

Supporting Information

Understanding the reactivity and selectivity of Diels-Alder reactions involving furans

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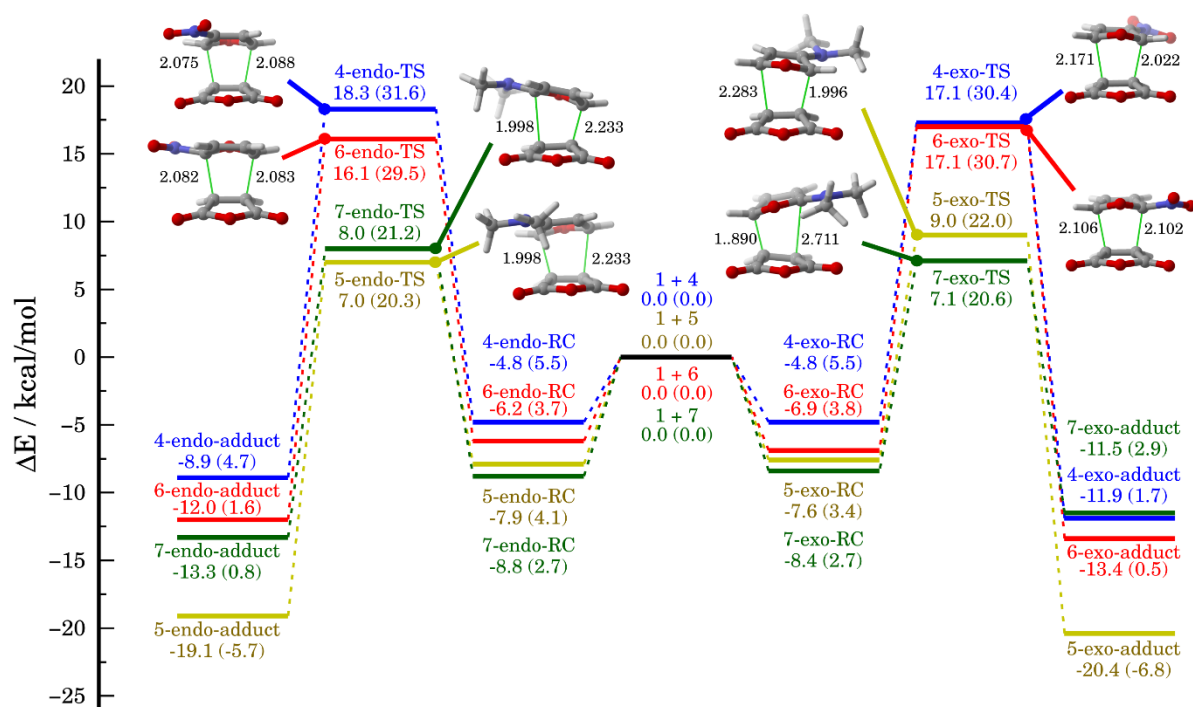


Figure S1. Relative energies of the stationary points, including the zero-point energies (in kcal/mol), on the potential energy surface for the **1 + 4** (blue), **1 + 5** (yellow), **1 + 6** (red), and **1 + 7** (green) reactions, calculated at DLPNO-CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPP. Values within parentheses refer to relative free energy computed at the same level of theory. Bond distances in the corresponding transition states are given in angstroms.

Table S1. Computed activation energies (without zero-point energy correction) calculated at DLPNO-CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPPa level of theory for the reactions between maleic anhydride (**1**), cyclopentadiene (**2**), furan (**3**), 3-nitrofurane (**4**), N,N-dimethylfuran-3-amine (**5**), 2-nitrofurane (**6**), and N,N-dimethylfuran-2-amine (**7**). All values are in kcal mol⁻¹.

Reactions	endo pathway			exo pathway		
	ΔE [‡]	ΔE [‡] _{strain}	ΔE [‡] _{int}	ΔE [‡]	ΔE [‡] _{strain}	ΔE [‡] _{int}
1 + 2	7.2	25.8	-18.6	9.1	26.2	-17.1
1 + 3	13.6	37.0	-23.4	14.1	35.2	-21.1
1 + 4	19.4	37.2	-17.8	17.4	34.9	-17.5
1 + 5	5.4	36.0	-30.6	7.8	31.6	-23.7
1 + 6	17.4	35.8	-18.4	18.6	34.1	-15.5
1 + 7	6.7	36.8	-30.2	4.5	34.0	-29.5

Cartesian coordinates at M06-2X/def2-TZVPP level of theory. The electronic energies, with zero-point energy correction, estimated at DLPNO-CCSD(T)/def2-TZVPP//M06-2X/def2-TZVPP.

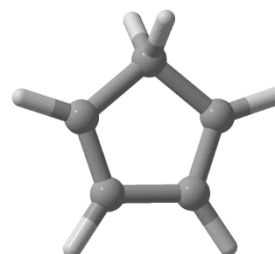
E = -378.670357404 ; 1-Maleic Anhydride

C	-0.000072000	0.162568000	1.121817000
C	0.000210000	-1.256513000	0.661869000
C	0.000210000	-1.256513000	-0.661869000
C	-0.000072000	0.162568000	-1.121817000
O	-0.000158000	0.963778000	0.000000000
O	-0.000072000	0.598630000	-2.221989000
O	-0.000072000	0.598630000	2.221989000
H	0.000378000	-2.080478000	-1.356341000
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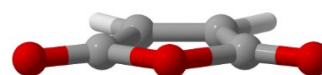
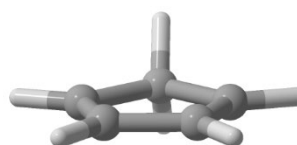
E = -193.643459927 ; 2-Cyclopentadiene

C	-0.000009000	0.279771000	1.173529000
C	-0.000009000	-0.985482000	0.733681000
C	-0.000009000	-0.985482000	-0.733681000
C	-0.000009000	0.279771000	-1.173529000
C	0.000023000	1.211946000	0.000000000
H	-0.000012000	-1.873977000	1.347924000
H	-0.000012000	-1.873977000	-1.347924000
H	-0.000011000	0.604776000	-2.202713000
H	-0.000011000	0.604776000	2.202713000
H	-0.876499000	1.867675000	0.000000000
H	0.876615000	1.867585000	0.000000000



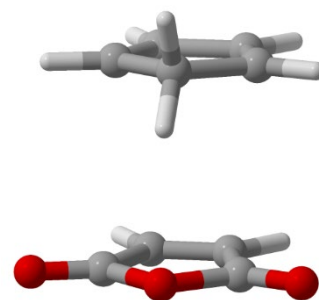
E = -572.322683010 ; 2-endo-RC

C	-0.032117000	-1.406918000	1.123199000
C	-1.334019000	-0.850836000	0.662677000
C	-1.334019000	-0.850836000	-0.662677000
C	-0.032117000	-1.406918000	-1.123199000
O	0.711159000	-1.708513000	0.000000000
O	0.364365000	-1.603855000	-2.222121000
O	0.364365000	-1.603855000	2.222121000
C	-0.003157000	1.993798000	1.172609000
C	1.127264000	1.419039000	0.731518000
C	1.127264000	1.419039000	-0.731518000
C	-0.003157000	1.993798000	-1.172609000
C	-0.818588000	2.446232000	0.000000000
H	1.913007000	1.004267000	1.345868000
H	1.913007000	1.004267000	-1.345868000
H	-0.288157000	2.141706000	-2.203300000
H	-2.091939000	-0.532186000	-1.359242000
H	-2.091939000	-0.532186000	1.359242000
H	-0.288157000	2.141706000	2.203300000
H	-1.830068000	2.028768000	0.000000000
H	-0.938988000	3.535057000	0.000000000



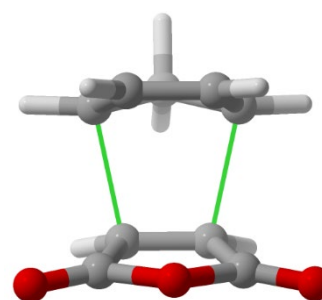
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C	0.591814000	2.483962000	0.731439000
C	0.591814000	2.483962000	-0.731439000
C	-0.504484000	1.846856000	-1.173333000
C	1.264245000	-0.782938000	-0.662766000
C	1.264245000	-0.782938000	0.662766000
C	-0.504484000	1.846856000	1.173333000
C	-1.327853000	1.414267000	0.000000000
C	0.059467000	-1.524722000	1.122974000
C	0.059467000	-1.524722000	-1.122974000
O	-0.618714000	-1.958821000	0.000000000
O	-0.325739000	-1.744515000	2.221599000
O	-0.325739000	-1.744515000	-2.221599000
H	1.358508000	2.931977000	1.346740000
H	1.358508000	2.931977000	-1.346740000
H	-0.788713000	1.684634000	-2.202020000
H	1.960878000	-0.344525000	-1.356925000
H	1.960878000	-0.344525000	1.356925000
H	-0.788713000	1.684634000	2.202020000
H	-1.568786000	0.347442000	0.000000000
H	-2.296409000	1.927689000	0.000000000



