SUPPORTING INFORMATION

A new, comprehensive insight on the competition between (4+2) and (2+4) cycloaddition schemes and molecular mechanism of Diels-Alder reaction of 2-nitrofuran with isoprene

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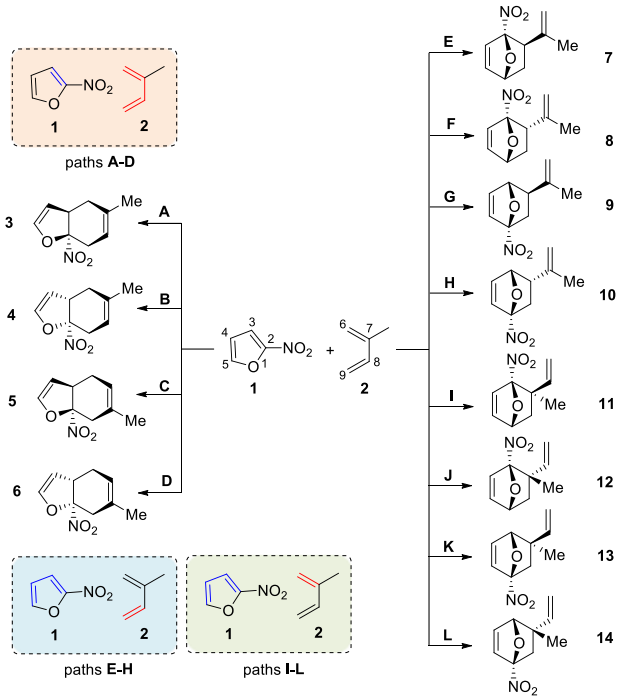


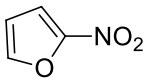
Scheme S1. Theoretically possible chemo-, regio-, and stereoselective pathways of the DA between 2-nitrofuran (**1**) and isoprene (**2**).

Table S1. ωB97XD/6-311+G(d) key parameters of the critical structures of the DA between 2-nitrofuran (**1**) and isoprene (**2**) in benzene (PCM).

Structure	Interatomic distances [Å]								l'	l''	Δl	GEDT [e]
path A-D	**C2-C3**	**C2-C6**	**C3-C6**	**C6-C7**	**C7-C8**	**C8-C9**	**C9-C2**	**C9-C3**				
MC_A	1.357		3.523	1.335	1.477	1.331	3.572					0.00
TS_A	1.419		2.244	1.378	1.409	1.379	2.156		0.54	0.59	0.04	0.14
3	1.554		1.542	1.510	1.332	1.506	1.526					
MC_B	1.357		3.624	1.335	1.478	1.332	3.232					0.00
TS_B	1.415		2.110	1.386	1.411	1.370	2.313		0.63	0.49	0.14	0.08
4	1.545		1.538	1.510	1.331	1.505	1.533					
MC_C	1.357	3.562		1.334	1.478	1.332		3.577				0.00
TS_C	1.417	2.097		1.388	1.409	1.372		2.328	0.62	0.49	0.13	0.02
5	1.553	1.524		1.512	1.332	1.505		1.544				
MC_D	1.357	3.206		1.335	1.478	1.332		3.750				0.00
TS_D	1.415	2.175		1.382	1.408	1.379		2.212	0.58	0.56	0.01	0.01
6	1.548	1.530		1.511	1.331	1.504		1.540				
path E-H	**C2-C3**	**C2-C8**	**C2-C9**	**C3-C4**	**C4-C5**	**C5-C8**	**C5-C9**	**C8-C9**				
MC_E	1.358	3.376		1.421	1.360		3.337	1.333				0.00
TS_E	1.404	2.408		1.369	1.428		1.980	1.402	0.48	0.73	0.25	0.01
7	1.516	1.581		1.328	1.519		1.556	1.554				
MC_F	1.358	3.266		1.421	1.361		3.371	1.334				0.00
TS_F	1.404	2.351		1.370	1.425		1.993	1.401	0.51	0.72	0.21	0.12
8	1.511	1.577		1.329	1.518		1.558	1.552				
MC_G	1.358		3.907	1.421	1.361	4.416		1.331				0.00
TS_G	1.418		2.006	1.371	1.410	2.363		1.397	0.72	0.50	0.22	0.06
9	1.518		1.564	1.328	1.519	1.576		1.550				
MC_H	1.358		3.225	1.421	1.360	3.794		1.332				0.00
TS_H	1.419		1.999	1.373	1.403	2.342		1.398	0.71	0.51	0.20	0.07
10	1.517		1.554	1.328	1.517	1.575		1.549				
path I-L	**C2-C3**	**C2-C6**	**C2-C7**	**C3-C4**	**C4-C5**	**C5-C6**	**C5-C7**	**C6-C7**				
MC_I	1.358		3.306	1.420	1.361	3.312		1.337				0.00
TS_I	1.402		2.500	1.370	1.431	1.944		1.408	0.43	0.75	0.32	0.04
11	1.515		1.594	1.328	1.518	1.554		1.564				
MC_J	1.358		3.361	1.421	1.361	3.329		1.337				0.00
TS_J	1.403		2.495	1.369	1.431	1.945		1.408	0.43	0.75	0.31	0.07
12	1.516		1.593	1.328	1.519	1.553		1.566				
MC_K	1.357	3.435		1.423	1.360		3.901	1.335				0.00
TS_K	1.419	2.003		1.372	1.406		2.414	1.402	0.71	0.48	0.23	0.11
13	1.518	1.554		1.328	1.519		1.585	1.556				
MC_L	1.357	3.562		1.423	1.360		4.251	1.334				0.00
TS_L	1.421	1.970		1.374	1.398		2.405	1.404	0.73	0.48	0.25	0.06
14	1.517	1.553		1.328	1.518		1.579	1.555				

Table S2. Thermochemistry and cartesian coordinates of 2-nitrofuran (**1**) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.073638 (Hartree/Particle)
Thermal correction to Energy =	0.079629 (Hartree/Particle)
Thermal correction to Enthalpy =	0.080574 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.042949 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-434.418 (Hartree/Particle)
Sum of electronic and thermal Energies =	-434.412 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-434.411 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-434.449 (Hartree/Particle)



1

Center	Coordinates (Angstroms) X	Y	Z
C	1.99438200	-0.71780900	0.00000400
C	2.13901700	0.63473200	-0.00002900
C	0.82156000	1.17286900	0.00003600
C	0.00577300	0.08767000	0.00001600
O	0.69213200	-1.06388800	-0.00000300
H	2.69320900	-1.53831500	-0.00000800
H	3.06876800	1.18158800	-0.00006100
H	0.51518400	2.20622500	0.00005300
N	-1.42008900	-0.00155300	0.00002200
O	-1.92759600	-1.10578600	-0.00000500
O	-2.02715200	1.05675000	-0.00003000

Table S3. Thermochemistry and cartesian coordinates of isoprene (**2**) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

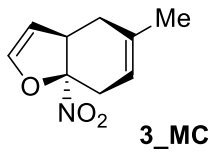
Zero-point correction =	0.113657 (Hartree/Particle)
Thermal correction to Energy =	0.119662 (Hartree/Particle)
Thermal correction to Enthalpy =	0.120607 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.084789 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-195.163 (Hartree/Particle)
Sum of electronic and thermal Energies =	-195.157 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-195.156 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-195.192 (Hartree/Particle)

2

Center	Coordinates (Angstroms) X	Y	Z
C	-2.016955000	-0.101522000	0.209816000
H	-2.944018000	-0.629529000	0.011834000
C	0.598177000	1.438330000	-0.093424000
H	1.562765000	1.908052000	0.074228000
H	-0.240361000	2.095960000	-0.299677000
H	-2.078895000	0.790881000	0.826201000
C	-0.855178000	-0.539207000	-0.271164000
C	0.456079000	0.111636000	-0.065632000
C	1.617366000	-0.821244000	0.153896000
H	1.730414000	-1.504760000	-0.694526000
H	2.555501000	-0.277519000	0.279208000
H	1.456948000	-1.441891000	1.041393000
H	-0.839293000	-1.469148000	-0.839612000

Table S4. Thermochemistry and cartesian coordinates of **MC** of product (**3**) (path A) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188263 (Hartree/Particle)
Thermal correction to Energy =	0.20223 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203174 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.144659 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.58941 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.57545 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.5745 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.63302 (Hartree/Particle)

