

Supporting Information

Predicting Reactivity for Bioorthogonal Cycloadditions Involving Nitrones

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1. General Computational methods

All calculations were carried with the Gaussian 16 program package*. Geometry optimizations were carried out at the M06-2X level of theory with the 6-31G(d) basis set. Solvent effects in methanol and acetonitrile were evaluated at the M06-2X/6-311++G(d,p) level at 298.15K with a self-consistent reaction field (SCRF) using the SMD model on the gas-phase-optimized structures. Harmonic vibrational analysis was performed at the same level of theory as the geometry optimization to confirm no imaginary vibration was observed for the optimized structure and only a single imaginary vibration was observed for the transition state.

D/I analysis was performed based on the following formula:

$$\text{Distortion_Nitron} = \text{TS_Nitron} - \text{SM_Nitron}$$

$$\text{Distortion_Dipolarophile} = \text{TS_Dipolarophile} - \text{SM_Dipolarophile}$$

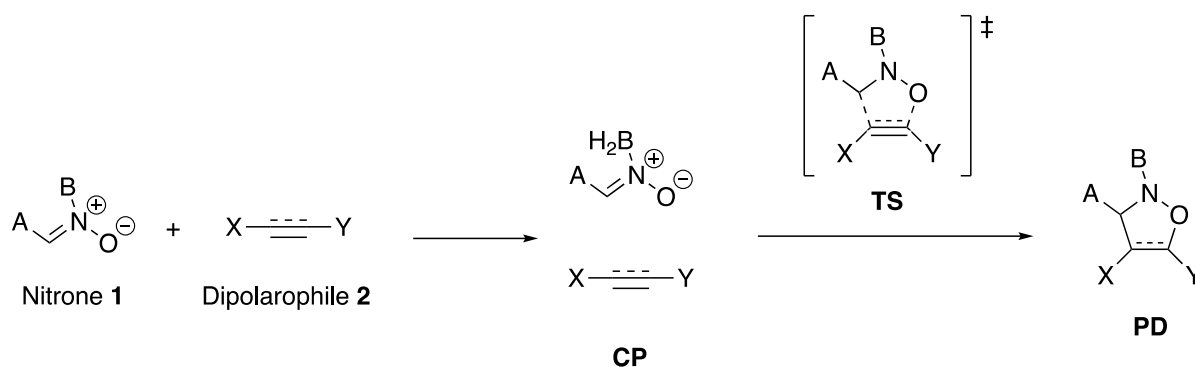
$$\text{Distortion_Total} = \text{Dis_Nitron} + \text{Distortion_Dipolarophile}$$

$$\text{Interaction} = \text{TS_Nitron} + \text{TS_Dipolarophile} - \text{TS_E}$$

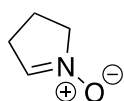
$$\Delta E_{\ddagger} = \text{TS_E} - (\text{SM_Nitron} + \text{SM_Dipolarophile})$$

* Gaussian 16, Revision B.01, 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. Cartesian Coordinates and Energies



Scheme S1

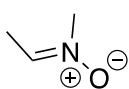


1a

1a_M062X6-31G*.log
 Energy (E) = -286.405311664 Hartree
 Enthalpy (H) = -286.286961 Hartree
 Gibbs free energy (G) = -286.321649 Hartree
 Charge = 0, Spin = 1

C	0.059964	1.142209	-0.032170
H	0.516814	2.120169	-0.090854
O	2.082501	0.018778	-0.048167
N	0.829055	0.092552	-0.007784
C	0.038662	-1.162519	0.136086
H	0.468657	-1.888213	-0.554315
H	0.196687	-1.511823	1.160129
C	-1.389645	0.796581	0.098254
H	-1.764131	1.033005	1.103113
H	-2.019127	1.339625	-0.612611
C	-1.393846	-0.728725	-0.166728
H	-2.130010	-1.258379	0.440049
H	-1.623090	-0.917749	-1.218342

1a_M062X6-311++g**_sp.log
 E = -179789.57230559012



1b

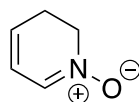
1b_M062X6-31G*.log

Energy (E) = -248.302979631 Hartree
 Enthalpy (H) = -248.192607 Hartree
 Gibbs free energy (G) = -248.228644 Hartree

Charge = 0, Spin = 1

C	0.662982	-0.700599	-0.000039
H	0.646810	-1.783607	-0.000097
O	-1.607915	-0.826499	0.000038
N	-0.523589	-0.168663	-0.000024
C	1.951110	0.064736	0.000032
H	2.066462	0.698879	-0.886344
H	2.065913	0.699789	0.885813
H	2.780104	-0.644938	0.000657
C	-0.720240	1.291664	-0.000007
H	-1.307231	1.525290	0.888059
H	0.221425	1.837396	-0.000614
H	-1.308154	1.525026	-0.887524

1b_M062X6-311++g**_sp.log
 E = -155875.3196361777



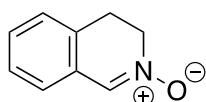
1c

1c_M062X6-31G*.log
 Energy (E) = -324.481832180 Hartree
 Enthalpy (H) = -324.357515 Hartree
 Gibbs free energy (G) = -324.393577 Hartree

Charge = 0, Spin = 1

C	-1.820792	0.131460	0.022223
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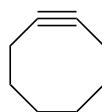
C -1.084925 1.247975 0.096069
 C 0.358747 1.217043 -0.065119
 N 1.023500 0.090886 -0.002737
 C 0.283104 -1.161522 0.315923
 C -1.121219 -1.169145 -0.269295
 O 2.273557 -0.023395 -0.105677
 H -2.901420 0.157609 0.111410
 H -1.540607 2.220632 0.250166
 H 0.963159 2.100947 -0.220435
 H 0.261295 -1.218980 1.409859
 H 0.913837 -1.960899 -0.069276
 H -1.667823 -2.022880 0.141546
 H -1.070883 -1.320338 -1.357492
 1c_M062X6-311++g**_sp.log
 E = -203688.17244651137



1d

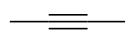
1d_M062X6-31G*.log
 Energy (E) = -478.082876078 Hartree
 Enthalpy (H) = -477.908221 Hartree
 Gibbs free energy (G) = -477.950257 Hartree
 Charge = 0, Spin = 1
 C -0.547640 0.765681 -0.108407
 C -0.327054 -0.622275 -0.088529
 C 1.031328 -1.136097 -0.179492
 N 2.077342 -0.378451 0.026717
 C 1.877230 1.049677 0.394121
 C 0.662944 1.642629 -0.302054
 O 3.273517 -0.775401 0.008777
 C -1.842754 1.257922 -0.011510
 C -2.925635 0.386252 0.096434
 C -2.709603 -0.989845 0.101508
 C -1.416934 -1.493326 0.009273
 H 1.248135 -2.179414 -0.373870
 H 2.809648 1.537551 0.114997
 H 1.773857 1.070646 1.484154
 H 0.877144 1.731473 -1.375853
 H 0.484034 2.653748 0.075646
 H -2.006914 2.332484 -0.026649
 H -3.933675 0.780763 0.173113
 H -3.549390 -1.672679 0.181890
 H -1.243663 -2.565916 0.021273
 1d_M062X6-311++g**_sp.log

E = -300098.48410381126



2a

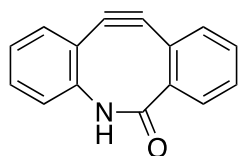
2a_M062X6-31G*.log
 Energy (E) = -311.848085077 Hartree
 Enthalpy (H) = -311.656524 Hartree
 Gibbs free energy (G) = -311.696727 Hartree
 Charge = 0, Spin = 1
 C 1.854065 0.580397 0.283751
 C 1.958221 -0.908630 -0.123907
 C 0.604142 -1.455012 -0.032129
 C -0.601462 -1.454317 0.031577
 C -1.956459 -0.910825 0.124224
 C -1.855565 0.578385 -0.283288
 H 2.800945 1.071079 0.029988
 H 1.752671 0.637500 1.374002
 H 2.675261 -1.433721 0.515275
 H 2.325067 -0.990717 -1.154205
 H -2.322229 -0.993664 1.154857
 H -2.672928 -1.437316 -0.514464
 H -2.802944 1.067403 -0.028217
 H -1.755509 0.636117 -1.373620
 C -0.684998 1.345032 0.372633
 H -0.545505 0.973781 1.396241
 H -1.004473 2.387675 0.475632
 C 0.682841 1.345178 -0.373151
 H 1.001305 2.387993 -0.477424
 H 0.543622 0.972628 -1.396321
 2a_M062X6-311++g**_sp.log
 E = -195748.27997587435



2b

2b_M062X6-31G*.log
 Energy (E) = -155.894169481 Hartree
 Enthalpy (H) = -155.801865 Hartree
 Gibbs free energy (G) = -155.837071 Hartree
 Charge = 0, Spin = 1
 C 2.066512 -0.000067 0.000039
 C 0.603022 0.000108 -0.000074

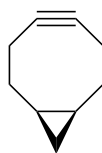
C -0.603026 0.000202 -0.000112
 C -2.066507 -0.000065 0.000052
 H 2.458416 1.014429 0.118144
 H 2.458159 -0.609636 0.819672
 H -2.458670 1.017501 0.086412
 H -2.457993 -0.583859 0.838274
 H -2.458313 -0.434332 -0.924397
 H 2.458394 -0.405175 -0.937537
 2b_M062X6-311++g**_sp.log
 E = -97858.42176730659



2c

2c_M062X6-31G*.log
 Energy (E) = -706.625204740 Hartree
 Enthalpy (H) = -706.411736 Hartree
 Gibbs free energy (G) = -706.465130 Hartree
 Charge = 0, Spin = 1
 C 1.875248 0.480629 -0.038921
 C 1.965334 -0.924029 -0.143438
 C 0.709342 -1.547914 -0.348191
 C -0.498295 -1.527755 -0.379099
 C -1.789415 -0.977814 -0.169258
 C -1.813564 0.423414 -0.002671
 C -0.678305 1.424208 -0.221928
 N 0.723067 1.273379 -0.275746
 C 3.053107 1.190579 0.225145
 C 4.270050 0.536449 0.372200
 C 4.348436 -0.850256 0.264115
 C 3.191915 -1.573203 0.009793
 C -2.956440 -1.734884 -0.054378
 C -4.161023 -1.115819 0.253948
 C -4.197701 0.261865 0.444845
 C -3.039006 1.020007 0.305436
 O -1.035049 2.578899 -0.400627
 H 1.021256 2.230268 -0.437591
 H 3.010532 2.272575 0.318707
 H 5.162091 1.119944 0.576238
 H 5.298518 -1.359983 0.380124
 H 3.216302 -2.654520 -0.073857
 H -2.899671 -2.808297 -0.198443
 H -5.065481 -1.708177 0.349285
 H -5.131983 0.754592 0.693095

H -3.070740 2.095901 0.422087
 2c_M062X6-311++g**_sp.log
 E = -443541.5055930105



2d

2d_M062X6-31G*.log
 Energy (E) = -349.915636731 Hartree
 Enthalpy (H) = -349.718297 Hartree
 Gibbs free energy (G) = -349.758963 Hartree
 Charge = 0, Spin = 1
 C 1.661031 0.293448 0.479432
 C 1.932041 -1.144131 -0.032749
 C 0.608001 -1.760676 -0.153845
 C -0.600044 -1.763479 -0.149927
 C -1.926859 -1.152464 -0.032865
 C -1.663096 0.286768 0.478583
 C -0.760333 1.094237 -0.436561
 C 0.755755 1.097280 -0.436447
 C -0.004688 2.290131 0.076318
 H 2.613635 0.827319 0.590815
 H 1.216455 0.221634 1.478688
 H 2.585381 -1.680360 0.663105
 H 2.444831 -1.114590 -1.001407
 H -2.580475 -1.690512 0.661324
 H -2.436493 -1.125779 -1.003282
 H -1.219737 0.218014 1.478597
 H -2.618314 0.816313 0.588081
 H -1.181625 1.215760 -1.433897
 H 1.177016 1.220068 -1.433633
 H -0.006610 3.212645 -0.494728
 H -0.004908 2.432811 1.154706
 2d_M062X6-311++g**_sp.log
 E = -219643.13394484657



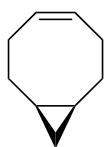
2e

2e_M062X6-31G*.log
 Energy (E) = -351.149066433 Hartree

Enthalpy (H) = -350.928175 Hartree
Gibbs free energy (G) = -350.968721
Hartree

Charge = 0, Spin = 1

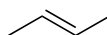
C -0.215313 -1.635119 -0.549598
C 1.218404 -1.814148 0.026817
C 1.577400 -0.453793 0.555671
C 1.711511 0.585930 -0.264989
C 1.057438 1.893011 0.061944
C -0.422915 1.688593 -0.368014
C -1.194510 0.675184 0.466430
C -1.126634 -0.841890 0.374418
C -2.334442 -0.108205 -0.133162
H -0.675988 -2.607214 -0.767957
H -0.126261 -1.102346 -1.504534
H 1.893493 -2.147441 -0.769096
H 1.227452 -2.576422 0.812731
H 1.318419 -0.255285 1.596279
H 1.897891 0.399021 -1.325748
H 1.484414 2.749549 -0.469625
H 1.102925 2.100971 1.137741
H -0.436306 1.385909 -1.423517
H -0.960841 2.644151 -0.318667
H -1.368943 1.025428 1.483382
H -1.265286 -1.324570 1.341872
H -3.274137 -0.187054 0.403620
H -2.442470 -0.042078 -1.213585
2e_M062X6-311++g**_sp.log
E = -220415.35903410387