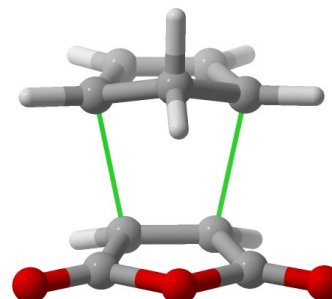
E = -572.29927930 ; 2-endo-TS

C	-0.128524000	-1.247275000	1.131291000
C	-1.122064000	-0.245592000	0.692657000
C	-1.122064000	-0.245592000	-0.692657000
C	-0.128524000	-1.247275000	-1.131291000
O	0.509974000	-1.725391000	0.000000000
O	0.156777000	-1.628418000	-2.219759000
O	0.156777000	-1.628418000	2.219759000
C	-0.004025000	1.583201000	1.149423000
C	1.259444000	1.207519000	0.697467000
C	1.259444000	1.207519000	-0.697467000
C	-0.004025000	1.583201000	-1.149423000
C	-0.700747000	2.254648000	0.000000000
H	2.059973000	0.842601000	1.323330000
H	2.059973000	0.842601000	-1.323330000
H	-0.253633000	1.750027000	-2.186936000
H	-1.931973000	0.028652000	-1.347542000
H	-1.931973000	0.028652000	1.347542000
H	-0.253633000	1.750027000	2.186936000
H	-1.785547000	2.202404000	0.000000000
H	-0.404910000	3.310729000	0.000000000



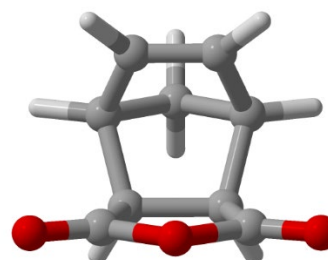
E = -572.295647970 ; 2-exo-TS

C	0.360006000	2.445978000	0.697567000
C	0.360006000	2.445978000	-0.697567000
C	-0.451504000	1.407760000	-1.150683000
C	0.982263000	-0.220102000	-0.692502000
C	0.982263000	-0.220102000	0.692502000
C	-0.451504000	1.407760000	1.150683000
C	-1.323779000	1.005923000	0.000000000
C	0.146180000	-1.360690000	1.129555000
C	0.146180000	-1.360690000	-1.129555000
O	-0.381591000	-1.964650000	0.000000000
O	-0.101272000	-1.758262000	2.221313000
O	-0.101272000	-1.758262000	-2.221313000
H	0.984623000	3.065522000	1.323716000
H	0.984623000	3.065522000	-1.323716000
H	-0.699688000	1.217252000	-2.184823000
H	1.749469000	0.148565000	-1.349536000
H	1.749469000	0.148565000	1.349536000
H	-0.699688000	1.217252000	2.184823000
H	-1.709829000	-0.008249000	0.000000000
H	-2.186575000	1.684079000	0.000000000



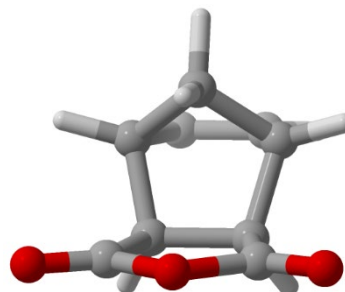
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C	-0.135670000	-1.214824000	1.141904000
C	-0.884635000	0.040976000	0.766298000
C	-0.884635000	0.040976000	-0.766298000
C	-0.135670000	-1.214824000	-1.141904000
O	0.254348000	-1.880758000	0.000000000
O	0.130667000	-1.627047000	-2.220485000
O	0.130667000	-1.627047000	2.220485000
C	-0.128140000	1.365660000	1.126279000
C	1.304976000	1.183741000	0.665752000
C	1.304976000	1.183741000	-0.665752000
C	-0.128140000	1.365660000	-1.126279000
C	-0.669538000	2.266708000	0.000000000
H	2.138403000	0.977270000	1.320811000
H	2.138403000	0.977270000	-1.320811000
H	-0.274023000	1.684642000	-2.152613000
H	-1.873157000	0.020824000	-1.220289000
H	-1.873157000	0.020824000	1.220289000
H	-0.274023000	1.684642000	2.152613000
H	-1.757024000	2.352758000	0.000000000
H	-0.212039000	3.253693000	0.000000000



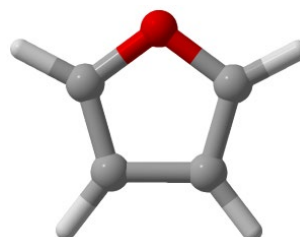
E = -572.358781828 ; 2-exo-adduct

C	-0.356305000	2.453520000	-0.665436000
C	-0.356305000	2.453520000	0.665436000
C	0.322500000	1.176704000	1.124913000
C	-0.685886000	0.034240000	0.767166000
C	-0.685886000	0.034240000	-0.767166000
C	0.322500000	1.176704000	-1.124913000
C	1.358068000	0.998045000	0.000000000
C	-0.146568000	-1.328160000	-1.140064000
C	-0.146568000	-1.328160000	1.140064000
O	0.143386000	-2.047850000	0.000000000
O	0.048209000	-1.775962000	-2.219430000
O	0.048209000	-1.775962000	2.219430000
H	-0.834356000	3.165678000	-1.321994000
H	-0.834356000	3.165678000	1.321994000
H	0.671979000	1.139013000	2.151857000
H	-1.652569000	0.177450000	1.243011000
H	-1.652569000	0.177450000	-1.243011000
H	0.671979000	1.139013000	-2.151857000
H	1.851338000	0.023948000	0.000000000
H	2.106821000	1.786039000	0.000000000

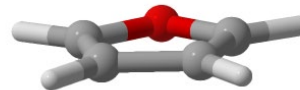


E = -229.566161708 ; 3-Furan

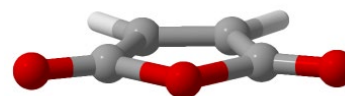
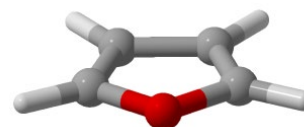
C	0.000053000	-0.346575000	1.086968000
C	0.000053000	0.952968000	0.716115000
C	0.000053000	0.952968000	-0.716115000
C	0.000053000	-0.346575000	-1.086968000
O	-0.000196000	-1.150465000	0.000000000
H	0.000101000	1.805425000	1.372172000
H	0.000101000	1.805425000	-1.372172000
H	0.000050000	-0.841922000	-2.041016000
H	0.000050000	-0.841922000	2.041016000



E = -608.245694987 ; 3-endo-RC
 C -0.018752000 -1.398630000 1.122313000
 C -1.314267000 -0.826840000 0.662554000
 C -1.314267000 -0.826840000 -0.662554000
 C -0.018752000 -1.398630000 -1.122313000
 O 0.715547000 -1.721881000 0.000000000
 O 0.381634000 -1.585707000 -2.221844000
 O 0.381634000 -1.585707000 2.221844000
 C -0.089699000 1.991911000 1.086833000
 C 1.107745000 1.479849000 0.714193000
 C 1.107745000 1.479849000 -0.714193000
 C -0.089699000 1.991911000 -1.086833000
 O -0.826167000 2.315459000 0.000000000
 H 1.886386000 1.133214000 1.371240000
 H 1.886386000 1.133214000 -1.371240000
 H -0.538103000 2.195192000 -2.042992000
 H -2.069043000 -0.494806000 -1.355910000
 H -2.069043000 -0.494806000 1.355910000
 H -0.538103000 2.195192000 2.042992000

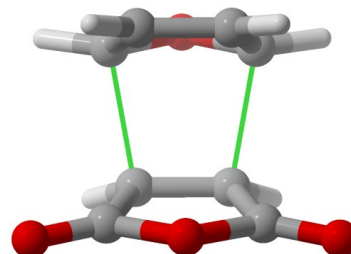


E = -608.244994266 ; 3-exo-RC
 C 0.427426000 2.551746000 0.714471000
 C 0.427426000 2.551746000 -0.714471000
 C -0.534763000 1.675006000 -1.088542000
 C 1.296235000 -0.758902000 -0.662540000
 C 1.296235000 -0.758902000 0.662540000
 C -0.534763000 1.675006000 1.088542000
 O -1.131580000 1.139368000 0.000000000
 C 0.062350000 -1.457380000 1.119565000
 C 0.062350000 -1.457380000 -1.119565000
 O -0.620518000 -1.878557000 0.000000000
 O -0.331805000 -1.653921000 2.220349000
 O -0.331805000 -1.653921000 -2.220349000
 H 1.053159000 3.129815000 1.371696000
 H 1.053159000 3.129815000 -1.371696000
 H -0.905948000 1.342893000 -2.042204000
 H 2.008132000 -0.347399000 -1.358079000
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 H -0.905948000 1.342893000 2.042204000