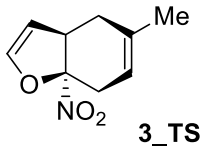


3_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-0.41732100	2.35178500	0.52398700
H	0.11307900	3.21021600	0.90544200
C	-0.58976400	1.09097300	1.15941100
H	-0.21313900	0.75702200	2.11160500
C	-1.32334900	0.36066900	0.28220100
C	-1.06113000	2.26357400	-0.67148400
H	-1.21123500	2.95478400	-1.48481000
C	0.94854700	-1.67131800	-1.57991300
H	0.29605400	-1.71424400	-2.44532900
C	2.16708700	-1.10246400	1.14802600
H	2.82196700	-0.96796200	2.00393900
O	-1.62145900	1.04890200	-0.83021500
N	-1.75974400	-0.99495800	0.34711000
O	-1.44690600	-1.61651100	1.34968500
O	-2.40151200	-1.43955300	-0.58483200
H	1.41105000	-1.87744200	1.22423800
H	1.21109600	-2.61641100	-1.11344300
C	1.40621100	-0.50979000	-1.11732900
C	2.27564600	-0.33164700	0.06390500
C	3.25724200	0.80579300	-0.02331200
H	2.72844800	1.75512100	-0.16738300
H	3.86500800	0.88768200	0.87971500
H	3.92753200	0.68362300	-0.88012500
H	1.14835800	0.40415300	-1.65367000

Table S5. Thermochemistry and cartesian coordinates of **TS** of product (**3**) (path A) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189464 (Hartree/Particle)
Thermal correction to Energy =	0.201329 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202273 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.151277 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.547 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.535 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.534 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.585 (Hartree/Particle)

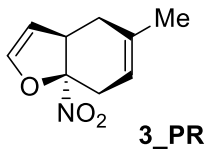


3_TS

Center	**Coordinates (Angstroms)** X	Y	Z
C	-0.56891300	1.75545600	-0.87952000
H	-1.29677600	2.26990900	-1.48783100
C	0.06844500	0.49884000	-1.17627900
H	0.31388300	0.13662500	-2.16204700
C	0.88255900	0.25678500	-0.03986200
C	-0.11417300	2.15056800	0.32600300
H	-0.33718300	3.00798600	0.94169000
C	0.01600400	-1.28994300	1.18776200
H	0.62579800	-1.23539000	2.08444500
C	-1.53494500	-1.07082800	-1.14646700
H	-2.10102300	-0.87931000	-2.05341900
O	0.84208200	1.32188000	0.81725500
N	2.17341500	-0.37721300	-0.15816600
O	2.25980800	-1.26303400	-0.99796300
O	3.06814000	-0.03693500	0.58949600
H	-0.72613000	-1.78242200	-1.25848600
H	0.34871200	-2.01971100	0.45707800
C	-1.30720500	-0.90396900	1.24366400
C	-2.09853900	-0.80140200	0.08216600
C	-3.41724900	-0.08140700	0.16527400
H	-3.25130700	1.00297300	0.16199200
H	-4.06914700	-0.32307800	-0.67608400
H	-3.94635800	-0.32655800	1.08908800
H	-1.69050700	-0.47041900	2.16399200

Table S6. Thermochemistry and cartesian coordinates of **PR** of product (**3**) (path A) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.194555 (Hartree/Particle)
Thermal correction to Energy =	0.205722 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206666 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.157085 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.639 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.628 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.627 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.677 (Hartree/Particle)

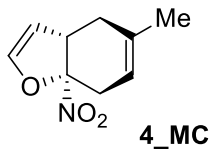


3_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.09151300	1.92900800	0.65384600
H	0.45724500	2.71805400	1.29420700
C	0.04424700	0.46949400	1.02922000
H	-0.56704700	0.30613900	1.91913500
C	-0.66659900	-0.11784000	-0.22102000
C	-0.37373000	2.07405800	-0.57661100
H	-0.48971900	2.94788100	-1.20042500
C	0.01004400	-1.33740400	-0.83922700
H	-0.47123400	-1.55868400	-1.79391300
C	1.42807800	-0.16734200	1.26859800
H	2.01611700	0.49756100	1.90718200
O	-0.76723200	0.89998900	-1.17060300
N	-2.11008500	-0.52095100	0.18006800
O	-2.19339400	-1.38914900	1.02703600
O	-3.04284400	0.02264800	-0.35761000
H	1.29215100	-1.09755400	1.83431400
H	-0.14710200	-2.19685300	-0.18009800
C	1.47696100	-1.04167300	-1.00610600
C	2.16206800	-0.47351000	-0.01549600
C	3.61934700	-0.13773500	-0.09056300
H	3.77336000	0.93937900	0.03622800
H	4.17546800	-0.63347800	0.71263500
H	4.05735500	-0.43748800	-1.04486800
H	1.95018400	-1.28854700	-1.95129300

Table S7. Thermochemistry and cartesian coordinates of **MC** of product (**4**) (path B) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188554 (Hartree/Particle)
Thermal correction to Energy =	0.202398 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203342 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145595 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.632 (Hartree/Particle)

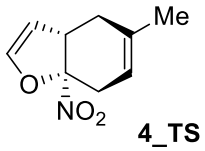


4_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.757720000	-0.501194000	1.258201000
C	-2.401781000	0.133323000	0.089417000
C	1.083013000	2.111154000	-0.821660000
H	0.770604000	3.050230000	-1.250505000
C	0.670085000	0.806551000	-1.208859000
H	-0.025160000	0.521863000	-1.981059000
C	1.333998000	-0.028153000	-0.370021000
C	1.953598000	1.941497000	0.209534000
H	2.524301000	2.624230000	0.817626000
C	-0.829371000	0.062438000	2.028771000
H	-0.461495000	1.067131000	1.836062000
H	-0.395609000	-0.467074000	2.870210000
C	-2.669212000	1.440469000	0.048270000
H	-3.127773000	1.896384000	-0.824291000
H	-2.457490000	2.093225000	0.889298000
O	2.116175000	0.634435000	0.494946000
N	1.282006000	-1.447306000	-0.243772000
O	0.568196000	-2.035972000	-1.040305000
O	1.933629000	-1.972649000	0.637099000
H	-2.053442000	-1.529651000	1.462408000
C	-2.746562000	-0.796272000	-1.043213000
H	-1.855793000	-1.320375000	-1.402731000
H	-3.448959000	-1.566796000	-0.707647000
H	-3.203524000	-0.263424000	-1.879537000

Table S8. Thermochemistry and cartesian coordinates of **TS** of product (**4**) (path B) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189600 (Hartree/Particle)
Thermal correction to Energy =	0.201471 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202415 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.151451 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.547 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.535 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.534 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.585 (Hartree/Particle)

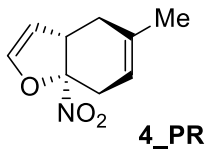


4_TS

Center	**Coordinates (Angstroms)** X	Y	Z
C	-1.604634000	-0.531862000	1.200543000
C	-2.116527000	0.437478000	0.312176000
C	1.310349000	2.017395000	-0.641056000
H	1.238324000	3.017926000	-1.039249000
C	0.356697000	0.937316000	-0.837292000
H	-0.174574000	0.756947000	-1.759796000
C	0.921136000	-0.125230000	-0.092232000
C	2.277489000	1.550310000	0.167614000
H	3.149997000	2.012384000	0.602517000
C	-0.380639000	-0.395346000	1.799928000
H	0.053501000	0.573694000	2.017822000
H	0.058400000	-1.224341000	2.345536000
C	-1.406640000	1.610407000	0.106706000
H	-1.771738000	2.329692000	-0.621042000
H	-0.833512000	2.048845000	0.913152000
O	2.106986000	0.237471000	0.476883000
N	0.799757000	-1.493581000	-0.471417000
O	-0.186263000	-1.779503000	-1.141826000
O	1.638620000	-2.293608000	-0.091852000
H	-2.085948000	-1.505806000	1.218520000
C	-3.223369000	0.051376000	-0.629395000
H	-2.801548000	-0.417904000	-1.526087000
H	-3.897227000	-0.677026000	-0.173294000
H	-3.811886000	0.914714000	-0.945752000

Table S9. Thermochemistry and cartesian coordinates of **PR** of product (**4**) (path B) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.194396 (Hartree/Particle)
Thermal correction to Energy =	0.205628 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206572 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.156632 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.638 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.627 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.626 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.676 (Hartree/Particle)