2f

2f_M062X6-31G*.log
Energy (E) = -351.161979936 Hartree
Enthalpy (H) = -350.940313 Hartree
Gibbs free energy (G) = -350.981930
Hartree
Charge = 0, Spin = 1
C 0.433765 -1.516575 0.542233
C -0.997524 -1.789260 0.090748
C -1.965952 -0.669480 -0.205364
C -1.966251 0.668835 -0.205706
C -0.998358 1.788977 0.090653
C 0.432818 1.516477 0.542543

C 1.243207 0.751345 -0.474900
C 1.243648 -0.750803 -0.475133
C 2.475532 0.000565 -0.053038
H 0.916806 -2.484702 0.725889
H 0.434743 -0.996850 1.505460
H -1.481699 -2.432538 0.838810
H -0.955079 -2.407673 -0.818762
H -2.927253 -1.093111 -0.502388
H -2.927721 1.091919 -0.502940
H -1.482972 2.431930 0.838711
H -0.955782 2.407596 -0.818705
H 0.433553 0.996242 1.505493
H 0.915624 2.484595 0.726848
H 1.283912 1.224840 -1.454250
H 1.284470 -1.224119 -1.454561
H 3.339255 0.000971 -0.709154
H 2.716830 0.000409 1.007327
2f_M062X6-311++g**_sp.log
E = -220424.1443523167



2g

2g_M062X6-31G*.log
Energy (E) = -157.132134884 Hartree
Enthalpy (H) = -157.016200 Hartree
Gibbs free energy (G) = -157.049995
Hartree
Charge = 0, Spin = 1
C -1.956345 -0.078518 -0.000025
C -0.533805 0.397396 0.000055
C 0.533905 -0.397544 0.000033
C 1.956273 0.078588 -0.000025
H -2.005845 -1.171107 0.000308
H -2.497163 0.287493 0.880013
H -0.381779 1.477798 0.000054
H 0.381770 -1.477919 0.000073
H 2.497208 -0.287330 0.879991
H 2.005530 1.171206 0.000403
H -2.496791 0.286902 -0.880532
H 2.496906 -0.286575 -0.880538
2g_M062X6-311++g**_sp.log
E = -98633.87235962052

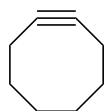
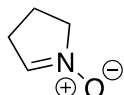


2h

2h_M062X6-31G*.log
 Energy (E) = -157.130297616 Hartree
 Enthalpy (H) = -157.014151 Hartree
 Gibbs free energy (G) = -157.048426 Hartree
 Charge = 0, Spin = 1

C 0.666971 0.666610 -0.000086
 C -0.666851 0.666521 0.000021
 H 1.168506 1.633576 -0.000020
 H -1.168571 1.633415 0.000271
 C 1.581406 -0.523780 -0.000001
 H 2.236249 -0.508224 -0.878512
 H 2.233086 -0.510494 0.880934
 H 1.040319 -1.471862 -0.002036
 C -1.581436 -0.523724 -0.000026
 H -1.040709 -1.472007 -0.003728
 H -2.232275 -0.511147 0.881535
 H -2.237145 -0.507015 -0.877894

2h_M062X6-311++g**_sp.log
 E = -98632.86874899197

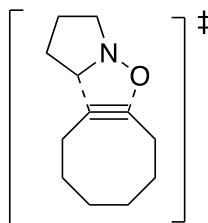


CP1

CP1_M062X6-31G*.log
 Energy (E) = -598.269253349 Hartree
 Enthalpy (H) = -597.957284 Hartree
 Gibbs free energy (G) = -598.015158 Hartree
 Charge = 0, Spin = 1

C 1.434906 -1.955527 0.037984
 C 0.571405 -1.599436 -1.194932
 C 0.495703 -0.137479 -1.220044
 C 0.769673 1.013713 -0.967762
 C 1.494051 2.112588 -0.323885
 C 2.821281 1.519191 0.202306
 H 1.679711 -3.022151 -0.021879
 H 0.804547 -1.831159 0.926076

H -0.408276 -2.077183 -1.095492
 H 1.042841 -1.962787 -2.115977
 H 0.906546 2.506441 0.516865
 H 1.686959 2.952622 -0.999011
 H 3.299708 2.271530 0.840403
 H 3.491362 1.357279 -0.650259
 C 2.672197 0.196057 0.986132
 H 1.743690 0.226703 1.572742
 H 3.481830 0.174548 1.723620
 C 2.736476 -1.136328 0.182069
 H 3.465376 -1.782490 0.682870
 H 3.151203 -0.940269 -0.815832
 C -2.678317 -0.396734 -0.661976
 H -2.977939 -1.159572 -1.368278
 O -1.807317 -1.927926 0.835176
 N -2.100199 -0.762590 0.440532
 C -1.710202 0.396165 1.283427
 H -2.083515 0.195436 2.288701
 H -0.617650 0.400222 1.296881
 C -2.753106 1.085401 -0.818490
 H -2.050550 1.415468 -1.592770
 H -3.752163 1.427906 -1.104427
 C -2.332100 1.605193 0.580835
 H -1.628173 2.436153 0.504450
 H -3.207389 1.956017 1.132187
 CP1_M062X6-311++g**_sp.log
 E = -375542.7368557001

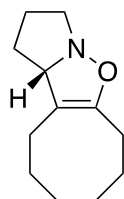


TS1

TS1_M062X6-31G*.log
 Energy (E) = -598.250471748 Hartree
 Enthalpy (H) = -597.939791 Hartree
 Gibbs free energy (G) = -597.994481 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -364.9696
 C 2.717029 -1.546443 0.535241
 C 1.371488 -1.928668 -0.102064
 C 0.497626 -0.753257 -0.191264
 C 0.211110 0.449254 -0.185327

C	0.636358	1.854009	-0.023754
C	2.141684	2.009304	-0.292049
H	3.388341	-2.409258	0.451099
H	2.568233	-1.373101	1.608342
H	0.886493	-2.729921	0.464408
H	1.531018	-2.322526	-1.114222
H	0.416181	2.185015	1.001324
H	0.073349	2.526512	-0.686092
H	2.416794	3.050858	-0.085121
H	2.328868	1.843176	-1.360007
C	3.040358	1.069923	0.534301
H	2.587260	0.921743	1.523955
H	3.981134	1.600848	0.716284
C	3.393176	-0.308871	-0.085258
H	4.475717	-0.446667	0.009556
H	3.188392	-0.291179	-1.164072
C	-1.936906	0.420009	-0.898604
H	-1.541183	0.567683	-1.893980
O	-1.295494	-1.752373	-0.762376
N	-2.096541	-0.812178	-0.450501
C	-2.738541	-0.814513	0.873700
H	-3.310677	-1.735215	0.993133
H	-1.924264	-0.792932	1.609526
C	-2.794309	1.389153	-0.134616
H	-2.161239	2.107691	0.399274
H	-3.465470	1.965444	-0.778192
C	-3.565307	0.470131	0.847456
H	-3.678493	0.913965	1.837713
H	-4.563313	0.261897	0.453013

TS1_M062X6-311++g**_sp.log
E = -375528.0359818919



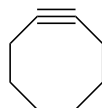
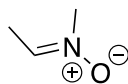
PD1

PD1_M062X6-31G*.log
Energy (E) = -598.354535313 Hartree
Enthalpy (H) = -598.040302 Hartree
Gibbs free energy (G) = -598.091318 Hartree
Charge = 0, Spin = 1

C	2.529064	-1.261015	0.707793
C	1.177863	-1.916181	0.422585

C	0.096158	-0.967038	0.021243
C	-0.065345	0.354569	0.118287
C	0.823655	1.436464	0.665070
C	1.942289	1.876914	-0.301073
H	3.228332	-2.058479	0.979697
H	2.451481	-0.624861	1.595896
H	0.840491	-2.496089	1.291089
H	1.285616	-2.636784	-0.398345
H	1.258561	1.155033	1.630322
H	0.187079	2.304950	0.875811
H	2.200415	2.921995	-0.092007
H	1.550275	1.851677	-1.326160
C	3.231825	1.054968	-0.229273
H	3.697541	1.205805	0.754998
H	3.932256	1.471633	-0.962913
C	3.096591	-0.452602	-0.480810
H	4.089705	-0.841126	-0.729560
H	2.474459	-0.615589	-1.370706
C	-1.371035	0.694375	-0.570066
H	-1.195660	1.209223	-1.525215
O	-0.937678	-1.603920	-0.629193
N	-1.980632	-0.641850	-0.828910
C	-2.982374	-0.844081	0.229293
H	-3.665452	-1.647936	-0.053256
H	-2.491848	-1.105275	1.179419
C	-2.405045	1.462797	0.287879
H	-2.015004	1.599093	1.302437
H	-2.633331	2.451099	-0.117596
C	-3.628285	0.531722	0.319145
H	-4.237575	0.654087	1.217190
H	-4.263661	0.700502	-0.555625

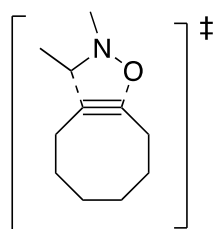
PD1_M062X6-311++g**_sp.log
E = -375586.0522237863



CP2

CP2_M062X6-31G*.log
Energy (E) = -560.165043536 Hartree
Enthalpy (H) = -559.861163 Hartree
Gibbs free energy (G) = -559.920789 Hartree

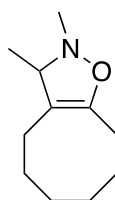
Charge = 0, Spin = 1
 C 1.318637 -2.189393 -0.200349
 C 0.116177 -1.862954 0.721729
 C 0.361600 -0.519570 1.251636
 C 0.848672 0.581359 1.370055
 C 1.790381 1.675581 1.116494
 C 2.425014 1.409243 -0.270328
 H 1.042571 -3.047368 -0.823248
 H 2.164475 -2.510553 0.419221
 H 0.032879 -2.610530 1.517136
 H -0.830729 -1.889382 0.167416
 H 2.569235 1.677629 1.888727
 H 1.319562 2.664777 1.139739
 H 3.294337 2.068297 -0.378059
 H 1.710945 1.705071 -1.048677
 C 2.849115 -0.056249 -0.509464
 H 3.237299 -0.469440 0.430298
 H 3.699397 -0.036643 -1.199657
 C 1.776305 -1.019571 -1.099761
 H 2.185465 -1.454192 -2.018084
 H 0.892522 -0.443911 -1.407647
 C -1.836569 0.429982 -1.192068
 H -1.694818 -0.273609 -2.004425
 O -2.935620 -1.260213 -0.145756
 N -2.506990 -0.060945 -0.194906
 C -1.276351 1.815921 -1.243872
 H -2.055345 2.586675 -1.278856
 H -0.628799 2.017464 -0.382744
 H -0.671921 1.920048 -2.147427
 C -2.804692 0.725820 1.012689
 H -2.228391 0.284698 1.826519
 H -2.543779 1.775335 0.889922
 H -3.870754 0.602941 1.199679
 CP2_M062X6-311++g**_sp.log
 E = -351628.1227706481



TS2

TS2_M062X6-31G*.log
 Energy (E) = -560.151019629 Hartree
 Enthalpy (H) = -559.848318 Hartree

Gibbs free energy (G) = -559.904271
 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -320.1318
 C 2.431640 -1.662441 0.339202
 C 1.040854 -1.925681 -0.262026
 C 0.231272 -0.703093 -0.216454
 C 0.003183 0.505300 -0.116113
 C 0.492894 1.880777 0.102364
 C 1.999638 1.977486 -0.190114
 H 3.056142 -2.543078 0.147674
 H 2.340001 -1.578432 1.429301
 H 0.538381 -2.744596 0.261940
 H 1.136202 -2.243678 -1.308354
 H 0.303512 2.173098 1.144868
 H -0.046433 2.608494 -0.518466
 H 2.335011 2.984655 0.086375
 H 2.154986 1.883092 -1.271813
 C 2.862195 0.929898 0.539690
 H 2.413323 0.718141 1.519486
 H 3.830108 1.396892 0.751897
 C 3.137084 -0.405160 -0.203935
 H 4.215634 -0.592332 -0.163832
 H 2.893625 -0.290430 -1.268581
 C -2.244955 0.559197 -0.646496
 H -1.904249 0.605517 -1.672727
 O -1.679100 -1.599535 -0.698540
 N -2.404713 -0.667821 -0.196014
 C -2.901368 1.750910 -0.017863
 H -3.984224 1.765751 -0.192427
 H -2.724940 1.795956 1.060483
 H -2.487428 2.659758 -0.459794
 C -2.869152 -0.926645 1.162931
 H -2.025462 -0.760667 1.843456
 H -3.706347 -0.278956 1.424872
 H -3.171769 -1.971435 1.198947
 TS2_M062X6-311++g**_sp.log
 E = -351615.4480130506



PD2

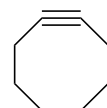
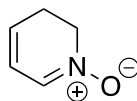
PD2_M062X6-31G*.log

Energy (E) = -560.256175457 Hartree
Enthalpy (H) = -559.949794 Hartree
Gibbs free energy (G) = -560.000465
Hartree

Charge = 0, Spin = 1

C	2.035116	-1.557385	0.295071
C	1.237052	-1.339990	-1.004193
C	-0.073251	-0.650902	-0.772734
C	-0.471409	0.609022	-0.589580
C	0.307190	1.885835	-0.541994
C	1.815782	1.719637	-0.342524
H	2.683692	-2.431233	0.165428
H	1.328341	-1.811582	1.095798
H	0.995896	-2.311151	-1.447484
H	1.840643	-0.799625	-1.738818
H	-0.081018	2.494855	0.287713
H	0.119011	2.476277	-1.450855
H	2.260797	2.720213	-0.323558
H	2.252140	1.223035	-1.215859
C	2.192259	0.959137	0.949850
H	1.289872	0.788072	1.552535
H	2.847232	1.593771	1.556065
C	2.910234	-0.379021	0.729398
H	3.414404	-0.666041	1.659922
H	3.705895	-0.231544	-0.014442
C	-1.986981	0.551834	-0.462933
H	-2.440332	0.716420	-1.452388
O	-1.120010	-1.555118	-0.698461
N	-2.245599	-0.867045	-0.118405
C	-2.614506	1.539538	0.510711
H	-3.682348	1.336836	0.634873
H	-2.131445	1.510624	1.492047
H	-2.510752	2.553555	0.114226
C	-2.149402	-1.156971	1.310693
H	-1.213794	-0.792905	1.763012
H	-3.002330	-0.703965	1.820353
H	-2.209135	-2.239763	1.427365

