click reaction of the dibenzannulated cyclooctynes with methylazide.

DIBC	2.19	2.17
DIBO1	2.23	2.16
DIBO2	2.25	2.16
DIBAC	2.23	2.17
DIBAC-Me	2.26	2.17
DIBONE	2.27	2.15
ODIBO	2.26	2.17
BARAC	2.24	2.16

Table S3. Interatomic distances between nitrogens of azide and alkynyl carbons for the 1,4-TS geometries. Distances in angstroms.

Calculated Geometries

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

Cyclohexane
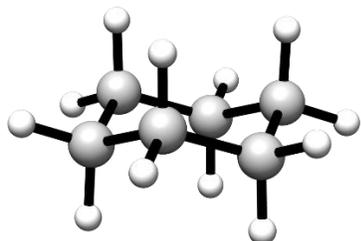
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C 1.456902 0.044215 -0.233780
C 0.766770 -1.239497 0.233600
C -0.690189 -1.283766 -0.233682
C -1.456903 -0.044216 0.233778
C -0.766771 1.239497 -0.233599
H 1.309255 -2.116562 -0.129679
H 1.506385 0.045643 -1.329837
H 2.487729 0.075244 0.129462
H 0.713909 1.327632 1.329712
H 1.178477 2.192040 -0.129781
H -0.713906 -1.327631 -1.329713
H -1.178478 -2.192041 0.129778
H -2.487728 -0.075245 -0.129470
H -1.506392 -0.045643 1.329835
H -0.792890 1.281644 -1.329631
H -1.309254 2.116561 0.129689
H 0.792889 -1.281638 1.329633

**Hexane**
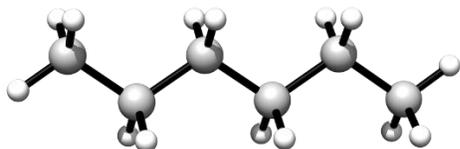
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H 4.056996 0.468353 0.000000
H 3.280410 -0.849875 -0.882309
C 1.878568 0.553356 -0.000000
H 1.830169 1.208276 0.876694
H 1.830170 1.208275 -0.876697
C 0.665296 -0.374065 -0.000000

H 0.712613 -1.030822 0.877330
H 0.712612 -1.030821 -0.877332
C -0.665296 0.374065 0.000001
H -0.712612 1.030824 -0.877329
H -0.712613 1.030819 0.877333
C -1.878568 -0.553356 -0.000002
H -1.830169 -1.208278 0.876691
H -1.830170 -1.208273 -0.876700
C -3.201079 0.209393 0.000001
H -3.280410 0.849877 -0.882308
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2-Pentyne
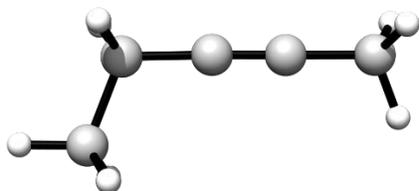
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C -1.215287 -0.086074 -0.000032
C -0.042370 -0.351299 -0.000444
C 1.393208 -0.641025 0.000177
H 1.633949 -1.249269 -0.876196
H 1.633402 -1.248539 0.877207
C 2.244669 0.634048 -0.000143
H 2.029194 1.237871 0.882384
H 2.029795 1.237011 -0.883407
H 3.307318 0.384900 0.000321
H -3.140892 -0.234438 -0.853466

3-Hexyne
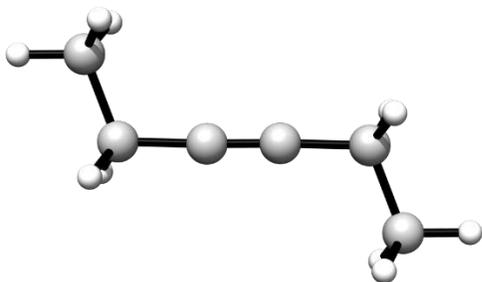
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C -0.562282 -0.214112 -0.000443
C -1.945618 -0.695211 -0.000468
H -2.102081 -1.330286 0.875957
H -2.102347 -1.329392 -0.877491
C -2.960925 0.453788 0.000272
H -2.829058 1.081088 -0.882316
H -2.828804 1.080182 0.883465
C 2.960917 -0.453808 0.000742
H 2.828667 -1.080200 0.883917
H 2.829154 -1.081104 -0.881864
H 3.980265 -0.063654 0.000824
H -3.980264 0.063612 0.000219

3-Heptyne
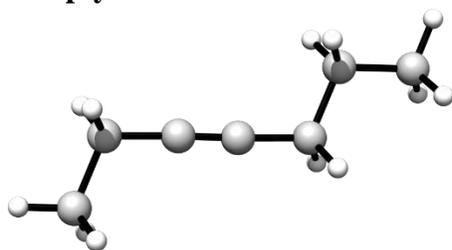
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C -1.272942 -0.657892 -0.000494
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C -2.282936 0.497978 0.000402
H -2.101381 1.125300 -0.876091
H -2.101200 1.124097 0.877717
C -3.721363 -0.010224 0.000202
H -3.919531 -0.624115 0.882719
H -4.434018 0.816293 0.000856
H -3.919722 -0.622884 -0.883127
C 3.635943 -0.473234 0.000613

H 3.496870 -1.098048 0.883833
H 3.497243 -1.099151 -0.881886
H 4.659530 -0.094335 0.000593

4-Octyne
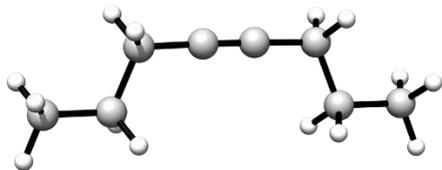
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H 2.409575 -1.234105 0.991854
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C -0.601354 -0.804981 -0.018812
C -2.064036 -0.774695 -0.059991
H -2.461218 -1.388326 0.755345
H -2.409346 -1.233791 -0.992206
C -2.630837 0.647618 0.049208
H -2.224646 1.252348 -0.765738
H -2.277002 1.097201 0.980590
C -4.155739 0.652160 0.003874
H -4.573190 0.064597 0.825745
H -4.551880 1.666017 0.082486
H -4.520476 0.221619 -0.932369
C 2.630797 0.647617 -0.049006
H 2.276720 1.097496 -0.980149
H 2.224804 1.252083 0.766237
C 4.155721 0.652218 -0.004071
H 4.572967 0.064912 -0.826228
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4-Nonyne
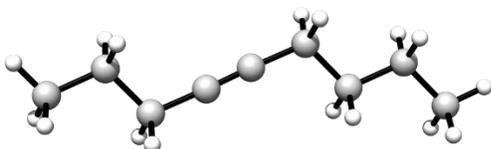
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C -0.090763 0.353067 -0.000029
C -1.191465 -0.133250 0.000039
C -2.548786 -0.680993 -0.000566
H -2.679871 -1.323760 0.876181
H -2.679908 -1.321783 -0.878753
C -3.628584 0.410057 0.000692
H -3.486150 1.047779 -0.875528
H -3.486124 1.045788 0.878354
C -5.032699 -0.186451 0.000039
H -5.192416 -0.811866 0.882273
H -5.795333 0.594202 0.000936
H -5.192443 -0.809863 -0.883607
C 2.345020 -0.190536 0.000100
H 2.205290 -0.829203 0.877918
H 2.205243 -0.829845 -0.877243
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C 3.882016 1.034781 0.876897
C 3.881963 1.034140 -0.877682
C 4.830251 -0.694361 0.000211
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5-Decyne
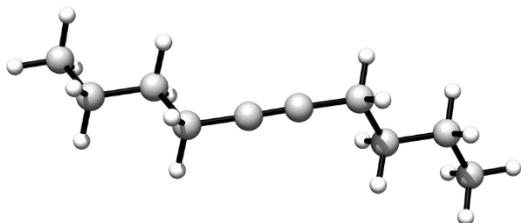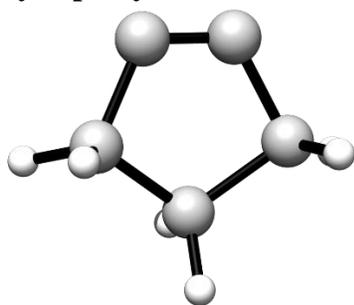

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H 1.967409 -0.511404 1.731506
C 0.564751 -0.836306 0.207450
C -0.564748 -0.836296 -0.207456
C -1.949715 -0.817765 -0.680480
H -2.355871 -1.833997 -0.645639
H -1.967393 -0.511350 -1.731510
C -2.844661 0.119556 0.140797
H -2.429885 1.131792 0.103325
H -2.817712 -0.190739 1.190094
C -4.286044 0.130014 -0.360897

H -4.687949 -0.888456 -0.326782
H -4.300106 0.433266 -1.413428
C 2.844659 0.119559 -0.140789
H 2.817702 -0.190709 -1.190094
H 2.429881 1.131793 -0.103287
C 4.286046 0.130007 0.360893
H 4.687953 -0.888461 0.326749
H 4.300116 0.433233 1.413432
C 5.177668 1.062597 -0.455075
H 6.204705 1.060793 -0.085218
H 5.198164 0.760354 -1.505206
H 4.807061 2.089933 -0.412595
C -5.177675 1.062581 0.455088
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Cyclopentyne

# of imaginary frequencies = 0
E = -193.922065
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C 0.090010 -1.148810 -0.607327
C 0.090010 0.211248 -1.262769
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H -0.613730 0.331570 2.085416
H 1.089678 0.446733 1.633078
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Cyclohexyne
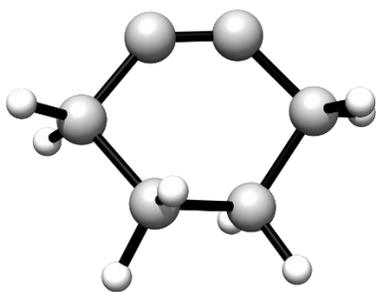
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C 0.073465 -0.600638 -1.292274
C 0.237807 -1.573727 -0.190928
C -0.237807 -0.733035 1.043691
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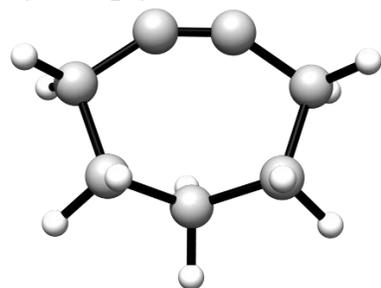H -0.109311 1.221711 1.958769
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H 0.109311 -1.221711 1.958769

Cycloheptyne

# of imaginary frequencies = 0
E = -272.614677
0 1
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C -0.091856 -1.382854 0.602229
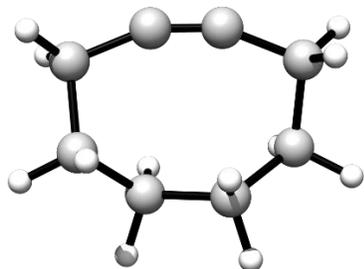C -0.091856 -0.565084 -1.821095
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H -1.096178 -0.541068 2.254108
H 1.411640 0.855746 -1.198009
H 0.589114 -0.924649 -2.594446
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H 0.589114 -0.924649 2.594446
H 0.091537 1.569808 -2.112894
H -1.096178 -0.541068 -2.254108

Cyclooctyne

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E = -311.934316
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C 0.600209 -1.454523 -0.033295
C -1.952796 -0.910218 0.124628
C -0.600230 -1.454532 0.033292
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H -1.753645 0.635679 -1.372336
H 2.315935 -0.994262 -1.153502
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H 0.545756 0.976528 -1.393692
C -0.684371 1.347085 0.372115
H -0.545741 0.976522 1.393691
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H -2.315941 -0.994236 1.153507
H -2.663687 -1.438559 -0.514209
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Cyclononyne
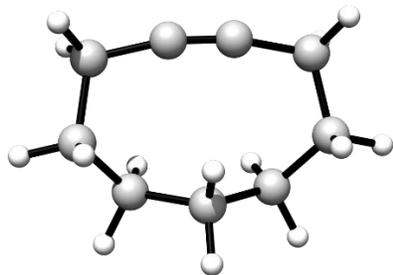
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C -2.034296 -1.195825 0.068885
C -0.600963 -1.485720 0.018246
H -2.256067 0.416358 -1.365612
H -3.329334 0.516358 0.019146
C -0.000196 1.462541 -0.400217
H -0.000081 0.778284 -1.250624
C -1.318173 1.260268 0.390379
H -1.094870 0.891507 1.397168
H -1.815655 2.223881 0.523978
H -0.000055 2.467435 -0.832098
H -2.392827 -1.397049 1.083507
H -2.594303 -1.852650 -0.601095
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H 1.093833 0.890532 1.397236
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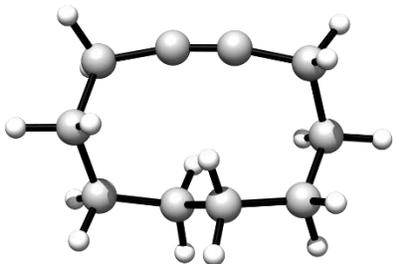C 2.303387 0.286439 -0.280177
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Cyclodecyne

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E = -390.558882
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C 0.184118 1.965870 -1.232665
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C -0.588966 -0.489570 -1.361162
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C -0.106308 -2.037036 1.368442
H -1.151265 -2.364889 1.337552
H 0.373174 -2.590739 2.179956
C 0.106308 2.037036 1.368442
H 1.151265 2.364889 1.337552
H -0.373174 2.590739 2.179956
C 0.049011 0.599313 1.642414
C -0.049011 -0.599313 1.642414
H 1.092370 2.576292 -1.290557
H -0.426044 2.244982 -2.099296
H 1.147121 0.369285 -2.296764
H 1.285097 0.240488 -0.558104
H -1.285097 -0.240488 -0.558104
H -1.147121 -0.369285 -2.296764
H -1.092370 -2.576292 -1.290557
H 0.426044 -2.244982 -2.099296
C -0.588966 2.371752 0.032345
H -0.747996 3.453515 -0.005866
H -1.582033 1.914238 0.036837
C 0.588966 -2.371752 0.032345
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3,3-Difluoro-4-octyne
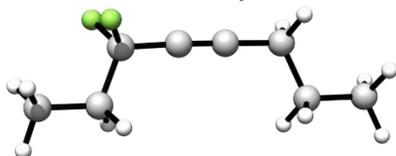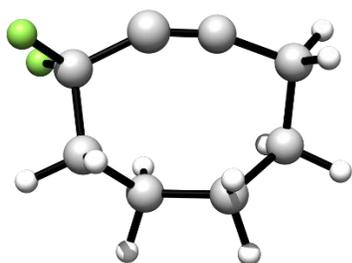

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C -1.075365 -0.594097 -0.045290
C -2.531977 -0.697917 -0.075936
H -2.855383 -1.355300 0.737215
H -2.830540 -1.183137 -1.010533
C -3.227153 0.665368 0.048660
H -2.887436 1.311272 -0.764904
H -2.911598 1.139099 0.981613
C -4.745376 0.522681 0.013662
H -5.098229 -0.107150 0.834178

H -5.234480 1.493831 0.102966
H -5.074126 0.066456 -0.923487
C 2.018920 1.124425 -0.077921
H 1.605300 1.527024 -1.005315
H 1.549938 1.658647 0.751494
C 3.537699 1.262865 -0.040427
H 3.996550 0.728780 -0.873001
H 3.940986 0.861350 0.889684
H 3.818598 2.314228 -0.110671
F 2.140706 -1.038040 -1.005511
F 2.074559 -0.875860 1.165885