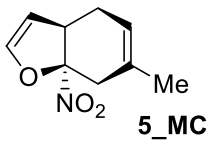


4_PR

Center	Coordinates (Angstroms) X	Y	Z
C	1.673706000	0.978842000	0.818381000
C	2.257240000	0.013237000	0.111716000
C	-0.948360000	-1.983439000	-0.688526000
H	-0.917209000	-2.817776000	-1.373133000
C	0.033899000	-0.840937000	-0.661605000
H	0.120247000	-0.332409000	-1.623327000
C	-0.652770000	0.092683000	0.359415000
C	-1.815353000	-1.814263000	0.298324000
H	-2.644125000	-2.416674000	0.639018000
C	0.271851000	0.821450000	1.341829000
H	0.275473000	0.205317000	2.247430000
H	-0.160544000	1.781551000	1.629186000
C	1.449989000	-1.224432000	-0.200307000
H	1.929719000	-1.822803000	-0.979579000
H	1.380616000	-1.866631000	0.687281000
O	-1.606130000	-0.668076000	1.034392000
N	-1.429110000	1.183345000	-0.443580000
O	-0.747676000	1.913057000	-1.134473000
O	-2.627460000	1.255375000	-0.320013000
H	2.203473000	1.895251000	1.059551000
C	3.660055000	0.089186000	-0.407633000
H	3.672641000	0.028795000	-1.501509000
H	4.154183000	1.016434000	-0.110435000
H	4.257896000	-0.751276000	-0.038234000

Table S10. Thermochemistry and cartesian coordinates of **MC** of product (**5**) (path C) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188661 (Hartree/Particle)
Thermal correction to Energy =	0.202435 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203379 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145905 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.632 (Hartree/Particle)

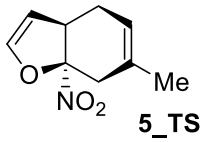


5_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.58355700	1.83380300	1.01592700
H	-1.59537000	2.71777900	1.63398500
C	-1.06186000	0.55335400	1.35065200
H	-0.58468900	0.23652900	2.26302600
C	-1.28327700	-0.20781900	0.24925200
C	-2.06694500	1.72534700	-0.25092600
H	-2.54686400	2.41804000	-0.92279500
C	1.86959100	-0.84422900	-1.28060900
H	1.40931000	-0.99561600	-2.25197800
C	2.41352500	-0.23475400	1.65404100
H	2.89305000	-0.01076900	2.60170900
O	-1.88698300	0.47978000	-0.73183400
N	-0.98231900	-1.57838400	-0.00443100
O	-0.44772900	-2.19188400	0.90510900
O	-1.27272600	-2.04120800	-1.08979300
H	1.82922400	-1.14887700	1.59756700
H	2.27829400	-1.72094500	-0.78854300
C	1.93319800	0.36591600	-0.72178300
C	2.53244400	0.58512000	0.61126500
H	3.08708000	1.51563900	0.73378800
C	1.42507000	1.60132600	-1.41648700
H	2.24640300	2.29974200	-1.61134100
H	0.94914500	1.36206900	-2.36919200
H	0.70100900	2.13320800	-0.79106300

Table S11. Thermochemistry and cartesian coordinates of **TS** of product (**5**) (path C) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189271 (Hartree/Particle)
Thermal correction to Energy =	0.20123 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202174 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.150951 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.545 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.533 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.532 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.583 (Hartree/Particle)

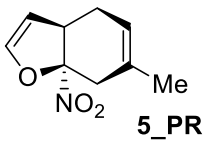


5_TS

Center	Coordinates (Angstroms) X	Y	Z
C	0.249090000	2.208258000	-0.095306000
H	0.732212000	3.126491000	0.201118000
C	-0.371596000	1.245248000	0.770014000
H	-0.845253000	1.447746000	1.716707000
C	-0.779759000	0.208464000	-0.105654000
C	0.158980000	1.724319000	-1.349386000
H	0.508676000	2.093364000	-2.300742000
C	0.425912000	-1.498706000	0.068590000
H	0.043342000	-2.113323000	-0.742521000
C	1.357732000	0.306036000	2.014405000
H	1.694596000	1.095944000	2.677874000
O	-0.553670000	0.566532000	-1.406463000
N	-2.034635000	-0.493842000	0.112442000
O	-2.313614000	-0.740120000	1.275485000
O	-2.699303000	-0.817831000	-0.848944000
H	0.554773000	-0.308605000	2.402615000
H	-0.005170000	-1.719879000	1.039080000
C	1.715487000	-0.993359000	-0.021336000
C	2.159991000	-0.110068000	0.982277000
H	3.090114000	0.425597000	0.806336000
C	2.540191000	-1.221365000	-1.261396000
H	3.074719000	-2.175111000	-1.202482000
H	1.906870000	-1.261847000	-2.151188000
H	3.284094000	-0.435094000	-1.407762000

Table S12. Thermochemistry and cartesian coordinates of **PR** of product (**5**) (path C) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.194623 (Hartree/Particle)
Thermal correction to Energy =	0.205773 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206717 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.157264 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.639 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.628 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.627 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.677 (Hartree/Particle)

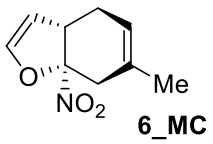


5_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.48386100	2.16472200	0.24839000
H	0.50817500	3.22410000	0.03998000
C	0.30999100	1.08811000	-0.79254700
H	1.09846800	1.13033300	-1.54665000
C	0.48294800	-0.17948800	0.08763100
C	0.58260100	1.60149500	1.44162000
H	0.69910800	2.02559500	2.42781700
C	-0.57860000	-1.25642300	-0.09807800
H	-0.43805500	-2.02232300	0.66884700
C	-1.05543800	1.11358300	-1.51196400
H	-1.29052400	2.14400700	-1.78797000
O	0.50823100	0.22892600	1.42163700
N	1.86549000	-0.81169300	-0.22975300
O	2.00821900	-1.20949600	-1.36952300
O	2.69425200	-0.88063000	0.64375700
H	-0.96024100	0.55695300	-2.45282900
H	-0.43703100	-1.73161900	-1.07342800
C	-1.94749100	-0.62009200	-0.00594800
C	-2.15373000	0.51052800	-0.67837500
H	-3.11997100	1.00575800	-0.64356700
C	-2.97363100	-1.30382300	0.84284700
H	-3.14288000	-2.33121700	0.50242800
H	-2.63490100	-1.36571100	1.88261700
H	-3.92927000	-0.77608300	0.82260400

Table S13. Thermochemistry and cartesian coordinates of **MC** of product (**6**) (path D) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188426 (Hartree/Particle)
Thermal correction to Energy =	0.202312 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203256 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145363 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.633 (Hartree/Particle)

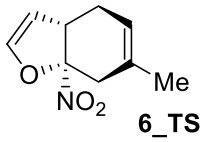


6_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.936593000	0.189141000	0.622538000
C	-2.079185000	1.013318000	-0.595615000
C	2.234216000	1.660036000	-0.212371000
H	-2.268251000	0.461778000	-1.515668000
H	2.539997000	2.672708000	-0.423540000
C	1.390691000	0.830297000	-1.001553000
H	0.895971000	1.059462000	-1.930524000
C	1.312646000	-0.335584000	-0.311574000
C	2.583167000	0.919489000	0.874350000
H	3.203842000	1.112495000	1.734094000
C	-1.104012000	0.525394000	1.610553000
H	-0.477407000	1.410760000	1.550865000
H	-1.006434000	-0.087119000	2.501450000
C	-2.021404000	2.342962000	-0.642676000
H	-2.128328000	2.878037000	-1.580780000
H	-1.883363000	2.942168000	0.252988000
O	2.026271000	-0.306038000	0.822961000
N	0.560473000	-1.516910000	-0.577029000
O	-0.099354000	-1.518002000	-1.604767000
O	0.612671000	-2.429181000	0.224162000
C	-2.750375000	-1.076497000	0.651530000
H	-2.484073000	-1.719891000	-0.193671000
H	-2.587561000	-1.640175000	1.571494000
H	-3.819319000	-0.857427000	0.562555000

Table S14. Thermochemistry and cartesian coordinates of **TS** of product (**6**) (path D) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189592 (Hartree/Particle)
Thermal correction to Energy =	0.201459 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202403 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.151465 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.546 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.534 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.533 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.584 (Hartree/Particle)

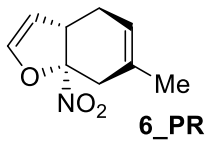


6_TS

Center	Coordinates (Angstroms) X	Y	Z
C	-1.81226700	-0.62024000	-0.57361500
C	-1.54770100	-1.68535100	0.30807200
C	2.35320300	-1.14335000	0.37182900
H	-2.24743200	-1.84739600	1.12482500
H	2.92914900	-1.98299500	0.72989000
C	1.06607900	-0.70391000	0.86814000
H	0.74065100	-0.76722800	1.89304400
C	0.74956100	0.39502900	0.03495900
C	2.68575100	-0.32680000	-0.64468300
H	3.52782400	-0.30333400	-1.31843100
C	-0.79002900	-0.17653700	-1.39068800
H	-0.03649100	-0.85846900	-1.77043700
H	-0.92085900	0.72023800	-1.98981400
C	-0.33283500	-2.33597500	0.34766300
H	-0.14502200	-3.06936400	1.12548600
H	0.25910700	-2.46893100	-0.54843800
O	1.77162800	0.66467600	-0.82953300
N	0.04507000	1.55318300	0.52983400
O	-0.71897000	1.35465600	1.46209800
O	0.21494000	2.62519200	-0.01881500
C	-3.08681300	0.16920600	-0.43220300
H	-3.39526900	0.25160600	0.61239200
H	-2.97688400	1.17931800	-0.83205300
H	-3.90075300	-0.31434800	-0.98215400