PD2_M062X6-311++g**_sp.log
E = -351673.25623726257



CP3

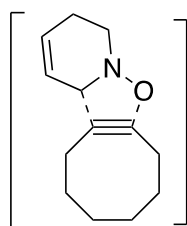
CP3_M062X6-31G*.log

Energy (E) = -636.343027743 Hartree
Enthalpy (H) = -636.025162 Hartree
Gibbs free energy (G) = -636.085493
Hartree

Charge = 0, Spin = 1

C	2.003136	1.959942	-0.180475
C	1.260110	1.905242	1.176855
C	0.876205	0.508975	1.390802
C	0.878939	-0.690957	1.243213
C	1.190406	-1.993657	0.652357
C	2.453395	-1.779936	-0.218623
H	2.528088	2.920238	-0.244133
H	1.255590	1.956248	-0.982362
H	0.397616	2.580595	1.164599
H	1.923507	2.239416	1.983730
H	0.340490	-2.337802	0.049828
H	1.371883	-2.764593	1.407878
H	2.567358	-2.652710	-0.871555
H	3.334221	-1.760024	0.434314
C	2.435088	-0.492139	-1.072521
H	1.406835	-0.310215	-1.412698
H	3.019758	-0.692622	-1.976878
C	2.999921	0.803792	-0.417263
H	3.793253	1.189731	-1.066551
H	3.487310	0.554043	0.533678
C	-2.169757	1.755778	-0.590375
C	-1.409777	0.980235	-1.374530
C	-1.432681	-0.467286	-1.259048
N	-1.977069	-1.057061	-0.227910
C	-2.551355	-0.233315	0.868800
C	-3.113177	1.094708	0.378635
O	-1.971837	-2.305162	-0.026938
H	-2.170762	2.835872	-0.694792
H	-0.767805	1.399781	-2.142840
H	-0.976333	-1.130354	-1.983316
H	-1.722591	-0.090456	1.569339
H	-3.306904	-0.870289	1.326535
H	-3.308618	1.730541	1.247063

H -4.081434 0.935027 -0.117934
 CP3_M062X6-311++g**_sp.log
 E = -399440.9523028708

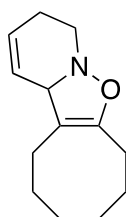


TS3

TS3_M062X6-31G*.log
 Energy (E) = -636.327597215 Hartree
 Enthalpy (H) = -636.010917 Hartree
 Gibbs free energy (G) = -636.067233
 Hartree
 Charge = 0, Spin = 1

Imaginary frequency: -355.3235
 C 2.329943 2.051719 -0.203617
 C 0.808237 1.857101 -0.107582
 C 0.439843 0.441553 -0.303084
 C 0.743237 -0.756757 -0.305314
 C 1.642009 -1.911395 -0.177630
 C 2.914651 -1.515112 0.588166
 H 2.555435 3.092954 0.057512
 H 2.637921 1.919071 -1.248042
 H 0.308716 2.507166 -0.838265
 H 0.453832 2.186230 0.879076
 H 1.903083 -2.265762 -1.183371
 H 1.134113 -2.744102 0.318628
 H 3.614876 -2.357285 0.537571
 H 2.666506 -1.381575 1.648471
 C 3.607219 -0.240778 0.069062
 H 3.501846 -0.195824 -1.023143
 H 4.680200 -0.351348 0.259636
 C 3.154701 1.107497 0.691396
 H 4.055426 1.651742 0.995371
 H 2.596712 0.915399 1.617734
 C -3.421225 1.205957 0.493226
 C -2.513440 1.423206 -0.464810
 C -1.723714 0.330519 -1.031478
 N -1.859531 -0.896588 -0.548038
 C -2.421536 -1.051341 0.798144
 C -3.670756 -0.197080 0.977604
 O -1.009495 -1.787619 -0.900311
 H -4.017301 2.020930 0.892018

H -2.333072 2.417362 -0.861710
 H -1.289547 0.396639 -2.020037
 H -1.622257 -0.748200 1.490462
 H -2.617863 -2.115623 0.927729
 H -3.964504 -0.206042 2.031488
 H -4.506454 -0.635199 0.413128
 TS3_M062X6-311++g**_sp.log
 E = -399427.8256640271

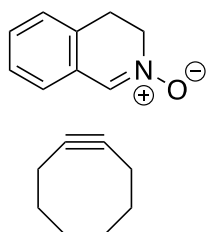


PD3

PD3_M062X6-31G*.log
 Energy (E) = -636.427598035 Hartree
 Enthalpy (H) = -636.107447 Hartree
 Gibbs free energy (G) = -636.159508
 Hartree
 Charge = 0, Spin = 1

C 2.203264 1.753428 -0.228657
 C 0.755392 1.851917 -0.715151
 C 0.044406 0.543888 -0.855875
 C 0.503744 -0.707345 -0.891437
 C 1.854189 -1.354405 -0.836662
 C 2.397844 -1.484737 0.598369
 H 2.604876 2.770820 -0.172855
 H 2.812933 1.240033 -0.980141
 H 0.721627 2.405597 -1.664962
 H 0.193149 2.464598 0.004922
 H 2.569126 -0.822690 -1.470656
 H 1.730752 -2.352152 -1.269348
 H 3.085332 -2.337405 0.635842
 H 1.560304 -1.731663 1.263824
 C 3.138425 -0.255134 1.129808
 H 4.055168 -0.107906 0.541544
 H 3.466554 -0.481973 2.151207
 C 2.349565 1.061011 1.146041
 H 2.856190 1.745623 1.834417
 H 1.354375 0.879239 1.573904
 C -3.109906 1.016548 0.789118
 C -2.300057 1.395069 -0.196835
 C -1.470225 0.432245 -1.001549
 N -1.746134 -0.978563 -0.657607

C -1.933560 -1.162554 0.786471
 C -3.188400 -0.419942 1.225669
 O -0.510998 -1.648920 -0.961142
 H -3.731441 1.749822 1.297046
 H -2.247281 2.436898 -0.504627
 H -1.741185 0.568221 -2.061666
 H -1.062339 -0.785120 1.346449
 H -2.021597 -2.237217 0.959676
 H -3.285457 -0.484948 2.314678
 H -4.078259 -0.898404 0.797267
 PD3_M062X6-311++g**_sp.log
 E = -399484.09674037056

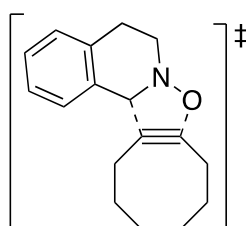


CP4

CP4_M062X6-31G*.log
 Energy (E) = -789.945105447 Hartree
 Enthalpy (H) = -789.577017 Hartree
 Gibbs free energy (G) = -789.641298
 Hartree
 Charge = 0, Spin = 1

C 3.815952 0.141024 -0.286474
 C 2.779300 1.022012 -1.022129
 C 1.638269 0.152814 -1.310158
 C 0.890628 -0.791792 -1.210869
 C 0.383559 -2.064934 -0.699935
 C 1.135031 -2.309753 0.628348
 H 4.604761 0.796520 0.100793
 H 4.291273 -0.524285 -1.017550
 H 3.220011 1.456617 -1.925000
 H 2.450773 1.861489 -0.395671
 H 0.603907 -2.871866 -1.409687
 H -0.700023 -2.057804 -0.538880
 H 0.911384 -3.327820 0.968562
 H 0.722186 -1.631029 1.387643
 C 2.668476 -2.118758 0.545054
 H 3.011178 -2.433410 -0.449348
 H 3.114041 -2.828364 1.250692
 C 3.259460 -0.715186 0.873955
 H 4.092432 -0.871729 1.568355
 H 2.523460 -0.126010 1.437306

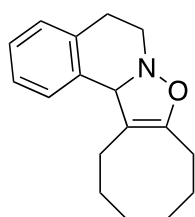
C -2.037522 0.155033 0.871394
 C -1.982536 0.647891 -0.443687
 C -1.218894 1.852336 -0.730938
 N -0.324402 2.314587 0.098770
 C -0.082847 1.602504 1.377856
 C -1.352880 0.978666 1.931379
 O 0.440654 3.295816 -0.132718
 C -2.743078 -1.011360 1.141251
 C -3.403013 -1.692473 0.118170
 C -3.354761 -1.200566 -1.185013
 C -2.646825 -0.036824 -1.466206
 H -1.280602 2.367290 -1.681738
 H 0.351866 2.351785 2.037748
 H 0.665646 0.838839 1.138603
 H -2.030327 1.774769 2.269110
 H -1.106526 0.369848 2.806838
 H -2.780628 -1.387801 2.160526
 H -3.951551 -2.602695 0.338423
 H -3.864329 -1.728061 -1.985121
 H -2.593275 0.341270 -2.483233
 CP4_M062X6-311++g**_sp.log
 E = -495852.49614759185



TS4

TS4_M062X6-31G*.log
 Energy (E) = -789.929816511 Hartree
 Enthalpy (H) = -789.562772 Hartree
 Gibbs free energy (G) = -789.624481
 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -350.8202
 C -4.253362 -0.508284 -0.208856
 C -3.067806 -1.484129 -0.159920
 C -1.802556 -0.752640 -0.299334
 C -1.073478 0.246177 -0.298555
 C -0.895493 1.695837 -0.095510
 C -2.035485 2.273614 0.757854
 H -5.165977 -1.074962 0.010962
 H -4.361295 -0.129896 -1.232851
 H -3.155759 -2.241811 -0.945847
 H -3.066696 -2.027540 0.794008

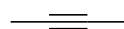
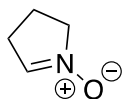
H -0.883775 2.198009 -1.074016
 H 0.072090 1.921503 0.370530
 H -1.896785 3.360249 0.815167
 H -1.937055 1.892862 1.782009
 C -3.452168 1.967555 0.235504
 H -3.432805 1.949507 -0.862681
 H -4.086455 2.818739 0.506270
 C -4.147898 0.683946 0.761509
 H -5.168443 0.958107 1.050314
 H -3.656494 0.352608 1.686418
 C 2.839522 -0.453544 0.450705
 C 2.043274 0.046020 -0.592921
 C 0.886281 -0.717183 -1.060692
 N 0.554866 -1.865152 -0.488158
 C 1.041147 -2.138142 0.868220
 C 2.527859 -1.832028 0.979655
 O -0.578971 -2.383490 -0.785140
 C 3.912111 0.302890 0.911531
 C 4.201670 1.544587 0.349696
 C 3.416046 2.036066 -0.690656
 C 2.342599 1.288417 -1.160784
 H 0.476117 -0.553604 -2.048656
 H 0.815822 -3.185864 1.067110
 H 0.437762 -1.508988 1.538334
 H 3.088261 -2.575959 0.397401
 H 2.848524 -1.931099 2.021090
 H 4.528792 -0.086440 1.717869
 H 5.039120 2.125792 0.722394
 H 3.638995 3.001147 -1.134291
 H 1.720189 1.666679 -1.967972
 TS4_M062X6-311++g**_sp.log
 E = -495838.3171870284



PD4

PD4_M062X6-31G*.log
 Energy (E) = -790.024350498 Hartree
 Enthalpy (H) = -789.653870 Hartree
 Gibbs free energy (G) = -789.712211
 Hartree
 Charge = 0, Spin = 1
 C -4.002391 -0.710665 -0.294863

C -2.851391 -1.220924 0.592049
 C -1.479693 -0.922924 0.059330
 C -0.690033 0.150393 -0.016456
 C -0.891948 1.556957 0.449890
 C -2.312150 1.903454 0.898495
 H -4.871440 -1.359038 -0.135431
 H -3.713851 -0.830173 -1.346536
 H -2.911656 -2.310835 0.665036
 H -2.959098 -0.834937 1.610423
 H -0.629676 2.236312 -0.374768
 H -0.174308 1.785815 1.249905
 H -2.294695 2.926191 1.289550
 H -2.601269 1.271465 1.745260
 C -3.356132 1.802510 -0.236685
 H -2.843564 1.617165 -1.190465
 H -3.856600 2.770593 -0.344764
 C -4.436201 0.733270 -0.038540
 H -5.276080 0.952591 -0.708491
 H -4.831930 0.813697 0.983819
 C 2.866885 -0.511828 0.165615
 C 1.877888 0.279526 -0.428476
 C 0.529951 -0.290271 -0.831408
 N 0.476162 -1.764066 -0.743948
 C 1.127707 -2.265426 0.473163
 C 2.616491 -1.983664 0.379223
 O -0.918687 -2.037719 -0.547737
 C 4.088832 0.066596 0.516672
 C 4.343010 1.410355 0.275006
 C 3.369528 2.192682 -0.342885
 C 2.152726 1.624116 -0.697279
 H 0.359241 -0.019336 -1.885798
 H 0.928166 -3.338119 0.515941
 H 0.704412 -1.792212 1.372844
 H 3.036385 -2.552416 -0.459675
 H 3.118899 -2.328096 1.289026
 H 4.849478 -0.555686 0.982305
 H 5.297555 1.843914 0.556680
 H 3.560976 3.239722 -0.555880
 H 1.406948 2.228665 -1.206568
 PD4_M062X6-311++g**_sp.log
 E = -495891.76389231766