DIFO

# of imaginary frequencies = 0
E = -510.426400
0 1
C -1.498430 -0.198792 -0.016150
C 2.540391 0.117165 0.307173
C -0.407066 -1.171631 -0.054747
C 2.211654 -1.345671 -0.080680
C 0.760010 -1.455143 -0.059440
H 2.420792 0.227034 1.388693
H 3.596459 0.292199 0.086158
C 0.338192 1.586654 0.270090
H 0.315411 1.223107 1.302180
C 1.677197 1.177757 -0.411280
H 1.484673 0.846717 -1.437798
H 2.288079 2.078808 -0.500031
H 0.320182 2.675968 0.341348
H 2.575904 -1.562104 -1.089094
H 2.690730 -2.049680 0.602056
C -0.970065 1.170293 -0.429844
H -0.839354 1.148676 -1.514756
H -1.770956 1.880153 -0.205645
F -2.542391 -0.547104 -0.819104
F -2.012412 -0.124526 1.249787

Cyclohexane (D3)
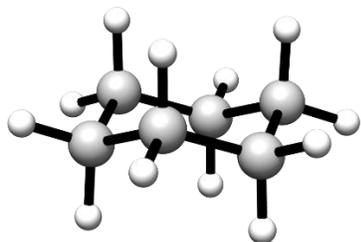
# of imaginary frequencies = 0
E = -235.817080
0 1
C 1.427297 -0.297538 0.233496
C 0.455943 -1.384808 -0.233619
C -0.971407 -1.087253 0.233492
C -1.427297 0.297538 -0.233496
C -0.455943 1.384808 0.233619
C 0.971407 1.087253 -0.233492
H -1.658228 -1.856280 -0.130462
H 0.471592 -1.432118 -1.329543
H 0.778556 -2.364188 0.130156
H 1.476290 -0.307731 1.329390
H 2.436653 -0.507848 -0.130620
H -1.476290 0.307731 -1.329390
H -2.436653 0.507848 0.130620
H -0.778556 2.364188 -0.130156
H -0.471592 1.432118 1.329543
H 1.004578 1.124591 -1.329399
H 1.658228 1.856280 0.130462
H -1.004578 -1.124591 1.329399

Hexane (D3)
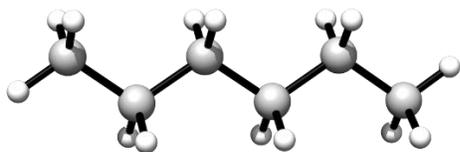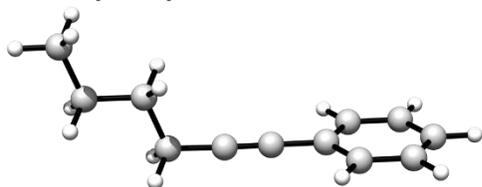

# of imaginary frequencies = 0
E = -237.011226
0 1
C -3.201079 0.209393 0.000001
H -3.280410 0.849872 0.882315
H -4.056996 -0.468353 -0.000000
H -3.280410 0.849875 -0.882309
C -1.878568 -0.553356 -0.000000
H -1.830169 -1.208276 0.876694
H -1.830170 -1.208275 -0.876697
C -0.665296 0.374065 -0.000000
H -0.712613 1.030822 0.877330

H -0.712612 1.030821 -0.877332
C 0.665296 -0.374065 0.000001
H 0.712612 -1.030824 -0.877329
H 0.712613 -1.030819 0.877333
C1.878568 0.553356 -0.000002
H 1.830169 1.208278 0.876691
H 1.830170 1.208273 -0.876700
C 3.201079 -0.209393 0.000001
H 3.280410 -0.849877 -0.882308
H 4.056996 0.468353 -0.000002
H 3.280410 -0.849870 0.882315

Hex-1-yn-1-ylbenzene
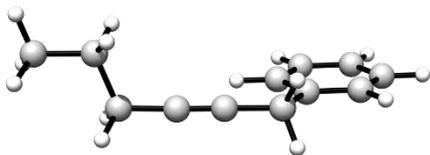

# of imaginary frequencies = 0
E = -465.560582
0 1
C 0.387708 -0.067675 -0.502801
C -0.784183 -0.106238 -0.779730
C -2.214729 -0.148344 -1.076563
H -2.454437 0.638776 -1.798752
H -2.452368 -1.101024 -1.560714
C 1.783330 -0.022550 -0.177366
C 2.489165 -1.203551 0.082322
H 1.966613 -2.150995 0.032959
C 3.840545 -1.156723 0.397912
H 4.377312 -2.076648 0.596979
C 4.504248 0.065228 0.459044
C 3.808883 1.243274 0.202280
H 4.320951 2.197029 0.248722
H 5.558651 0.099356 0.705676
C 2.457411 1.203050 -0.113960
H 1.910307 2.115983 -0.314905
C -3.083490 0.022354 0.177797
H -2.831823 -0.764560 0.895501
H -2.834455 0.974212 0.656998
C -4.574774 -0.023995 -0.143723
H -4.812720 0.761123 -0.869579
H -4.810354 -0.977082 -0.629521
C -5.440627 0.146885 1.101882
H -6.504030 0.110937 0.858312
H -5.235487 -0.642793 1.829035

H -5.239082 1.105392 1.586714

Hex-2-yn-1-ylbenzene

# of imaginary frequencies = 0
E = -465.557201
0 1
C 0.738280 -1.082812 0.238539
C 1.840060 -0.653518 0.458192
C 3.187686 -0.130355 0.685120
H 3.131017 0.733956 1.355084
H 3.783765 -0.887491 1.205005
C 3.893543 0.274521 -0.616422
H 3.939807 -0.594885 -1.277219
H 3.286194 1.025530 -1.128215
C 5.295201 0.815575 -0.352370
H 5.790707 1.101522 -1.281656
H 5.259433 1.697052 0.293126
H 5.917600 0.065224 0.142095
C -0.601283 -1.607077 -0.021201
H -0.598611 -2.120345 -0.988277
H -0.833464 -2.370592 0.728479
C -1.714622 -0.571213 -0.022461
C -1.485179 0.778630 0.222630
C -3.019171 -0.998661 -0.279008
C -2.541951 1.686891 0.211695
H -0.475512 1.117866 0.422210
C -4.073595 -0.095492 -0.290509
H -3.207391 -2.050666 -0.471509
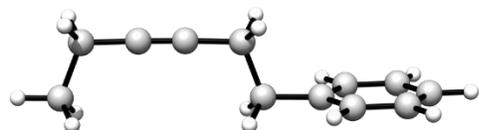C -3.836940 1.254959 -0.044188
H -2.348216 2.735650 0.404518
H -5.079957 -0.443817 -0.491349
H -4.657539 1.962310 -0.052385

**Hex-3-yn-1-ylbenzene**

# of imaginary frequencies = 0
E = -465.558901
0 1
C -2.114473 -0.075669 -0.746610

C -3.309554 -0.071200 -0.606726
C -4.760874 -0.061256 -0.412480
H -5.196084 0.734305 -1.023630
H -5.176017 -1.002796 -0.782583
C -5.148340 0.138277 1.057607
H -6.233899 0.141007 1.170283
H -4.737397 -0.662787 1.673507
H -4.758216 1.086224 1.430594
C -0.657427 -0.078435 -0.877345
H -0.333534 -0.992244 -1.384610
H -0.341054 0.757959 -1.507890
C 0.049276 0.021061 0.489640
H -0.278011 0.935611 0.989839
H -0.267460 -0.819291 1.111962
C 1.547771 0.019330 0.329001
C 2.259148 -1.180850 0.296518
C 2.247209 1.214477 0.156530
C 3.635748 -1.188403 0.098082
H 1.727534 -2.117578 0.433301
C 3.623874 1.212496 -0.042210
H 1.706284 2.155410 0.183808
C 4.322268 0.009694 -0.072232
H 4.173128 -2.129366 0.080170
H 4.151934 2.150275 -0.169619
H 5.395039 0.006146 -0.223780

3,4-MOBO
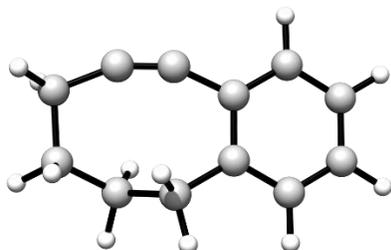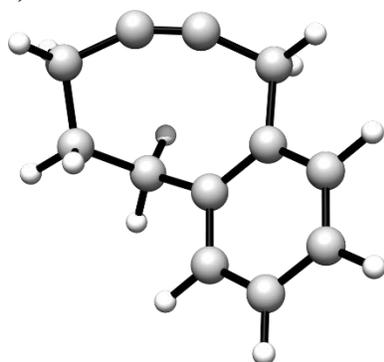

# of imaginary frequencies = 0
E = -464.345126
0 1
C -3.023039 0.595479 0.023672
C -0.507432 -1.401419 -0.197793
C -3.065829 -0.955982 0.101045
C -1.711647 -1.435197 -0.160674
H -3.154222 0.899975 -1.018812
H -3.884790 0.983407 0.572929
C -0.571344 1.356780 -0.480134
H -0.940416 0.986224 -1.442935

C -1.722612 1.229863 0.566361
H -1.376765 0.670197 1.439985
H -1.963617 2.233537 0.923363
H -0.340138 2.414116 -0.627052
H -3.363473 -1.272375 1.105517
H -3.804373 -1.358200 -0.595131
C 0.777169 -0.774271 -0.129984
C 0.732507 0.638472 -0.195608
C 1.986148 -1.442883 0.054928
H 1.989742 -2.525046 0.100844
C 1.929374 1.335748 -0.056862
H 1.917899 2.419590 -0.104970
C 3.136751 0.667567 0.135128
H 4.054174 1.234395 0.240896
C 3.166692 -0.721449 0.185742
H 4.105555 -1.242063 0.330437

4,5-MOBO

# of imaginary frequencies = 0
E = -464.338706
0 1
C 0.189903 2.005557 0.444289
C 1.918870 -1.442803 -0.253461
C 1.491321 1.636461 -0.108190
C 3.036156 -0.402049 -0.529236
C 2.380495 0.902926 -0.448560

H 0.300724 2.212638 1.515006
H 1.348427 -1.590293 -1.173638
H -0.222916 2.907098 -0.011368
H 2.389022 -2.399199 -0.010722
C 0.934354 -1.040520 0.883787
H 1.416871 -0.331884 1.559445
H 0.724327 -1.933474 1.476955
H 3.819292 -0.469213 0.231486
H 3.505253 -0.589813 -1.496572
C -0.774971 0.839198 0.225968
C -0.420108 -0.513684 0.414063
C -1.395196 -1.482693 0.155454
H -1.134976 -2.526745 0.301386
C -2.067067 1.153758 -0.197844
C -2.676227 -1.160008 -0.273424
H -3.398403 -1.944813 -0.464459
C -3.018865 0.173436 -0.446911
H -2.327606 2.196830 -0.344402
H -4.012010 0.451391 -0.778726

**5,6-MOBO**
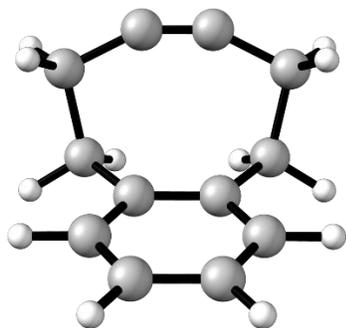
# of imaginary frequencies = 0
E = -464.342730
0 1
C -1.705274 -1.909732 -0.320501
C -0.754420 1.586884 0.864302
C -2.178235 -0.601430 -0.777944
C -1.705264 1.909736 -0.320508
C -2.178225 0.601428 -0.777924
H -2.520391 -2.556841 0.010435

H -0.361934 2.521304 1.274497
H -1.162461 -2.432316 -1.112836
H -1.345579 1.110510 1.649061
H -2.520379 2.556851 0.010422
H -1.162452 2.432304 -1.112855
C -0.754436 -1.586865 0.864309
H -1.345599 -1.110476 1.649056
H -0.361957 -2.521280 1.274522
C 0.416189 -0.706427 0.452732
C 0.416197 0.706433 0.452730
C 1.566503 -1.371365 0.017818
H 1.569755 -2.457249 0.025512
C 2.697125 -0.694017 -0.419451
H 3.569160 -1.246481 -0.748431
C 2.697133 0.693995 -0.419453
C 1.566519 1.371357 0.017814
H 3.569175 1.246449 -0.748434
H 1.569782 2.457241 0.025505

Methylazide
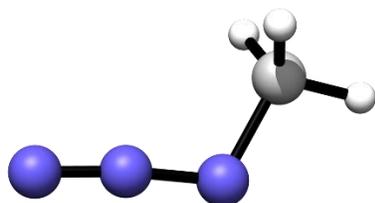
# of imaginary frequencies = 0
E = -204.058143
0 1
N -1.765340 -0.284391 0.000097
N -0.711569 0.109609 -0.000181
N 0.392041 0.647193 0.000084
C 1.522531 -0.294028 0.000008
H 1.516562 -0.925454 -0.892692
H 2.426079 0.308799 0.000372
H 1.516244 -0.926051 0.892279

3,4-MOBO (1,4-TS)
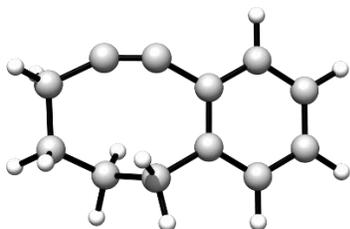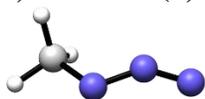
# of imaginary frequencies = 1
E = -668.388160
0 1
C 0.915357 2.882701 -0.005793
C 0.323625 -0.354766 0.070774
C 1.906346 1.726127 -0.257169
C 1.286531 0.415004 0.005373
H 0.922748 3.136121 1.058532
H 1.287374 3.762783 -0.537161
C -1.362262 1.844134 0.659220
H -0.723233 1.679521 1.533173
C -0.529601 2.574713 -0.433146
H -0.520879 1.981860 -1.352932
H -1.029196 3.514220 -0.679213
H -2.177616 2.492188 0.987952
H 2.224589 1.743487 -1.306509
H 2.805598 1.865987 0.347687
C -1.099344 -0.589235 0.009208
C -1.946759 0.512698 0.257998
C -1.647575 -1.828771 -0.327009
H -0.982952 -2.664803 -0.501953
C -3.323385 0.330543 0.153496
H -3.981762 1.170723 0.348577
C -3.864304 -0.903941 -0.194333
H -4.938827 -1.020287 -0.272855
C -3.023826 -1.985014 -0.434141
H -3.437965 -2.950165 -0.700192
N 1.302356 -2.333825 0.505349
N 2.359240 -1.896664 0.459627
N 3.011191 -0.830400 0.404170
C 4.130249 -0.792547 -0.538570
H 4.445859 0.247648 -0.595021
H 4.970393 -1.387316 -0.175160
H 3.836057 -1.135622 -1.534401