Table S15. Thermochemistry and cartesian coordinates of **PR** of product (**6**) (path D) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.194454 (Hartree/Particle)
Thermal correction to Energy =	0.205644 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206589 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.156727 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.638 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.627 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.626 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.676 (Hartree/Particle)

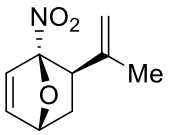


6_PR

Center	Coordinates (Angstroms) X	Y	Z
C	-2.049361000	-0.170121000	-0.275571000
C	-1.920353000	-1.286606000	0.437939000
C	1.923914000	-1.505789000	0.459889000
H	-2.760015000	-1.682719000	1.001997000
H	2.428193000	-2.252909000	1.054266000
C	0.537174000	-0.977969000	0.721294000
H	0.424541000	-0.564974000	1.725665000
C	0.469770000	0.161936000	-0.323747000
C	2.391732000	-0.937114000	-0.640418000
H	3.320166000	-1.063895000	-1.176829000
C	-0.858519000	0.318543000	-1.067541000
H	-0.757635000	-0.279480000	-1.979574000
H	-0.989608000	1.353141000	-1.391943000
C	-0.595565000	-1.996841000	0.500253000
H	-0.575483000	-2.734467000	1.305418000
H	-0.403718000	-2.546187000	-0.430932000
O	1.525722000	-0.030581000	-1.213088000
N	0.747283000	1.500058000	0.427407000
O	-0.131522000	1.873207000	1.178086000
O	1.789800000	2.074513000	0.230204000
C	-3.311711000	0.627176000	-0.381814000
H	-4.127508000	0.166774000	0.178954000
H	-3.156172000	1.640310000	0.003694000
H	-3.628227000	0.727597000	-1.425895000

Table S16. Thermochemistry and cartesian coordinates of **MC** of product (**7**) (path E) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188959 (Hartree/Particle)
Thermal correction to Energy =	0.202588 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203532 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.146657 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.594 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.58 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.579 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.636 (Hartree/Particle)

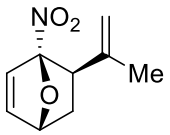


7_MC

Center	Coordinates (Angstroms) X	Y	Z
C	1.25346400	0.44831200	0.03748000
C	1.88156800	-1.46965000	0.76095300
H	1.93967600	-2.23372300	1.51860100
O	1.21696100	-0.35252500	1.11185400
N	0.62836700	1.72539300	0.15371200
O	0.10821400	2.01707700	1.21280200
O	0.66346400	2.43696100	-0.83625200
C	-1.15063100	-2.50983000	-0.16691700
H	-0.67825900	-3.35741800	-0.65189600
H	-1.37994500	-2.61883900	0.88878700
C	2.34693100	-1.38106700	-0.51421700
C	1.93058900	-0.11142900	-0.99792100
H	2.10103000	0.33241900	-1.96519700
H	2.91050000	-2.13217300	-1.04498000
C	-2.06461200	-0.19169700	-0.29142800
C	-2.27655300	0.86463100	-1.08307000
H	-1.99428400	0.85316800	-2.13190100
H	-2.72613400	1.77849500	-0.70847600
C	-1.43181700	-1.39739800	-0.84623300
H	-1.17454100	-1.35037700	-1.90316000
C	-2.43954200	-0.18512300	1.16446600
H	-1.56135100	-0.35008200	1.79531100
H	-2.88310800	0.76868700	1.45233500
H	-3.15764900	-0.98050400	1.38868500

Table S17. Thermochemistry and cartesian coordinates of **TS** of product (**7**) (path E) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189996 (Hartree/Particle)
Thermal correction to Energy =	0.201615 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202559 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.15258 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.553 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.541 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.54 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.59 (Hartree/Particle)

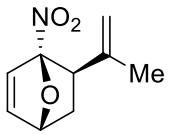


7_TS

Center	Coordinates (Angstroms) X	Y	Z
C	0.746911000	0.764994000	0.135256000
C	1.929385000	-0.919631000	0.633997000
H	2.346896000	-1.612636000	1.350887000
O	0.996315000	-0.067809000	1.160849000
N	-0.314826000	1.693655000	0.288484000
O	-1.003020000	1.628510000	1.290884000
O	-0.511951000	2.454434000	-0.651079000
C	0.673152000	-2.016579000	-0.433680000
H	1.374077000	-2.466590000	-1.127109000
H	0.359536000	-2.685877000	0.362154000
C	2.649900000	-0.207472000	-0.372641000
C	1.858032000	0.854469000	-0.719084000
H	1.975073000	1.564089000	-1.522725000
H	3.549781000	-0.552064000	-0.859737000
C	-1.623751000	-0.947262000	-0.405459000
C	-2.519501000	-0.215229000	-1.084926000
H	-2.269225000	0.253530000	-2.031648000
H	-3.528016000	-0.065997000	-0.714472000
C	-0.278182000	-1.124817000	-0.948518000
H	-0.117975000	-0.722463000	-1.944045000
C	-1.965540000	-1.590594000	0.911473000
H	-1.253266000	-1.299333000	1.687041000
H	-2.961531000	-1.293822000	1.242027000
H	-1.944762000	-2.682777000	0.834492000

Table S18. Thermochemistry and cartesian coordinates of **PR** of product (**7**) (path E) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193892 (Hartree/Particle)
Thermal correction to Energy =	0.205071 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206015 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.156638 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.603 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.592 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.591 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.64 (Hartree/Particle)

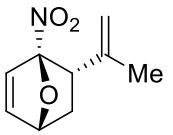


7_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.54352100	0.48677800	-0.00089000
C	1.85922200	-1.05466100	0.51867600
H	2.41079100	-1.63460500	1.25291500
O	1.00481000	-0.10432000	1.17849100
N	-0.36618100	1.63747100	0.26319700
O	-0.82745600	1.77400000	1.37054300
O	-0.60805900	2.33815900	-0.70018700
C	0.82462600	-1.83499400	-0.34182900
H	1.28054800	-2.32784600	-1.20042300
H	0.33501600	-2.59166600	0.26951700
C	2.64561600	-0.15882500	-0.42277000
C	1.81424300	0.82174600	-0.75646100
H	1.91344700	1.61589700	-1.48166900
H	3.63332000	-0.36572000	-0.81169900
C	-1.60902500	-0.90425000	-0.35326100
C	-2.57030100	-0.57385200	-1.21447300
H	-2.34494300	-0.19422800	-2.20660100
H	-3.62028500	-0.66592100	-0.95419900
C	-0.16372400	-0.70920400	-0.75598700
H	-0.12082900	-0.51030600	-1.82667200
C	-1.92196000	-1.42877300	1.02346100
H	-1.34416600	-0.91044800	1.79114100
H	-2.98272400	-1.30969900	1.24922600
H	-1.68457500	-2.49426100	1.10650900

Table S19. Thermochemistry and cartesian coordinates of **MC** of product (**8**) (path F) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188833 (Hartree/Particle)
Thermal correction to Energy =	0.202543 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203487 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145914 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.594 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.58 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.579 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.637 (Hartree/Particle)

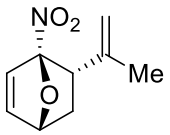


8_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.306997000	-0.085377000	-0.229567000
C	-1.614230000	1.985790000	0.225421000
C	1.602608000	0.383486000	1.178972000
H	-1.876274000	2.790033000	0.893124000
O	-1.664692000	0.750212000	0.755296000
N	-1.245420000	-1.475731000	0.080361000
O	-1.396304000	-1.815091000	1.239392000
O	-1.028992000	-2.229686000	-0.852682000
C	1.569413000	1.711340000	1.298549000
H	1.921296000	2.375802000	0.515411000
H	1.185691000	2.181036000	2.198080000
C	2.095615000	-0.357548000	0.009049000
C	2.067939000	-1.694036000	0.012900000
H	1.690086000	-2.251258000	0.865353000
H	2.410151000	-2.276036000	-0.836716000
C	-1.238278000	1.942241000	-1.081988000
C	-1.036056000	0.569215000	-1.387656000
H	-0.724743000	0.121099000	-2.317120000
H	-1.118521000	2.786126000	-1.743197000
C	2.608751000	0.424607000	-1.168115000
H	3.470853000	1.038433000	-0.888216000
H	2.913393000	-0.237298000	-1.980365000
H	1.842342000	1.106125000	-1.551415000
H	1.230980000	-0.225736000	2.001092000