CP5

CP5_M062X6-31G*.log

Energy (E) = -442.313221281 Hartree

Enthalpy (H) = -442.100446 Hartree

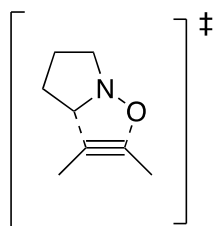
Gibbs free energy (G) = -442.152810 Hartree

Charge = 0, Spin = 1

C	0.680494	2.468899	0.279320
C	1.484323	1.259846	0.080665
C	2.151310	0.266504	-0.088871
C	2.967921	-0.931875	-0.296087
H	-0.311777	2.361772	-0.175554
H	0.550769	2.673031	1.346657
H	2.770849	-1.379066	-1.275849
H	2.760478	-1.689145	0.467609
C	-1.380899	-0.104155	1.057800
H	-1.740891	0.568777	1.824492
O	-2.173152	1.213973	-0.667793
N	-1.593176	0.199872	-0.186094
C	-0.987061	-0.787699	-1.116463
H	-1.746041	-1.028441	-1.861780
H	-0.153174	-0.272389	-1.599131
C	-0.575548	-1.350704	1.222889
H	0.437323	-1.101560	1.562833
H	-1.011772	-2.038978	1.953055
C	-0.565880	-1.944858	-0.209198
H	0.413875	-2.341871	-0.481461
H	-1.289592	-2.760498	-0.278515
H	4.034497	-0.693304	-0.247393
H	1.174936	3.335037	-0.170295

CP5_M062X6-311++g**_sp.log

E = -277652.7589307745



TS5

TS5_M062X6-31G*.log

Energy (E) = -442.279540037 Hartree

Enthalpy (H) = -442.068046 Hartree

Gibbs free energy (G) = -442.115120 Hartree

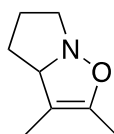
Charge = 0, Spin = 1

Imaginary frequency: -459.1513

C	-2.950194	-0.868215	-0.301883
C	-1.791446	0.015092	-0.106313
C	-1.087258	1.035152	-0.062856
C	-0.840759	2.480663	-0.250696
H	-2.742415	-1.610928	-1.077078
H	-3.163313	-1.415372	0.620636
H	-0.189368	2.660730	-1.113656
H	-0.345687	2.924220	0.621791
C	0.750002	0.291644	0.904161
H	0.322988	0.586199	1.854048
O	-0.586710	-1.511227	0.635283
N	0.547595	-0.947191	0.473573
C	1.315072	-1.204728	-0.754125
H	1.537469	-2.270115	-0.824501
H	0.670855	-0.910914	-1.593585
C	2.008137	0.862138	0.307963
H	1.775174	1.751725	-0.287800
H	2.736893	1.165675	1.065409
C	2.531619	-0.296684	-0.579898
H	2.932304	0.051709	-1.533109
H	3.325008	-0.835506	-0.055416
H	-1.772416	3.028283	-0.422852
H	-3.838014	-0.295917	-0.589285

TS5_M062X6-311++g**_sp.log

E = -277627.4860728287



PD5

PD5_M062X6-31G*.log

Energy (E) = -442.384541843 Hartree

Enthalpy (H) = -442.170011 Hartree

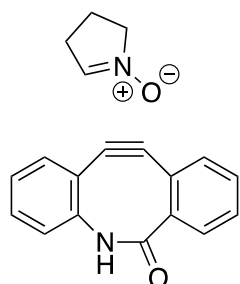
Gibbs free energy (G) = -442.215024 Hartree

Charge = 0, Spin = 1

C	2.724340	-0.919795	0.434738
C	1.388985	-0.448493	-0.024881
C	0.853834	0.766827	-0.143812

C	1.454983	2.100876	0.147005
H	2.619615	-1.575065	1.304927
H	3.210637	-1.497028	-0.357603
H	0.856140	2.661752	0.875014
H	1.509378	2.713877	-0.761288
C	-0.533643	0.597353	-0.714222
H	-0.585401	0.955831	-1.751558
O	0.558730	-1.464231	-0.434813
N	-0.730014	-0.884528	-0.689842
C	-1.579556	-1.164697	0.477967
H	-2.014131	-2.162882	0.391753
H	-0.989687	-1.107700	1.405511
C	-1.690377	1.184141	0.129794
H	-1.296802	1.583709	1.070754
H	-2.213467	1.993431	-0.384421
C	-2.590865	-0.028018	0.416256
H	-3.167493	0.073361	1.338215
H	-3.287409	-0.195435	-0.411000
H	2.467008	2.010192	0.550122
H	3.365652	-0.077665	0.699903

PD5_M062X6-311++g**_sp.log
E = -277686.5573510512



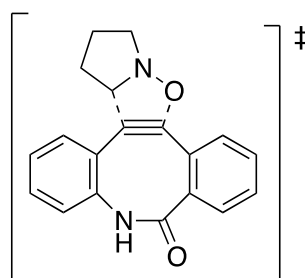
CP6

CP6_M062X6-31G*.log
Energy (E) = -993.045204938 Hartree
Enthalpy (H) = -992.711334 Hartree
Gibbs free energy (G) = -992.784913 Hartree
Charge = 0, Spin = 1

C	0.633916	2.411467	0.085808
C	1.367733	1.323495	-0.433716
C	0.621975	0.119688	-0.505774
C	-0.430724	-0.473549	-0.437280
C	-1.834242	-0.643650	-0.327395
C	-2.543433	0.511039	0.069995
C	-1.988851	1.844528	0.569895
N	-0.669253	2.357093	0.643390
C	1.274359	3.655303	0.154884

C	2.588234	3.814859	-0.269116
C	3.303399	2.736430	-0.784535
C	2.684301	1.496987	-0.866709
C	-2.496445	-1.833520	-0.634906
C	-3.883994	-1.880725	-0.585560
C	-4.603595	-0.744388	-0.227860
C	-3.938857	0.431663	0.105575
O	-2.805701	2.593328	1.083370
H	-0.830994	3.226754	1.141978
H	0.730087	4.511917	0.544113
H	3.050463	4.794406	-0.200569
H	4.325958	2.862886	-1.122943
H	3.206155	0.638103	-1.278254
H	-1.893691	-2.692741	-0.907965
H	-4.401964	-2.802558	-0.831398
H	-5.688092	-0.770763	-0.196369
H	-4.495652	1.307983	0.411706
C	2.454503	-2.353667	-0.646247
H	2.592927	-2.148273	-1.699070
O	0.327331	-3.199011	-0.943954
N	1.338920	-2.891038	-0.256921
C	1.269790	-3.014452	1.220184
H	0.593341	-2.219110	1.549777
H	0.825849	-3.983684	1.448006
C	3.363277	-2.035637	0.500226
H	4.399638	-2.334545	0.318749
H	3.364567	-0.955701	0.701274
C	2.718057	-2.824667	1.664900
H	3.206729	-3.796965	1.767090
H	2.797544	-2.301860	2.619047

CP6_M062X6-311++g**_sp.log
E = -623335.3496867309



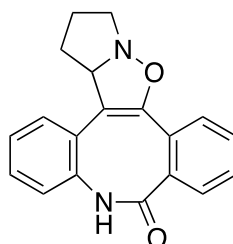
TS6

TS6_M062X6-31G*.log
Energy (E) = -993.041138596 Hartree
Enthalpy (H) = -992.708360 Hartree
Gibbs free energy (G) = -992.774752 Hartree
Charge = 0, Spin = 1

Imaginary frequency: -216.1101

C	-0.438436	-2.229215	0.209226
C	-1.201170	-1.257974	-0.475879
C	-0.702432	0.080995	-0.456936
C	0.339731	0.732859	-0.379301
C	1.765932	0.800209	-0.383045
C	2.473954	-0.283908	0.175391
C	1.921082	-1.370217	1.077894
N	0.633770	-1.918205	1.092606
C	-0.846024	-3.563815	0.158867
C	-1.982329	-3.943284	-0.549492
C	-2.734805	-2.987485	-1.225202
C	-2.341185	-1.655403	-1.182010
C	2.454596	1.843702	-1.010101
C	3.836530	1.798497	-1.128253
C	4.543984	0.717742	-0.605453
C	3.867285	-0.297722	0.058973
O	2.671597	-1.793366	1.943391
H	0.666205	-2.591119	1.852312
H	-0.257570	-4.313341	0.681467
H	-2.273337	-4.988509	-0.572810
H	-3.620258	-3.276720	-1.781608
H	-2.910563	-0.895401	-1.709922
H	1.876517	2.672929	-1.401401
H	4.362711	2.606341	-1.627510
H	5.624554	0.674476	-0.696293
H	4.411731	-1.114485	0.518166
C	-2.341659	1.897872	-0.681718
H	-2.205918	1.744479	-1.742524
O	-0.280059	2.839000	-0.400556
N	-1.472504	2.623736	-0.025888
C	-1.821944	2.740714	1.403270
H	-1.237833	1.968841	1.918034
H	-1.514825	3.724546	1.758456
C	-3.559783	1.610904	0.143860
H	-4.491675	1.862488	-0.370444
H	-3.596467	0.542162	0.387863
C	-3.327308	2.477822	1.407076
H	-3.869969	3.421943	1.312949
H	-3.660571	1.983808	2.320546

TS6_M062X6-311++g**_sp.log
E = -623332.2627303521

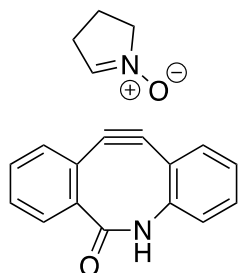


PD6

PD6_M062X6-31G*.log
Energy (E) = -993.154264023 Hartree
Enthalpy (H) = -992.818328 Hartree
Gibbs free energy (G) = -992.881666 Hartree
Charge = 0, Spin = 1

C	-0.035814	1.940152	0.483608
C	0.763789	1.331780	-0.495203
C	1.018952	-0.107306	-0.492372
C	0.115996	-1.092451	-0.433828
C	-1.354855	-1.054775	-0.463235
C	-2.135430	-0.315331	0.435474
C	-1.619399	0.369248	1.671716
N	-0.527721	1.204978	1.600575
C	-0.253980	3.320099	0.452032
C	0.328771	4.108311	-0.531006
C	1.138206	3.516311	-1.499397
C	1.348958	2.145043	-1.476477
C	-1.987429	-1.823103	-1.450027
C	-3.368912	-1.821475	-1.573971
C	-4.144767	-1.072547	-0.690274
C	-3.528780	-0.349220	0.320318
O	-2.175706	0.186165	2.739022
H	-0.375918	1.647320	2.501487
H	-0.880185	3.767464	1.218854
H	0.154010	5.179270	-0.539911
H	1.601511	4.122929	-2.270849
H	1.975268	1.680847	-2.233160
H	-1.372814	-2.418465	-2.117221
H	-3.841437	-2.410324	-2.353774
H	-5.226720	-1.073375	-0.774438
H	-4.117465	0.187592	1.056726
C	2.376197	-0.743731	-0.688899
H	2.743837	-0.602669	-1.713632
O	0.663366	-2.343611	-0.553660
N	2.088542	-2.191181	-0.461758
C	2.473179	-2.460831	0.935189
H	1.720027	-2.054618	1.626673
H	2.562474	-3.537350	1.091921

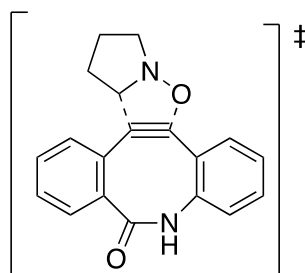
C 3.449965 -0.362106 0.356739
H 4.323417 0.107613 -0.100303
H 3.024421 0.348006 1.072870
C 3.783358 -1.693505 1.052694
H 4.573355 -2.223638 0.512365
H 4.101161 -1.564989 2.089289
PD6_M062X6-311++g**_sp.log
E = -623397.6253780263



CP7

CP7_M062X6-31G*.log
Energy (E) = -993.046008750 Hartree
Enthalpy (H) = -992.712352 Hartree
Gibbs free energy (G) = -992.781552 Hartree
Charge = 0, Spin = 1
C 2.120358 -1.205051 -0.072552
C 2.154195 -0.116013 -0.969607
C 0.886896 0.157222 -1.544420
C -0.302554 -0.029748 -1.663838
C -1.574772 -0.497430 -1.242842
C -1.554184 -1.251515 -0.049361
C -0.324813 -1.684033 0.732885
N 0.959297 -2.010637 0.159984
C 3.305454 -1.559739 0.577252
C 4.482087 -0.854910 0.344951
C 4.497155 0.237955 -0.519281
C 3.327531 0.611509 -1.166478
C -2.785677 -0.207784 -1.876137
C -3.982929 -0.652885 -1.328368
C -3.977124 -1.379770 -0.139528
C -2.772404 -1.670896 0.493517
O -0.492678 -2.021203 1.888554
H 1.265209 -2.748443 0.791376
H 3.304940 -2.393427 1.274881
H 5.389096 -1.155311 0.860014
H 5.411311 0.799537 -0.677727
H 3.292292 1.475707 -1.819827

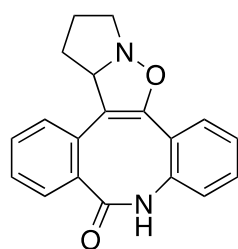
H -2.772096 0.379103 -2.788259
H -4.921147 -0.424710 -1.824411
H -4.909919 -1.721957 0.296388
H -2.757949 -2.232396 1.420530
C -1.244703 2.629123 -0.004871
H -1.485710 3.161401 -0.915155
O 1.035308 2.785542 -0.351285
N 0.006023 2.438899 0.288646
C 0.174899 1.648659 1.534744
H 0.655379 0.711870 1.237070
H 0.874674 2.199566 2.165128
C -2.184494 2.042618 0.997594
H -2.877475 2.793801 1.391785
H -2.796374 1.248263 0.552770
C -1.238870 1.494010 2.102359
H -1.347369 2.075343 3.020154
H -1.459450 0.451187 2.340606
CP7_M062X6-311++g**_sp.log
E = -623338.2981623203