3,4-MOBO (1,5-TS)
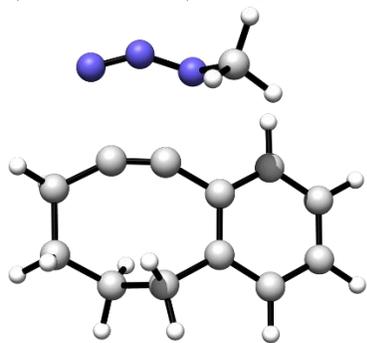
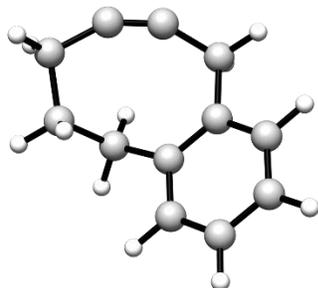# of imaginary frequencies = 1
E = -668.390153
0 1
C 1.320679 2.990018 0.123501
C 0.588477 -0.172596 -0.270642
C 2.186854 1.891333 -0.525144
C 1.575054 0.563566 -0.353375
H 1.507022 3.007442 1.201874
H 1.656801 3.955205 -0.265184
C -0.908366 1.906141 0.914443
H -0.171854 1.565910 1.649866
C -0.188982 2.818623 -0.122659
H -0.348880 2.427523 -1.132366
H -0.660801 3.803302 -0.098110
H -1.648130 2.493416 1.462800
H 2.266396 2.079689 -1.601711
H 3.204156 1.917518 -0.128699
C -0.840072 -0.360083 -0.215462
C -1.598389 0.689932 0.346042
C -1.480665 -1.484530 -0.741578
H -0.875228 -2.267009 -1.184401
C -2.985651 0.564847 0.370590
H -3.577909 1.363103 0.805778
C -3.620562 -0.557746 -0.153049
H -4.701422 -0.629076 -0.125237
C -2.866062 -1.582831 -0.713558
H -3.354628 -2.455202 -1.130936
N 3.268994 -0.859054 -0.225822
N 2.602312 -1.773253 -0.047773
N 1.423118 -2.187477 -0.058194
C 0.993665 -2.950410 1.117906
H -0.094106 -2.972692 1.082095
H 1.368641 -3.974839 1.076616
H 1.313085 -2.473402 2.048042

4,5-MOBO (1,4-TS)
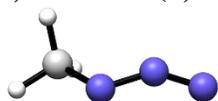
# of imaginary frequencies = 1
E = -668.382492
0 1
C 0.319280 -1.361836 0.897750
C 0.131966 2.322670 -0.220964
C -0.836656 -0.641434 0.338789
C -1.336932 1.852918 -0.243928
C -1.373390 0.397130 -0.036765
H 0.281075 -1.268194 1.990328
H 0.585898 2.097189 -1.188951
H 0.273030 -2.429768 0.678232
H 0.145408 3.409923 -0.108544
C 0.991094 1.667062 0.896119
H 0.342845 1.285530 1.688412
H 1.615072 2.439502 1.351528
H -1.899445 2.343319 0.559051
H -1.811842 2.137372 -1.186184
C 1.632081 -0.794194 0.376946
C 1.928021 0.581194 0.391343
C 3.164628 0.995895 -0.110929
H 3.401209 2.055715 -0.095845
C 2.573337 -1.688118 -0.135436
C 4.094257 0.098973 -0.622216
H 5.042313 0.458231 -1.004585
C 3.796773 -1.257110 -0.633357
H 2.334597 -2.746442 -0.148704
H 4.506159 -1.974648 -1.028054
N -2.489467 -2.166674 0.076422
N -3.239715 -1.384175 -0.288019
N -3.381571 -0.201966 -0.667704
C -4.522973 0.533613 -0.122798
H -4.372095 1.575228 -0.400778
H -5.460938 0.191767 -0.564838

H -4.576932 0.454402 0.966728

4,5-MOBO (1,5-TS)
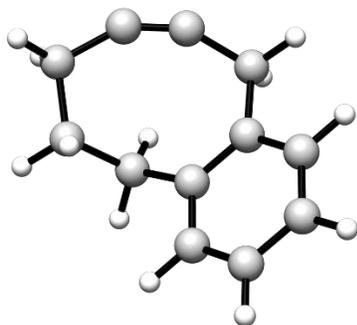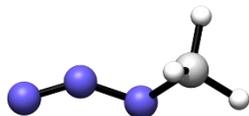
# of imaginary frequencies = 1
E = -668.382065
0 1
C -0.132288 -0.999525 0.950698
C 0.638717 2.553674 -0.338929
C -1.060870 -0.030382 0.344066
C -0.900337 2.476873 -0.345701
C -1.321173 1.092975 -0.078810
H -0.149436 -0.851968 2.037571
H 1.015366 2.172528 -1.291483
H -0.440861 -2.031678 0.776314
H 0.934143 3.604461 -0.278096
C 1.301870 1.752867 0.815985
H 0.577535 1.590835 1.617648
H 2.105905 2.356924 1.242580
H -1.315318 3.120941 0.436766
H -1.301609 2.842408 -1.293610
C 1.282184 -0.812941 0.419363
C 1.923304 0.438576 0.372701
C 3.224329 0.493727 -0.135914
H 3.726255 1.456097 -0.169229
C 1.960390 -1.943666 -0.038955
C 3.890037 -0.636300 -0.593275
H 4.898276 -0.552900 -0.981286
C 3.252889 -1.868893 -0.542555
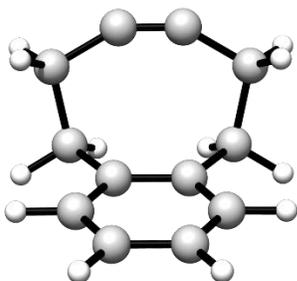H 1.458301 -2.905040 -0.002379
H 3.752936 -2.764006 -0.892592
N -3.494856 1.012859 -0.514865
N -3.604230 -0.087621 -0.216693

N -3.034019 -1.055548 0.329398
C -3.178930 -2.356501 -0.324716
H -2.512865 -3.040274 0.197645
H -4.198507 -2.734845 -0.227432
H -2.899106 -2.314228 -1.381035

5,6-MOBO (TS)
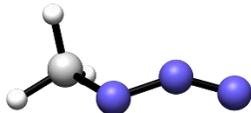
# of imaginary frequencies = 1
E = -668.387756
0 1
C 0.139538 2.119810 0.503770
C -0.619586 -1.466780 1.337671
C 1.007958 0.965842 0.225463
C 0.726969 -1.601251 0.590868
C 1.197164 -0.246175 0.266496
H 0.669722 2.875134 1.089766
H -0.974717 -2.463993 1.611755
H -0.161294 2.595951 -0.434596
H -0.442743 -0.921217 2.266791
H 1.446304 -2.138332 1.216583
H 0.594800 -2.181326 -0.327916
C -1.105888 1.619115 1.269439
H -0.776707 1.197231 2.221334
H -1.750826 2.471557 1.500303
C -1.905119 0.606776 0.470482
C -1.684102 -0.784428 0.498815
C -2.901127 1.107674 -0.373027
H -3.075775 2.179319 -0.389289
C -3.667672 0.281292 -1.183618
H -4.431587 0.704822 -1.824740
C -3.449600 -1.090197 -1.155335
C -2.469663 -1.604124 -0.316840
H -4.040543 -1.755280 -1.773737
H -2.303770 -2.676982 -0.287658

N 2.879500 1.736048 -0.790695
N 3.333908 0.690698 -0.883315
N 3.126781 -0.536010 -0.775206
C 4.167367 -1.323020 -0.112982
H 3.751671 -2.318679 0.029163
H 5.057374 -1.408908 -0.739600
H 4.439338 -0.901665 0.859137

3,4-MOBO (1,4-Triazole)
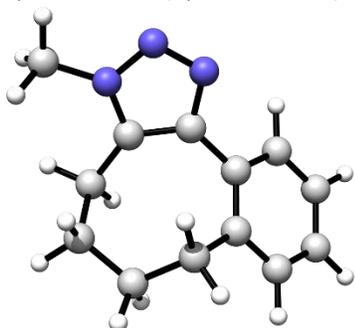
# of imaginary frequencies = 0
E = -668.541082
0 1
C -1.178412 2.424381 0.315291
C -1.359148 1.140988 1.144187
H -1.853701 2.394495 -0.547401
H -1.490684 3.274047 0.929114
C 0.849547 1.615070 -1.105940
H 0.056748 1.192234 -1.729828
C 0.250278 2.683376 -0.164964
H 0.909207 2.807592 0.701429
H 0.248274 3.641933 -0.691292
H 1.543763 2.115959 -1.784744
H -0.531510 1.051936 1.855147
H -2.275534 1.215061 1.736234
C 1.034796 -0.719825 -0.062126
C 1.622242 0.499548 -0.433417
C 1.826954 -1.753828 0.446026
H 1.350000 -2.693321 0.700369
C 2.996280 0.659681 -0.229972
H 3.463113 1.596447 -0.518400
C 3.775709 -0.359084 0.300935
H 4.839497 -0.208340 0.442270
C 3.190740 -1.579775 0.626898
H 3.793863 -2.387779 1.023130
C -1.410163 -0.112076 0.334834
C -0.415797 -0.919929 -0.173989
N -0.997428 -1.988581 -0.784532

N -2.281296 -1.877141 -0.695768
N -2.550309 -0.748675 -0.026445
C -3.923819 -0.379395 0.251330
H -4.120591 0.633602 -0.101015
H -4.555788 -1.084589 -0.283413
H -4.128667 -0.443294 1.321059

3,4-MOBO (1,5-Triazole)
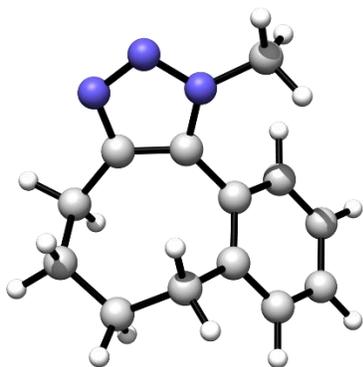
# of imaginary frequencies = 0
E = -668.541926
0 1
C 1.215901 2.763557 -0.177017
C 0.733790 -0.619726 -0.121500
C 1.475252 1.630677 -1.182478
C 1.674378 0.289171 -0.556254
H 1.943327 2.683345 0.637795
H 1.412139 3.715981 -0.678035
C -0.642288 1.609250 1.248644
H 0.229489 1.181455 1.751644
C -0.199140 2.826073 0.402081
H -0.921664 2.979474 -0.407251
H -0.254473 3.715146 1.036307
H -1.314660 1.964274 2.033142
H 0.646299 1.580693 -1.896888
H 2.381350 1.853304 -1.749455
C -0.731531 -0.549647 -0.127625
C -1.382108 0.532711 0.486517
C -1.475248 -1.539202 -0.780150
H -0.953275 -2.358566 -1.262652
C -2.776215 0.594115 0.402644
H -3.291659 1.423827 0.875708
C -3.511014 -0.385344 -0.251824
H -4.591141 -0.311499 -0.295960
C -2.858653 -1.464190 -0.841804
H -3.422708 -2.233857 -1.354299
N 2.776725 -1.411509 0.208127

N 2.905090 -0.242488 -0.333361
N 1.472776 -1.660270 0.342401
C 1.025284 -2.910727 0.926017
H 1.830430 -3.282838 1.555466
H 0.131965 -2.728541 1.522174
H 0.802006 -3.642637 0.148624

4,5-MOBO (1,4-Triazole)
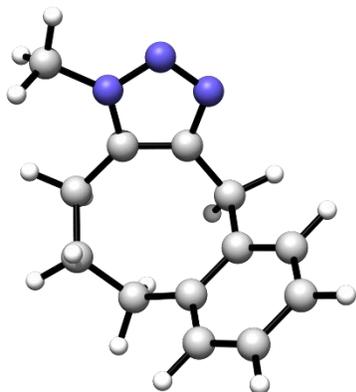
\# of imaginary frequencies = 0
E = -668.537668
0 1
C 0.282320 -0.807476 1.546515
C -0.300053 2.321354 -0.119700
C -1.591826 1.701954 0.440356
H 0.208827 -0.062998 2.344118
H -0.170453 2.027785 -1.165369
H 0.405093 -1.783473 2.017947
H -0.439443 3.405919 -0.108982
C 0.989042 2.001387 0.671086
H 0.746865 1.929091 1.735817
H 1.657999 2.859655 0.575241
H -1.658976 1.936272 1.508605
H -2.448781 2.190454 -0.030908
C 1.465488 -0.520939 0.645203
C 1.762240 0.781500 0.214610
C 2.821818 0.965523 -0.677076
H 3.063769 1.972455 -1.003148
C 2.227193 -1.589634 0.172494
C 3.573820 -0.104331 -1.147315
H 4.390349 0.068819 -1.838228
C 3.275393 -1.391576 -0.717740
H 1.980034 -2.593391 0.501494
H 3.852884 -2.236767 -1.072744
C -1.721373 0.223295 0.263729
C -0.984115 -0.833912 0.750381
N -1.534314 -1.988610 0.297329

N -2.566105 -1.711008 -0.431635
N -2.692082 -0.380677 -0.467431
C -3.779996 0.218087 -1.215102
H -4.314273 -0.596858 -1.697673
H -4.455493 0.753717 -0.546932
H -3.390601 0.899991 -1.971732

4,5-MOBO (1,5-Triazole)
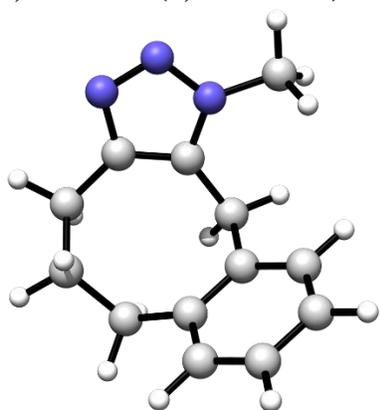
# of imaginary frequencies = 0
E = -668.537965
0 1
C -0.193674 -0.488797 1.429414
C 0.069139 2.639927 -0.308152
C -1.365344 2.337189 0.151227
H -0.192267 0.293703 2.192344
H 0.204811 2.298375 -1.338290
H -0.330919 -1.440170 1.948675
H 0.184015 3.727296 -0.317909
C 1.192319 2.063444 0.584887
H 0.863240 2.084878 1.628961
H 2.044774 2.744447 0.530712
H -1.463852 2.607135 1.209210
H -2.061759 2.970806 -0.401935
C 1.116923 -0.505800 0.668193
C 1.715076 0.686218 0.228147
C 2.870419 0.595795 -0.551040
H 3.344343 1.511663 -0.889585
C 1.698486 -1.731158 0.344243
C 3.431805 -0.629230 -0.892407
H 4.327915 -0.663816 -1.500324
C 2.848468 -1.802661 -0.433189
H 1.244216 -2.645079 0.714414
H 3.284079 -2.765019 -0.673469
C -1.809886 0.927358 -0.062749
C -1.333535 -0.238616 0.493735

N -2.962438 -0.679714 -0.945140
N -2.804407 0.603654 -0.931487
N -2.077379 -1.207041 -0.093056
C -2.000272 -2.643884 0.074939
H -2.802770 -3.074055 -0.519799
H -1.038540 -3.014893 -0.281886
H -2.137261 -2.912271 1.123176

5,6-MOBO (Triazole)
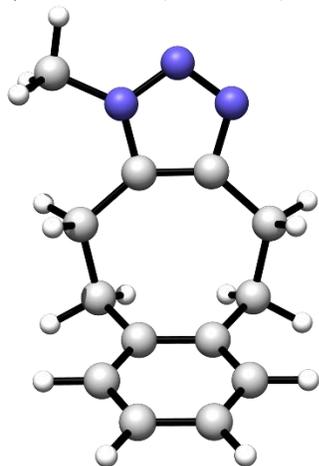
# of imaginary frequencies = 0
E = -668.536063
0 1
C 0.252103 2.093657 0.238222
C -0.469556 -1.283093 1.374620
C 0.818906 -1.481361 0.571375
H 0.720031 2.975871 0.682288
H -0.767488 -2.264362 1.752334
H -0.130396 2.412299 -0.737599
H -0.264665 -0.662625 2.247967
H 1.507640 -2.077766 1.179397
H 0.582485 -2.089509 -0.310865
C -0.934124 1.666363 1.105335
H -0.579488 1.308239 2.073463
H -1.530004 2.560013 1.306761
C -1.819027 0.650844 0.425643
C -1.600987 -0.725907 0.547297
C -2.863849 1.099983 -0.386558
H -3.036314 2.168246 -0.475226
C -3.680307 0.212905 -1.074575
H -4.485098 0.586229 -1.696530
C -3.463163 -1.155666 -0.951776
C -2.432069 -1.612461 -0.142404
H -4.097209 -1.861094 -1.475374
H -2.266354 -2.680425 -0.035050