Table S20. Thermochemistry and cartesian coordinates of **TS** of product (**8**) (path F) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.190007 (Hartree/Particle)
Thermal correction to Energy =	0.201636 (Hartree/Particle)
Thermal correction to Enthalpy =	0.20258 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.152413 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.553 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.541 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.54 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.59 (Hartree/Particle)

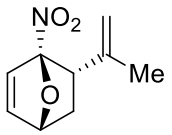


8_TS

Center	Coordinates (Angstroms) X	Y	Z
C	1.00303600	0.26463300	0.29788200
C	0.34837800	2.21250800	-0.20064800
C	-0.88487700	-0.04986800	-1.06691300
H	0.47897000	3.17007700	-0.68441400
O	1.31106200	1.28960300	-0.51604800
N	1.69212700	-0.96253700	0.11525800
O	2.41201100	-1.09257300	-0.86289500
O	1.45088200	-1.84021600	0.93371600
C	-1.10969000	1.32361900	-1.22809400
H	-2.00642000	1.76544500	-0.80574200
H	-0.81025200	1.76062200	-2.17523900
C	-1.71252100	-0.95235000	-0.26786200
C	-1.48255300	-2.27276000	-0.31177200
H	-0.69573700	-2.69244200	-0.93082100
H	-2.07647600	-2.97386800	0.26524900
C	-0.04149200	1.99559300	1.15321100
C	0.35318900	0.71968700	1.45683900
H	0.14049700	0.12404200	2.33003200
H	-0.66095500	2.65801800	1.73917800
C	-2.81690900	-0.36835700	0.57233600
H	-3.58933200	0.08359300	-0.05848700
H	-3.29065500	-1.13528500	1.18683800
H	-2.44643500	0.41660900	1.23736900
H	-0.21909900	-0.52978700	-1.77882200

Table S21. Thermochemistry and cartesian coordinates of **PR** of product (**8**) (path F) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193920 (Hartree/Particle)
Thermal correction to Energy =	0.205108 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206052 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.156121 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.601 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.639 (Hartree/Particle)

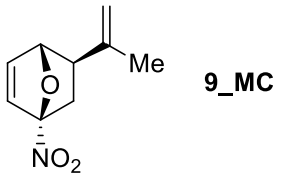


8_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.722275000	0.031977000	0.095956000
C	0.737858000	2.064232000	-0.405020000
C	-0.566000000	0.080958000	-0.812937000
H	1.220816000	2.945869000	-0.816146000
O	1.572072000	0.907965000	-0.591121000
N	1.303187000	-1.342636000	0.163059000
O	1.950293000	-1.726330000	-0.784727000
O	1.028050000	-2.000595000	1.145360000
C	-0.577138000	1.605515000	-1.103748000
H	-1.448686000	2.121585000	-0.701620000
H	-0.527260000	1.794573000	-2.176032000
C	-1.801935000	-0.576451000	-0.244208000
C	-2.041981000	-1.854605000	-0.534821000
H	-1.390150000	-2.424491000	-1.191142000
H	-2.897657000	-2.380991000	-0.123668000
C	0.487476000	2.020160000	1.091197000
C	0.474954000	0.730554000	1.412893000
H	0.234203000	0.241838000	2.344641000
H	0.256013000	2.871575000	1.716855000
C	-2.729429000	0.219176000	0.633687000
H	-3.270787000	0.971372000	0.050430000
H	-3.470225000	-0.428754000	1.104723000
H	-2.192592000	0.753921000	1.420930000
H	-0.275778000	-0.445465000	-1.724476000

Table S22. Thermochemistry and cartesian coordinates of **MC** of product (**9**) (path G) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188595 (Hartree/Particle)
Thermal correction to Energy =	0.20237 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203314 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145894 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.632 (Hartree/Particle)

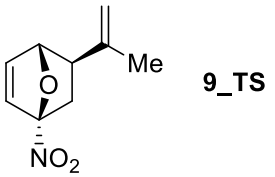


9_MC

Center	Coordinates (Angstroms) X	Y	Z
C	1.27369400	0.40987500	0.14516700
C	0.69363200	2.26829400	-0.75034000
H	0.55609600	2.91919600	-1.59808200
O	1.18859200	1.04784100	-1.02926600
N	1.74995900	-0.93454900	0.12655600
O	2.03020200	-1.43266500	-0.94569700
O	1.83218800	-1.49270100	1.20866700
C	-1.47374800	-1.40529700	0.39285200
C	0.47586700	2.41402300	0.58470600
C	0.85892800	1.18263700	1.18198300
H	0.83241000	0.89830100	2.22135500
H	0.08549000	3.28940600	1.07951300
C	-1.26826600	-2.52308100	-0.30077000
H	-0.79029200	-3.38420800	0.15345900
H	-1.56792200	-2.61728800	-1.34048300
C	-2.07980800	-0.16121300	-0.12669100
C	-1.94420900	0.22374800	-1.39747500
H	-2.40883300	1.13439800	-1.76354000
H	-1.35453000	-0.34602600	-2.10845400
C	-2.82955200	0.66370200	0.88410300
H	-3.23269400	1.57734700	0.44327600
H	-3.65759400	0.09530400	1.31974900
H	-2.17009200	0.94768500	1.71193100
H	-1.18884200	-1.38820000	1.44455800

Table S23. Thermochemistry and cartesian coordinates of **TS** of product (**9**) (path G) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189617 (Hartree/Particle)
Thermal correction to Energy =	0.201426 (Hartree/Particle)
Thermal correction to Enthalpy =	0.20237 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.15133 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.547 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.535 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.534 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.585 (Hartree/Particle)

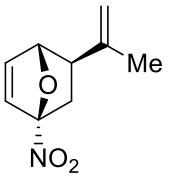


9_TS

Center	Coordinates (Angstroms) X	Y	Z
C	1.199263000	0.290512000	-0.093144000
C	-0.498051000	1.171739000	-0.984095000
H	-1.328829000	1.197723000	-1.672533000
O	0.328064000	0.107676000	-1.111156000
N	2.289452000	-0.667142000	-0.028753000
O	2.254572000	-1.633892000	-0.759128000
O	3.144495000	-0.440495000	0.808427000
C	-1.336913000	0.214827000	0.886828000
C	0.204050000	2.230398000	-0.371446000
C	1.334778000	1.677092000	0.171503000
H	2.079258000	2.123737000	0.810979000
H	-0.153520000	3.244432000	-0.272152000
C	-0.128190000	-0.300292000	1.361147000
H	0.346254000	0.164259000	2.216755000
H	0.054922000	-1.367889000	1.279029000
C	-2.371507000	-0.590875000	0.199874000
C	-2.132124000	-1.770312000	-0.379868000
H	-2.923052000	-2.317137000	-0.882801000
H	-1.148338000	-2.227736000	-0.387715000
C	-3.736926000	0.043709000	0.168133000
H	-4.457889000	-0.569492000	-0.374930000
H	-4.117499000	0.201868000	1.182576000
H	-3.697466000	1.029269000	-0.310350000
H	-1.703337000	1.123859000	1.353673000

Table S24. Thermochemistry and cartesian coordinates of **PR** of product (**9**) (path G) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193776 (Hartree/Particle)
Thermal correction to Energy =	0.204976 (Hartree/Particle)
Thermal correction to Enthalpy =	0.20592 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.155799 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.601 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.639 (Hartree/Particle)

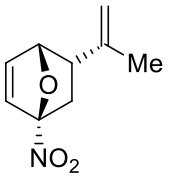


9_PR

Center	Coordinates (Angstroms) X	Y	Z
C	1.07016000	0.18943000	0.03417800
C	-0.65558200	1.02487600	-0.79529000
H	-1.35743900	1.16228400	-1.61312700
O	0.34311800	0.06048000	-1.15323800
N	2.30059600	-0.65638800	0.02484100
O	2.43242600	-1.48710800	-0.84064000
O	3.07491000	-0.45248500	0.94066400
C	-1.24783200	0.37382000	0.51196700
C	0.19436500	2.20875300	-0.36841800
C	1.29702100	1.68556000	0.15568700
H	2.12121000	2.15065700	0.67642700
H	-0.11198400	3.24557400	-0.39592600
C	0.03976900	-0.24369300	1.11405200
H	0.29262700	0.14495200	2.09879400
H	-0.01296300	-1.33064600	1.16792200
C	-2.37607400	-0.57899400	0.17510400
C	-2.18724500	-1.82807100	-0.24247600
H	-3.02714400	-2.45690500	-0.52133700
H	-1.20156900	-2.26917300	-0.34367300
C	-3.74623700	0.03464800	0.26930400
H	-4.52574700	-0.65458800	-0.05956800
H	-3.96706500	0.33792000	1.29852500
H	-3.81216300	0.94002600	-0.34543500
H	-1.63563700	1.15953100	1.16457400