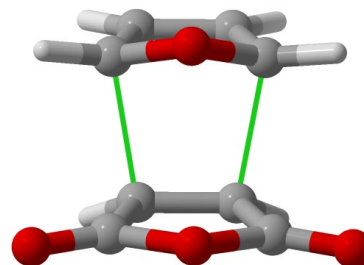
E = -608.213362425 ; 3-endo-TS

C	-0.121361000	1.238404000	1.131516000
C	-1.068968000	-0.185994000	0.701173000
C	-1.068968000	-0.185994000	-0.701173000
C	-0.121361000	-1.238404000	-1.131516000
O	0.487105000	-1.752728000	0.000000000
O	0.158282000	-1.623473000	-2.220017000
O	0.158282000	-1.623473000	2.220017000
C	-0.07452800	1.600561000	1.068834000
C	1.240969000	1.232717000	0.682588000
C	1.240969000	1.232717000	-0.682588000
C	-0.07452800	1.600561000	-1.068834000
O	-0.68840700	2.173928000	0.000000000
H	2.011559000	0.883192000	1.349097000
H	2.011559000	0.883192000	-1.349097000
H	-0.414529000	1.925185000	-2.038465000
H	-1.914741000	0.041323000	-1.329366000
H	-1.914741000	0.041323000	1.329366000
H	-0.414529000	1.925185000	2.038465000



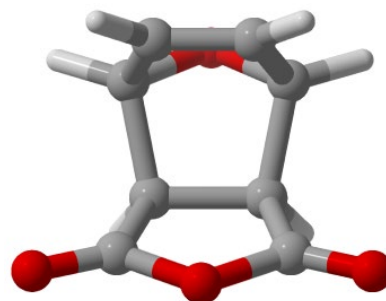
E = -608.212562010 ; 3-exo-TS

C	0.293377000	2.427978000	0.683062000
C	0.293377000	2.427978000	-0.683062000
C	-0.490141000	1.311138000	-1.070073000
C	0.955444000	-0.156301000	-0.700541000
C	0.955444000	-0.156301000	0.700541000
C	-0.490141000	1.311138000	1.070073000
O	-1.226514000	0.919356000	0.000000000
C	0.143547000	-1.322746000	1.127872000
C	0.143547000	-1.322746000	-1.127872000
O	-0.381715000	-1.920834000	0.000000000
O	-0.087618000	-1.731153000	2.219417000
O	-0.087618000	-1.731153000	-2.219417000
H	0.869366000	3.046330000	1.350628000
H	0.869366000	3.046330000	-1.350628000
H	-0.903502000	1.074986000	-2.037766000
H	1.754637000	0.173402000	-1.342232000
H	1.754637000	0.173402000	1.342232000
H	-0.903502000	1.074986000	2.037766000



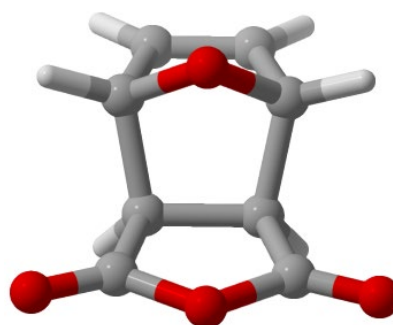
E = -608.25413060 ; 3-endo-adduct

C	-0.122509000	-1.201135000	1.141789000
C	-0.902256000	0.033754000	0.763446000
C	-0.902256000	0.033754000	-0.763446000
C	-0.122509000	-1.201135000	-1.141789000
O	0.289386000	-1.854427000	0.000000000
O	0.151651000	-1.604962000	-2.221195000
O	0.151651000	-1.604962000	2.221195000
C	-0.169429000	1.393746000	1.065143000
C	1.283844000	1.216375000	0.663739000
C	1.283844000	1.216375000	-0.663739000
C	-0.169429000	1.393746000	-1.065143000
O	-0.683797000	2.181528000	0.000000000
H	2.101138000	1.025360000	1.341124000
H	2.101138000	1.025360000	-1.341124000
H	-0.388851000	1.830938000	-2.031448000
H	-1.885750000	0.018552000	-1.224131000
H	-1.885750000	0.018552000	1.224131000
H	-0.388851000	1.830938000	2.031448000



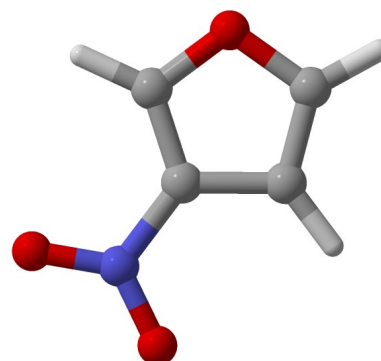
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C	0.297839000	2.464878000	0.663333000
C	0.297839000	2.464878000	-0.663333000
C	-0.359042000	1.156710000	-1.065173000
C	0.693255000	0.036241000	-0.765687000
C	0.693255000	0.036241000	0.765687000
C	-0.359042000	1.156710000	1.065173000
O	-1.275206000	0.937824000	0.000000000
C	0.137487000	-1.320922000	1.136832000
C	0.137487000	-1.320922000	-1.136832000
O	-0.160428000	-2.034199000	0.000000000
O	-0.052329000	-1.762098000	2.219267000
O	-0.052329000	-1.762098000	-2.219267000
H	0.741648000	3.176165000	1.341739000
H	0.741648000	3.176165000	-1.341739000
H	-0.843405000	1.086018000	-2.032513000
H	1.645691000	0.198657000	-1.260749000
H	1.645691000	0.198657000	1.260749000
H	-0.843405000	1.086018000	2.032513000



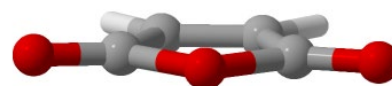
E = -433.791539968 ; 4-3-Nitrofuran

O	-2.042388000	-0.716039000	0.000567000
C	-0.759412000	-1.092924000	-0.000285000
C	0.019052000	0.014917000	0.000057000
C	-0.831664000	1.156653000	0.000089000
C	-2.079230000	0.643809000	-0.000408000
N	1.457462000	0.011641000	-0.000031000
H	-0.531785000	2.188552000	-0.000015000
H	-3.058449000	1.086104000	-0.000834000
H	-0.534590000	-2.143526000	-0.000571000
O	2.009390000	1.088736000	0.000142000
O	2.011762000	-1.066116000	-0.000095000



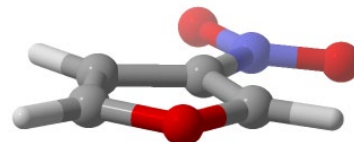
E = -812.469487057 ; 4-endo-RC

O	-0.209173000	2.335237000	-0.427827000
C	-1.221438000	1.544357000	-0.799040000
C	-1.461800000	0.649677000	0.190062000
C	-0.541775000	0.897401000	1.246693000
C	0.203528000	1.934657000	0.806789000
C	0.873824000	-1.565957000	-0.229593000
C	1.014170000	-0.722937000	-1.451814000
C	2.004002000	0.132419000	-1.244400000
C	2.552565000	-0.121654000	0.118020000
O	1.850441000	-1.173400000	0.663229000
O	0.090131000	-2.418885000	0.013056000
O	3.421025000	0.438258000	0.698302000
N	-2.484601000	-0.365513000	0.149367000
H	-0.458279000	0.359765000	2.174341000
H	1.026417000	2.482516000	1.229710000
H	2.397352000	0.907710000	-1.881354000
H	0.369172000	-0.852523000	-2.305927000
H	-1.682792000	1.716712000	-1.754230000
O	-2.683269000	-0.985150000	1.165464000
O	-3.068920000	-0.513981000	-0.903275000



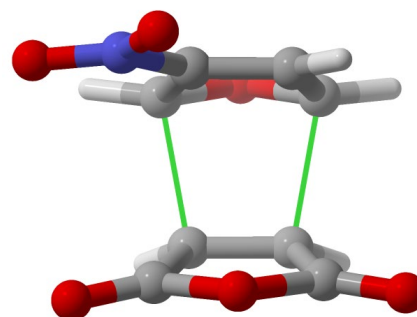
E = -812.469561404 ; 4-exo-RC

O	2.718278000	0.293696000	0.242512000
C	1.898000000	1.344290000	-0.109909000
C	1.023599000	0.880633000	-1.225444000
C	1.318310000	-0.387158000	-1.473318000
C	2.402978000	-0.797709000	-0.536948000
O	1.933327000	2.395689000	0.433985000
O	2.938948000	-1.847382000	-0.413946000
C	-0.147466000	-1.429830000	1.227739000
C	-1.246280000	-1.558054000	0.451127000
C	-1.783596000	-0.243869000	0.378645000
C	-0.989120000	0.582078000	1.102880000
O	0.008753000	-0.139678000	1.626982000
N	-2.943992000	0.172047000	-0.364171000
H	-1.637903000	-2.446590000	-0.009938000
H	0.595636000	-2.123516000	1.578923000
H	0.899916000	-1.069195000	-2.195175000
H	0.296700000	1.528886000	-1.687935000
H	-1.017798000	1.636585000	1.312012000
O	-3.218876000	1.352185000	-0.349777000
O	-3.553825000	-0.688607000	-0.956922000

