Electronic Supplementary Information

For

Unraveling High-Precision Stereocontrol in a Triple Cascade

Organocatalytic Reaction

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Department of Chemistry

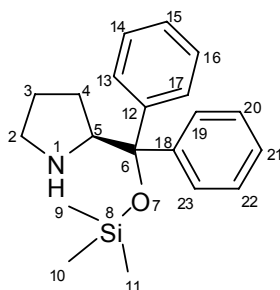Indian Institute of Technology Bombay

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Table S1 Comparison of geometric parameters of catalyst optimized at the B3LYP/6-31G* and

ONIOM(B3LYP/6-31G*:AM1) levels of theory

Bond distances (in Å)	DFT	ONIOM	Bond angles/Dihedral angles	DFT	ONIOM
C_5-C_6	1.55	1.53	$C_5C_6C_{12}$	107	107
C_6-C_{12}	1.54	1.52	$C_5C_6C_{18}$	112	112
C_6-C_{18}	1.54	1.52	$C_5C_6O_7$	110	111
C_6-O_7	1.41	1.39	$N_1C_5C_6O_7$	-58	-50
O_7-Si_8	1.68	1.80	$N_1C_5C_6C_{18}$	65	72
Si_8-C_9	1.88	1.82	$N_1C_5C_6C_{12}$	-175	-168
Si_8-C_{10}	1.88	1.83	$C_5C_6C_{12}C_{17}$	111	112
Si_8-C_{11}	1.86	1.81	$C_5C_6C_{12}C_{23}$	16	14
C_{12}-C_{17}	1.39	1.40	$C_5C_6O_7Si_8$	62	50

Table S2 Computed Relative Energies (ΔE) obtained at the B3LYP/6-31G* level for the catalyst
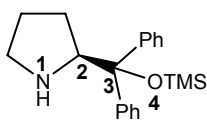
Dihedral angle ($N_1C_2C_3O_4$)	Relative ΔE in kcal/mol
+60	0.0
180	3.2
-60	2.9
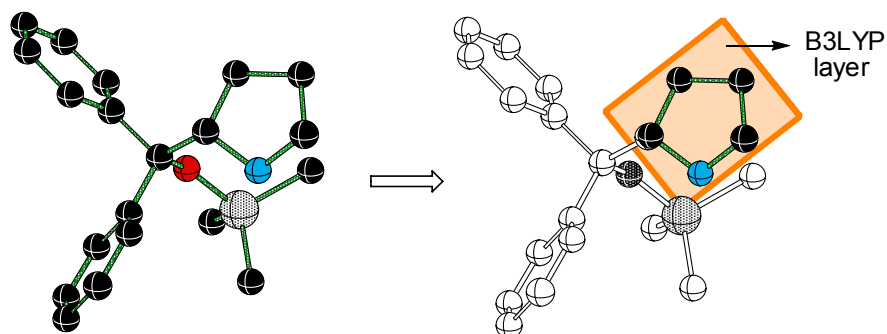
B3LYP
layer

Figure S1. Two-layered ONIOM partition scheme employed for diphenylsiloxytrimethyl

prolinol ether catalyst. Atoms separated by white bonds represents the lower AM1 layer and the

dark bond the higher B3LYP layer (hydrogens are omitted for clarity).

Table S3 Relative energies of enamine conformers formed between propanal and the catalyst

calculated at the B3LYP/6-31G* level of theory

Enamine	Relative energy in kcal/mol
(E)-anti-enamine	0.0
(Z)-anti-enamine	2.2
(E)-syn-enamine	0.2
(Z)-syn-enamine	10.7