Table S25. Thermochemistry and cartesian coordinates of **MC** of product (**10**) (path H) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188267 (Hartree/Particle)
Thermal correction to Energy =	0.202302 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203246 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.143656 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.574 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.574 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.633 (Hartree/Particle)

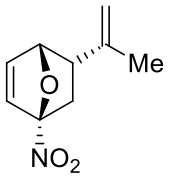


10_MC

Center	Coordinates (Angstroms) X	Y	Z
C	1.353975000	0.508146000	0.238132000
C	0.294850000	2.182505000	-0.578130000
C	-0.516458000	-1.747160000	-1.110143000
H	0.005296000	-2.003945000	-2.025575000
H	-0.077139000	-2.103452000	-0.182586000
C	-1.640814000	-1.032924000	-1.134393000
H	0.083390000	2.890465000	-1.362831000
O	1.253960000	1.278572000	-0.854630000
N	2.293029000	-0.563438000	0.196258000
O	2.960573000	-0.708165000	-0.809574000
O	2.350355000	-1.272380000	1.189100000
C	-2.444327000	-0.619699000	0.035507000
C	-2.396186000	-1.253449000	1.209655000
H	-2.987503000	-0.917423000	2.055911000
H	-1.783561000	-2.135912000	1.364468000
C	0.493869000	0.886684000	1.217869000
C	-0.203690000	1.998783000	0.674070000
H	0.374623000	0.422921000	2.182953000
H	-0.980010000	2.578344000	1.148098000
H	-2.010890000	-0.688372000	-2.099427000
C	-3.348276000	0.561919000	-0.194479000
H	-2.779838000	1.424480000	-0.556606000
H	-4.095652000	0.330619000	-0.961145000
H	-3.876680000	0.853285000	0.715240000

Table S26. Thermochemistry and cartesian coordinates of **TS** of product (**10**) (path H) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189526 (Hartree/Particle)
Thermal correction to Energy =	0.201389 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202333 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.151017 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.549 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.537 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.536 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.587 (Hartree/Particle)

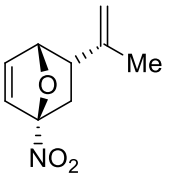


10_TS

Center	Coordinates (Angstroms) X	Y	Z
C	1.15541300	0.16999600	0.20341100
C	-0.36202300	1.64033600	0.27475200
C	-0.02997100	-0.82983500	-1.05798000
H	0.60700400	-0.69818200	-1.92778100
H	0.02236200	-1.82228600	-0.62426900
C	-1.22625900	-0.10821700	-1.02228600
H	-0.85280500	2.54587700	-0.04650100
O	0.84340700	1.39358300	-0.29583200
N	2.49948200	-0.29776700	-0.11095800
O	3.16357400	0.33841400	-0.89970300
O	2.83480100	-1.33987900	0.42146000
C	-2.42756100	-0.53110700	-0.28717500
C	-2.47151700	-1.60969200	0.50352300
H	-3.37173400	-1.86446300	1.05348300
H	-1.62805400	-2.28056300	0.62777200
C	0.55239400	0.01177700	1.47789400
C	-0.45972000	0.93953700	1.48582800
H	0.76777000	-0.77451700	2.18325400
H	-1.25151600	1.04494800	2.21133100
H	-1.38817900	0.62439200	-1.80726500
C	-3.62221800	0.37116700	-0.44689800
H	-3.39366200	1.38327700	-0.09394200
H	-3.90527900	0.46054100	-1.50059600
H	-4.48775400	0.00463400	0.10740400

Table S27. Thermochemistry and cartesian coordinates of **PR** of product (**10**) (path H) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193838 (Hartree/Particle)
Thermal correction to Energy =	0.205065 (Hartree/Particle)
Thermal correction to Enthalpy =	0.206009 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.155787 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.602 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.591 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.64 (Hartree/Particle)

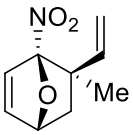


10_PR

Center	Coordinates (Angstroms) X	Y	Z
C	-1.092175000	-0.067813000	0.071613000
C	0.594231000	-1.299481000	0.016723000
C	-0.124563000	0.878226000	-0.691338000
H	-0.513984000	1.095899000	-1.686641000
H	0.010654000	1.813139000	-0.153469000
C	1.124027000	-0.035434000	-0.758512000
H	1.088397000	-2.238626000	-0.214461000
O	-0.766516000	-1.330548000	-0.435170000
N	-2.532297000	0.262571000	-0.142088000
O	-3.205297000	-0.467978000	-0.827207000
O	-2.910309000	1.289025000	0.390424000
C	2.450067000	0.481325000	-0.258800000
C	2.668058000	1.725824000	0.157997000
H	3.654228000	2.036053000	0.489881000
H	1.896789000	2.486765000	0.182959000
C	-0.643136000	-0.135466000	1.518573000
C	0.433217000	-0.912768000	1.474968000
H	-1.059329000	0.447321000	2.327295000
H	1.129305000	-1.137989000	2.270937000
H	1.261798000	-0.360715000	-1.794849000
C	3.555526000	-0.542095000	-0.289780000
H	3.359592000	-1.362227000	0.410055000
H	3.645119000	-0.991952000	-1.284305000
H	4.518971000	-0.103563000	-0.025834000

Table S28. Thermochemistry and cartesian coordinates of **MC** of product (**11**) (path I) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189078 (Hartree/Particle)
Thermal correction to Energy =	0.202629 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203573 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.14705 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.594 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.58 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.579 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.636 (Hartree/Particle)

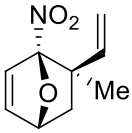


11_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.20843300	0.46857900	0.12850000
C	-2.09303000	-1.26729000	-0.76372200
H	-2.40809700	-1.85092600	-1.61312400
O	-1.53520500	-0.07696000	-1.05110500
N	-0.59477800	1.75589000	0.10615800
O	-0.48276700	2.32294500	-0.96202200
O	-0.22172700	2.19413800	1.18283800
C	1.07455600	-2.23453300	-0.75896100
H	0.73367400	-3.12753900	-0.24471700
H	0.94848000	-2.21169000	-1.83769500
C	-2.14002700	-1.47365400	0.58073800
C	-1.55335600	-0.32491100	1.17537600
H	-1.40283900	-0.10780400	2.22022000
H	-2.53836600	-2.34110100	1.08313700
C	2.07322600	-0.02195900	-0.84222400
H	1.89612500	-0.04221000	-1.91601400
C	2.64643900	1.05560900	-0.30593100
H	2.84259700	1.14355700	0.75797900
H	2.93019500	1.90162900	-0.92197700
C	1.62939500	-1.21131200	-0.10063000
C	1.81627300	-1.23533200	1.39120400
H	2.87807400	-1.19545200	1.65431000
H	1.33898300	-0.37081100	1.86296300
H	1.39196000	-2.14105600	1.82801000

Table S29. Thermochemistry and cartesian coordinates of **TS** of product (**11**) (path I) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189685 (Hartree/Particle)
Thermal correction to Energy =	0.20142 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202364 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.152297 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.554 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.542 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.541 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.592 (Hartree/Particle)

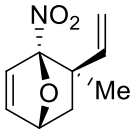


11_TS

Center	Coordinates (Angstroms) X	Y	Z
C	-0.293567000	1.001225000	0.043729000
C	-2.040871000	0.173373000	-0.827860000
H	-2.730323000	0.071232000	-1.654796000
O	-0.882105000	0.830228000	-1.154091000
N	1.041079000	1.453118000	0.071057000
O	1.613839000	1.657136000	-0.986367000
O	1.565177000	1.534258000	1.179931000
C	-1.290098000	-1.609961000	-0.641617000
H	-2.098203000	-2.114204000	-0.120590000
H	-1.249527000	-1.840977000	-1.703036000
C	-2.392573000	0.546348000	0.508171000
C	-1.242449000	1.028253000	1.075030000
H	-1.045244000	1.297297000	2.100498000
H	-3.332529000	0.327425000	0.992182000
C	1.166192000	-1.417847000	-0.759364000
H	1.034137000	-1.246555000	-1.825336000
C	2.410143000	-1.525811000	-0.277950000
H	2.616476000	-1.698778000	0.773209000
H	3.267019000	-1.452398000	-0.937592000
C	-0.056529000	-1.487233000	0.026371000
C	0.027506000	-1.744603000	1.503053000
H	0.352800000	-2.774427000	1.690425000
H	0.742399000	-1.079657000	1.995308000
H	-0.946368000	-1.616225000	1.979170000