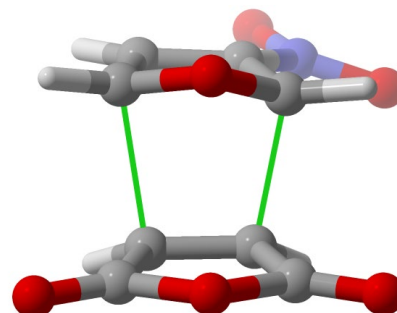


E = -812.432780524 ; 4-endo-TS

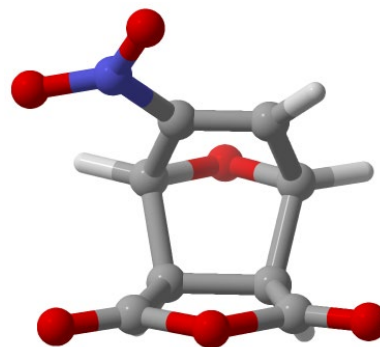
O	0.141984000	2.162599000	-1.011944000
C	-0.711620000	1.113390000	-1.110506000
C	-1.076319000	0.772625000	0.216664000
C	-0.152373000	1.310010000	1.059455000
C	0.739609000	1.997829000	0.200816000
C	0.877448000	-0.188599000	-1.401571000
C	0.459636000	-1.478887000	-0.796333000
O	1.050044000	-1.569036000	0.456137000
C	1.966908000	-0.550462000	0.615222000
C	1.824389000	0.374204000	-0.537574000
O	-0.252955000	-2.326543000	-1.215069000
O	2.686608000	-0.487504000	1.556683000
N	-2.157035000	-0.124823000	0.562310000
H	-0.045220000	1.141832000	2.117826000
H	1.474255000	2.737691000	0.471489000
H	2.668444000	0.976690000	-0.832015000
H	0.874690000	-0.093675000	-2.475573000
H	-1.325789000	1.047731000	-1.992645000
O	-2.314737000	-0.370190000	1.733591000
O	-2.825094000	-0.538972000	-0.357183000



E = -812.434607256 ; 4-exo-TS
 O 2.668323000 0.536309000 0.086794000
 C 1.633374000 1.423803000 -0.113153000
 C 0.496120000 0.683322000 -0.738276000
 C 0.958804000 -0.615861000 -0.975028000
 C 2.357184000 -0.681909000 -0.483439000
 O 1.704644000 2.562024000 0.209225000
 O 3.132924000 -1.579736000 -0.513188000
 C 0.087387000 -1.581416000 0.763493000
 C -1.213753000 -1.614501000 0.219377000
 C -1.667474000 -0.336160000 0.357312000
 C -0.624832000 0.440102000 0.927177000
 O 0.233099000 -0.448987000 1.492685000
 N -2.857501000 0.221256000 -0.230294000
 H -1.683770000 -2.429896000 -0.303256000
 H 0.744314000 -2.398844000 1.013037000
 H 0.650330000 -1.282559000 -1.761950000
 H -0.197348000 1.240199000 -1.349638000
 H -0.696162000 1.415467000 1.381446000
 O -2.922410000 1.431514000 -0.268096000
 O -3.688545000 -0.550804000 -0.646465000

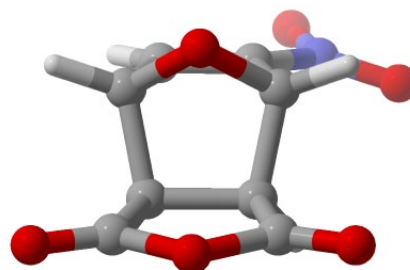


E = -812.476049854 ; 4-endo-adduct
 O -0.075110000 -1.963612000 -1.309385000
 C 0.544431000 -0.683958000 -1.292170000
 C -0.734403000 0.229100000 -1.309212000
 C -1.685124000 -0.581978000 -0.431186000
 C -0.799259000 -1.834127000 -0.090551000
 C -1.979598000 0.320334000 0.745021000
 O -1.326367000 1.517703000 0.579778000
 C -0.606518000 1.558742000 -0.601098000
 C 1.097627000 -0.672296000 0.116063000
 C 0.275336000 -1.373374000 0.880263000
 O -0.006951000 2.521951000 -0.928892000
 O -2.637063000 0.088955000 1.702383000
 N 2.264165000 0.074525000 0.539162000
 H 0.301930000 -1.507240000 1.949970000
 H -1.343095000 -2.737776000 0.154134000
 H -2.607184000 -0.892396000 -0.913884000
 H -1.065295000 0.376994000 -2.332702000
 H 1.242260000 -0.541122000 -2.106586000
 O 2.602361000 -0.023003000 1.694059000
 O 2.811538000 0.733656000 -0.316423000



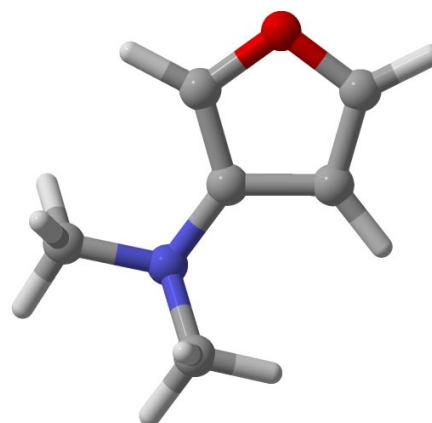
E = **-812.480901766** ; **4-exo-adduct**

O	2.761439000	0.588520000	-0.068449000
C	1.674208000	1.431566000	-0.110431000
C	0.434223000	0.654240000	-0.505362000
C	0.935041000	-0.782428000	-0.682991000
C	2.418163000	-0.701538000	-0.382763000
C	-0.515282000	0.492785000	0.722265000
C	-1.685127000	-0.331176000	0.231197000
C	-1.266222000	-1.576476000	0.073554000
C	0.192545000	-1.511803000	0.488068000
O	0.186266000	-0.487324000	1.475965000
O	1.762466000	2.581170000	0.149170000
O	3.207569000	-1.583066000	-0.385343000
N	-2.948328000	0.223820000	-0.193842000
H	-1.794375000	-2.412660000	-0.355949000
H	0.669252000	-2.416578000	0.847164000
H	0.774570000	-1.247298000	-1.651033000
H	-0.050388000	1.125432000	-1.355733000
H	-0.720232000	1.393355000	1.288000000
O	-2.991965000	1.433609000	-0.271405000
O	-3.846504000	-0.540411000	-0.452035000

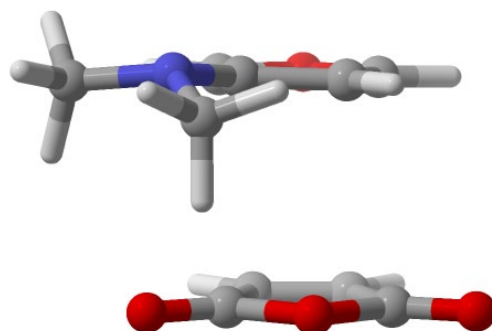


E= **-363.225795215** ; **5-N,N-dimethylfuran-3-amine**

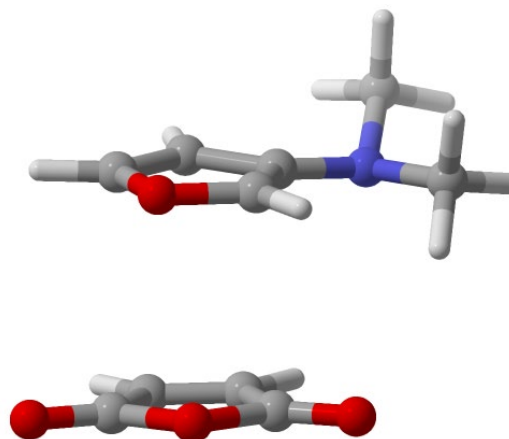
C	2.204683000	-0.610478000	-0.018994000
O	2.144250000	0.718628000	0.173024000
C	0.829840000	1.071203000	0.114154000
C	0.059199000	-0.022967000	-0.134119000
C	0.973488000	-1.130943000	-0.212105000
N	-1.320813000	-0.073068000	-0.324693000
C	-1.987616000	1.188625000	-0.093228000
C	-1.986827000	-1.197560000	0.306328000
H	0.741849000	-2.164284000	-0.400208000
H	3.185364000	-1.051324000	0.005416000
H	0.610632000	2.113794000	0.247184000
H	-3.045344000	1.085700000	-0.328624000
H	-1.889846000	1.527296000	0.949247000
H	-1.562455000	1.951834000	-0.744928000
H	-3.025693000	-1.223376000	-0.019612000
H	-1.516079000	-2.130251000	0.004908000
H	-1.963341000	-1.134215000	1.403062000