C 1.560099 -0.254827 0.118653
C 1.365482 1.111941 -0.005500
N 2.511489 1.646538 -0.524360
N 3.379984 0.719813 -0.729286
N7 2.830211 -0.431870 -0.350792
C 3.588545 -1.661579 -0.455921
H 4.519136 -1.414355 -0.961187
H 3.806701 -2.067169 0.533506
H 3.036912 -2.399748 -1.039277

DIBC
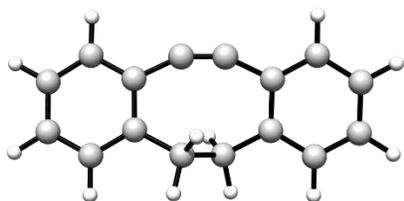
# of imaginary frequencies = 0
E = -616.758295
0 1
C 1.846804 -0.601419 -0.273053
C -0.604344 1.405671 -0.007087
C 1.893635 0.792984 -0.023186
C 0.604396 1.405691 0.007319
C -1.893578 0.792987 0.023307
C -1.846904 -0.601437 0.273148
C -3.107482 1.438129 -0.210084
H -3.113170 2.505009 -0.396300
C -3.046160 -1.306687 0.258379
H -3.033101 -2.375305 0.445303
C 4.258212 -0.662324 -0.020474
H 5.179012 -1.233397 -0.019019
C 4.290033 0.709230 0.208462
H 5.233496 1.209556 0.389519
C -4.289957 0.709290 -0.208662
H -5.233383 1.209636 -0.389863
C -4.258243 -0.662250 0.020301
H -5.179081 -1.233261 0.018656
C 3.046080 -1.306698 -0.258372
C 3.107580 1.438096 0.210055
H 3.113293 2.504962 0.396346
H 3.032973 -2.375332 -0.445232
C -0.527520 -1.277680 0.581069
H -0.086361 -0.785274 1.452439
H -0.731461 -2.309305 0.873023
C 0.527497 -1.277493 -0.581025
H 0.086251 -0.784765 -1.452175

H 0.731240 -2.309072 -0.873286

_S_-DIBO
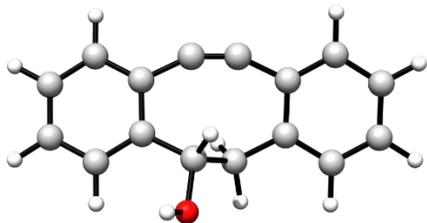
# of imaginary frequencies = 0
E = -691.977869
0 1
C -1.808282 0.398261 -0.147929
C 0.688504 -1.575526 -0.131913
C -1.822799 -1.016096 -0.076248
C -0.520458 -1.601783 -0.128184
C 1.964412 -0.941460 -0.021853
C 1.881327 0.413848 0.385463
C 3.194807 -1.524006 -0.322349
H 3.230159 -2.561748 -0.630098
C 3.058954 1.150298 0.454403
H 3.013657 2.190839 0.756846
C -4.204452 0.388025 0.174250
H -5.131967 0.937826 0.281382
C -4.213067 -1.001769 0.215589
H -5.145112 -1.536861 0.350420
C 4.356672 -0.767733 -0.231864
H 5.313667 -1.218683 -0.464336
C 4.287666 0.568015 0.150018
H 5.193008 1.159622 0.215539
C -3.008995 1.082363 -0.006906
C -3.021278 -1.706451 0.096161
H -3.007591 -2.788216 0.145897
H -3.006091 2.165512 -0.031046
C 0.541217 1.006596 0.761697
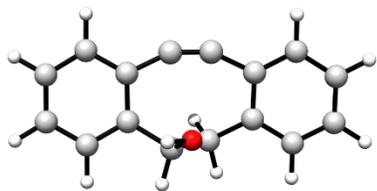H 0.109733 0.407294 1.567297
H 0.682659 2.019785 1.140480
C -0.487325 1.116098 -0.407229
H -0.040149 0.655943 -1.296312
O -0.674615 2.502990 -0.642083
H -1.136470 2.612688 -1.478048

_R_-DIBO

# of imaginary frequencies = 0
E = -691.972191
0 1
C -1.845739 -0.550610 0.042018
C 0.613278 1.494937 -0.036431
C -1.878035 0.864047 -0.028477
C -0.593981 1.482227 -0.034151
C 1.899745 0.886334 -0.089461
C 1.849749 -0.482738 -0.443293
C 3.109774 1.503326 0.224692
H 3.115991 2.552767 0.491999
C 3.042072 -1.198784 -0.444199
H 3.027135 -2.251500 -0.705342
C -4.268404 -0.561888 -0.118119
H -5.195844 -1.120444 -0.155311
C -4.286686 0.827072 -0.170715
H -5.228480 1.356505 -0.249733
C 4.286128 0.765993 0.205137
H 5.227321 1.242385 0.451098
C 4.250416 -0.585309 -0.123353
H 5.166137 -1.164406 -0.134727
C -3.054712 -1.238182 -0.011196
C -3.094462 1.539402 -0.129228
H -3.093236 2.621087 -0.182673
H -3.048069 -2.322502 0.037308
C 0.548044 -1.127513 -0.874998
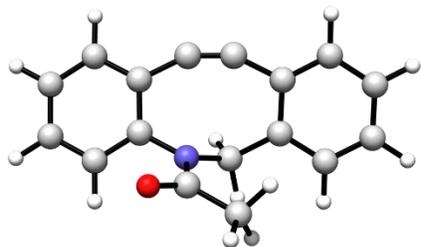H 0.118098 -0.535242 -1.687063
H 0.787161 -2.108106 -1.289588
C -0.547029 -1.330835 0.227728
H -0.831479 -2.389270 0.193365
O 0.050971 -1.063676 1.486763
H -0.633468 -1.096746 2.160833

DIBAC

# of imaginary frequencies = 0
E = -785.436745
0 1
C 1.788738 0.130788 -0.203216
C -0.653707 -1.766645 0.496234
C 1.832380 -1.234273 0.158241
C 0.551894 -1.793748 0.437213
C -1.929514 -1.192825 0.217195
C -1.854696 -0.037593 -0.595248
C -3.160420 -1.661924 0.673762
H -3.191873 -2.547015 1.296751
C -3.037851 0.607501 -0.936156
H -2.999572 1.491698 -1.564658
C 4.180730 0.101552 -0.494396
H 5.095968 0.625524 -0.741455
C 4.222230 -1.245852 -0.144435
H 5.168094 -1.772885 -0.122421
C -4.327679 -0.994530 0.323948
H -5.283970 -1.358809 0.678994
C -4.268067 0.137184 -0.482353
H -5.178005 0.655653 -0.759045
C 2.971221 0.785024 -0.526910
C 3.050897 -1.914646 0.177912
H 3.064120 -2.962372 0.450584
H 2.937233 1.837179 -0.779171
N 0.540305 0.835081 -0.213600
C -0.521082 0.430849 -1.163487
H -0.096883 -0.384503 -1.751984
H -0.710436 1.255190 -1.856661
C 0.429411 1.955563 0.594893
O 1.328230 2.307690 1.327271
C -0.877889 2.716086 0.536864
H -1.177190 2.950966 -0.485947
H -1.677588 2.130685 0.993822
H -0.737454 3.636530 1.097847

DIBAC-Me
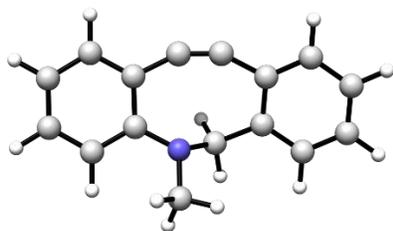
# of imaginary frequencies = 0
E = -672.089498
0 1
C -1.756876 -0.422641 0.052570
C 0.670432 1.633422 0.105759
C -1.811706 0.998956 -0.045350
C -0.534178 1.628067 0.002417
C 1.939601 0.980591 0.047500
C 1.842881 -0.356236 -0.410050
C 3.170629 1.513939 0.419923
H 3.224947 2.539603 0.763176
C 2.997164 -1.125224 -0.466142
H 2.937169 -2.149562 -0.820461
C -4.183486 -0.445056 0.040560
H -5.105502 -1.013233 0.080388
C -4.226413 0.939583 -0.084432
H -5.176159 1.456260 -0.139104
C 4.313516 0.723122 0.354237
H 5.270958 1.136687 0.647234
C 4.228598 -0.593733 -0.081950
H 5.119382 -1.208546 -0.127945
C -2.968336 -1.119532 0.102535
C -3.037826 1.655963 -0.126772
H -3.044334 2.736559 -0.200930
H -2.962572 -2.199364 0.182799
N -0.515370 -1.064843 0.169398
C -0.485572 -2.390120 0.754776
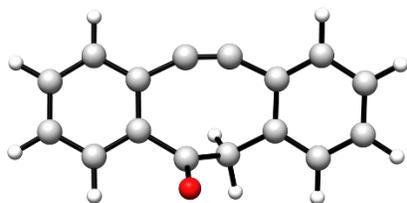H -0.829094 -3.176627 0.065039
H 0.544657 -2.614243 1.040723
H -1.100260 -2.414439 1.654964
C 0.502215 -0.885154 -0.884654
H 0.103892 -0.203239 -1.638073
H 0.660643 -1.851645 -1.379156

DIBONE

# of imaginary frequencies = 0
E = -690.771735
0 1
C 1.824340 0.481092 0.052815
C -0.637684 -1.550518 -0.010664
C 1.859156 -0.926343 -0.055449
C 0.569499 -1.539569 -0.057689
C -1.923574 -0.932248 -0.029301
C -1.874636 0.425723 -0.426788
C -3.124251 -1.517798 0.367118
H -3.134684 -2.558182 0.667088
C -3.047711 1.169070 -0.380927
H -3.025666 2.213942 -0.669227
C 4.236094 0.520366 0.075545
H 5.162047 1.079326 0.133448
C 4.266026 -0.866204 -0.047156
H 5.216068 -1.385098 -0.088278
C -4.286234 -0.756848 0.389478
H -5.220655 -1.208133 0.699711
C -4.245668 0.584759 0.024858
H -5.150162 1.180422 0.051524
C 3.018022 1.189857 0.137046
C 3.083133 -1.592624 -0.102919
H 3.097082 -2.672987 -0.173290
H 2.980418 2.266587 0.255122
C -0.575349 1.014499 -0.939587
H -0.183724 0.384009 -1.740894
H -0.778532 2.006902 -1.348371
C 0.521503 1.248847 0.120795
O 0.382728 2.122606 0.938765

ODIBO
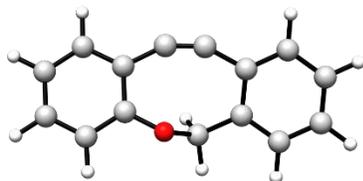
# of imaginary frequencies = 0
E = -652.654928
0 1
C 1.743154 -0.565921 -0.217022

C -0.614174 1.478273 0.048592
C 1.854782 0.823348 0.033855
C 0.593235 1.483254 0.092796
C -1.880058 0.820245 0.031645
C -1.775036 -0.574502 0.250588
C -3.117867 1.407352 -0.218093
H -3.176566 2.475885 -0.383250
C -2.928639 -1.345029 0.191676
H -2.860966 -2.416248 0.349090
C 4.142425 -0.754186 -0.154509
H 5.032730 -1.366342 -0.234229
C 4.257073 0.609819 0.100123
H 5.234290 1.060146 0.221336
C -4.260087 0.615367 -0.261237
H -5.223164 1.071029 -0.457002
C -4.167101 -0.757231 -0.061984
H -5.057275 -1.373040 -0.103676
C 2.890725 -1.342299 -0.308384
C 3.116387 1.395826 0.195358
H 3.189068 2.459055 0.387559
H 2.783292 -2.400151 -0.514562
C -0.442944 -1.193110 0.613515
H -0.032191 -0.687804 1.491913
H -0.590956 -2.247766 0.855697
O 0.528812 -1.147750 -0.454300

BARAC
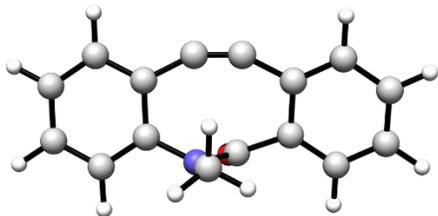
# of imaginary frequencies = 0
E = -746.116134
0 1
C -1.795426 -0.459211 0.180631
C 0.613247 1.595891 -0.027585
C -1.870782 0.942281 -0.041136
C -0.595962 1.590130 -0.066241
C 1.889533 0.942435 -0.024941
C 1.802066 -0.452815 -0.248982
C 3.134914 1.535263 0.172479
H 3.197312 2.603798 0.336427
C 2.954354 -1.221604 -0.290169
H 2.883107 -2.283602 -0.495078

C -4.188045 -0.607301 -0.011766
H -5.090233 -1.206717 -0.007370
C -4.266411 0.765312 -0.222926
H -5.229961 1.234163 -0.380639
C 4.281249 0.748621 0.152322
H 5.249218 1.208804 0.309022
C 4.193991 -0.621095 -0.078198
H 5.094119 -1.223117 -0.103748
C -2.952315 -1.219031 0.188440
C -3.113157 1.540971 -0.241322
H -3.165659 2.608221 -0.416015
H -2.872594 -2.287842 0.345769
N -0.511247 -1.037033 0.460028
C -0.086877 -0.911165 1.854156
H 0.882572 -1.390995 1.982014
H -0.016988 0.134209 2.173041
H -0.813078 -1.428196 2.482262
C 0.420000 -0.980466 -0.577797
O 0.117330 -1.229848 -1.718458

DIBC (TS)
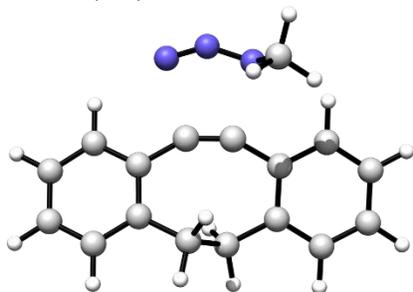
# of imaginary frequencies = 1
E = -820.802024
0 1
C 1.534685 -1.621516 -0.141840
C -0.662552 0.733076 -0.338046
C 1.744674 -0.230094 -0.291536
C 0.571965 0.610734 -0.295006
C -1.979050 0.166193 -0.208738
C -2.069415 -1.072192 0.467199
C -3.132731 0.776431 -0.707951
H -3.046443 1.731990 -1.208941
C -3.321409 -1.662182 0.613135
H -3.399935 -2.611504 1.132680
C 3.939546 -1.957247 -0.186472
H 4.786610 -2.630900 -0.134937
C 4.136567 -0.598360 -0.403280
H 5.137302 -0.205406 -0.536837

C -4.369776 0.163790 -0.559170
H -5.258300 0.640275 -0.955498
C -4.466137 -1.055001 0.104427
H -5.430886 -1.532412 0.228830
C 2.646222 -2.457341 -0.069742
C 3.044624 0.257725 -0.456156
H 3.183515 1.311998 -0.658488
H 2.492475 -3.523904 0.056196
C -0.817503 -1.731856 0.985124
H -0.285420 -1.032196 1.635729
H -1.094096 -2.591024 1.598456
C 0.139705 -2.195765 -0.158480
H -0.314804 -1.924471 -1.116334
H 0.213830 -3.284634 -0.147609
N -0.956880 2.906003 -0.308081
N 0.139207 3.140926 -0.074274
N 1.287450 2.641491 0.004924
C 1.950240 2.881400 1.298139
H 2.801711 2.207063 1.343515
H 2.308909 3.910227 1.361000
H 1.279166 2.669189 2.134620