TS7

TS7_M062X6-31G*.log
Energy (E) = -993.038878720 Hartree
Enthalpy (H) = -992.706454 Hartree
Gibbs free energy (G) = -992.773551 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -235.3998
C 2.121949 -0.815985 0.444034
C 2.096608 0.080204 -0.646694
C 0.810030 0.600457 -0.972319
C -0.394600 0.359190 -1.059676
C -1.367111 -0.681816 -0.912761
C -1.224595 -1.525526 0.207351
C -0.314034 -1.263852 1.390457
N 1.038939 -0.966716 1.359343
C 3.318375 -1.455834 0.766421
C 4.475991 -1.211383 0.033685

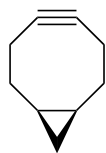
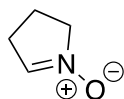
C 4.452275 -0.316018 -1.032671
 C 3.266170 0.324768 -1.368735
 C -2.401239 -0.915647 -1.826862
 C -3.257332 -1.997135 -1.660445
 C -3.111919 -2.839653 -0.560313
 C -2.119100 -2.583232 0.379120
 O -0.821167 -1.362874 2.500062
 H 1.353026 -0.967495 2.324668
 H 3.335297 -2.147774 1.603974
 H 5.396079 -1.720573 0.301652
 H 5.355308 -0.117139 -1.600320
 H 3.224358 1.029407 -2.192322
 H -2.508716 -0.247090 -2.675577
 H -4.043435 -2.178777 -2.386916
 H -3.783646 -3.680298 -0.421468
 H -2.031331 -3.195589 1.270186
 C -1.371619 2.535214 -0.740373
 H -1.355570 2.678957 -1.811780
 O 0.883345 2.796721 -0.539226
 N -0.286002 2.790227 -0.054419
 C -0.477006 2.613202 1.401463
 H 0.271344 1.880903 1.716594
 H -0.272064 3.568395 1.891189
 C -2.565876 2.370340 0.144007
 H -3.200758 3.264637 0.129789
 H -3.181767 1.525459 -0.179536
 C -1.925292 2.120493 1.533530
 H -2.463521 2.633777 2.331834
 H -1.932633 1.051129 1.761571
 TS7_M062X6-311++g**_sp.log
 E = -623331.7411201947



PD7

PD7_M062X6-31G*.log
 Energy (E) = -993.155237937 Hartree
 Enthalpy (H) = -992.819579 Hartree
 Gibbs free energy (G) = -992.883259
 Hartree
 Charge = 0, Spin = 1

C 1.903721 0.792531 0.634520
 C 1.129908 1.399395 -0.362047
 C -0.311118 1.140384 -0.452792
 C -0.960654 -0.021318 -0.556432
 C -0.385673 -1.372262 -0.639083
 C 0.471091 -1.909169 0.334206
 C 0.792330 -1.249669 1.646902
 N 1.308535 0.026225 1.673504
 C 3.274314 1.055422 0.694855
 C 3.868473 1.918528 -0.217266
 C 3.096871 2.531798 -1.203118
 C 1.734727 2.273019 -1.270606
 C -0.741251 -2.180594 -1.729745
 C -0.238953 -3.465913 -1.871288
 C 0.618057 -3.987970 -0.903399
 C 0.949117 -3.216894 0.200797
 O 0.629757 -1.856549 2.690037
 H 1.582931 0.280888 2.616576
 H 3.864844 0.579649 1.472309
 H 4.934333 2.113863 -0.156563
 H 3.556314 3.210831 -1.913791
 H 1.114319 2.748518 -2.023537
 H -1.412288 -1.776753 -2.482436
 H -0.518380 -4.062713 -2.734044
 H 1.007311 -4.996292 -0.999906
 H 1.569920 -3.622279 0.993289
 C -2.434037 0.280886 -0.674749
 H -2.879935 -0.141058 -1.582070
 O -1.103541 2.239191 -0.537376
 N -2.471129 1.781849 -0.757039
 C -3.232045 2.234053 0.424204
 H -2.865534 3.216528 0.722728
 H -4.275618 2.332959 0.103793
 C -3.221208 -0.120448 0.596562
 H -4.271821 -0.314476 0.353331
 H -2.802208 -1.021990 1.052279
 C -3.098463 1.128494 1.472341
 H -3.857595 1.183398 2.255990
 H -2.109398 1.169628 1.942334
 PD7_M062X6-311++g**_sp.log
 E = -623398.4658391924



CP8

CP8_M062X6-31G*.log

Energy (E) = -636.339342363 Hartree

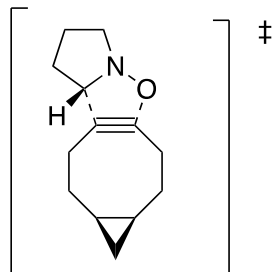
Enthalpy (H) = -636.021313 Hartree

Gibbs free energy (G) = -636.078605 Hartree

Charge = 0, Spin = 1

C	2.429051	1.571008	0.117883
C	1.155719	2.307279	-0.373688
C	0.394418	1.309014	-1.135930
C	0.179813	0.185969	-1.534594
C	0.423833	-1.255091	-1.666864
C	1.792456	-1.482771	-0.975784
C	1.806298	-1.042133	0.477382
C	2.119443	0.357959	0.975501
C	3.112735	-0.756222	1.164616
H	3.050744	2.268179	0.694263
H	3.011655	1.273466	-0.761192
H	1.424689	3.181155	-0.975893
H	0.578795	2.675555	0.485407
H	0.461299	-1.576612	-2.712620
H	-0.344096	-1.842904	-1.150137
H	2.565722	-0.950533	-1.542751
H	2.040338	-2.550618	-1.017931
H	1.049128	-1.554994	1.070177
H	1.570972	0.621320	1.880722
H	3.293316	-1.143544	2.161769
H	3.995167	-0.729660	0.528835
C	-2.759012	-0.644939	-0.474128
H	-3.040052	-1.438015	-1.154447
O	-1.468952	-2.043718	0.837586
N	-1.985354	-0.929743	0.526834
C	-1.652075	0.264588	1.341856
H	-1.861426	0.006116	2.381237
H	-0.577827	0.415589	1.214544
C	-3.079341	0.809384	-0.571516
H	-2.570519	1.247518	-1.437770
H	-4.152049	0.994464	-0.683506
C	-2.518766	1.382687	0.756894

H -1.938517 2.290907 0.582687
 H -3.335673 1.630172 1.438297
 CP8_M062X6-311++g**_sp.log
 E = -399437.9689465105



TS8

TS8_M062X6-31G*.log

Energy (E) = -636.321480167 Hartree

Enthalpy (H) = -636.004948 Hartree

Gibbs free energy (G) = -636.059944 Hartree

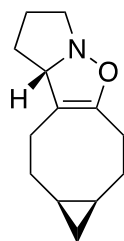
Charge = 0, Spin = 1

Imaginary frequency: -313.2196

C	-2.045045	-1.710890	-0.570835
C	-0.505102	-1.755163	-0.509422
C	0.027117	-0.378352	-0.470072
C	-0.222269	0.823786	-0.357925
C	-1.106922	1.983492	-0.201975
C	-2.564891	1.493048	-0.300935
C	-2.914016	0.461644	0.753546
C	-2.668684	-1.025404	0.628056
C	-4.070298	-0.480987	0.563518
H	-2.439239	-2.733791	-0.636587
H	-2.340131	-1.198015	-1.493626
H	-0.112416	-2.312556	-1.370286
H	-0.189035	-2.313156	0.383579
H	-0.893963	2.734586	-0.970164
H	-0.928764	2.468863	0.765635
H	-2.727904	1.076215	-1.301844
H	-3.247264	2.346874	-0.200537
H	-2.788591	0.837364	1.768375
H	-2.405240	-1.503765	1.570883
H	-4.752681	-0.663952	1.386964
H	-4.542936	-0.476016	-0.416106
C	2.317566	-0.315333	-0.916366
H	2.030759	-0.295083	-1.957863
O	1.686348	1.834570	-0.518965
N	2.404047	0.818982	-0.253859
C	2.872448	0.598703	1.124420

H	3.433293	1.473904	1.454032
H	1.968976	0.492240	1.738155
C	3.047578	-1.419529	-0.208008
H	2.338172	-2.191867	0.111899
H	3.796654	-1.908987	-0.837475
C	3.682609	-0.691348	1.004251
H	3.652949	-1.289206	1.916439
H	4.727710	-0.455094	0.787737

TS8_M062X6-311++g**_sp.log
E = -399425.40945747995



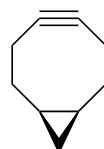
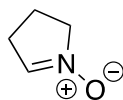
PD8

PD8_M062X6-31G*.log
Energy (E) = -636.420445961 Hartree
Enthalpy (H) = -636.100331 Hartree
Gibbs free energy (G) = -636.152745 Hartree
Charge = 0, Spin = 1

C	-2.001808	-1.538920	-0.678843
C	-0.477253	-1.613060	-0.691066
C	0.347071	-0.362468	-0.572887
C	0.142693	0.950423	-0.404408
C	-0.976965	1.926734	-0.176475
C	-2.423754	1.451366	-0.235935
C	-2.768722	0.452387	0.841767
C	-2.561236	-1.020050	0.623326
C	-3.954124	-0.457371	0.679405
H	-2.388437	-2.550735	-0.853381
H	-2.355085	-0.933588	-1.519751
H	-0.162617	-2.109968	-1.621662
H	-0.166636	-2.301082	0.110138
H	-0.825830	2.731668	-0.906001
H	-0.789419	2.387160	0.803458
H	-2.648169	1.045327	-1.227134
H	-3.065949	2.333061	-0.121388
H	-2.577451	0.810896	1.851621
H	-2.239959	-1.584891	1.496740
H	-4.572006	-0.672145	1.544499
H	-4.500313	-0.395219	-0.258833
C	1.843159	-0.556962	-0.755722

H	2.068719	-0.851822	-1.790820
O	1.316605	1.686809	-0.462040
N	2.418673	0.782615	-0.477880
C	2.978166	0.722352	0.880816
H	3.673722	1.550010	1.035342
H	2.174989	0.781786	1.631339
C	2.525816	-1.518415	0.248500
H	1.807046	-1.825304	1.015837
H	2.911113	-2.421684	-0.229995
C	3.622602	-0.657101	0.893088
H	3.893671	-0.988625	1.897775
H	4.525197	-0.651103	0.274296

PD8_M062X6-311++g**_sp.log
E = -399480.0713396493

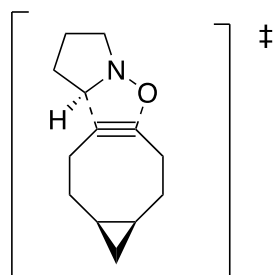


CP8'

CP8'_M062X6-31G*.log
Energy (E) = -636.336595548 Hartree
Enthalpy (H) = -636.018870 Hartree
Gibbs free energy (G) = -636.077617 Hartree
Charge = 0, Spin = 1

C	1.493651	1.638609	0.036547
C	0.482947	1.526185	1.205481
C	0.206718	0.090092	1.319157
C	0.347446	-1.087591	1.076032
C	1.002592	-2.216646	0.403542
C	1.947791	-1.581957	-0.648418
C	2.970119	-0.633496	-0.051142
C	2.763733	0.837196	0.255423
C	3.631336	0.419089	-0.899845
H	1.760240	2.693542	-0.104324
H	0.973476	1.325258	-0.875480
H	-0.409378	2.109574	0.958525
H	0.911888	1.918348	2.134994
H	0.289670	-2.891260	-0.084676
H	1.576371	-2.820610	1.116402
H	1.338009	-1.049529	-1.388450
H	2.475737	-2.378867	-1.188207

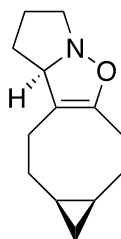
H 3.630519 -1.127869 0.660555
H 3.312386 1.159517 1.139959
H 4.706161 0.556035 -0.843577
H 3.212963 0.569682 -1.892495
C -2.837418 0.734371 0.545034
H -3.004284 1.601249 1.170536
O -1.653959 1.928647 -1.043250
N -2.175085 0.881866 -0.561062
C -1.992260 -0.403566 -1.281211
H -2.281116 -0.229944 -2.318690
H -0.922598 -0.620418 -1.234528
C -3.182903 -0.689612 0.830153
H -2.547984 -1.070544 1.639022
H -4.226486 -0.819573 1.131400
C -2.865529 -1.396712 -0.512238
H -2.358169 -2.350629 -0.357075
H -3.789468 -1.591973 -1.061544
CP8b_M062X6-311++g**_sp.log
E = -399437.61848468555



TS8'

TS8'_M062X6-31G*.log
Energy (E) = -636.321280016 Hartree
Enthalpy (H) = -636.004801 Hartree
Gibbs free energy (G) = -636.059828 Hartree
Charge = 0, Spin = 1
Imaginary frequency: -316.7216
C -2.466977 1.479194 0.594464
C -1.075733 1.962002 0.139352
C -0.212949 0.787947 -0.033413
C 0.024729 -0.421499 -0.074579
C -0.509521 -1.791483 0.060597
C -1.974987 -1.732635 0.536134
C -2.879006 -0.973984 -0.413963
C -3.110917 0.519761 -0.386366
C -4.198923 -0.421365 0.052428
H -3.128506 2.344449 0.730290
H -2.370209 1.001595 1.576759