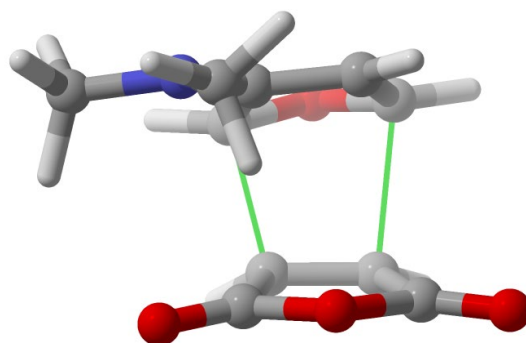
E = -741.908671785 ; 5-endo-RC
O 1.259933000 -1.471158000 0.435664000
C 0.620682000 -1.436749000 -0.783452000
C 1.257810000 -0.371372000 -1.600213000
C 2.223334000 0.177085000 -0.874172000
C 2.249593000 -0.503993000 0.446552000
O -0.267404000 -2.177817000 -1.053977000
O 2.954230000 -0.330212000 1.383230000
C -1.230583000 0.822716000 0.281247000
C -1.004467000 1.506493000 -0.885196000
O 0.034065000 2.376894000 -0.729906000
C 0.498910000 2.212056000 0.519877000
C -0.222054000 1.285251000 1.193793000
N -2.242069000 -0.073052000 0.542478000
C -3.039373000 -0.465567000 -0.598088000
C -2.025689000 -1.077844000 1.566718000
H -0.050669000 0.966407000 2.206739000
H 1.336018000 2.824400000 0.806757000
H 2.906276000 0.973060000 -1.119669000
H 0.934886000 -0.153310000 -2.604047000
H -1.507546000 1.525970000 -1.833714000
H -3.850077000 -1.108310000 -0.261809000
H -3.477467000 0.422442000 -1.057814000
H -2.454542000 -1.003399000 -1.353842000
H -2.984007000 -1.531648000 1.814385000
H -1.334184000 -1.865932000 1.253885000
H -1.639759000 -0.608438000 2.469303000



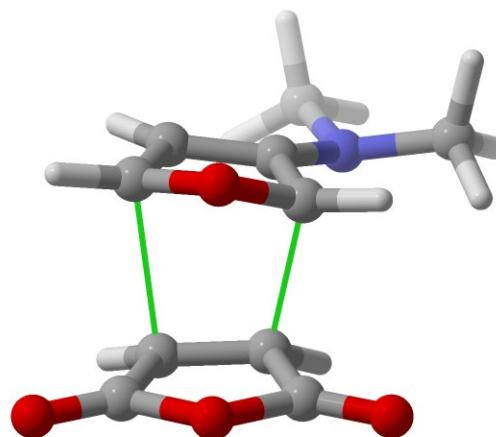
E = -741.908233256 ; 5-exo-RC
O 0.231020000 -1.282710000 1.248670000
C -0.151473000 -2.214516000 0.356175000
C -1.242394000 -1.807472000 -0.332228000
C -1.559796000 -0.498495000 0.166028000
C -0.639110000 -0.242878000 1.140992000
N -2.543776000 0.358263000 -0.315694000
C -3.820799000 -0.264880000 -0.615663000
C -2.662688000 1.597041000 0.427823000
C 0.934444000 0.713225000 -1.263905000
C 1.418307000 1.541988000 -0.126190000
O 2.475984000 0.881224000 0.454437000
C 2.699020000 -0.295369000 -0.236300000
C 1.703642000 -0.363699000 -1.339707000
O 1.025779000 2.590622000 0.269280000
O 3.555289000 -1.056936000 0.063436000
H -1.746761000 -2.358741000 -1.106195000
H 0.437560000 -3.114505000 0.328894000
H 1.668867000 -1.192210000 -2.026758000
H 0.087320000 1.008359000 -1.862039000
H -0.470593000 0.590472000 1.798118000
H -3.389363000 2.240277000 -0.064512000
H -2.987634000 1.428396000 1.464370000
H -1.701391000 2.111448000 0.442853000
H -4.452388000 0.454053000 -1.134926000
H -3.676956000 -1.122002000 -1.269309000
H -4.341618000 -0.600663000 0.290616000



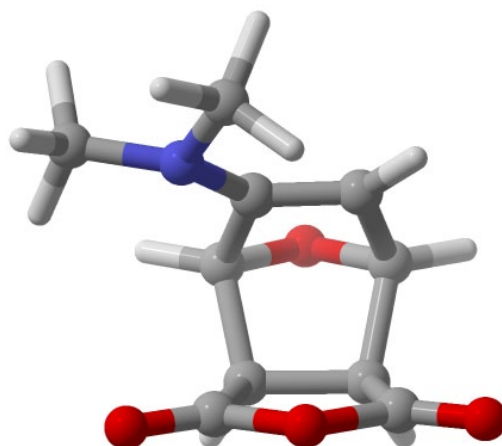
E = -741.885051461 ; 5-endo-TS
 C 1.940006000 0.271816000 -0.670199000
 C 0.793471000 0.012238000 -1.440823000
 C 0.253929000 -1.282447000 -0.937579000
 O 0.963958000 -1.644626000 0.172485000
 C 2.072382000 -0.788949000 0.317223000
 O -0.65446200 -1.939283000 -1.345797000
 O 2.883573000 -1.000763000 1.160890000
 C -0.511139000 1.403724000 -0.847225000
 O 0.463225000 2.317586000 -0.559878000
 C 1.002785000 1.857123000 0.593380000
 C 0.052568000 1.117453000 1.304131000
 C -0.968690000 0.844432000 0.401499000
 N -2.074958000 0.090747000 0.563273000
 C -3.014127000 -0.048274000 -0.533428000
 C -2.111201000 -0.855235000 1.662462000
 H 0.184174000 0.728518000 2.298554000
 H 1.858058000 2.392498000 0.970487000
 H 2.794862000 0.856106000 -0.963406000
 H 0.708186000 0.209879000 -2.498523000
 H -1.127027000 1.644928000 -1.698813000
 H -3.231394000 0.933148000 -0.956182000
 H -2.636989000 -0.707336000 -1.319022000
 H -3.944496000 -0.457851000 -0.147545000
 H -1.383378000 -1.659889000 1.523910000
 H -1.900308000 -0.344956000 2.602780000
 H -3.107235000 -1.284862000 1.726600000



E = -741.881760027 ; 5-exo-TS
O 0.331522000 -0.445474000 1.486549000
C 0.147250000 -1.617482000 0.850958000
C -1.137613000 -1.657214000 0.296097000
C -1.587503000 -0.346194000 0.293488000
C -0.515180000 0.419572000 0.859244000
N -2.683521000 0.184082000 -0.318980000
C -3.685600000 -0.744244000 -0.798630000
C -3.148501000 1.485546000 0.124801000
C 0.596321000 0.588427000 -0.789574000
C 1.674948000 1.437700000 -0.198433000
O 2.751582000 0.642485000 0.073372000
C 2.522789000 -0.639880000 -0.438812000
C 1.159675000 -0.680263000 -0.967668000
O 1.656604000 2.601696000 0.051461000
O 3.369452000 -1.474311000 -0.382683000
H -1.592589000 -2.519476000 -0.158649000
H 0.799817000 -2.425178000 1.139861000
H 0.882219000 -1.428364000 -1.688068000
H -0.116822000 1.062655000 -1.448582000
H -0.567846000 1.403126000 1.298391000
H -2.327041000 2.200383000 0.112831000
H -3.907950000 1.842846000 -0.566753000
H -3.575559000 1.455277000 1.133224000
H -4.425825000 -0.199235000 -1.379541000
H -3.222616000 -1.485221000 -1.448568000
H -4.193934000 -1.266369000 0.020299000