_S_-DIBO (1,4-TS)
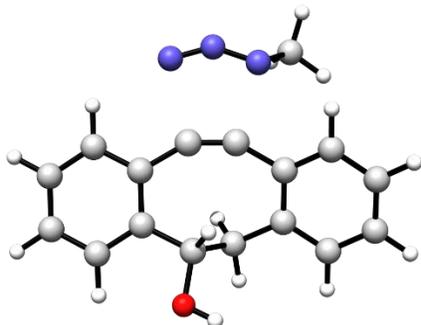
# of imaginary frequencies = 1
E = -896.024114
0 1
C 2.129395 -0.846013 -0.115934
C -0.688152 0.744019 -0.199624
C 1.898451 0.548564 -0.112691
C 0.527284 0.995296 -0.200024
C -1.768766 -0.209782 -0.129104
C -1.460586 -1.461976 0.450298
C -3.046647 0.020777 -0.645156
H -3.252744 0.970070 -1.124979
C -2.455667 -2.432726 0.520000
H -2.226708 -3.391402 0.974107
C 4.495385 -0.444788 0.145287

H 5.502610 -0.832270 0.243726
C 4.273574 0.927572 0.139693
H 5.105117 1.615394 0.235353
C -4.023721 -0.964196 -0.570016
H -5.009774 -0.777146 -0.977990
C -3.732795 -2.188914 0.021526
H -4.494807 -2.956237 0.088279
C 3.426592 -1.326801 0.013521
C 2.982446 1.422183 0.009747
H 2.801753 2.488116 0.005417
H 3.590053 -2.396439 -0.003580
C -0.053046 -1.720132 0.912533
H 0.253494 -0.937864 1.610645
H 0.010514 -2.674005 1.439745
C 0.955297 -1.780841 -0.285693
H 0.424361 -1.467599 -1.192795
O 1.445817 -3.099553 -0.463263
H 0.719257 -3.651179 -0.763092
N 0.540214 3.225290 -0.338152
N -0.596279 3.309873 -0.238406
N -1.670120 2.668125 -0.227032
C -2.551428 2.948083 0.915750
H -1.996235 2.957080 1.857075
H -3.286162 2.146335 0.940213
H -3.069683 3.898596 0.778424

S-DIBO (1,5-TS)
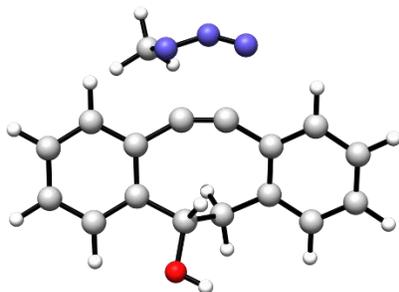
# of imaginary frequencies = 1
E = -896.021071
0 1
C 1.546168 -1.414438 -0.122944
C -0.676621 0.925998 -0.345508
C 1.739278 -0.021201 -0.268957
C 0.559192 0.811620 -0.292915
C -1.987403 0.348021 -0.197965
C -2.055307 -0.877772 0.504357
C -3.153866 0.930482 -0.699055
H -3.087034 1.876437 -1.220821

C -3.295611 -1.484901 0.675434
H -3.356094 -2.420691 1.221750
C 3.942185 -1.733289 -0.127255
H 4.794442 -2.399392 -0.063518
C 4.133674 -0.372594 -0.338036
H 5.133876 0.027368 -0.453914
C -4.380110 0.301555 -0.525310
H -5.279332 0.756643 -0.922602
C -4.453622 -0.904235 0.164220
H -5.410756 -1.391150 0.308480
C 2.653263 -2.250894 -0.038097
C 3.037777 0.476512 -0.411985
H 3.172656 1.530760 -0.615758
H 2.492720 -3.315475 0.069652
C -0.780889 -1.499343 1.007423
H -0.245004 -0.780647 1.632213
H -0.998423 -2.371782 1.626679
C 0.141962 -1.974331 -0.162247
H -0.300258 -1.619166 -1.101813
O 0.224403 -3.390079 -0.193119
H -0.645476 -3.734415 -0.410068
N -0.991203 3.090788 -0.374362
N 0.100358 3.341532 -0.135517
N 1.251956 2.855600 -0.030739
C 1.895676 3.134226 1.264983
H 1.214313 2.939812 2.097374
H 2.750755 2.467426 1.340158
H 2.246148 4.166960 1.304612

_R_-DIBO (1,4-TS)
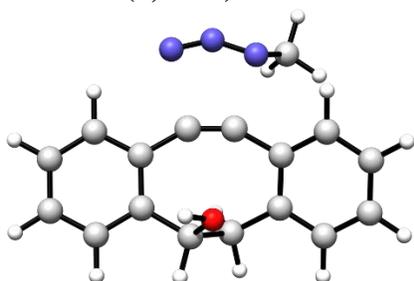
\# of imaginary frequencies = 1
E = -896.019672
0 1
C 2.112170 -1.063967 0.051957
C -0.593674 0.713539 -0.166267
C 1.966571 0.336619 -0.094331
C 0.633654 0.878681 -0.172207
C -1.733764 -0.160080 -0.103255

C -1.525003 -1.411422 0.511562
C -2.976663 0.146611 -0.663336
H -3.101898 1.098490 -1.165701
C -2.584253 -2.312453 0.565188
H -2.431920 -3.277971 1.035739
C 4.522236 -0.785297 0.172455
H 5.506945 -1.224335 0.278904
C 4.376825 0.586785 0.009958
H 5.248993 1.229243 -0.011399
C -4.017908 -0.769329 -0.603739
H -4.976118 -0.527835 -1.048035
C -3.824473 -1.998384 0.019255
H -4.635122 -2.715377 0.072234
C 3.391956 -1.596740 0.189073
C 3.110298 1.141787 -0.119160
H 2.993103 2.210389 -0.233185
H 3.504062 -2.670134 0.304424
C -0.174104 -1.759191 1.082581
H 0.158552 -0.956777 1.745462
H -0.275151 -2.659477 1.690493
C 0.931046 -2.015628 0.005501
H 1.334572 -3.017389 0.193117
O 0.314470 -2.010312 -1.274409
H 1.007704 -2.016081 -1.940273
N 0.796343 3.124513 -0.262228
N -0.333768 3.272875 -0.166034
N -1.444324 2.699288 -0.175873
C -2.329407 3.017130 0.952829
H -1.798462 2.958059 1.906417
H -2.768029 4.008901 0.830502
H -3.123787 2.274096 0.937137

_R_-DIBO (1,5-TS)
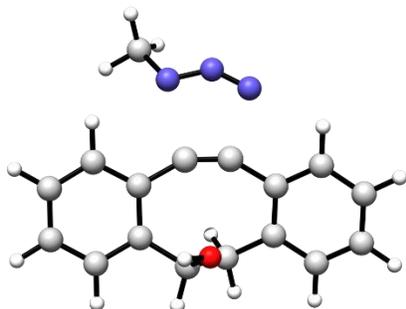
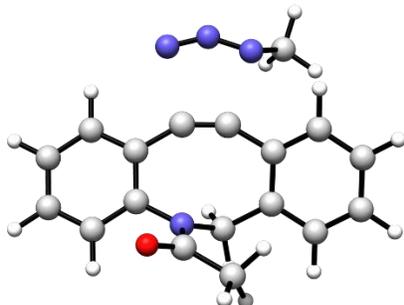# of imaginary frequencies = 1
E = -896.016758
0 1
C -1.418619 -1.668470 -0.017909
C 0.590089 0.899013 0.066960

C -1.720316 -0.288541 0.092640
C -0.623711 0.645986 0.071815
C 1.947176 0.414843 -0.013288
C 2.136823 -0.876506 -0.552593
C 3.048018 1.147453 0.440783
H 2.890847 2.135710 0.849097
C 3.427784 -1.393129 -0.610769
H 3.579284 -2.386105 -1.020337
C -3.796381 -2.177840 -0.021367
H -4.592401 -2.910231 -0.078842
C -4.087016 -0.831522 0.156828
H -5.114613 -0.502027 0.253523
C 4.325320 0.609178 0.376402
H 5.169435 1.183642 0.738543
C 4.518167 -0.662282 -0.152536
H 5.514307 -1.085055 -0.208797
C -2.467298 -2.582901 -0.091209
C -3.058132 0.098682 0.214365
H -3.280331 1.141308 0.384600
H -2.233359 -3.638309 -0.187560
C 0.970062 -1.682968 -1.064253
H 0.412741 -1.092221 -1.791676
H 1.359706 -2.550204 -1.599224
C 0.000359 -2.198052 0.042714
H -0.070681 -3.285958 -0.071567
O 0.588372 -1.914681 1.304195
H -0.047722 -2.143714 1.988384
N -0.365404 3.212894 0.139058
N 0.740516 2.882386 0.228470
N -1.502489 2.719292 0.097277
C -2.484964 3.497199 -0.666292
H -2.071371 3.873505 -1.604674
H -3.314108 2.834564 -0.897351
H -2.861230 4.339679 -0.075055

DIBAC (1,4-TS)

# of imaginary frequencies = 1
E = -989.484471

0 1
C 2.08488300 -0.39920500 0.23953500
C -0.80025500 0.93524200 -0.19742600
C 1.76954100 0.95988500 0.04135000
C 0.38488800 1.29156200 -0.16619200
C -1.79939700 -0.08846100 -0.04155600
C -1.42036100 -1.23099700 0.69306700
C -3.08542000 -0.01130800 -0.58387400
H -3.34210600 0.84684200 -1.19305100
C -2.36724000 -2.22092100 0.93435100
H -2.08533600 -3.09239900 1.51681900
C 4.41104300 0.17403400 0.50736100
H 5.43477900 -0.13519500 0.67998800
C 4.10693900 1.51946700 0.31890500
H 4.89255100 2.26463900 0.34766200
C -4.00733200 -1.02479900 -0.35700200
H -4.99958000 -0.95679200 -0.78668400
C -3.65743900 -2.12221800 0.42305100
H -4.37856600 -2.90672800 0.61764400
C 3.40252800 -0.77887800 0.47058200
C 2.79634100 1.90916400 0.09047900
H 2.55001100 2.95125500 -0.05898700
H 3.62954600 -1.82995700 0.59608400
N 1.05742500 -1.39324000 0.19537500
C -0.00582700 -1.36408400 1.22032200
H 0.21956100 -0.50963200 1.86066200
H 0.06322300 -2.25950100 1.84517300
C 1.19164200 -2.41543500 -0.73000900
O 2.09832400 -2.43293100 -1.53425200
C 0.14959300 -3.51293200 -0.70977300
H -0.05599700 -3.87940500 0.29681800
H -0.78813900 -3.14870100 -1.13305500
H 0.53040200 -4.32343300 -1.32636200
N 0.24292100 3.48002900 -0.56704400
N -0.90018500 3.48441000 -0.53280900
N -1.92698600 2.77163700 -0.49349400
C -2.88281100 3.12365400 0.56729000
H -3.56910500 2.28456100 0.65557600
H -2.37907800 3.27962800 1.52461000
H -3.44888500 4.01579000 0.29415000

DIBAC (1,5-TS)
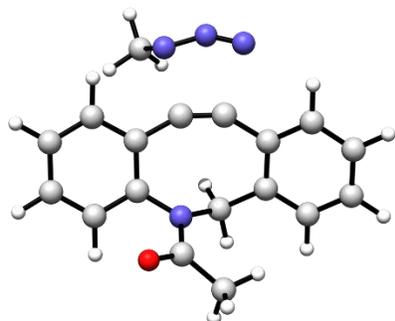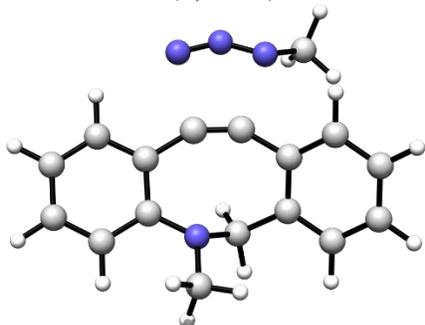
# of imaginary frequencies = 1
E = -989.481907
0 1
C 1.416078 -1.232727 0.148111
C -0.510506 1.293174 -0.464582
C 1.753726 0.071667 -0.254120
C 0.689642 1.023377 -0.371607
C -1.867394 0.867798 -0.287963
C -2.057506 -0.237218 0.569900
C -2.965742 1.519368 -0.851604
H -2.792916 2.372290 -1.495975
C -3.361208 -0.615552 0.880357
H -3.528628 -1.427491 1.581418
C 3.763984 -1.815860 0.135058
H 4.540155 -2.553735 0.297213
C 4.091935 -0.543782 -0.333472
H 5.121084 -0.290399 -0.556815
C -4.254708 1.091720 -0.564895
H -5.103040 1.597124 -1.010344
C -4.455178 0.035155 0.317420
H -5.459724 -0.281848 0.570001
C 2.438476 -2.157271 0.361209
C 3.088585 0.390472 -0.521639
H 3.285903 1.379274 -0.916054
H 2.178199 -3.163040 0.666082
N 0.056197 -1.652096 0.284651
C -0.867334 -0.944192 1.201730
H -0.259103 -0.208960 1.731320
H -1.233616 -1.653586 1.949079
C -0.286964 -2.845089 -0.353675
O 0.476339 -3.397694 -1.119225
C -1.616233 -3.483282 -0.016444
H -2.418632 -2.784125 0.184523
H -1.886173 -4.120796 -0.854404
H -1.471842 -4.119276 0.861712
N -0.543907 3.517278 -0.377255
N 0.574344 3.592986 -0.147253

N 1.660592 2.982451 -0.098943
C 2.480497 3.194234 1.097736
H 3.201386 2.380392 1.117962
H 3.024464 4.137486 1.040393
H 1.880277 3.161955 2.010178

DIBAC-Me (1,4-TS)

# of imaginary frequencies = 1
E = -876.138160
0 1
C 2.096220 -0.828770 0.017026
C -0.680907 0.775848 -0.228509
C 1.886340 0.576682 -0.079882
C 0.526433 1.039497 -0.174045
C -1.725033 -0.213929 -0.209680
C -1.413692 -1.411594 0.468628
C -2.966277 -0.070753 -0.830101
H -3.180599 0.845423 -1.368390
C -2.363349 -2.422894 0.530000
H -2.127614 -3.340356 1.060520
C 4.491722 -0.437635 -0.063769
H 5.498413 -0.839374 -0.061648
C 4.286771 0.934894 -0.137504
H 5.127640 1.614243 -0.199143
C -3.899922 -1.100623 -0.771693
H -4.857897 -0.986457 -1.265038
C -3.605638 -2.273307 -0.085441
H -4.334829 -3.072945 -0.035599
C 3.411030 -1.307742 0.018814
C 2.989709 1.430573 -0.143937
H 2.812087 2.494653 -0.219949
H 3.590149 -2.373133 0.090999
N 1.002570 -1.702044 0.028713
C 1.203740 -3.074466 -0.384980
H 1.685746 -3.694450 0.387217
H 0.227464 -3.510445 -0.610604
H 1.807093 -3.106435 -1.292507

C -0.033477 -1.561505 1.062526
H 0.202013 -0.692202 1.677756
H -0.006435 -2.442011 1.717619
N -0.642098 3.293252 -0.032991
N 0.497994 3.253132 -0.067343
N -1.705285 2.659274 -0.183656
C -2.766164 2.903703 0.809331
H -3.375022 2.002564 0.798736
H -2.365690 3.073548 1.811045
H -3.399824 3.754199 0.515225