Table S30. Thermochemistry and cartesian coordinates of **PR** of product (**11**) (path I) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193866 (Hartree/Particle)
Thermal correction to Energy =	0.204802 (Hartree/Particle)
Thermal correction to Enthalpy =	0.205747 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.157541 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.601 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.637 (Hartree/Particle)

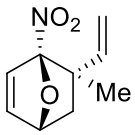


11_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.33767700	-0.54484400	-0.00038800
C	1.94959900	0.50027900	-0.83089500
H	2.64752000	0.69632800	-1.63977300
O	0.97592200	-0.47501400	-1.24174700
N	-0.73980000	-1.57621400	0.00707100
O	-1.09817400	-2.05398800	-1.04143000
O	-1.20541500	-1.83274200	1.10182200
C	1.02831300	1.68049600	-0.41369200
H	1.50129700	2.34441000	0.31130100
H	0.74901300	2.26788300	-1.28903300
C	2.49240400	-0.12733200	0.44055400
C	1.47271600	-0.79166900	0.97230000
H	1.38094900	-1.29855100	1.92134200
H	3.47614300	0.04171200	0.85704400
C	-1.40633000	1.11222500	-0.72389900
H	-1.21771500	0.87797600	-1.76928000
C	-2.62372200	1.49531000	-0.35872400
H	-2.88325500	1.73688900	0.66678900
H	-3.41797900	1.58074000	-1.09268500
C	-0.21287900	0.93999900	0.18451200
C	-0.49518800	1.30945800	1.63434600
H	-0.81448800	2.35248000	1.69905600
H	-1.27881700	0.68340900	2.06587200
H	0.40172600	1.20064200	2.24603900

Table S31. Thermochemistry and cartesian coordinates of **MC** of product (**12**) (path J) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189135 (Hartree/Particle)
Thermal correction to Energy =	0.202649 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203593 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.147488 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.594 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.58 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.579 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.636 (Hartree/Particle)

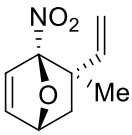


12_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.282614000	0.336400000	-0.031002000
C	-1.754789000	-1.685656000	-0.561673000
C	1.799679000	-0.998048000	0.082161000
H	-1.806332000	-2.504130000	-1.260793000
O	-1.264761000	-0.532558000	-1.052012000
N	-0.797802000	1.652528000	-0.283288000
O	-0.339651000	1.897268000	-1.383827000
O	-0.871822000	2.443905000	0.640758000
C	1.374837000	-2.213164000	0.444292000
H	1.105212000	-2.437322000	1.472324000
H	1.284376000	-3.023909000	-0.272151000
C	1.908694000	0.064276000	1.093422000
H	1.631931000	-0.221147000	2.107209000
C	2.303397000	1.317036000	0.863803000
H	2.582674000	1.667046000	-0.125104000
H	2.347003000	2.045383000	1.665959000
C	2.166041000	-0.675627000	-1.339781000
H	3.207436000	-0.346592000	-1.412085000
H	2.038728000	-1.545570000	-1.986266000
H	1.543309000	0.133508000	-1.732361000
C	-2.091749000	-1.555454000	0.750465000
C	-1.779905000	-0.215893000	1.105653000
H	-1.896289000	0.276126000	2.057470000
H	-2.505110000	-2.323221000	1.385411000

Table S32. Thermochemistry and cartesian coordinates of **TS** of product (**12**) (path J) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189986 (Hartree/Particle)
Thermal correction to Energy =	0.201681 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202626 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.152415 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.552 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.54 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.539 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.59 (Hartree/Particle)

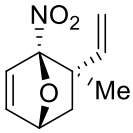


12_TS

Center	**Coordinates (Angstroms)** X	Y	Z
C	0.31530800	-0.96239000	0.24788800
C	2.18190700	-0.11671900	-0.29797800
C	-0.08972500	1.37466100	-0.52696300
H	3.07485800	-0.10575600	-0.90777400
O	1.21781600	-0.98187300	-0.74984200
N	-0.92735800	-1.59077800	0.03330700
O	-1.15424300	-2.08933700	-1.06052300
O	-1.73211900	-1.53510800	0.95949400
C	1.28986100	1.55259800	-0.74723900
H	1.82158000	2.24844200	-0.10556700
H	1.61050700	1.59199600	-1.78511000
C	-0.68485500	1.87158600	0.70593000
H	0.01940200	2.16834200	1.48103800
C	-1.99422700	1.98637800	0.95441700
H	-2.75279300	1.72509900	0.22454000
H	-2.34738800	2.36097900	1.90865900
C	-0.97055700	0.99631700	-1.68345700
H	-1.31080700	1.90205400	-2.19863700
H	-0.42751000	0.38573100	-2.40651800
H	-1.86331700	0.44383500	-1.38384100
C	2.14893200	-0.13500400	1.13238700
C	0.91769200	-0.62806700	1.47011600
H	0.44312500	-0.68634600	2.43653600
H	2.88620100	0.31544700	1.77988500

Table S33. Thermochemistry and cartesian coordinates of **PR** of product (**12**) (path J) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193844 (Hartree/Particle)
Thermal correction to Energy =	0.204769 (Hartree/Particle)
Thermal correction to Enthalpy =	0.205713 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.157483 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.6 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.588 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.636 (Hartree/Particle)

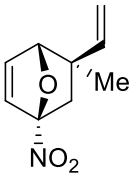


12_PR

Center	Coordinates (Angstroms) X	Y	Z
C	-0.436850000	-0.453038000	-0.142025000
C	-1.953621000	0.876216000	0.414954000
C	0.472909000	0.742123000	0.387661000
H	-2.857067000	1.120664000	0.966306000
O	-1.499568000	-0.441722000	0.765257000
N	0.268402000	-1.767166000	-0.140963000
O	0.052892000	-2.543190000	0.759665000
O	1.055171000	-1.937021000	-1.052495000
C	-0.693846000	1.723121000	0.744347000
H	-0.656730000	2.650798000	0.171868000
H	-0.667856000	1.971358000	1.806149000
C	1.375685000	1.302066000	-0.678567000
H	0.867708000	1.645723000	-1.577494000
C	2.694741000	1.433450000	-0.606616000
H	3.272252000	1.121081000	0.257069000
H	3.252532000	1.865870000	-1.430482000
C	1.218600000	0.301509000	1.646047000
H	1.705604000	1.160401000	2.113373000
H	0.526786000	-0.131305000	2.369692000
H	1.989963000	-0.441058000	1.425819000
C	-2.048905000	0.773031000	-1.097590000
C	-1.086798000	-0.068881000	-1.456553000
H	-0.730500000	-0.355450000	-2.434807000
H	-2.700964000	1.359957000	-1.730117000

Table S34. Thermochemistry and cartesian coordinates of **MC** of product (**13**) (path K) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188501 (Hartree/Particle)
Thermal correction to Energy =	0.201474 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202418 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.147182 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.589 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.63 (Hartree/Particle)

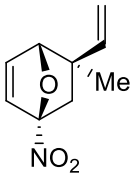


13_MC

Center	Coordinates (Angstroms) X	Y	Z
C	1.32832900	0.41217700	0.00082700
C	0.29108700	2.23497700	-0.44389600
H	-0.22395900	2.90307200	-1.11422700
O	0.74109000	1.09224400	-0.99418900
N	1.87319600	-0.86626700	-0.31504900
O	1.82618400	-1.24473300	-1.46887200
O	2.34893400	-1.49678400	0.61610900
C	-1.81212000	-0.92912400	0.43936300
C	0.59417900	2.29199200	0.88074200
C	1.28088200	1.08242700	1.17988000
H	1.67718400	0.74542600	2.12380900
H	0.35359000	3.09412700	1.56057800
C	-1.65137200	-0.70429500	1.91931000
H	-1.35533000	0.32775200	2.13115700
H	-2.60025700	-0.87621500	2.43932500
H	-0.90277500	-1.37242900	2.34938400
C	-1.18733400	-1.91724000	-0.20469000
H	-0.49843300	-2.58123600	0.30935500
H	-1.34967500	-2.10297700	-1.26117500
C	-2.73677200	-0.00608700	-0.25194000
C	-2.58981900	0.45013100	-1.49443300
H	-3.32315200	1.11487500	-1.93968100
H	-1.73131800	0.18141200	-2.10299100
H	-3.59026500	0.33450300	0.33444500

Table S35. Thermochemistry and cartesian coordinates of **TS** of product (**13**) (path K) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189173 (Hartree/Particle)
Thermal correction to Energy =	0.201103 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202048 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.151139 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.545 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.533 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.532 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.583 (Hartree/Particle)