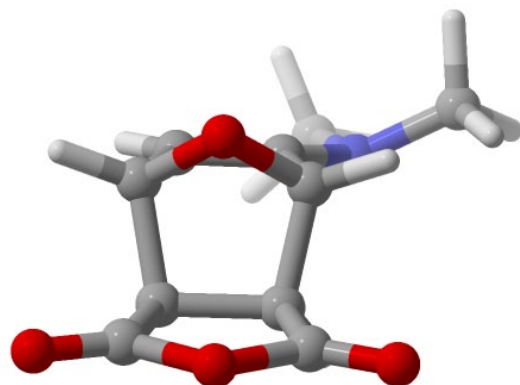


E = -741.926600669 ; 5-endo-adduct
 C 0.091745000 -1.282172000 1.053804000
 C -1.020738000 -1.777193000 0.163526000
 O -0.322984000 -2.151165000 -1.024885000
 C 0.402556000 -0.949716000 -1.182820000
 C 0.979884000 -0.718745000 0.212629000
 C -1.809353000 -0.524541000 -0.385126000
 C -0.783846000 0.066702000 -1.350867000
 C -2.015256000 0.558444000 0.644039000
 O -1.217559000 1.647140000 0.340293000
 C -0.504353000 1.449998000 -0.819034000
 O -2.716860000 0.558546000 1.598165000
 O 0.207642000 2.286704000 -1.265852000
 N 2.043051000 0.089635000 0.461720000
 C 3.081712000 0.266545000 -0.533295000
 C 2.399071000 0.274490000 1.850414000
 H 0.065420000 -1.254306000 2.129729000
 H -1.648501000 -2.583162000 0.524601000
 H -2.756264000 -0.809932000 -0.835558000
 H -1.098892000 0.114470000 -2.389149000
 H 1.085108000 -1.005037000 -2.022297000
 H 3.686481000 1.127042000 -0.255688000
 H 3.736140000 -0.607409000 -0.622755000
 H 2.638872000 0.483298000 -1.503329000
 H 3.170124000 1.037237000 1.926523000
 H 1.522670000 0.609232000 2.406596000
 H 2.767044000 -0.651543000 2.307895000



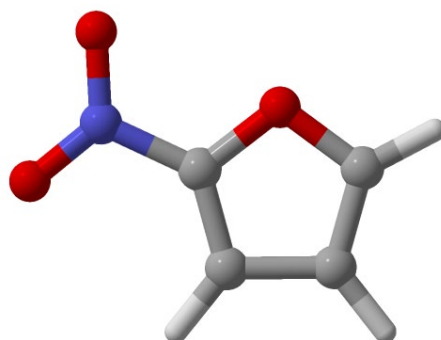
E = -741.928699227 ; 5-exo-adduct

O	0.275971000	-0.369654000	1.477695000
C	-0.420914000	0.521610000	0.629915000
C	0.544907000	0.583928000	-0.598561000
C	1.087589000	-0.847946000	-0.615977000
C	0.294392000	-1.480478000	0.579149000
C	2.552216000	-0.692243000	-0.277256000
O	2.853573000	0.638818000	-0.088286000
C	1.750061000	1.435284000	-0.269447000
C	-1.606946000	-0.319369000	0.163826000
C	-1.150830000	-1.582668000	0.154763000
O	1.802122000	2.613473000	-0.150078000
O	3.373713000	-1.537344000	-0.159603000
N	-2.767647000	0.219692000	-0.322970000
C	-3.737622000	-0.738996000	-0.809256000
C	-3.341949000	1.364118000	0.366088000
H	-1.635258000	-2.477423000	-0.198041000
H	0.767893000	-2.345723000	1.030014000
H	0.973262000	-1.406795000	-1.539431000
H	0.056898000	0.946358000	-1.499006000
H	-0.602345000	1.473118000	1.116502000
H	-4.103302000	1.811402000	-0.270234000
H	-3.803747000	1.083494000	1.319615000
H	-2.581021000	2.116596000	0.554524000
H	-4.563741000	-0.208430000	-1.278013000
H	-3.270444000	-1.384976000	-1.551391000
H	-4.133129000	-1.367249000	-0.001041000

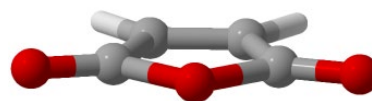


E = -433.788601436 ; 6-2-Nitrofuran

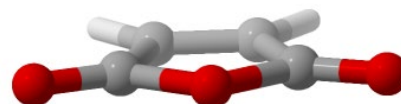
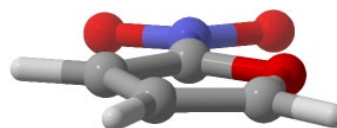
O	-0.693059000	-1.062206000	0.000030000
C	-0.007726000	0.085959000	-0.000161000
C	-0.815510000	1.170444000	-0.000007000
C	-2.135310000	0.635808000	0.000102000
C	-1.995368000	-0.714102000	-0.000006000
H	-0.496896000	2.197013000	-0.000054000
H	-3.061563000	1.182272000	0.000163000
H	-2.696831000	-1.528869000	-0.000029000
N	1.425885000	-0.003094000	-0.000400000
O	1.922395000	-1.103582000	0.000187000
O	2.020361000	1.053611000	0.000177000



E = -812.468763309 ; 6-endo-RC
 O 1.087846000 1.506508000 -0.191384000
 C 1.609440000 0.306497000 -0.462103000
 C 1.030142000 -0.282786000 -1.534674000
 C 0.047506000 0.652219000 -1.968703000
 C 0.129816000 1.710358000 -1.120933000
 C -1.639149000 -1.433979000 -0.010387000
 C -0.764650000 -1.046185000 1.133514000
 C -1.123460000 0.166339000 1.528844000
 C -2.251739000 0.614798000 0.663724000
 O -2.530457000 -0.403273000 -0.223311000
 O -1.627572000 -2.414802000 -0.673904000
 O -2.845455000 1.640224000 0.665004000
 H 1.265392000 -1.253962000 -1.932360000
 H -0.636090000 0.545675000 -2.792428000
 H -0.401503000 2.643117000 -1.050929000
 H -0.715500000 0.789086000 2.308456000
 H 0.011227000 -1.697457000 1.504335000
 N 2.595370000 -0.195875000 0.451995000
 O 2.859043000 0.478275000 1.420046000
 O 3.066777000 -1.279293000 0.181456000

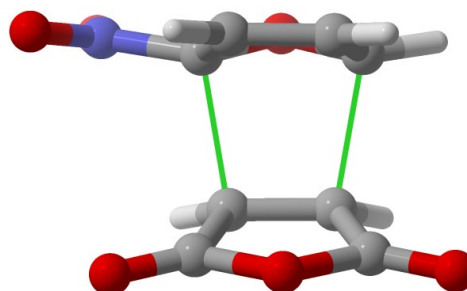


E = -812.469961744 ; 6-exo-RC
 O 1.584012000 1.033450000 0.180797000
 C 1.728886000 0.326833000 -0.998538000
 C 1.763303000 -1.123036000 -0.651643000
 C 1.656636000 -1.231937000 0.665049000
 C 1.535438000 0.141328000 1.232049000
 O 1.805172000 0.861123000 -2.051719000
 O 1.410614000 0.490231000 2.357476000
 C -1.432147000 1.961471000 -0.699408000
 C -1.638096000 2.025748000 0.641711000
 C -1.653634000 0.682146000 1.105485000
 C -1.460708000 -0.065925000 -0.007611000
 O -1.325736000 0.682977000 -1.109706000
 H -1.767185000 0.311102000 2.108269000
 H -1.746769000 2.919333000 1.229594000
 H -1.327674000 2.706958000 -1.467132000
 H 1.629448000 -2.111213000 1.287395000
 H 1.848875000 -1.887712000 -1.405833000
 N -1.327474000 -1.480810000 -0.162776000
 O -1.150439000 -1.915627000 -1.277620000
 O -1.366428000 -2.136224000 0.858843000



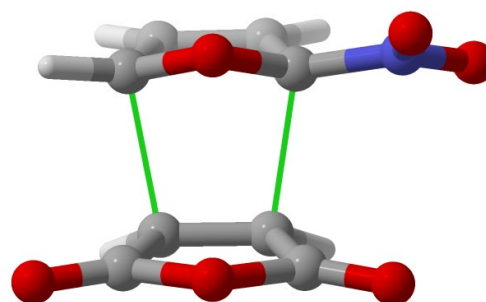
E = -812.433345959 ; 6-endo-TS

O	0.881847000	-1.646113000	-0.401793000
C	1.140861000	-0.480407000	0.220353000
C	0.488212000	-0.444051000	1.476390000
C	-0.489298000	-1.390517000	1.373637000
C	-0.350010000	-1.964366000	0.079554000
C	-0.216289000	0.515287000	-1.004540000
C	-0.762654000	1.602336000	-0.150113000
O	-1.995929000	1.186983000	0.323453000
C	-2.361867000	0.005458000	-0.290554000
C	-1.206142000	-0.469222000	-1.090878000
O	-0.295240000	2.649069000	0.146958000
O	-3.427453000	-0.488724000	-0.122403000
H	0.663911000	0.288271000	2.245519000
H	-1.296488000	-1.589807000	2.058621000
H	-0.773966000	-2.883612000	-0.289310000
H	-1.379378000	-1.112775000	-1.938078000
H	0.510573000	0.750214000	-1.767676000
N	2.437407000	0.123973000	-0.076558000
O	2.999627000	-0.242900000	-1.077620000
O	2.806726000	0.970785000	0.699372000