DIBAC-Me (1,5-TS)
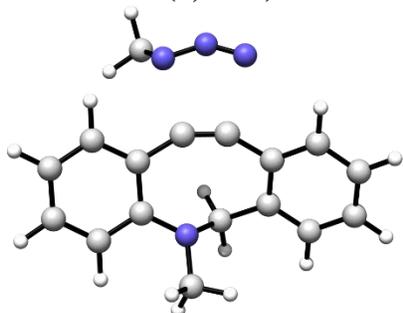
# of imaginary frequencies = 1
E = -876.136232
0 1
C 1.462029 -1.453322 -0.027917
C -0.642737 0.962894 -0.348849
C 1.721799 -0.062047 -0.188282
C 0.581592 0.813795 -0.234503
C -1.957266 0.395544 -0.226535
C -2.035080 -0.810957 0.503386
C -3.115271 0.961934 -0.759127
H -3.043777 1.898044 -1.298427
C -3.271108 -1.420181 0.675185
H -3.334777 -2.342315 1.244765
C 3.843453 -1.880199 -0.267148
H 4.660064 -2.592304 -0.292731
C 4.092781 -0.524025 -0.442743
H 5.098632 -0.167596 -0.625705
C -4.341676 0.328079 -0.591275
H -5.236151 0.768251 -1.015646
C -4.423674 -0.860446 0.125335
H -5.380455 -1.350676 0.259493
C 2.547627 -2.337820 -0.063159
C 3.032003 0.370517 -0.403693
H 3.196424 1.422483 -0.600184
H 2.373691 -3.398222 0.068458
N 0.148909 -1.919519 0.064146

C -0.126590 -3.297790 -0.283917
H 0.146823 -4.008097 0.511660
H -1.198475 -3.393593 -0.472819
H 0.403826 -3.566806 -1.197632
C -0.767977 -1.392917 1.084902
H -0.246143 -0.628489 1.662944
H -1.024869 -2.204209 1.777968
N -0.890789 3.169229 -0.414466
N 0.205224 3.370591 -0.157279
N 1.341195 2.861627 -0.024185
C 1.981083 3.140680 1.271243
H 2.805138 2.437511 1.367185
H 2.377661 4.157248 1.294974
H 1.284696 2.992844 2.100770

DIBONE (1,4-TS)
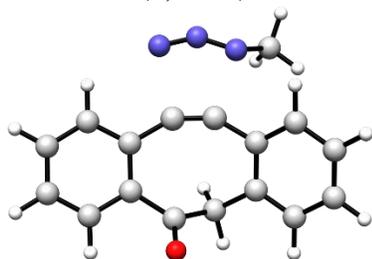
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E = -894.820712
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C -0.643085 0.751584 -0.163707
C 1.923347 0.452222 -0.074656
C 0.575777 0.960311 -0.113843
C -1.730747 -0.189038 -0.174687
C -1.483182 -1.421704 0.463785
C -2.943640 0.028849 -0.832867
H -3.101661 0.975185 -1.336953
C -2.459695 -2.411547 0.415383
H -2.269040 -3.365894 0.893157
C 4.504682 -0.641025 -0.131335
H 5.501586 -1.063874 -0.158538
C 4.323125 0.735967 -0.223109
H 5.180390 1.391432 -0.320348
C -3.907712 -0.969500 -0.865614
H -4.842710 -0.800190 -1.385905
C -3.666149 -2.189817 -0.241275
H -4.415448 -2.971767 -0.268941
C 3.399905 -1.473723 -0.014149
C 3.045371 1.277468 -0.203520

H 2.899786 2.344871 -0.297697
H 3.517015 -2.549604 0.040125
C -0.166722 -1.644412 1.168888
H 0.074425 -0.789676 1.803084
H -0.238606 -2.539048 1.790499
C 0.985213 -1.929886 0.191882
O 1.030258 -2.996238 -0.370976
N 0.640290 3.228810 -0.102524
N -0.498871 3.308099 -0.063897
N -1.579358 2.689134 -0.158081
C -2.547568 2.920135 0.922021
H -3.279306 2.118099 0.849717
H -2.069740 2.886657 1.904210
H -3.055907 3.875878 0.785123

DIBONE (1,5-TS)
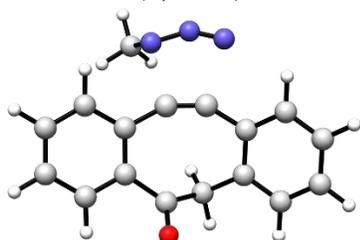
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E = -894.818569
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C -0.635988 0.962235 -0.264026
C 1.697819 -0.144738 -0.226229
C 0.584547 0.768991 -0.198356
C -1.958831 0.412146 -0.197590
C -2.089013 -0.793418 0.524270
C -3.069733 0.979915 -0.825189
H -2.951395 1.916888 -1.355020
C -3.329622 -1.421209 0.563144
H -3.434210 -2.354644 1.104653
C 3.781290 -2.014103 -0.398664
H 4.585090 -2.737147 -0.463511
C 4.024237 -0.667725 -0.656480
H 5.018596 -0.337797 -0.933228
C -4.299365 0.338448 -0.773579
H -5.157380 0.775765 -1.269517
C -4.428226 -0.864254 -0.084681
H -5.387164 -1.366887 -0.044815
C 2.495090 -2.430766 -0.086110
C 2.991547 0.255414 -0.580365
H 3.161648 1.294520 -0.832146

H 2.275322 -3.478982 0.077247
C -0.893920 -1.366895 1.251479
H -0.382711 -0.582077 1.812044
H -1.236855 -2.134298 1.947868
C 0.087857 -2.090171 0.320762
O -0.202664 -3.182685 -0.102956
N -0.806505 3.180247 -0.235335
N 0.309071 3.326423 -0.034277
N 1.428926 2.770857 0.015853
C 2.175018 2.993909 1.263512
H 2.619373 3.990565 1.274109
H 1.537731 2.859824 2.141218
H 2.971310 2.252859 1.281733

ODIBO (1,4-TS)
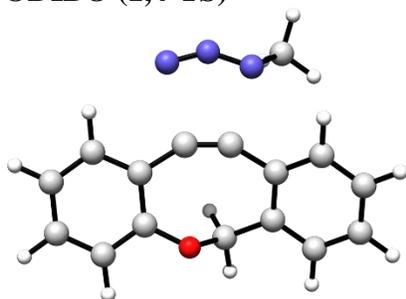
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C 1.963151 0.253761 -0.127948
C 0.646054 0.823028 -0.182314
C -1.685068 -0.276157 -0.193505
C -1.418094 -1.553099 0.345181
C -2.949620 0.007548 -0.711431
H -3.127014 0.979742 -1.155968
C -2.430635 -2.503962 0.366879
H -2.225124 -3.487382 0.776310
C 4.447154 -1.030373 -0.049629
H 5.408646 -1.529382 -0.026809
C 4.381523 0.360027 -0.067979
H 5.290571 0.948494 -0.057484
C -3.949540 -0.957755 -0.682782
H -4.926332 -0.732590 -1.094132
C -3.695682 -2.211348 -0.137237
H -4.474637 -2.963770 -0.115235
C 3.280565 -1.786656 -0.060574
C 3.147763 0.995199 -0.105534

H 3.082108 2.075133 -0.127632
H 3.305826 -2.869488 -0.054211
C -0.043934 -1.865960 0.876235
H 0.267517 -1.109491 1.601474
H -0.048213 -2.842061 1.367017
O 0.922544 -1.932501 -0.190194
N 0.789240 3.083023 -0.175582
N -0.344251 3.201494 -0.100607
N -1.454480 2.631763 -0.155045
C -2.346718 2.889935 0.984166
H -2.805244 3.876588 0.899299
H -3.127075 2.133384 0.939045
H -1.816373 2.804341 1.935978

ODIBO (1,5-TS)
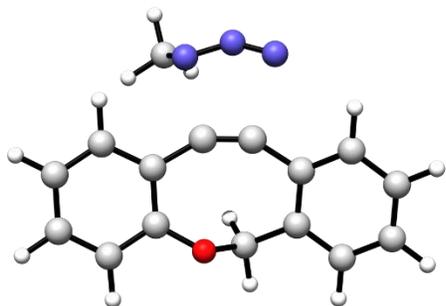
# of imaginary frequencies = 1
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C -0.658110 0.792966 -0.313783
C 1.697512 -0.239518 -0.247761
C 0.569243 0.649523 -0.252738
C -1.961085 0.200223 -0.205676
C -2.014209 -1.057851 0.432969
C -3.132054 0.786646 -0.686766
H -3.077592 1.758979 -1.159703
C -3.239028 -1.701040 0.559638
H -3.282136 -2.670221 1.045331
C 3.765772 -2.127045 -0.277060
H 4.563540 -2.859987 -0.288516
C 4.052937 -0.776912 -0.457269
H 5.073158 -0.452754 -0.621042
C -4.346986 0.124615 -0.555775
H -5.251783 0.581637 -0.938280
C -4.403956 -1.117515 0.067038
H -5.351570 -1.632417 0.169175
C 2.451844 -2.543651 -0.101460
C 3.024639 0.154863 -0.443868

H 3.227588 1.201788 -0.631931
H 2.199260 -3.590997 0.009498
C -0.755075 -1.671569 0.986101
H -0.239972 -0.961875 1.639047
H -1.002724 -2.564227 1.564798
O 0.138850 -2.092837 -0.061866
N -0.903640 3.009153 -0.317577
N 0.202575 3.196252 -0.099651
N 1.341796 2.684988 -0.017195
C 2.021251 2.934465 1.265055
H 1.348849 2.771581 2.111282
H 2.845499 2.227636 1.322562
H 2.421623 3.949184 1.297386

BARAC (1,4-TS)
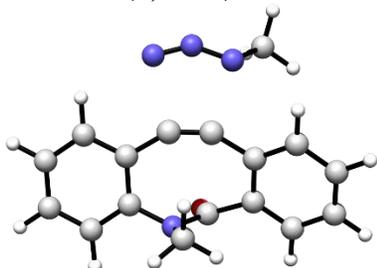
# of imaginary frequencies = 1
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C 1.944493 0.441454 -0.155466
C 0.609536 0.979171 -0.254463
C -1.737682 -0.118625 -0.222121
C -1.481864 -1.391462 0.330702
C -3.022256 0.170517 -0.687544
H -3.210381 1.135826 -1.142699
C -2.501412 -2.321577 0.464878
H -2.292258 -3.282468 0.920966
C 4.455255 -0.768724 0.121525
H 5.427086 -1.233665 0.234981
C 4.348513 0.615230 0.032529
H 5.239092 1.230593 0.073810
C -4.032595 -0.778353 -0.580184
H -5.024178 -0.549273 -0.951843
C -3.780209 -2.015517 0.006290
H -4.576883 -2.743153 0.102252
C 3.311107 -1.559688 0.068755
C 3.103990 1.218341 -0.101766
H 3.017349 2.294923 -0.160399

H 3.367735 -2.639094 0.141271
N 0.880990 -1.756586 -0.215331
C 0.480551 -1.978779 -1.605053
H -0.393237 -2.627878 -1.635597
H 0.252923 -1.040430 -2.122570
H 1.301905 -2.478926 -2.119179
C -0.065260 -1.611596 0.794483
O 0.238826 -1.547901 1.961094
N 0.740337 3.218171 -0.284424
N -0.390507 3.341769 -0.177095
N -1.499209 2.764504 -0.192363
C -2.331313 2.998300 0.999557
H -3.128886 2.259793 0.968010
H -1.754651 2.866727 1.918329
H -2.770713 3.996527 0.969994

BARAC (1,5-TS)
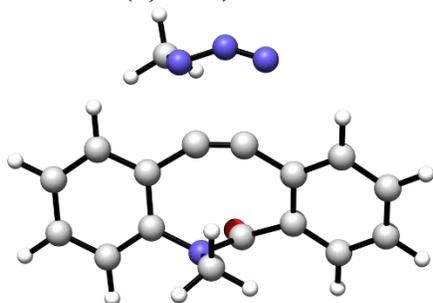
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C 1.762906 -0.059942 -0.299191
C 0.607780 0.803049 -0.360946
C -1.938894 0.353833 -0.272102
C -2.000383 -0.875408 0.420203
C -3.124825 0.946079 -0.709498
H -3.081387 1.898689 -1.222020
C -3.220863 -1.475592 0.687933
H -3.251435 -2.402478 1.249187
C 3.888093 -1.876494 -0.106758
H 4.711362 -2.575159 -0.020780
C 4.134988 -0.533575 -0.373046
H 5.151903 -0.186244 -0.510292
C -4.342365 0.319259 -0.471474
H -5.258443 0.780097 -0.820879
C -4.394842 -0.881713 0.230768
H -5.350176 -1.352100 0.429598

C 2.578741 -2.327497 0.030885
C 3.082193 0.367873 -0.468837
H 3.266881 1.408693 -0.703955
H 2.359355 -3.372158 0.216168
N 0.167710 -1.900723 -0.098552
C -0.333885 -2.162766 -1.448818
H -1.348433 -2.553860 -1.392400
H -0.328340 -1.260306 -2.070102
H 0.304708 -2.917039 -1.909603
C -0.670831 -1.402517 0.893679
O -0.310805 -1.287898 2.040704
N -0.895251 3.128632 -0.424190
N 0.203114 3.326514 -0.176311
N 1.342254 2.815533 -0.069958
C 1.949186 3.002170 1.262087
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H 2.282840 4.033198 1.387804
H 1.247335 2.732119 2.055078

DIBC (Triazole)
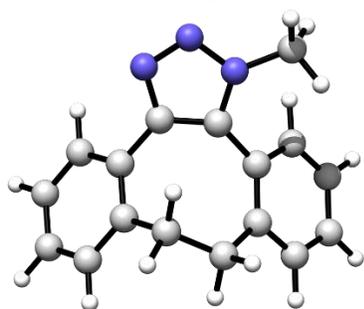
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C -1.717508 0.591501 -0.221070
C -1.962816 -0.455191 0.678134
C -2.603088 0.840477 -1.270071
H -2.404088 1.671673 -1.936459
C -3.081785 -1.263290 0.474354
H -3.285383 -2.071104 1.170652
C 2.701157 -2.720328 -0.826029
H 3.185015 -3.654223 -1.085829
C 3.055673 -1.538365 -1.468383
H 3.813416 -1.533029 -2.242177
C -3.716187 0.031922 -1.454700
H -4.398988 0.227487 -2.272693
C -3.949036 -1.031174 -0.586429

H -4.814505 -1.668150 -0.726033
C 1.711306 -2.698989 0.142125
C 2.407349 -0.366781 -1.121035
H 2.646093 0.551804 -1.645495
H 1.434871 -3.625318 0.635109
C -1.069929 -0.669461 1.877298
H -0.662701 0.286190 2.209676
H -1.682381 -1.048245 2.700243
C 0.057295 -1.686796 1.665484
H -0.403041 -2.671148 1.537489
H 0.637148 -1.747396 2.594209
C 0.784638 0.982350 0.097693
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N 1.484392 2.133680 0.280722
C 2.905383 2.326364 0.512227
H 3.312361 1.436194 0.988334
H 3.429035 2.510359 -0.426533
H 3.017197 3.189642 1.164555