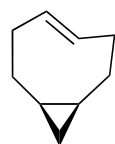
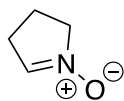
H -0.648300 2.659176 0.867753
H -1.146488 2.509425 -0.808778
H 0.082677 -2.387967 0.767031
H -0.451747 -2.317716 -0.903026
H -1.998865 -1.268541 1.529073
H -2.362941 -2.753181 0.654581
H -2.886662 -1.397404 -1.417756
H -3.249045 0.956118 -1.374758
H -5.079693 -0.547669 -0.568416
H -4.394641 -0.471172 1.121247
C 2.188112 -0.410058 -0.959105
H 1.703928 -0.489975 -1.921736
O 1.607729 1.768829 -0.651273
N 2.382283 0.783078 -0.437282
C 3.113589 0.696022 0.837360
H 3.709328 1.599880 0.968747
H 2.348783 0.645492 1.622773
C 3.064569 -1.440024 -0.307265
H 2.447403 -2.177454 0.219150
H 3.684100 -1.988505 -1.022975
C 3.911376 -0.597657 0.680811
H 4.075056 -1.105059 1.632727
H 4.887833 -0.380987 0.239738
TS8b_M062X6-311++g**_sp.log
E = -399425.19587566634



PD8'

PD8'_M062X6-31G*.log
Energy (E) = -636.420311138 Hartree
Enthalpy (H) = -636.100282 Hartree
Gibbs free energy (G) = -636.152742 Hartree
Charge = 0, Spin = 1
C -2.315501 1.371811 0.709237
C -0.942666 1.873847 0.277377
C 0.127712 0.890197 -0.103625
C 0.330846 -0.431362 -0.179975
C -0.457945 -1.694074 0.021875
C -1.910912 -1.639047 0.487914

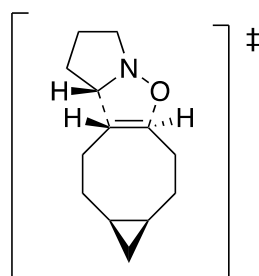
C -2.819489 -0.909013 -0.470921
 C -3.021206 0.576193 -0.361602
 C -4.137088 -0.362102 0.003727
 H -2.922670 2.249222 0.962957
 H -2.233705 0.789437 1.632193
 H -0.516310 2.504687 1.067405
 H -1.059950 2.538328 -0.589291
 H 0.100926 -2.333787 0.719700
 H -0.428918 -2.237053 -0.937172
 H -1.969315 -1.196446 1.487462
 H -2.265563 -2.671496 0.597360
 H -2.804877 -1.309015 -1.483154
 H -3.132757 1.107884 -1.304749
 H -4.999317 -0.429896 -0.650662
 H -4.365873 -0.471288 1.061228
 C 1.743338 -0.631966 -0.703329
 H 1.719376 -1.035963 -1.725871
 O 1.227078 1.626824 -0.517747
 N 2.321733 0.735103 -0.716818
 C 3.202394 0.827042 0.457409
 H 3.885854 1.671621 0.346562
 H 2.608839 0.961943 1.374648
 C 2.684242 -1.472082 0.195018
 H 2.187431 -1.695824 1.145324
 H 2.969252 -2.420724 -0.265656
 C 3.876673 -0.538184 0.451406
 H 4.399638 -0.756095 1.385126
 H 4.596807 -0.593405 -0.370774
 PD8b_M062X6-311++g**_sp.log
 E = -399480.02956317103



CP9

CP9_M062X6-31G*.log
 Energy (E) = -637.564865696 Hartree
 Enthalpy (H) = -637.223743 Hartree
 Gibbs free energy (G) = -637.284850 Hartree
 Charge = 0, Spin = 1
 C 2.066676 1.493959 -0.764076

C 0.620304 1.623595 -0.208334
 C 0.377093 0.313234 0.480492
 C 0.331304 -0.830889 -0.203569
 C 1.092048 -2.028278 0.280905
 C 2.554032 -1.754764 -0.171230
 C 3.227723 -0.583197 0.529827
 C 3.034397 0.899899 0.248904
 C 4.304045 0.213312 -0.163565
 H 2.447240 2.467290 -1.099495
 H 2.034266 0.843607 -1.647478
 H -0.084653 1.796211 -1.028976
 H 0.525696 2.465718 0.481150
 H 0.625748 0.268599 1.541936
 H 0.157976 -0.783231 -1.283065
 H 0.744571 -2.978005 -0.139787
 H 1.053959 -2.105836 1.374585
 H 2.551397 -1.585214 -1.256197
 H 3.170162 -2.647752 -0.003596
 H 3.421178 -0.788589 1.582341
 H 3.121822 1.507620 1.149426
 H 5.228648 0.435877 0.358953
 H 4.427867 0.022819 -1.227433
 C -2.760746 0.538631 -1.022139
 H -2.490034 1.267387 -1.774026
 O -2.220682 1.926498 0.747122
 N -2.639359 0.856445 0.232161
 C -2.995670 -0.277324 1.125075
 H -2.047572 -0.647035 1.524061
 H -3.599856 0.130979 1.935596
 C -3.212363 -0.874133 -1.215100
 H -3.999010 -0.969258 -1.969330
 H -2.375162 -1.508637 -1.533952
 C -3.705972 -1.263042 0.199687
 H -4.788130 -1.123825 0.264027
 H -3.482378 -2.301845 0.447894
 CP9_M062X6-311++g**_sp.log
 E = -400208.1597525145



TS9

TS9_M062X6-31G*.log
Energy (E) = -637.552915179 Hartree
Enthalpy (H) = -637.212791 Hartree
Gibbs free energy (G) = -637.266968
Hartree

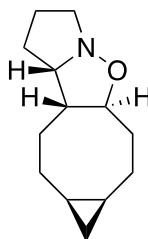
Charge = 0, Spin = 1

Imaginary frequency: -332.1715

C	2.588024	1.337104	-0.590626
C	1.186070	1.951726	-0.356210
C	0.302975	0.830827	0.105720
C	0.028759	-0.226639	-0.718227
C	0.299349	-1.622442	-0.222674
C	1.829134	-1.850319	-0.295961
C	2.641751	-1.027518	0.691678
C	3.022452	0.435176	0.551529
C	4.061883	-0.633941	0.374612
H	3.338947	2.123885	-0.738928
H	2.558657	0.750042	-1.516999
H	0.805753	2.389211	-1.286196
H	1.228785	2.753617	0.388363
H	0.335686	0.625499	1.175951
H	0.247868	-0.085560	-1.780777
H	-0.205777	-2.395597	-0.816855
H	-0.038217	-1.739589	0.817370
H	2.158032	-1.629608	-1.320200
H	2.062005	-2.909521	-0.122209
H	2.470011	-1.327793	1.725068
H	3.064732	0.955693	1.508288
H	4.833477	-0.758235	1.127376
H	4.396237	-0.823853	-0.642938
C	-2.298377	0.136835	-0.987755
H	-2.023457	0.578798	-1.934139
O	-1.558989	1.898462	0.257428
N	-2.339460	0.906058	0.083615
C	-2.857331	0.173289	1.249621
H	-1.985300	-0.237144	1.776905
H	-3.374090	0.872073	1.908436
C	-3.101449	-1.115910	-0.787275
H	-3.853285	-1.271320	-1.566504
H	-2.440135	-1.990155	-0.793341
C	-3.736567	-0.899903	0.609956
H	-4.757071	-0.524050	0.499124
H	-3.774756	-1.816202	1.201151

TS9_M062X6-311++g**_sp.log

E = -400196.8241043946



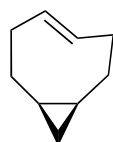
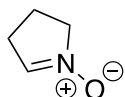
PD9

PD9_M062X6-31G*.log
Energy (E) = -637.638814213 Hartree
Enthalpy (H) = -637.294014 Hartree
Gibbs free energy (G) = -637.345611
Hartree

Charge = 0, Spin = 1

C	2.485894	1.220268	-0.596622
C	1.138325	1.917281	-0.395250
C	0.027233	0.997856	0.096097
C	-0.350428	-0.180321	-0.829880
C	0.132248	-1.549635	-0.338180
C	1.651568	-1.765370	-0.360652
C	2.436516	-1.052025	0.721788
C	2.878449	0.384208	0.599640
C	3.886994	-0.722364	0.489291
H	3.256719	1.975061	-0.792176
H	2.449217	0.588438	-1.491802
H	0.802210	2.379391	-1.330835
H	1.245277	2.727341	0.336365
H	0.278955	0.609656	1.094066
H	0.092469	-0.008461	-1.820382
H	-0.311157	-2.321921	-0.977385
H	-0.247844	-1.734925	0.677654
H	2.037722	-1.490535	-1.350283
H	1.847172	-2.840138	-0.257530
H	2.178281	-1.373537	1.729696
H	2.893039	0.939191	1.536945
H	4.596949	-0.865215	1.296757
H	4.284189	-0.934715	-0.500564
C	-1.905738	-0.011487	-0.966126
H	-2.116152	0.389965	-1.960652
O	-1.141932	1.824557	0.183696
N	-2.278777	1.015003	0.026036
C	-2.609879	0.283654	1.254969
H	-1.715275	-0.142497	1.736872
H	-3.100547	0.953760	1.964002
C	-2.833533	-1.199233	-0.634063
H	-3.574912	-1.346635	-1.422171
H	-2.280130	-2.134550	-0.540226

C -3.508186 -0.819996 0.708638
 H -4.509951 -0.421204 0.529350
 H -3.596110 -1.666965 1.392589
 PD9_M062X6-311++g**_sp.log
 E = -400246.3419909092

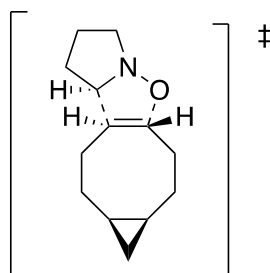


CP9'

CP9'_M062X6-31G*.log
 Energy (E) = -637.566012131 Hartree
 Enthalpy (H) = -637.224783 Hartree
 Gibbs free energy (G) = -637.284573 Hartree
 Charge = 0, Spin = 1

C -2.668407 -1.444886 -0.767376
 C -1.363907 -2.137229 -0.277845
 C -0.624997 -1.057035 0.463751
 C -0.187242 0.027099 -0.176620
 C -0.417087 1.398719 0.373361
 C -1.884592 1.712118 -0.033162
 C -2.936918 0.847206 0.648246
 C -3.318956 -0.585368 0.305639
 C -4.246621 0.545811 -0.034183
 H -3.393464 -2.184824 -1.130393
 H -2.405917 -0.808723 -1.621563
 H -0.805038 -2.512499 -1.142939
 H -1.596240 -2.992919 0.364734
 H -0.838106 -0.970685 1.530367
 H -0.035569 -0.012838 -1.258939
 H 0.263457 2.138622 -0.059903
 H -0.325374 1.413820 1.467320
 H -1.966868 1.608459 -1.123019
 H -2.115144 2.761736 0.189433
 H -3.018038 1.057388 1.714435
 H -3.612231 -1.160947 1.183741
 H -5.177145 0.657546 0.512710
 H -4.311086 0.820729 -1.084693
 C 2.773169 0.892306 0.743936
 H 2.506080 1.853887 1.160484
 O 2.296588 1.525961 -1.429414
 N 2.679705 0.717062 -0.539891

C 3.018178 -0.678263 -0.930641
 H 2.071875 -1.158452 -1.193288
 H 3.654135 -0.619151 -1.814244
 C 3.133804 -0.366007 1.465314
 H 3.870996 -0.211764 2.257984
 H 2.236984 -0.805397 1.923140
 C 3.670246 -1.258770 0.322109
 H 4.757138 -1.162282 0.257443
 H 3.428895 -2.313027 0.466552
 CP9b_M062X6-311++g**_sp.log
 E = -400208.9439649392



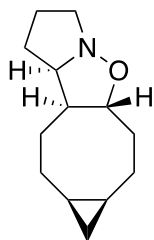
TS9'

TS9'_M062X6-31G*.log
 Energy (E) = -637.552300780 Hartree
 Enthalpy (H) = -637.212210 Hartree
 Gibbs free energy (G) = -637.266419 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -334.0303

C -1.732058 -1.643478 -0.756681
 C -0.273050 -1.586222 -0.235900
 C -0.088125 -0.248243 0.438633
 C -0.241084 0.894910 -0.296357
 C -1.190113 1.962365 0.146295
 C -2.607329 1.481980 -0.252388
 C -3.116974 0.274262 0.520467
 C -2.738207 -1.174202 0.278426
 C -4.103073 -0.676994 -0.106457
 H -1.991416 -2.659017 -1.084514
 H -1.802937 -0.998381 -1.641476
 H 0.416271 -1.722915 -1.080906
 H -0.091477 -2.414848 0.460935
 H -0.465236 -0.207848 1.461618
 H -0.117594 0.819402 -1.379875
 H -0.973427 2.928337 -0.320961
 H -1.130396 2.096736 1.233636
 H -2.608134 1.258133 -1.327847
 H -3.329542 2.297003 -0.113937

H	-3.300043	0.498192	1.570966
H	-2.712208	-1.767122	1.192871
H	-4.968580	-1.004593	0.460142
H	-4.290599	-0.542634	-1.169502
C	2.157805	0.004782	1.077131
H	1.762594	0.351807	2.020538
O	1.654849	1.921881	-0.050363
N	2.377450	0.887794	0.119623
C	3.052692	0.273054	-1.034487
H	2.265427	-0.029325	-1.737966
H	3.686337	1.020223	-1.513885
C	2.956390	-1.247516	0.853995
H	3.585038	-1.510773	1.709681
H	2.284743	-2.094153	0.670690
C	3.792582	-0.907379	-0.406471
H	4.798927	-0.598809	-0.111783
H	3.884582	-1.752943	-1.090110

TS9b_M062X6-311++g**_sp.log
E = -400196.6687391937



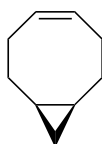
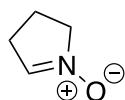
PD9'