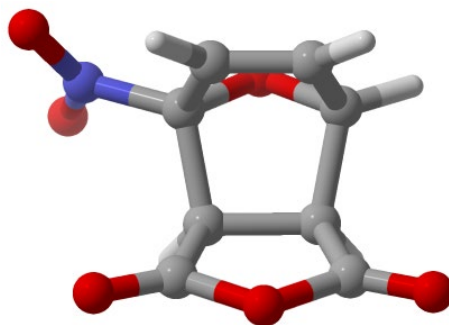
E = -812.431650525 ; 6-exo-TS

O	1.676250000	-1.442219000	-0.303910000
C	0.540700000	-1.552853000	0.474437000
C	0.334101000	-0.255411000	1.179525000
C	1.433927000	0.547538000	0.868135000
C	2.303645000	-0.245465000	-0.042865000
O	-0.105111000	-2.544422000	0.518999000
O	3.351543000	0.040322000	-0.521680000
C	0.589173000	1.787651000	-0.610153000
C	-0.198565000	2.581369000	0.265128000
C	-1.290624000	1.826382000	0.582080000
C	-1.086739000	0.607461000	-0.106535000
O	-0.184457000	0.780291000	-1.088644000
H	-2.080722000	2.010986000	1.288760000
H	0.094125000	3.534098000	0.673172000
H	1.418696000	2.077643000	-1.235161000
H	1.889391000	1.288406000	1.503037000
H	-0.240227000	-0.253076000	2.091297000
N	-2.116822000	-0.400258000	-0.338292000
O	-2.056902000	-1.035948000	-1.354916000
O	-2.933474000	-0.502560000	0.548703000



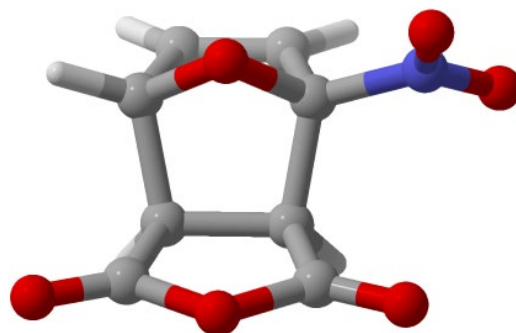
E = -812.478125204 ; 6-endo-adduct

O	0.849168000	-1.634983000	-0.501256000
C	0.992264000	-0.354401000	0.054548000
C	-0.046877000	0.449863000	-0.792236000
C	-1.148886000	-0.599971000	-0.920809000
C	-0.520428000	-1.802358000	-0.124791000
C	-2.350052000	0.034248000	-0.259187000
O	-2.014892000	1.289517000	0.199365000
C	-0.697417000	1.599015000	-0.056395000
C	0.473393000	-0.514377000	1.463171000
C	-0.491136000	-1.418986000	1.345051000
O	-0.211197000	2.618095000	0.294496000
O	-3.431116000	-0.420494000	-0.102555000
H	0.780234000	0.081832000	2.306157000
H	-1.191594000	-1.757727000	2.091808000
H	-0.886531000	-2.784097000	-0.396750000
H	-1.382877000	-0.895161000	-1.939324000
H	0.409144000	0.773156000	-1.724051000
N	2.408117000	0.116921000	-0.116098000
O	3.013527000	0.400029000	0.885420000
O	2.813216000	0.173504000	-1.248128000



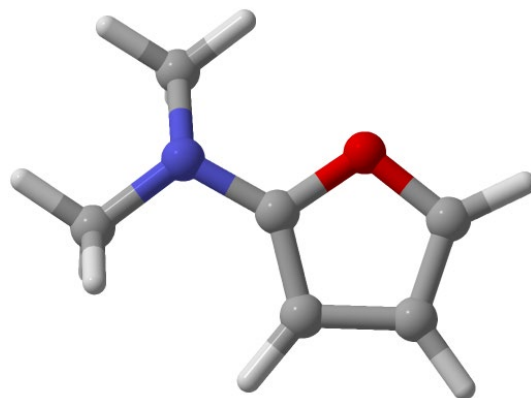
E = -812.480318553 ; 6-exo-adduct

O	-1.792087000	-1.490954000	0.101946000
C	-0.531248000	-1.553246000	-0.440779000
C	-0.116969000	-0.178868000	-0.939096000
C	-1.319106000	0.714078000	-0.616929000
C	-2.313389000	-0.223370000	0.037778000
C	0.945871000	0.473100000	0.003192000
C	1.308370000	1.821624000	-0.583039000
C	0.261911000	2.584579000	-0.300044000
C	-0.706710000	1.685689000	0.447576000
O	0.179275000	0.789369000	1.127150000
O	0.090047000	-2.556758000	-0.485654000
O	-3.385142000	0.041757000	0.462658000
H	2.190501000	2.013173000	-1.171259000
H	0.065502000	3.601305000	-0.600762000
H	-1.418659000	2.129608000	1.133300000
H	-1.783429000	1.230994000	-1.450994000
H	0.217815000	-0.231934000	-1.969696000
N	2.095488000	-0.426298000	0.319873000
O	2.150574000	-0.913097000	1.412140000
O	2.868266000	-0.582890000	-0.597197000



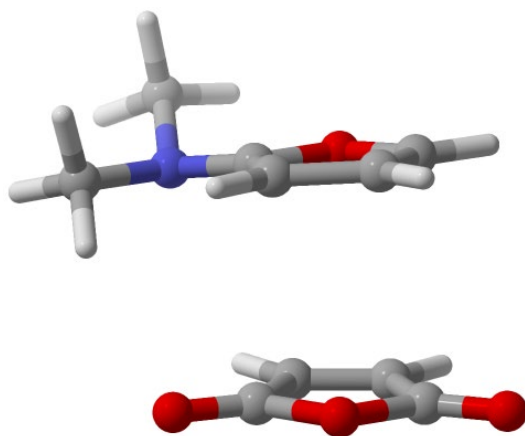
E= -363.232426609 ; 7-N,N-dimethylfuran-2-amine

C	2.133753000	-0.680104000	-0.050106000
O	0.825330000	-1.040759000	-0.210302000
C	0.085685000	0.082925000	-0.098554000
C	0.884859000	1.159660000	0.138376000
C	2.225751000	0.646872000	0.156895000
N	-1.271879000	-0.052739000	-0.295632000
C	-2.013294000	1.172790000	-0.093689000
C	-1.890865000	-1.228939000	0.295264000
H	0.569037000	2.176390000	0.284159000
H	3.132675000	1.203966000	0.315359000
H	2.849341000	-1.479375000	-0.102268000
H	-3.051333000	1.006556000	-0.374859000
H	-1.980114000	1.512696000	0.950658000
H	-1.603661000	1.957638000	-0.727779000
H	-2.898188000	-1.330475000	-0.104816000
H	-1.321668000	-2.115703000	0.033407000
H	-1.950905000	-1.155679000	1.388868000



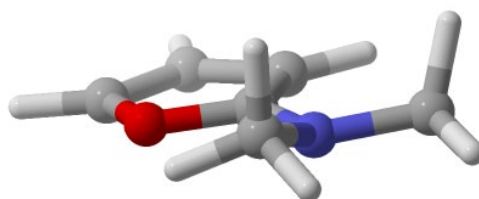
E = -741.916864110 ; 7-endo-RC

O	2.346954000	0.917978000	-0.456711000
C	1.252964000	1.559470000	0.080061000
C	0.801687000	0.775340000	1.260735000
C	1.613980000	-0.263614000	1.394370000
C	2.619862000	-0.205206000	0.299918000
O	0.819251000	2.567199000	-0.374291000
O	3.520799000	-0.934156000	0.052161000
C	-0.621028000	-0.356502000	-1.384429000
C	-1.407019000	-0.486742000	-0.275670000
O	-1.098196000	-1.620476000	0.390573000
C	-0.079618000	-2.224426000	-0.292493000
C	0.247095000	-1.494505000	-1.379244000
N	-2.363443000	0.322425000	0.295843000
C	-2.654161000	1.515610000	-0.477951000
C	-3.542927000	-0.352005000	0.820980000
H	-0.649466000	0.444540000	-2.101018000
H	1.016629000	-1.729564000	-2.094358000
H	0.266369000	-3.159769000	0.107440000
H	1.608787000	-1.058307000	2.121545000
H	-0.063251000	1.061482000	1.836797000
H	-3.324687000	2.149369000	0.098735000
H	-1.732887000	2.065172000	-0.665892000
H	-3.132115000	1.277613000	-1.437169000
H	-4.101350000	0.351698000	1.435356000
H	-4.195763000	-0.714541000	0.017487000
H	-3.243643000	-1.193530000	1.438650000