S-DIBO (1,4-Triazole)
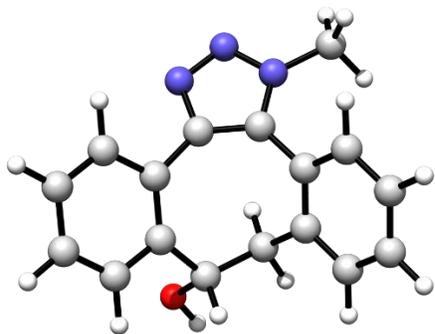
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E = -896.162372
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C -1.616535 -0.260514 -0.279190
C -1.206259 -1.406870 0.414001
C -2.564489 -0.358021 -1.301440
H -2.859190 0.535652 -1.840427
C -1.751843 -2.638360 0.048971
H -1.444790 -3.531188 0.584484
C 3.918025 -0.359018 -1.258761
H 4.828207 -0.790496 -1.657491
C 3.575497 0.960339 -1.539099
H 4.214651 1.576798 -2.159710

C -3.101084 -1.589868 -1.647829
H -3.829763 -1.658658 -2.446201
C -2.688909 -2.734931 -0.971896
H -3.101101 -3.700968 -1.237678
C 3.085823 -1.115013 -0.452559
C 2.400982 1.480259 -1.026645
H 2.116009 2.502373 -1.243429
H 3.365918 -2.132569 -0.201496
C -0.200245 -1.316795 1.530297
H -0.254122 -0.358171 2.047637
H -0.431219 -2.094959 2.265783
C 1.239705 -1.564770 1.073594
C 0.303619 1.415188 0.184175
C -1.017877 1.027008 0.079415
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H -3.610370 1.413054 0.885799
H -3.326308 3.147858 1.206295
H -3.572296 2.578045 -0.461206
H 1.258271 -2.554458 0.594834
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H 1.800732 -2.261988 2.814611

_S_-DIBO (1,5-Triazole)
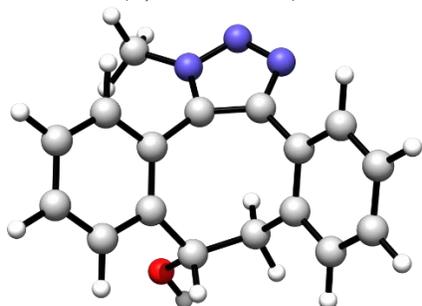
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C -1.808566 0.640633 -0.220251
C -1.953217 -0.537608 0.525890
C -2.756917 0.980661 -1.185269
H -2.637489 1.909211 -1.731097
C -3.033283 -1.377301 0.252130
H -3.159070 -2.286324 0.832280
C 2.722688 -2.307128 -1.454206

H 3.240655 -3.166160 -1.862963
C 2.995907 -1.027152 -1.924724
H 3.721898 -0.871288 -2.713380
C -3.829886 0.137890 -1.441586
H -4.560854 0.405293 -2.195062
C -3.961321 -1.051019 -0.729308
H -4.795104 -1.714328 -0.926460
C 1.773246 -2.476040 -0.460088
C 2.313472 0.050929 -1.388388
H 2.493013 1.046210 -1.779216
H 1.564496 -3.472129 -0.084874
C -0.993830 -0.861335 1.644231
H -0.588369 0.050267 2.085178
H -1.548328 -1.378863 2.435224
C 0.162068 -1.785497 1.254964
C 0.678466 1.122649 0.066447
C -0.649255 1.502735 0.034299
N -0.725859 2.826713 0.327476
N 0.465639 3.278755 0.549026
N 1.327434 2.271044 0.391788
C 2.744525 2.495833 0.621312
H 3.236169 2.831523 -0.292330
H 2.834116 3.264844 1.385343
H 3.199088 1.567793 0.963473
O 1.032517 -1.973665 2.369413
H 0.507738 -2.268714 3.119654
H -0.278661 -2.752188 0.974596

_R_-DIBO (1,4-Triazole)
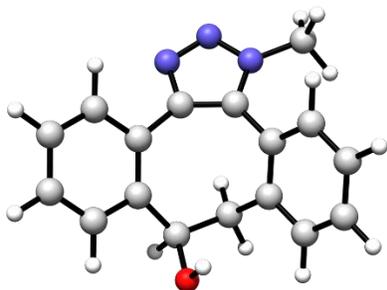
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E = -896.167514
0 1
C -1.947105 -0.563430 -0.310827
C -1.616116 0.749625 0.069377
C 1.569396 -0.181681 0.264271
C 1.228051 -1.295853 -0.514733
C 2.476491 -0.308832 1.319461
H 2.716431 0.559703 1.922876

C 1.811050 -2.527766 -0.206555
H 1.560074 -3.391465 -0.812898
C -4.070255 -0.345848 0.879331
H -5.012367 -0.785255 1.184828
C -3.747895 0.959921 1.235630
H -4.431768 1.558176 1.825552
C 3.044698 -1.540590 1.613094
H 3.741452 -1.633507 2.437158
C 2.708998 -2.653181 0.847110
H 3.150143 -3.617895 1.067656
C -3.180792 -1.080736 0.115432
C -2.536498 1.489458 0.832660
H -2.266984 2.502149 1.105426
H -3.437303 -2.090379 -0.181831
C 0.253817 -1.175909 -1.657797
H 0.299542 -0.186327 -2.114331
H 0.520032 -1.908370 -2.423127
C -1.191894 -1.502382 -1.260213
H -1.771563 -1.524399 -2.188227
O -1.252897 -2.841028 -0.784462
H -0.857677 -2.861879 0.094422
C -0.363209 1.476763 -0.226130
C 0.957779 1.109107 -0.059752
N 0.822028 3.251130 -0.611895
N -0.386234 2.801330 -0.549686
N 1.650693 2.247274 -0.316948
C 3.086088 2.464411 -0.323074
H 3.582223 1.578169 -0.716538
H 3.279829 3.321940 -0.963267
H 3.450072 2.670961 0.683983

_R_-DIBO (1,5-Triazole)
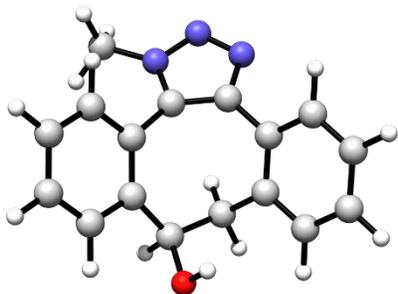
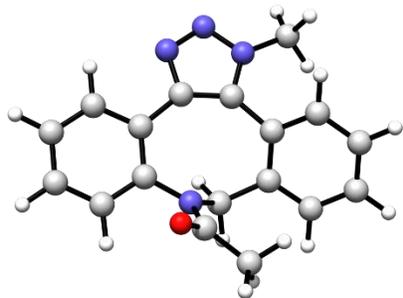# of imaginary frequencies = 0
E = -896.166733
0 1
C -1.028987 -1.471567 -0.297139
C -1.457179 -0.225667 0.194027
C 1.650094 0.857520 0.255824

C 1.959285 -0.247394 -0.550571
C 2.529858 1.264869 1.258862
H 2.280864 2.139122 1.848864
C 3.146013 -0.943415 -0.305596
H 3.406706 -1.781970 -0.943587
C -2.752168 -2.560348 1.051510
H -3.244594 -3.472429 1.366677
C -3.157830 -1.328081 1.553468
H -3.960606 -1.259802 2.277442
C 3.702650 0.559525 1.492806
H 4.379189 0.878224 2.276562
C 4.007229 -0.552687 0.713748
H 4.923894 -1.104042 0.886439
C -1.704005 -2.617821 0.149168
C -2.509399 -0.184205 1.126775
H -2.794064 0.775778 1.542154
H -1.377704 -3.576865 -0.233424
C1.061923 -0.652619 -1.695200
H 0.542260 0.214323 -2.104916
H 1.680167 -1.069656 -2.493596
C 0.056730 -1.754911 -1.344673
H -0.466064 -2.018995 -2.269521
O 0.761291 -2.937979 -0.995385
H 1.253799 -2.758579 -0.185532
C -0.867280 1.087484 -0.132295
C 0.410247 1.597276 -0.001084
N 0.364956 2.938219 -0.213880
N -0.852077 3.282019 -0.481106
N -1.612615 2.185976 -0.433514
C -3.029042 2.292802 -0.741612
H -3.599898 2.560278 0.148101
H -3.142934 3.071512 -1.492597
H -3.382015 1.338861 -1.128605

DIBAC (1,4-Triazole)

# of imaginary frequencies = 0
E = -989.619043
0 1

C -1.969761 -0.489588 -0.194923
C -1.821291 0.886714 0.007307
C 1.713525 0.163744 0.089257
C 1.503954 -0.915827 -0.782729
C 2.873391 0.176166 0.871040
H 3.001594 0.950813 1.616650
C 2.525029 -1.838840 -0.982151
H 2.370090 -2.647872 -1.688165
C -4.381793 -0.285351 -0.176279
H -5.359197 -0.746504 -0.247801
C -4.252602 1.084262 0.038772
H -5.131044 1.709833 0.140470
C 3.862550 -0.785856 0.707285
H 4.750781 -0.755814 1.326424
C 3.712770 -1.769516 -0.262150
H 4.493464 -2.501740 -0.427995
C -3.242272 -1.056984 -0.295980
C -2.996479 1.654406 0.119280
H -2.896294 2.718981 0.273060
H -3.315852 -2.126114 -0.447924
N -0.853593 -1.372843 -0.314117
C 0.134322 -1.128227 -1.374802
H -0.200637 -0.240460 -1.913950
H 0.149805 -1.956284 -2.088913
C -0.806396 -2.460231 0.548357
O -1.576813 -2.566803 1.477044
C 0.229835 -3.533889 0.293589
H 0.423371 -3.709097 -0.764192
H 1.169517 -3.261443 0.776752
H -0.147275 -4.443675 0.755708
C 0.823939 1.342548 0.100273
C -0.542294 1.637015 0.060678
N 0.501222 3.548209 0.048971
N -0.656595 3.000348 0.045985
N 1.413381 2.582818 0.081451
C 2.807531 2.979679 -0.069549
H 3.308377 3.045292 0.895712
H 3.327281 2.265885 -0.705366
H 2.795847 3.961555 -0.536493

DIBAC (1,5-Triazole)
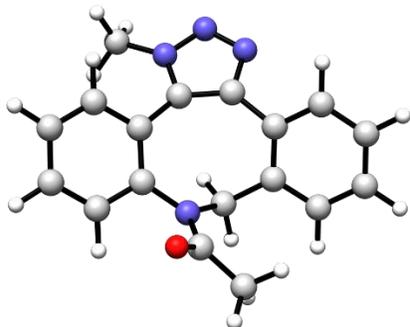
# of imaginary frequencies = 0
E = -989.613903
0 1
C -1.248081 -1.264250 -0.216406
C -1.714715 0.013387 0.148741
C 1.630624 1.092958 0.284092
C 1.982282 0.040094 -0.572176
C 2.612642 1.703371 1.068198
H 2.327143 2.530237 1.706423
C 3.324449 -0.322312 -0.676898
H 3.611591 -1.093152 -1.383380
C -3.442495 -2.210637 0.254651
H -4.100655 -3.070562 0.256288
C -3.868965 -0.984463 0.753309
H -4.854747 -0.870354 1.186435
C 3.935284 1.291291 0.995756
H 4.685117 1.771042 1.613021
C 4.299052 0.291235 0.100447
H 5.335745 -0.008381 0.004776
C -2.148503 -2.337420 -0.210320
C -3.014110 0.098187 0.684948
H -3.342095 1.046136 1.088504
H -1.792785 -3.301143 -0.547172
N 0.099766 -1.583465 -0.549365
C 0.923566 -0.683341 -1.373413
H 0.243657 0.027464 -1.844042
H 1.388456 -1.254842 -2.178477
C 0.670265 -2.673472 0.116616
O 0.110365 -3.236180 1.029719
C 2.016133 -3.178189 -0.357251
H 2.210972 -3.006953 -1.414161
H 2.805632 -2.706644 0.228862
H 2.029385 -4.246366 -0.149321
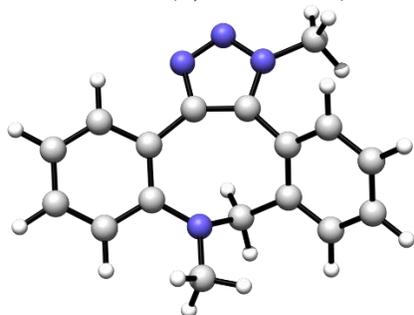C 0.313787 1.741132 0.186340
C -0.988717 1.291888 0.007667
N 0.316249 3.100299 0.065086
N -0.869768 3.510021 -0.212730

N -1.675716 2.451025 -0.261452
C -3.027032 2.675060 -0.762696
H -3.373271 1.786012 -1.284606
H -3.714484 2.917670 0.047318
H -2.969086 3.517018 -1.448633

DIBAC-Me (1,4-Triazole)
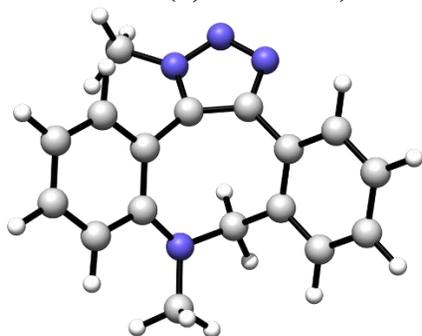

# of imaginary frequencies = 0
E = -876.277163
0 1
C 1.953294 -0.838874 0.049569
C 1.833142 0.567305 -0.057939
C -1.676979 -0.039296 -0.193342
C -1.473402 -1.188909 0.584311
C -2.784683 0.020359 -1.040782
H -2.920514 0.881899 -1.683724
C -2.415014 -2.210857 0.558074
H -2.260091 -3.086528 1.180496
C 4.343858 -0.663973 -0.400345
H 5.301573 -1.154537 -0.529656
C 4.235327 0.717142 -0.493912
H 5.101614 1.330162 -0.708128
C -3.707265 -1.020387 -1.081722
H -4.556696 -0.960125 -1.751232
C -3.537322 -2.128898 -0.262884
H -4.260533 -2.935318 -0.277255
C 3.219211 -1.423421 -0.123690
C 2.995436 1.308869 -0.316500
H 2.898558 2.382781 -0.394657
H 3.321331 -2.495427 -0.021457
N 0.852309 -1.666841 0.268212
C 0.926622 -3.069852 -0.074036
H 1.440037 -3.673169 0.690050
H -0.089329 -3.454811 -0.187813
H 1.438983 -3.196643 -1.027719
C -0.149170 -1.352801 1.280983
H 0.141301 -0.446101 1.811969
H -0.197372 -2.164588 2.016925

C 0.584774 1.364019 0.068883
C -0.787199 1.125973 -0.036502
N -0.405279 3.284485 0.352100
N 0.738804 2.704345 0.297088
N -1.341906 2.362746 0.153415
C -2.735209 2.761604 0.278447
H -3.294604 1.984138 0.795616
H -2.742833 3.681662 0.858013
H -3.181449 2.945433 -0.698814

DIBAC-Me (1,5-Triazole)
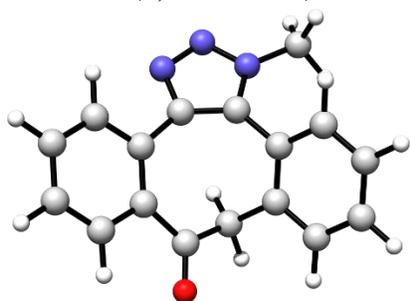

# of imaginary frequencies = 0
E = -876.277445
0 1
C 1.062834 -1.449617 0.236797
C 1.425422 -0.146917 -0.210891
C -1.718437 0.821441 -0.256600
C -1.920289 -0.351528 0.482235
C -2.668678 1.231754 -1.192414
H -2.504830 2.156010 -1.733907
C -3.064729 -1.112602 0.244452
H -3.237686 -2.013160 0.825620
C 2.856035 -2.349392 -1.183423
H 3.390508 -3.220507 -1.544102
C 3.199761 -1.078366 -1.624509
H 3.995058 -0.924093 -2.341726
C -3.801419 0.462687 -1.420989
H -4.533413 0.782542 -2.152860
C -3.996253 -0.717748 -0.708156
H -4.880194 -1.319389 -0.883140
C 1.814850 -2.526278 -0.291036
C 2.471350 -0.009680 -1.136041
H 2.690440 0.987886 -1.500235
H 1.581491 -3.536221 0.006484
N 0.064524 -1.741645 1.157756
C -0.348780 -3.131304 1.292098
H 0.460153 -3.746596 1.691950