PD9'_M062X6-31G*.log
Energy (E) = -637.639755531 Hartree
Enthalpy (H) = -637.294884 Hartree
Gibbs free energy (G) = -637.346397 Hartree
Charge = 0, Spin = 1

C	-1.528029	-1.519313	-0.812954
C	-0.094760	-1.513341	-0.264078
C	0.253319	-0.254621	0.536679
C	0.056232	1.054224	-0.260551
C	-1.123211	1.929720	0.144978
C	-2.496728	1.399177	-0.276798
C	-2.998810	0.212387	0.521985
C	-2.555234	-1.203574	0.250353
C	-3.947080	-0.768828	-0.111271
H	-1.738281	-2.503362	-1.249506
H	-1.617738	-0.800597	-1.635891
H	0.610450	-1.641511	-1.096669
H	0.030529	-2.390088	0.384525

H	-0.399311	-0.227687	1.416200
H	-0.015310	0.828989	-1.338045
H	-0.962253	2.913837	-0.309504
H	-1.086187	2.075263	1.232435
H	-2.479233	1.153695	-1.346436
H	-3.231124	2.206926	-0.173500
H	-3.184731	0.442814	1.569835
H	-2.479623	-1.836663	1.133966
H	-4.780601	-1.149520	0.469067
H	-4.163069	-0.628292	-1.167782
C	1.733280	-0.135284	1.025970
H	1.725416	0.154629	2.079812
O	1.230761	1.842968	-0.017179
N	2.308794	0.980173	0.252753
C	2.844520	0.379412	-0.976936
H	2.043228	0.092106	-1.674651
H	3.498648	1.093547	-1.481776
C	2.702602	-1.303372	0.769258
H	3.326529	-1.483342	1.647191
H	2.171134	-2.233447	0.560650
C	3.567667	-0.853447	-0.438761
H	4.570057	-0.578376	-0.101603
H	3.671208	-1.632715	-1.197406

PD9b_M062X6-311++g**_sp.log
E = -400247.0622399845

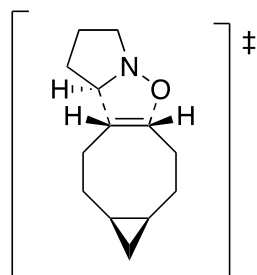


CP10

CP10_M062X6-31G*.log
Energy (E) = -637.580374347 Hartree
Enthalpy (H) = -637.238640 Hartree
Gibbs free energy (G) = -637.298393 Hartree
Charge = 0, Spin = 1

C	-2.350476	1.521162	0.250042
C	-0.803040	1.524956	0.127110
C	-0.122768	0.754291	1.229348
C	-0.097468	-0.576639	1.345810
C	-0.750778	-1.547197	0.391871
C	-2.298081	-1.593112	0.520576
C	-2.995034	-0.891821	-0.626551

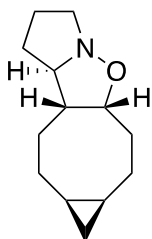
C -3.018723 0.607465 -0.756658
 C -4.282005 -0.139091 -0.425560
 H -2.739386 2.535221 0.101067
 H -2.639693 1.232278 1.266842
 H -0.414023 2.544350 0.126928
 H -0.523223 1.098358 -0.846022
 H 0.356627 1.348812 2.005950
 H 0.384172 -1.009019 2.223182
 H -0.335434 -2.546447 0.561434
 H -0.498577 -1.275386 -0.643224
 H -2.596457 -1.143637 1.473844
 H -2.643457 -2.633196 0.551058
 H -2.908911 -1.425812 -1.571636
 H -2.945647 0.970983 -1.780332
 H -5.063457 -0.218335 -1.173968
 H -4.645790 -0.055484 0.595481
 C 2.139286 -0.073908 -1.274181
 H 1.490745 0.205556 -2.093467
 O 2.144377 2.043843 -0.343193
 N 2.476322 0.830577 -0.404043
 C 3.318156 0.264689 0.682280
 H 4.128427 0.971985 0.860828
 H 2.673846 0.220852 1.564270
 C 2.678259 -1.426887 -0.933765
 H 1.883141 -2.072274 -0.537409
 H 3.111668 -1.940166 -1.797133
 C 3.737659 -1.103067 0.147679
 H 3.779700 -1.861657 0.931011
 H 4.726541 -1.036814 -0.312867
 CP10_M062X6-311++g**_sp.log
 E = -400218.36565924087



TS10

TS10_M062X6-31G*.log
 Energy (E) = -637.556768835 Hartree
 Enthalpy (H) = -637.215937 Hartree
 Gibbs free energy (G) = -637.269919
 Hartree
 Charge = 0, Spin = 1

Imaginary frequency: -447.4597
 C -2.473024 1.463199 0.362281
 C -1.054253 1.635913 -0.239531
 C 0.006597 0.936664 0.567155
 C 0.240077 -0.427132 0.539095
 C -0.627616 -1.415064 -0.214263
 C -2.023111 -1.633696 0.425607
 C -3.130276 -0.991974 -0.384971
 C -3.339686 0.498546 -0.421271
 C -4.344756 -0.387333 0.263989
 H -2.986932 2.431187 0.397155
 H -2.393120 1.128617 1.403633
 H -0.789089 2.694997 -0.302360
 H -1.042224 1.257930 -1.269016
 H 0.358799 1.487902 1.436638
 H 0.745832 -0.848407 1.410549
 H -0.093087 -2.371502 -0.282190
 H -0.775389 -1.076801 -1.248662
 H -2.023383 -1.233371 1.445596
 H -2.238893 -2.705095 0.517798
 H -3.311087 -1.493601 -1.334457
 H -3.643426 0.886040 -1.392295
 H -5.318007 -0.537642 -0.191410
 H -4.357712 -0.361013 1.350802
 C 2.002762 -0.498931 -0.772166
 H 1.358875 -0.622134 -1.634187
 O 1.608198 1.720855 -0.553514
 N 2.413014 0.729619 -0.470544
 C 3.414016 0.695160 0.603479
 H 4.070041 1.562173 0.517271
 H 2.864808 0.756802 1.554465
 C 2.992300 -1.524165 -0.287308
 H 2.512351 -2.200053 0.429891
 H 3.393941 -2.143065 -1.094816
 C 4.089551 -0.659133 0.387669
 H 4.455901 -1.094677 1.318635
 H 4.939643 -0.544780 -0.289716
 TS10_M062X6-311++g**_sp.log
 E = -400199.30343217263



PD10

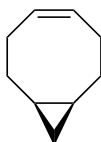
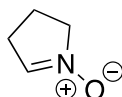
PD10_M062X6-31G*.log
 Energy (E) = -637.630932989 Hartree
 Enthalpy (H) = -637.286227 Hartree
 Gibbs free energy (G) = -637.338970 Hartree

Charge = 0, Spin = 1

C	-2.340421	1.425475	0.356931
C	-1.027617	1.629672	-0.428780
C	0.211584	1.043370	0.243768
C	0.507340	-0.477359	0.123494
C	-0.558204	-1.400676	-0.465485
C	-1.820092	-1.581684	0.407501
C	-3.060881	-1.026361	-0.255065
C	-3.305319	0.457327	-0.293735
C	-4.184539	-0.430295	0.545313
H	-2.851261	2.387336	0.476082
H	-2.114336	1.090819	1.377277
H	-0.817568	2.698700	-0.535669
H	-1.117233	1.234078	-1.447200
H	0.188223	1.325671	1.306788
H	0.747032	-0.854626	1.126993
H	-0.077663	-2.373879	-0.630312
H	-0.846147	-1.038581	-1.460479
H	-1.672709	-1.098888	1.381302
H	-1.980357	-2.643396	0.626571
H	-3.356081	-1.567233	-1.152375
H	-3.748883	0.831187	-1.214375
H	-5.206108	-0.610920	0.228538
H	-4.052494	-0.376799	1.623174
C	1.802193	-0.499454	-0.720675
H	1.543026	-0.600736	-1.780863
O	1.334191	1.705268	-0.383335
N	2.415306	0.813717	-0.503448
C	3.161750	0.684605	0.756423
H	3.837513	1.533618	0.877237
H	2.486705	0.652571	1.625977
C	2.865234	-1.506810	-0.258269
H	2.408911	-2.295488	0.347911
H	3.357302	-1.991577	-1.103969

C	3.874190	-0.654274	0.560041
H	4.151799	-1.118222	1.508688
H	4.788346	-0.503017	-0.019244

PD10_M062X6-311++g**_sp.log
 E = -400242.03307301225



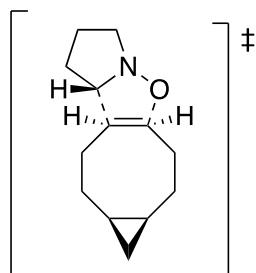
CP10'

CP10'_M062X6-31G*.log
 Energy (E) = -637.583248445 Hartree
 Enthalpy (H) = -637.240951 Hartree
 Gibbs free energy (G) = -637.299051 Hartree

Charge = 0, Spin = 1

C	1.718170	-0.901239	1.196692
C	1.039298	-2.081422	0.505749
C	0.187823	-1.890686	-0.728038
C	-0.023134	-0.933783	-1.643257
C	0.489469	0.455995	-1.939987
C	1.250614	1.270031	-0.895489
C	2.638379	0.741791	-0.626845
C	2.867152	-0.327091	0.404139
C	3.331229	1.078801	0.663714
H	2.107987	-1.261885	2.157365
H	0.980136	-0.129263	1.443031
H	0.404026	-2.593414	1.242737
H	1.805793	-2.828034	0.244501
H	-0.376801	-2.803932	-0.932885
H	-0.718539	-1.246451	-2.427039
H	-0.381391	1.040607	-2.268118
H	1.116884	0.369637	-2.841516
H	0.679965	1.343379	0.037162
H	1.339067	2.295891	-1.277590
H	3.273914	0.689217	-1.509620
H	3.647877	-1.048580	0.167436
H	4.394941	1.290935	0.647478
H	2.762701	1.656102	1.388637
C	-2.112677	1.356923	-0.140785
H	-1.749953	2.337214	-0.421409
O	-0.846630	1.296071	1.789731
N	-1.676061	0.825573	0.958095

C -2.274409 -0.506620 1.222556
 H -1.439826 -1.197988 1.351339
 H -2.811234 -0.420076 2.169750
 C -3.087745 0.492737 -0.868096
 H -4.064620 0.981200 -0.958853
 H -2.744712 0.274754 -1.886229
 C -3.154131 -0.793611 0.001497
 H -4.180425 -1.022554 0.292946
 H -2.760560 -1.645282 -0.554750
 CP10b_M062X6-311++g**_sp.log
 E = -400219.04175294755

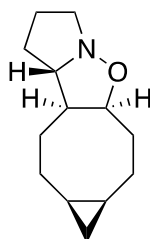


TS10'

TS10'_M062X6-31G*.log
 Energy (E) = -637.551342878 Hartree
 Enthalpy (H) = -637.210354 Hartree
 Gibbs free energy (G) = -637.264303
 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -494.3642

C 2.031900 1.388113 -0.474382
 C 1.149231 1.855353 0.687397
 C -0.055641 1.026009 1.062051
 C -0.299732 -0.342095 1.125509
 C 0.597755 -1.563479 0.959664
 C 1.629105 -1.640908 -0.175154
 C 2.953931 -0.993152 0.146514
 C 3.155429 0.484404 -0.025469
 C 3.820502 -0.476493 -0.969846
 H 2.473705 2.268449 -0.956599
 H 1.404051 0.913346 -1.235767
 H 0.758043 2.849416 0.449721
 H 1.776391 1.982093 1.583348
 H -0.744868 1.611297 1.669686
 H -1.113870 -0.582720 1.814111
 H -0.079030 -2.423375 0.853449
 H 1.128712 -1.738133 1.907117
 H 1.230537 -1.212145 -1.101125
 H 1.815267 -2.699553 -0.396332

H 3.475428 -1.449681 0.985836
 H 3.815519 0.948517 0.705646
 H 4.894921 -0.612346 -0.907450
 H 3.417031 -0.542508 -1.977343
 C -1.583237 -0.617504 -0.616236
 H -0.735884 -0.907097 -1.222747
 O -1.125264 1.598503 -0.650837
 N -1.987661 0.651195 -0.673845
 C -3.264614 0.820309 0.031437
 H -3.026741 1.043798 1.081973
 H -3.807429 1.664806 -0.394853
 C -2.737544 -1.526360 -0.288201
 H -2.913775 -2.286484 -1.054510
 H -2.542350 -2.055344 0.652548
 C -3.929884 -0.543271 -0.152420
 H -4.518821 -0.546543 -1.073185
 H -4.594302 -0.797736 0.674912
 TS10b_M062X6-311++g**_sp.log
 E = -400195.7578519528

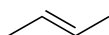
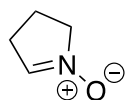


PD10'

PD10'_M062X6-31G*.log
 Energy (E) = -637.630883423 Hartree
 Enthalpy (H) = -637.286264 Hartree
 Gibbs free energy (G) = -637.338312
 Hartree
 Charge = 0, Spin = 1

C 2.137329 1.492042 0.122160
 C 1.060674 1.445095 1.229920
 C -0.299422 0.837892 0.841815
 C -0.548459 -0.676802 0.982332
 C 0.647200 -1.605346 0.768451
 C 1.420937 -1.410957 -0.556160
 C 2.851552 -1.021881 -0.263234
 C 3.179112 0.391021 0.137739
 C 3.675799 -0.163063 -1.174603
 H 2.672715 2.444037 0.212508
 H 1.638554 1.523821 -0.849471
 H 0.862064 2.473130 1.548506
 H 1.440212 0.920227 2.115642