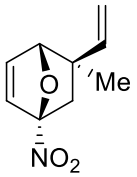


13_TS

Center	Coordinates (Angstroms) X	Y	Z
C	1.004061000	0.295411000	-0.172402000
C	-0.674546000	0.666522000	-1.394816000
H	-1.419552000	0.398615000	-2.127887000
O	0.303596000	-0.249512000	-1.194027000
N	2.215225000	-0.421439000	0.197944000
O	2.417625000	-1.509317000	-0.296420000
O	2.917082000	0.120802000	1.032221000
C	-1.584400000	0.011711000	0.629351000
C	-0.212582000	1.932287000	-0.991661000
C	0.910546000	1.710195000	-0.234704000
H	1.499569000	2.404238000	0.343103000
H	-0.718319000	2.870040000	-1.166197000
C	-2.403429000	1.211015000	1.050473000
H	-3.082838000	1.540580000	0.259423000
H	-3.014794000	0.967861000	1.927115000
H	-1.763747000	2.053716000	1.321595000
C	-0.345617000	-0.207026000	1.248885000
H	-0.033649000	0.461791000	2.043759000
H	-0.002190000	-1.229153000	1.379918000
C	-2.344970000	-1.107297000	0.036815000
C	-1.893892000	-2.321216000	-0.283813000
H	-2.555972000	-3.058723000	-0.724125000
H	-0.861355000	-2.622701000	-0.137043000
H	-3.391166000	-0.881595000	-0.168228000

Table S36. Thermochemistry and cartesian coordinates of **PR** of product (**13**) (path K) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193296 (Hartree/Particle)
Thermal correction to Energy =	0.204501 (Hartree/Particle)
Thermal correction to Enthalpy =	0.205446 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.155937 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.598 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.587 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.586 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.635 (Hartree/Particle)

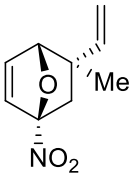


13_PR

Center	Coordinates (Angstroms) X	Y	Z
C	-0.87160200	-0.21866700	-0.03657900
C	0.89190200	-0.61570300	-1.08139300
H	1.55053600	-0.49413600	-1.93733200
O	-0.25202300	0.24067900	-1.20308800
N	-2.20313300	0.42445600	0.17319500
O	-2.50071200	1.38300400	-0.49713600
O	-2.88175200	-0.06631500	1.05554200
C	1.48691400	-0.11383500	0.29879900
C	0.23928000	-1.97092400	-0.87125800
C	-0.88778000	-1.72586300	-0.21283700
H	-1.60824900	-2.39823700	0.22956500
H	0.67422900	-2.92821600	-1.12297700
C	2.37438300	-1.15425400	0.98187900
H	3.21704400	-1.43236400	0.34082300
H	2.78433000	-0.75173600	1.91199100
H	1.81826400	-2.06171400	1.22526500
C	0.15902600	0.14127600	1.06904600
H	0.04492200	-0.49032300	1.94923200
H	0.04671200	1.18202900	1.37152300
C	2.29776000	1.13665200	0.02916000
C	1.85384200	2.38050400	-0.10462000
H	2.53854700	3.18943300	-0.33728300
H	0.80640700	2.64775400	-0.00845200
H	3.36273900	0.95226000	-0.11044300

Table S37. Thermochemistry and cartesian coordinates of **MC** of product (**14**) (path L) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.188659 (Hartree/Particle)
Thermal correction to Energy =	0.202434 (Hartree/Particle)
Thermal correction to Enthalpy =	0.203378 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.145899 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.59 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.576 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.575 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.632 (Hartree/Particle)

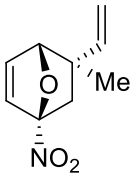


14_MC

Center	Coordinates (Angstroms) X	Y	Z
C	-1.283207000	-0.207606000	-0.249202000
C	-2.066654000	1.725655000	0.250973000
C	1.869408000	-0.844610000	1.280519000
H	1.409138000	-0.995977000	2.251898000
H	2.277846000	-1.721378000	0.788329000
C	1.933290000	0.365564000	0.721807000
H	-2.546472000	2.418415000	0.922845000
O	-1.886844000	0.480062000	0.731881000
N	-0.982613000	-1.578271000	0.004405000
O	-1.273209000	-2.041092000	1.089714000
O	-0.448122000	-2.191842000	-0.905149000
C	2.532590000	0.584762000	-0.611223000
C	2.413330000	-0.234842000	-1.654165000
H	2.892919000	-0.010831000	-2.601797000
H	3.087598000	1.515084000	-0.733556000
H	1.828669000	-1.148749000	-1.597909000
C	1.425483000	1.601061000	1.416595000
H	2.246949000	2.299385000	1.611214000
H	0.701331000	2.132993000	0.791323000
H	0.949747000	1.361900000	2.369418000
C	-1.061715000	0.553531000	-1.350613000
C	-1.583262000	1.834041000	-1.015885000
H	-0.584604000	0.236699000	-2.263014000
H	-1.595005000	2.717985000	-1.633991000

Table S38. Thermochemistry and cartesian coordinates of **TS** of product (**14**) (path L) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.189160 (Hartree/Particle)
Thermal correction to Energy =	0.201125 (Hartree/Particle)
Thermal correction to Enthalpy =	0.202069 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.150956 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.545 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.533 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.532 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.583 (Hartree/Particle)

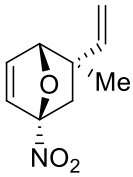


14_TS

Center	Coordinates (Angstroms) X	Y	Z
C	-0.98039200	0.15420700	0.26612500
C	0.49483100	-0.52705100	1.61849300
C	0.28349400	-0.20443100	-1.20208100
H	-0.28873900	-1.00318200	-1.66866600
H	0.21537600	0.73706900	-1.73513900
C	1.48391700	-0.57174100	-0.57329900
H	1.01060600	-1.28082800	2.19283200
O	-0.64910900	-0.93320600	1.00965300
N	-2.29351700	0.08375600	-0.36868500
O	-2.91094800	-0.95663900	-0.30963500
O	-2.64722900	1.08725600	-0.95977500
C	2.58511500	0.38715800	-0.43464500
C	2.58812400	1.67655300	-0.78604200
H	3.45847000	2.29825000	-0.60604200
H	3.48619800	-0.01410600	0.02835200
H	1.74277900	2.15997000	-1.26582200
C	1.84467100	-2.03875900	-0.49179400
H	2.29833500	-2.37468300	-1.43146800
H	2.56606100	-2.23960700	0.30486300
H	0.96143700	-2.65678400	-0.31565700
C	-0.49580900	1.32758500	0.90473500
C	0.49643800	0.86623500	1.73620300
H	-0.75774700	2.33991400	0.64272300
H	1.21778600	1.44987400	2.28671300

Table S39. Thermochemistry and cartesian coordinates of **PR** of product (**14**) (path L) (ωB97XD/6-311+G(d), in benzene solution (PCM)).

Zero-point correction =	0.193283 (Hartree/Particle)
Thermal correction to Energy =	0.204527 (Hartree/Particle)
Thermal correction to Enthalpy =	0.205471 (Hartree/Particle)
Thermal correction to Gibbs Free Energy =	0.155771 (Hartree/Particle)
Sum of electronic and zero-point Energies =	-629.6 (Hartree/Particle)
Sum of electronic and thermal Energies =	-629.588 (Hartree/Particle)
Sum of electronic and thermal Enthalpies =	-629.587 (Hartree/Particle)
Sum of electronic and thermal Free Energies =	-629.637 (Hartree/Particle)



14_PR

Center	Coordinates (Angstroms) X	Y	Z
C	0.921510000	-0.121840000	0.122999000
C	-0.694479000	0.544226000	1.262169000
C	-0.151173000	-0.035434000	-0.997039000
H	0.153908000	0.685091000	-1.757817000
H	-0.301847000	-1.003111000	-1.469768000
C	-1.357725000	0.492847000	-0.169861000
H	-1.159640000	1.235756000	1.960922000
O	0.630071000	0.983645000	0.929187000
N	2.320870000	-0.074720000	-0.396504000
O	2.975976000	0.924057000	-0.224637000
O	2.683607000	-1.071602000	-0.992110000
C	-2.601481000	-0.355613000	-0.170151000
C	-2.914357000	-1.352261000	-0.988690000
H	-3.866909000	-1.864154000	-0.900537000
H	-3.333692000	-0.060283000	0.582849000
H	-2.254740000	-1.698607000	-1.777937000
C	-1.731233000	1.920463000	-0.593725000
H	-2.069217000	1.934540000	-1.632798000
H	-2.542688000	2.311012000	0.027650000
H	-0.873194000	2.589418000	-0.498053000
C	0.590522000	-1.307562000	1.009628000
C	-0.443076000	-0.879293000	1.724817000
H	1.036171000	-2.288325000	0.930287000
H	-1.062517000	-1.440294000	2.410318000