H -1.174353 -3.182158 1.998513
H -0.680769 -3.561924 0.338716
C -0.939204 -0.759086 1.564935
H -0.440793 0.116885 1.975500
H -1.493118 -1.208061 2.389588
C 0.778889 1.133514 0.146156
C -0.511434 1.610346 0.004595
N -0.515936 2.942416 0.262859
N 0.684605 3.317077 0.563739
N 1.479786 2.244377 0.501088
C 2.885412 2.384050 0.841897
H 3.261132 1.425316 1.193900
H 3.464100 2.706892 -0.024117
H 2.959436 3.133360 1.627073

DIBONE (1,4-Triazole)
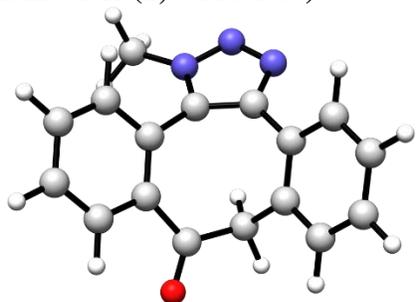

# of imaginary frequencies = 0
E = -894.967889
0 1
C 1.937141 -0.720071 0.186098
C 1.675717 0.642007 -0.078183
C -1.609985 -0.150949 -0.242566
C -1.311175 -1.295135 0.506069
C -2.575499 -0.208803 -1.253254
H -2.784764 0.677385 -1.841895
C -1.974696 -2.487891 0.214777
H -1.727210 -3.378123 0.782323
C 4.142409 -0.500056 -0.825895
H 5.084700 -0.949315 -1.114688
C 3.896549 0.849647 -1.062808
H 4.646333 1.470357 -1.538998
C -3.236964 -1.396850 -1.523878
H -3.977486 -1.436337 -2.313250
C -2.933615 -2.539904 -0.787057
H -3.442447 -3.472674 -0.998278
C 3.170364 -1.262409 -0.207678
C 2.682725 1.402224 -0.696694
H 2.483159 2.448440 -0.887407

H 3.343654 -2.309400 0.004325
C -0.246413 -1.261672 1.574741
H -0.163290 -0.273692 2.026966
H -0.465351 -2.000308 2.344845
C 1.061855 -1.696217 0.930707
O 1.381602 -2.859586 1.016346
C 0.438864 1.401677 0.202116
C -0.904946 1.095732 0.061150
N -0.655320 3.233544 0.598197
N 0.526131 2.727303 0.519358
N -1.535771 2.269749 0.321295
C -2.958729 2.558572 0.365768
H -3.336614 2.794762 -0.629382
H -3.488743 1.694268 0.763187
H -3.091634 3.417736 1.019055

DIBONE (1,5-Triazole)
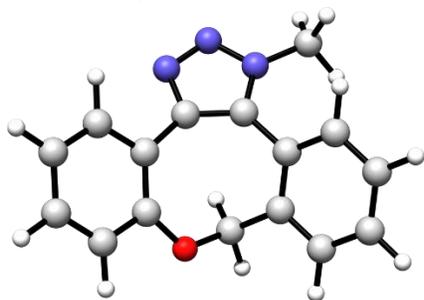

# of imaginary frequencies = 0
E = -894.965178
0 1
C 1.074244 -1.450850 0.218013
C 1.422783 -0.162690 -0.235114
C -1.738491 0.733393 -0.231126
C -1.961853 -0.424531 0.523744
C -2.651831 1.113821 -1.216103
H -2.473459 2.028119 -1.769693
C -3.076999 -1.214033 0.240687
H -3.249317 -2.113924 0.821787
C 2.820717 -2.411449 -1.181828
H 3.349147 -3.284875 -1.543569
C 3.163004 -1.140920 -1.633679
H 3.956632 -1.008383 -2.359181
C -3.764103 0.327345 -1.478876
H -4.467942 0.624866 -2.246689
C -3.970110 -0.846072 -0.756868
H -4.834216 -1.466402 -0.962595
C 1.790481 -2.552032 -0.269473
C 2.468951 -0.039324 -1.163614

H 2.712433 0.945480 -1.544574
H 1.510605 -3.530637 0.098560
C -1.045090 -0.803690 1.666430
H -0.567749 0.084583 2.085087
H -1.615292 -1.295825 2.453867
C 0.008274 -1.805578 1.235499
O -0.020242 -2.926433 1.686902
C 0.763509 1.101939 0.140029
C -0.545256 1.538574 0.041217
N -0.572836 2.874737 0.285138
N 0.626156 3.281153 0.544576
N 1.449359 2.235094 0.457050
C 2.860140 2.417741 0.758405
H 3.406524 2.741684 -0.127824
H 2.933499 3.182517 1.528411
H 3.272102 1.477511 1.119788

ODIBO (1,4-Triazole)
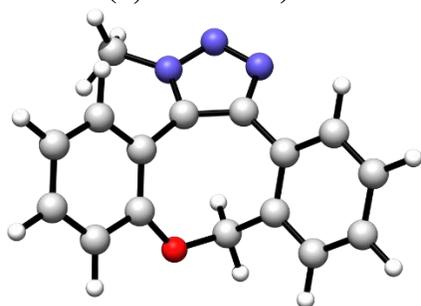

# of imaginary frequencies = 0
E = -856.848461
0 1
C1.916477 -0.928673 0.376016
C 1.724990 0.397927 -0.046082
C -1.557947 -0.209395 -0.197018
C -1.246455 -1.330567 0.581235
C -2.559885 -0.292176 -1.168408
H -2.779435 0.572055 -1.784962
C -1.943770 -2.518516 0.368597
H -1.700249 -3.387406 0.970649
C 4.112062 -0.971343 -0.660597
H 5.020560 -1.514168 -0.892633
C 3.949406 0.351238 -1.069529
H 4.726598 0.860923 -1.624551
C -3.247959 -1.480778 -1.367127
H -4.017723 -1.538192 -2.127121
C -2.938784 -2.598697 -0.597087
H -3.471210 -3.529409 -0.751044
C 3.107300 -1.592802 0.052368

C 2.774029 1.006823 -0.761397
H 2.628278 2.034336 -1.070321
H 3.209143 -2.613868 0.398258
C -0.161814 -1.278587 1.629458
H -0.071600 -0.287832 2.077653
H -0.390991 -1.993146 2.420223
O 1.088905 -1.718245 1.122979
C -0.810722 1.029042 0.027604
C 0.544676 1.263580 0.167194
N -0.444119 3.175436 0.437883
N 0.708706 2.595875 0.406547
N -1.377147 2.249699 0.212291
C -2.779876 2.624023 0.218331
H -3.365582 1.821118 0.663980
H -2.867987 3.530487 0.812701
H -3.133490 2.817392 -0.795064

ODIBO (1,5-Triazole)
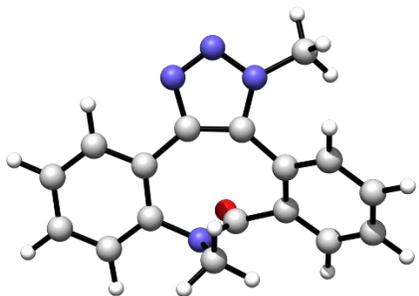

# of imaginary frequencies = 0
E = -856.849358
0 1
C 1.070756 -1.512625 0.484299
C 1.397273 -0.291747 -0.132075
C -1.759769 0.559176 -0.190989
C -1.891483 -0.570526 0.626471
C -2.740680 0.853885 -1.139000
H -2.631986 1.745858 -1.744507
C -2.988121 -1.413878 0.447992
H -3.093150 -2.287662 1.082678
C 2.838574 -2.626188 -0.757074
H 3.385519 -3.533489 -0.983558
C 3.157695 -1.428813 -1.397289
H 3.946512 -1.386280 -2.137182
C -3.830000 0.009802 -1.300814
H -4.586553 0.240736 -2.041195
C -3.948283 -1.134929 -0.515639
H -4.795107 -1.798216 -0.644424
C 1.808765 -2.660782 0.160324

C 2.436070 -0.294636 -1.082847
H 2.653850 0.635031 -1.596495
H 1.532470 -3.578662 0.663891
C -0.919712 -0.836553 1.750854
H -0.498396 0.092409 2.137851
H -1.441127 -1.338538 2.565262
O 0.125019 -1.754379 1.425242
C -0.582892 1.415571 -0.032186
C 0.730908 1.004482 0.089059
N -0.627682 2.767683 0.075904
N 0.570419 3.213766 0.267801
N 1.405017 2.170495 0.278926
C 2.820440 2.396180 0.519309
H 3.248314 1.508159 0.980636
H 3.342056 2.611721 -0.413656
H 2.905933 3.249846 1.187984

BARAC (1,4-Triazole)

# of imaginary frequencies = 0
E = -950.301374
0 1
C-1.976405 -0.923896 0.081559
C -1.930038 0.474181 0.148793
C 1.703623 0.005081 0.152561
C 1.511921 -1.217423 -0.509435
C 2.907330 0.187615 0.841048
H 3.059969 1.083394 1.429363
C 2.517599 -2.168778 -0.580406
H 2.335600 -3.093122 -1.116409
C -4.380878 -0.929451 0.138062
H -5.320608 -1.467869 0.126935
C -4.360741 0.460201 0.215241
H -5.289943 1.014528 0.269989
C 3.906387 -0.779435 0.803127
H 4.826045 -0.617898 1.352200
C 3.729988 -1.943771 0.064453
H 4.517933 -2.685357 0.016768
C -3.179425 -1.618041 0.071035

C -3.158625 1.150637 0.215005
H -3.153455 2.230406 0.259901
H -3.148239 -2.699125 0.005007
N -0.743778 -1.639148 0.111549
C -0.273387 -1.936322 1.465603
H 0.625141 -2.549302 1.430578
H -0.065878 -1.022320 2.034309
H -1.057520 -2.495534 1.977052
C 0.106552 -1.444333 -0.964354
O -0.271740 -1.331872 -2.104215
C -0.688208 1.295601 0.096361
C 0.707354 1.104391 0.072742
N 0.205253 3.268541 -0.141052
N -0.903539 2.640398 -0.017745
N 1.190084 2.378148 -0.091864
C 2.532006 2.859238 -0.398719
H 3.064670 2.112071 -0.982950
H 2.404400 3.768798 -0.980468
H 3.089358 3.087768 0.509155

BARAC (1,5-Triazole)
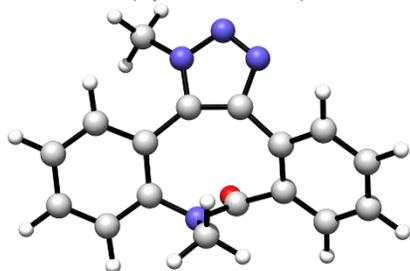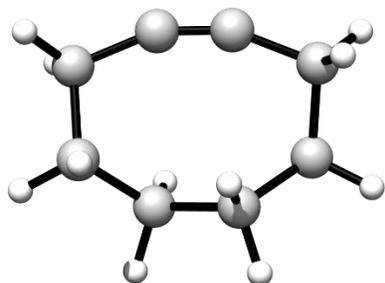

# of imaginary frequencies = 0
E = -950.295210
0 1
C 1.422764 -1.378621 0.047742
C 1.727210 -0.025641 -0.195231
C -1.872915 0.457488 -0.285397
C -2.024985 -0.687363 0.510000
C -2.996707 0.955323 -0.948604
H -2.900337 1.858896 -1.536958
C -3.258040 -1.304139 0.661868
H -3.344180 -2.177835 1.297709
C 3.721541 -2.031670 -0.298481
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C 4.025101 -0.721118 -0.645008
H 5.025403 -0.455603 -0.964286
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C -0.471889 -2.204349 -1.177777
H -1.480880 -2.592063 -1.057524
H -0.488631 -1.377676 -1.897216
H 0.164886 -2.999551 -1.565856
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Cyclooctyne
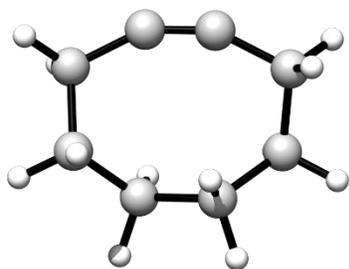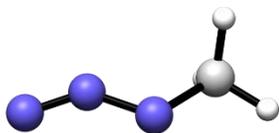

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C 0.600209 -1.454523 -0.033295
C -1.952796 -0.910218 0.124628
C -0.600230 -1.454532 0.033292
H 2.663660 -1.438588 0.514219
H -1.753645 0.635679 -1.372336
H 2.315935 -0.994262 -1.153502
H -2.799045 1.065627 -0.028199
C 0.684387 1.347083 -0.372113
H 0.545756 0.976528 -1.393692
C -0.684371 1.347085 0.372115
H -0.545741 0.976522 1.393691

H -1.003260 2.387535 0.473066
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C 1.853453 0.578910 0.284115
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Cyclooctyne (TS)

# of imaginary frequencies = 1
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C 0.315307 0.319537 -0.036885
C -1.001380 -1.933436 0.255699
C -0.008428 -0.860758 0.085254
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H 0.183250 2.051588 -1.211457
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Cyclooctyne (Triazole)
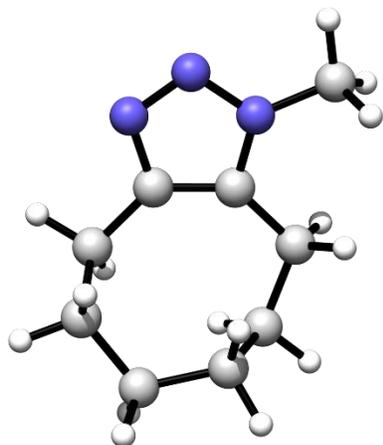
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BONO
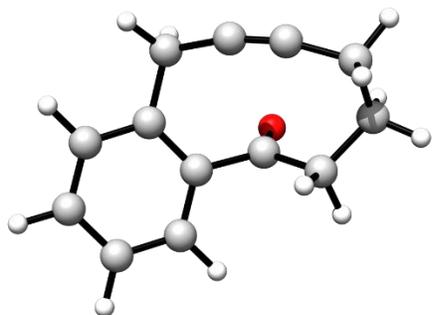
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C 1.255206 0.860795 0.194568
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C 2.573893 1.107484 -0.175434
H 2.928653 2.131907 -0.216323
O -0.921693 -0.668313 1.828519

References

1. Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2. a) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215-241 b) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res.* **2008**, *41*, 157-167.

3. Grimme, S.; Antony, J.; Ehrlich, S.; Krieg, H. *J. Chem. Phys.* **2010**, *132*, 154104.

4. Pettersen, E. F.; Goddard, T. D.; Huang, C. C.; Couch, G. S.; Greenblatt, D. M.; Meng, E. C.; Ferrin, T. E. *J. Comput. Chem.* **2004**, *25*, 1605-1612.

[5] NBO Version 3.1, E. D. Glendening, A. E. Reed, J. E. Carpenter, and F. Weinhold.