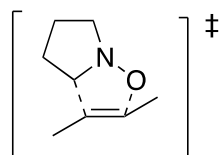
H -1.071823 1.338574 1.450288
 H -0.943164 -0.871800 1.987097
 H 0.278504 -2.635178 0.849235
 H 1.342629 -1.471343 1.606632
 H 0.939180 -0.642951 -1.171345
 H 1.406171 -2.333356 -1.147345
 H 3.405541 -1.787381 0.278522
 H 3.924454 0.491505 0.924470
 H 4.730566 -0.389739 -1.288701
 H 3.197244 0.217218 -2.073289
 C -1.673676 -0.883615 -0.054961
 H -1.463942 -1.766991 -0.668469
 O -0.553121 1.118660 -0.534317
 N -1.648035 0.317203 -0.945895
 C -2.910599 1.049923 -0.754388
 H -2.840692 1.738173 0.101299
 H -3.140591 1.632721 -1.649397
 C -3.103958 -0.938479 0.509798
 H -3.481000 -1.959946 0.601422
 H -3.125403 -0.483878 1.508528
 C -3.907959 -0.064842 -0.459772
 H -4.135824 -0.616624 -1.377649
 H -4.845362 0.304147 -0.037259
 PD10b_M062X6-311++g**_sp.log
 E = -400240.08586430154



CP11

CP11_M062X6-31G*.log
 Energy (E) = -443.549537657 Hartree
 Enthalpy (H) = -443.313256 Hartree
 Gibbs free energy (G) = -443.365003 Hartree
 Charge = 0, Spin = 1
 C 1.880732 2.079031 -0.465058
 C 1.939903 0.796105 0.312937
 C 1.931204 -0.424267 -0.223037
 C 1.970543 -1.705949 0.552155
 H 1.851339 1.885379 -1.542049
 H 0.993513 2.669137 -0.200252
 H 1.998148 0.888543 1.399269
 H 1.869896 -0.524612 -1.308342
 H 1.099688 -2.317911 0.290036

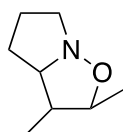
H 1.976872 -1.516896 1.630314
 C -1.227680 -0.707279 0.950203
 H -1.034712 -1.548320 1.602192
 O -0.824284 -1.909004 -0.985988
 N -1.131176 -0.873366 -0.334289
 C -1.359344 0.395273 -1.075086
 H -0.380299 0.706371 -1.449361
 H -2.009445 0.161217 -1.918536
 C -1.508551 0.712834 1.324007
 H -2.277343 0.806156 2.096378
 H -0.598619 1.194071 1.706765
 C -1.950591 1.332288 -0.023771
 H -3.041450 1.328493 -0.091334
 H -1.608876 2.361944 -0.143458
 H 2.751517 2.711987 -0.260406
 H 2.864981 -2.288189 0.302617
 CP11_M062X6-311++g**_sp.log
 E = -278428.2740988875



TS11

TS11_M062X6-31G*.log
 Energy (E) = -443.519808728 Hartree
 Enthalpy (H) = -443.284340 Hartree
 Gibbs free energy (G) = -443.331863 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -479.99
 C 0.204483 2.119783 -0.643033
 C 0.979963 1.130924 0.197393
 C 1.805966 0.187151 -0.391958
 C 2.977958 -0.409091 0.332145
 H -0.015984 1.703394 -1.632710
 H -0.746333 2.422549 -0.189243
 H 1.260349 1.481468 1.191115
 H 1.829702 0.132577 -1.478644
 H 3.188871 -1.418853 -0.026883
 H 2.771482 -0.470611 1.406146
 C -0.512046 -0.237786 1.048553
 H 0.109588 -0.429783 1.914554
 O 0.702269 -1.569323 -0.312827
 N -0.438258 -1.107644 0.043643
 C -1.477545 -0.878311 -0.968368

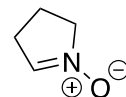
H -0.981847 -0.428360 -1.836396
H -1.896098 -1.840198 -1.272964
C -1.885444 0.359851 1.123866
H -2.474280 -0.101729 1.924601
H -1.844538 1.431780 1.337913
C -2.483734 0.060697 -0.279528
H -3.470596 -0.398072 -0.196823
H -2.596905 0.982164 -0.854557
H 0.780353 3.039734 -0.801768
H 3.878276 0.202721 0.198356
TS11_M062X6-311++g**_sp.log
E = -278405.29166248185



PD11

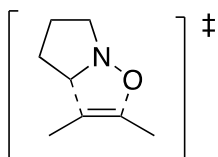
PD11_M062X6-31G*.log
Energy (E) = -443.599163409 Hartree
Enthalpy (H) = -443.360212 Hartree
Gibbs free energy (G) = -443.404500 Hartree
Charge = 0, Spin = 1
C 1.408226 2.060609 -0.163759
C 0.972113 0.751607 0.479202
C 1.240103 -0.507845 -0.341572
C 2.678196 -0.978659 -0.380813
H 0.988691 2.178856 -1.167725
H 1.092817 2.919927 0.436187
H 1.497585 0.623068 1.434064
H 0.859021 -0.361187 -1.369681
H 2.757586 -1.926599 -0.918724
H 3.047610 -1.125847 0.638102
C -0.533794 0.596797 0.744197
H -0.792890 0.966490 1.741865
O 0.469037 -1.493632 0.333034
N -0.765513 -0.883327 0.713993
C -1.782069 -1.155696 -0.318672
H -1.297495 -1.338677 -1.288610
H -2.361133 -2.042422 -0.049355
C -1.493998 1.189139 -0.298785
H -1.847286 2.187223 -0.027291
H -1.006507 1.259945 -1.278795
C -2.599940 0.131670 -0.371172
H -3.255292 0.200558 0.503765
H -3.216916 0.204899 -1.269843

H 2.498324 2.101310 -0.252380
H 3.309161 -0.240926 -0.885548
PD11_M062X6-311++g**_sp.log
E = -278451.4702746118



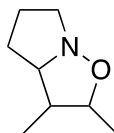
CP12

CP12_M062X6-31G*.log
Energy (E) = -443.546106196 Hartree
Enthalpy (H) = -443.309586 Hartree
Gibbs free energy (G) = -443.364184 Hartree
Charge = 0, Spin = 1
C 1.780649 -0.433028 1.023743
C 2.084705 0.777531 0.547417
H 1.549445 -0.505183 2.087420
H 2.082382 1.613378 1.247489
C -0.974394 0.400758 -1.127535
H -0.601436 0.308699 -2.138639
O -1.295986 -1.877373 -0.875888
N -1.319610 -0.677016 -0.489307
C -1.747881 -0.383794 0.903580
H -2.650743 -0.966723 1.087491
H -0.947529 -0.751207 1.551883
C -1.128272 1.637140 -0.302588
H -0.149184 2.032813 -0.006708
H -1.655720 2.432597 -0.837694
C -1.923996 1.133921 0.928301
H -1.563500 1.575515 1.858756
H -2.980575 1.390076 0.820061
C 1.742363 -1.730360 0.269709
H 2.371246 -2.475060 0.770128
H 0.725838 -2.138642 0.216703
H 2.098636 -1.627007 -0.757144
C 2.448184 1.126175 -0.867303
H 2.404014 0.263401 -1.534410
H 1.773401 1.892898 -1.268163
H 3.460726 1.542489 -0.916861
CP12_M062X6-311++g**_sp.log
E = -278426.6378584049



TS12

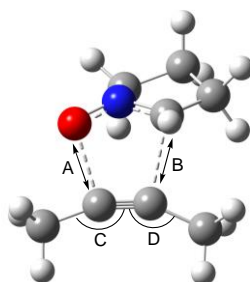
TS12_M062X6-31G*.log
 Energy (E) = -443.520485644 Hartree
 Enthalpy (H) = -443.285077 Hartree
 Gibbs free energy (G) = -443.331824 Hartree
 Charge = 0, Spin = 1
 Imaginary frequency: -478.1151
 C 1.596139 -0.493042 0.667956
 C 1.028064 0.768883 0.674382
 H 1.370794 -1.159333 1.495713
 H 0.392306 1.013894 1.526619
 C -0.605103 0.465885 -0.738703
 H 0.041488 0.746875 -1.561662
 O 0.257531 -1.615154 -0.523850
 N -0.752332 -0.830616 -0.478195
 C -1.791626 -1.041115 0.537724
 H -2.237764 -2.027303 0.403519
 H -1.293140 -1.006225 1.517544
 C -1.822836 1.237638 -0.306789
 H -1.545466 1.992343 0.438384
 H -2.308604 1.764152 -1.133368
 C -2.734916 0.138848 0.301456
 H -3.231873 0.463594 1.217004
 H -3.506283 -0.142632 -0.419839
 C 2.791386 -0.854459 -0.166646
 H 3.715171 -0.430913 0.247734
 H 2.903605 -1.939013 -0.225127
 H 2.678547 -0.483109 -1.189823
 C 1.661334 1.961330 -0.006343
 H 2.118660 1.685795 -0.962085
 H 0.924497 2.748134 -0.207966
 H 2.449500 2.405477 0.613296
 TS12_M062X6-311++g**_sp.log
 E = -278406.36350541026



PD12

PD12_M062X6-31G*.log
 Energy (E) = -443.596387368 Hartree
 Enthalpy (H) = -443.357193 Hartree
 Gibbs free energy (G) = -443.403194 Hartree
 Charge = 0, Spin = 1
 C 1.420685 -0.637260 0.469192
 C 0.686922 0.712773 0.483745
 H 1.671109 -0.952787 1.489426
 H 0.165888 0.812435 1.444601
 C -0.373071 0.495925 -0.607564
 H 0.063947 0.701077 -1.592836
 O 0.477993 -1.590121 -0.065674
 N -0.701094 -0.933896 -0.508838
 C -1.752338 -1.022959 0.513672
 H -2.219366 -2.009558 0.480948
 H -1.346066 -0.865341 1.524510
 C -1.708005 1.225787 -0.379919
 H -1.585793 2.006950 0.377600
 H -2.070698 1.709806 -1.288897
 C -2.679890 0.116889 0.099019
 H -3.331528 0.443213 0.912143
 H -3.311990 -0.208710 -0.731165
 C 2.667272 -0.689363 -0.401000
 H 3.465075 -0.059895 0.005618
 H 3.028662 -1.719302 -0.452944
 H 2.440748 -0.360000 -1.420250
 C 1.544360 1.952772 0.271285
 H 2.046095 1.927830 -0.700984
 H 0.921549 2.853052 0.302254
 H 2.310471 2.052082 1.046662
 PD12_M062X6-311++g**_sp.log
 E = -278449.8586526015

3. Calculated barriers and distortion energies for selected reactions of nitrones with dipolarophiles (Acetonitrile data)



Entry	Nitrone	Dipolarophile	k2 (M ⁻¹ s ⁻¹)	ΔG^\ddagger (kcal/mol)	Dis_Nitron	Dis_total	C-O distance A (Å)	CCC angle_C (°)	CCC angle_D (°)
				ΔE^\ddagger (kcal/mol)	Dis_Dipolarophile	Int	C-C distance B (Å)	Δ angle_C	Δ angle_D
1	1a	2a	1.95	23.0	9.5	12.8	2.13	156.48	149.23
				9.9	3.3	-2.9	2.26	-1.72	-8.79
2	1b	2a	N/A	21.3	7.7	10.5	2.16	157.03	149.68
				8.0	2.8	-2.5	2.31	-1.17	-8.34
3	1c	2a	N/A	22.0	8.5	11.6	2.12	155.80	150.33
				9.0	3.1	-2.7	2.29	-2.41	-7.70
4	1d	2a	1.5	22.1	8.7	11.9	2.10	155.57	149.92
				8.7	3.2	-3.2	2.31	-2.63	-8.11
5	1a	2b	N/A	35.3	12.8	24.9	2.08	161.15	153.43
				20.5	12.1	-4.4	2.21	-18.85	-26.55
6	1a	2c	41.7	12.6	3.8	5.4	2.20	150.46	142.38
				-1.6	1.6	-7.0	2.46	-5.35	-9.52
7	1a	2c	39.9	13.3	4.7	6.6	2.24	145.84	143.06
				-0.3	1.9	-6.9	2.41	-12.75	-8.84
8	1a	2d	0.05	20.7	7.3	9.5	2.17	154.49	147.00
				7.4	2.3	-2.1	2.33	-0.29	-7.70
9	1a	2d	0.05	20.8	7.3	9.7	2.16	154.42	146.83
				7.6	2.4	-2.2	2.34	-0.36	-7.88
10	1a	2e	0.08	22.0	7.8	10.3	2.15		
				8.3	2.6	-2.1	2.37		
11	1a	2e	0.08	22.2	8.0	10.6	2.17		
				8.5	2.6	-2.1	2.35		
12	1a	2f	N/A	29.0	13.3	19.3	2.11		
				14.4	6.0	-4.9	2.20		
13	1a	2f	N/A	32.6	14.9	23.9	2.10		
				18.0	8.9	-5.9	2.18		
14	1a	2g	N/A	32.0	15.0	24.6	2.08		
				18.1	9.7	-6.5	2.20		
15	1a	2h	N/A	30.7	13.8	21.6	2.11		
				16.2	7.8	-5.4	2.18		

Geometry optimizations were carried out at the M06-2X level of theory with the 6-31G(d) basis set. Solvent effects in acetonitrile were evaluated at the M06-2X/6-311++G(d,p) level at 298.15K with a self-consistent reaction field (SCRF) using the SMD model on the gas-phase-optimized structures. Dis_Nitron is the distortion energy for the nitrones shown, Dis_Dipolarophile is the distortion energy for the different dipolarophiles shown, Dis_total refers to the total distortion energy, and Int represents the interaction energy for the given reaction. The C-O and C-C bond distances are for the bond lengths at the transition states for the bonds forming in the reactions. The bond angles represent those in the illustration above the table.