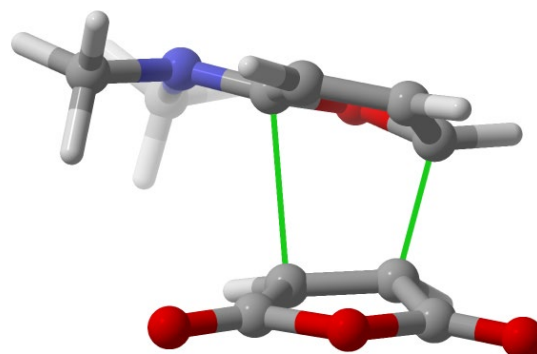


E = -741.916136674 ; 7-exo-RC

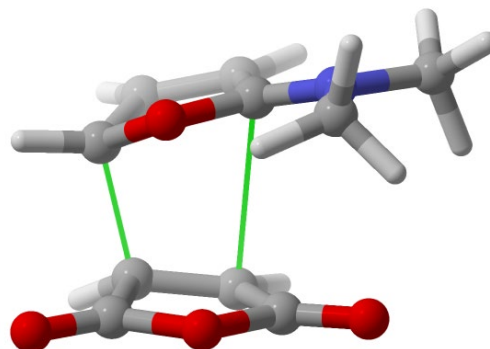
O	-0.404290000	1.244428000	-0.948211000
C	-0.139707000	2.463119000	-0.374700000
C	-0.834034000	2.586367000	0.773813000
C	-1.576769000	1.374328000	0.946835000
C	-1.265210000	0.596431000	-0.137733000
N	-1.593306000	-0.677639000	-0.484192000
C	-2.569184000	-1.335548000	0.351458000
C	-1.496752000	-1.099518000	-1.867646000
C	1.261897000	-0.139777000	1.607614000
C	0.907646000	-1.388973000	0.881325000
O	1.454681000	-1.307660000	-0.381004000
C	2.142495000	-0.113998000	-0.492265000
C	2.011791000	0.603464000	0.805246000
O	0.296767000	-2.335569000	1.253171000
O	2.714138000	0.199309000	-1.481537000
H	-2.261975000	1.128138000	1.737112000
H	-0.831647000	3.443424000	1.425123000
H	0.517469000	3.105520000	-0.930990000
H	2.472214000	1.561303000	0.976954000
H	0.936965000	0.043135000	2.618030000
H	-2.376513000	-0.805625000	-2.451209000
H	-0.609061000	-0.671005000	-2.323582000
H	-1.401537000	-2.183739000	-1.889208000
H	-2.579402000	-2.395049000	0.106263000
H	-2.279510000	-1.237984000	1.397697000
H	-3.577278000	-0.924084000	0.220119000



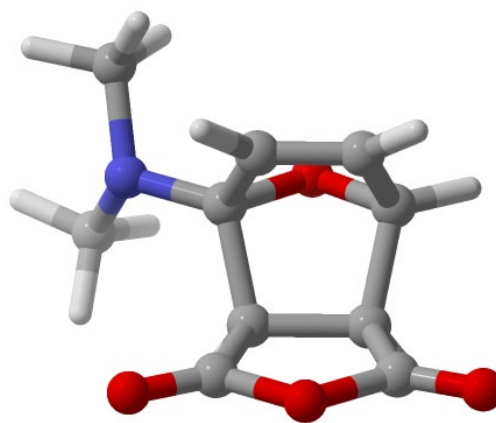
E = -741.890096204 ; 7-endo-TS
 C -1.241050000 -0.562466000 -1.031402000
 C -0.370613000 0.547425000 -1.074436000
 C -0.928394000 1.602828000 -0.272382000
 O -2.165131000 1.138887000 0.243980000
 C -2.450770000 -0.080621000 -0.286240000
 O -0.551548000 2.702796000 0.006680000
 O -3.486727000 -0.641020000 -0.104804000
 C 1.286661000 -0.602263000 0.391665000
 O 0.844611000 -1.670718000 -0.275097000
 C -0.487890000 -1.829197000 0.123256000
 C -0.593604000 -1.220221000 1.411636000
 C 0.454363000 -0.358066000 1.521482000
 N 2.506474000 -0.121318000 0.110555000
 C 2.848149000 1.161456000 0.708238000
 C 3.076640000 -0.384880000 -1.198591000
 H 0.613180000 0.401984000 2.265690000
 H -1.459871000 -1.279298000 2.049805000
 H -0.900207000 -2.790167000 -0.141929000
 H -1.428269000 -1.203989000 -1.881994000
 H 0.413133000 0.736582000 -1.786835000
 H 2.692891000 0.319315000 -1.944296000
 H 4.156869000 -0.274880000 -1.135345000
 H 2.840673000 -1.397003000 -1.510149000
 H 3.893546000 1.370777000 0.497032000
 H 2.222347000 1.962323000 0.301581000
 H 2.719805000 1.120060000 1.787124000



E = -741.891445562 ; 7-exo-TS
O -0.021177000 0.801300000 1.093717000
C -0.925884000 1.697823000 0.506468000
C -0.144907000 2.565098000 -0.306159000
C 1.049871000 1.942819000 -0.526238000
C 1.065649000 0.800101000 0.329881000
N 2.002501000 -0.107808000 0.547172000
C 3.124655000 -0.194265000 -0.370207000
C 1.799621000 -1.225669000 1.464248000
C -0.715828000 -0.095845000 -1.506270000
C -0.407351000 -1.358783000 -0.926374000
O -1.326094000 -1.594054000 0.133873000
C -2.183614000 -0.544720000 0.213745000
C -1.722570000 0.525724000 -0.744412000
O 0.455152000 -2.169046000 -1.135662000
O -3.104753000 -0.511079000 0.968593000
H 1.831394000 2.224191000 -1.208863000
H -0.521721000 3.440180000 -0.809341000
H -1.717130000 1.988572000 1.181072000
H -2.498395000 1.160031000 -1.151303000
H -0.262769000 0.239114000 -2.421498000
H 2.513384000 -1.154951000 2.285935000
H 0.788145000 -1.206317000 1.855561000
H 1.939849000 -2.159137000 0.923958000
H 3.496624000 0.798340000 -0.613874000
H 3.923877000 -0.747388000 0.116898000
H 2.826353000 -0.718638000 -1.281013000



E = -741.924011635 ; 7-endo-adduct
 C -0.492341000 -1.602046000 1.113989000
 C -0.446140000 -1.756438000 -0.395596000
 O 0.895983000 -1.432165000 -0.701252000
 C 0.971790000 -0.197196000 0.061329000
 C 0.375792000 -0.640321000 1.392082000
 C -1.173924000 -0.499199000 -0.997486000
 C -0.165806000 0.601125000 -0.687327000
 C -2.426465000 -0.082583000 -0.266492000
 O -2.207527000 1.113974000 0.378116000
 C -0.923424000 1.581126000 0.173542000
 N 2.246738000 0.395585000 0.112191000
 C 2.751976000 0.937632000 -1.140786000
 O -3.466117000 -0.647273000 -0.194593000
 O -0.555528000 2.603855000 0.642253000
 C 3.237664000 -0.452963000 0.764548000
 H 0.572342000 -0.143796000 2.329934000
 H -1.188740000 -2.097222000 1.772366000
 H -0.745372000 -2.705624000 -0.823661000
 H -1.381711000 -0.645137000 -2.053864000
 H 0.229438000 1.101250000 -1.564589000
 H 3.763364000 1.300229000 -0.968717000
 H 2.786426000 0.189797000 -1.942082000
 H 2.156431000 1.789351000 -1.461814000
 H 4.124648000 0.141346000 0.977028000
 H 2.844502000 -0.832627000 1.705216000
 H 3.522286000 -1.308607000 0.141834000



E = -741.921058817 ; 7-exo-adduct
O 0.384645000 0.779637000 1.016725000
C 0.984712000 0.255358000 -0.183777000
C -0.320492000 -0.122418000 -1.023943000
C -1.302640000 0.934460000 -0.514673000
C -0.397397000 1.795759000 0.418694000
C -2.290299000 0.142583000 0.316490000
O -2.045753000 -1.201152000 0.175002000
C -0.989515000 -1.430113000 -0.685804000
C 1.444685000 1.539250000 -0.870053000
C 0.599146000 2.486301000 -0.491207000
O -0.740243000 -2.519823000 -1.076245000
O -3.160133000 0.553875000 1.007269000
N 1.946534000 -0.753422000 0.044355000
C 3.291005000 -0.252078000 0.310633000
C 1.573337000 -1.711998000 1.083285000
H 2.226743000 1.592451000 -1.610177000
H 0.535101000 3.507313000 -0.833103000
H -0.934515000 2.381753000 1.156225000
H -1.828773000 1.513223000 -1.269375000
H -0.091560000 -0.115150000 -2.084522000
H 2.221696000 -2.582480000 1.000882000
H 1.682197000 -1.277347000 2.082728000
H 0.549711000 -2.050051000 0.973032000
H 3.947121000 -1.108298000 0.456804000
H 3.671707000 0.316181000 -0.533650000
H 3.331456000 0.373453000 1.210804000