-60°	180°	+60°
2a	**2b**[a]	**2c**[a]
2d[a]	**2e**[a]	**2f**
3a	**3b**[a]	**3c**
3d[a]	**3e**	**3f**
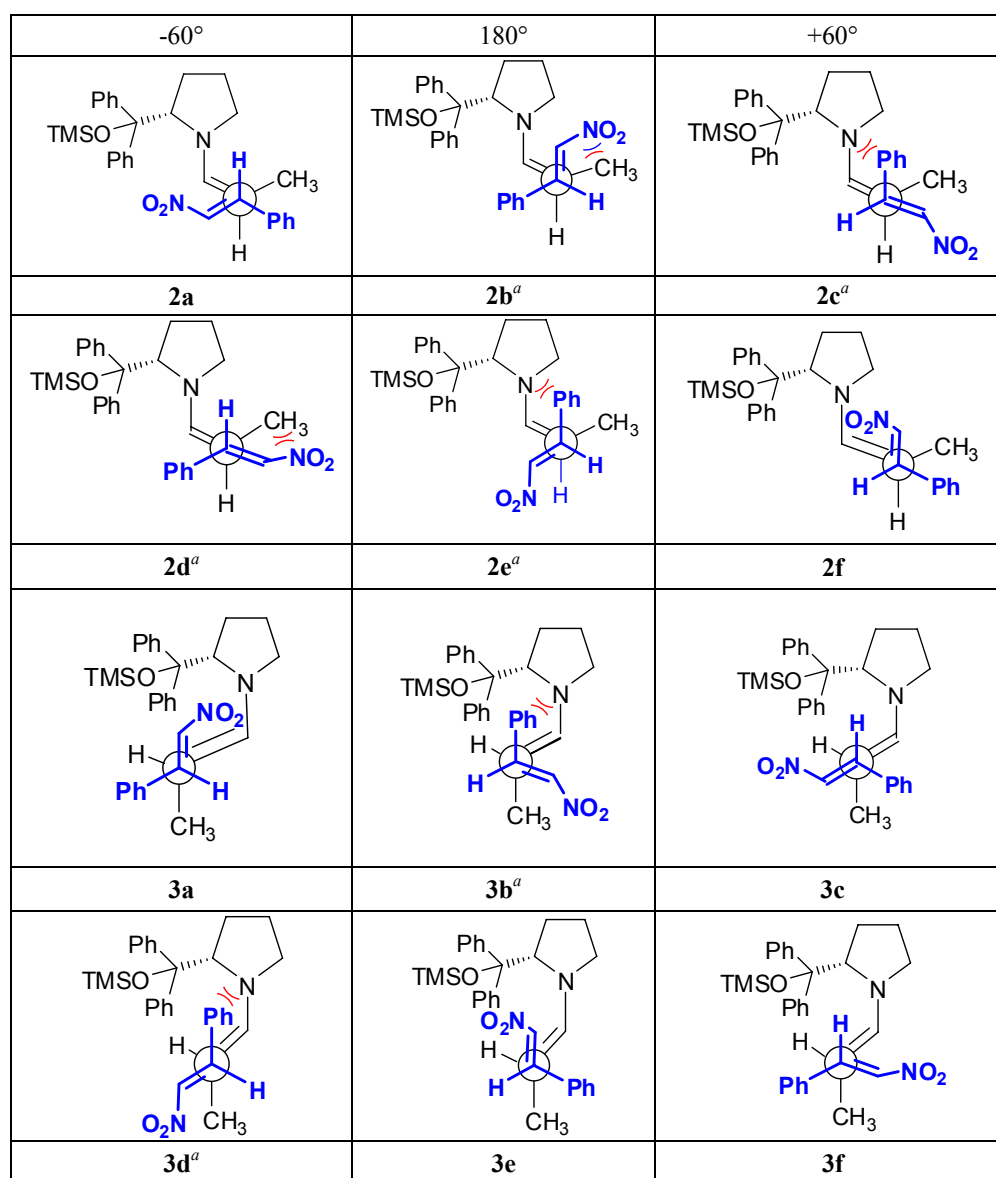
[a]*In spite of repeated attempts we could not locate transition states corresponding to these rotamers. Different initial guess sets were tried varying the crucial dihedral angles, bond lengths etc.,. These rotamers are highly detstabilized because of the gauche interactions between both phenyl group on nucleophile and pyrrolidine nitrogen or nitro group on nucleophiles and methyl group on electrophiles.*

Figure S2. Various rotamers for the addition of (*Z*)-*anti*-enamine (**2a-f**) as well as (*E*)-*syn*-

enamine (**3a-f**) on the *re/si* face of nitrostyrene grouped on the basis of the dihedral angles

between H of the nitrostyrene and the enamine double bond

	ρ(bcp)
C_1-C_2	0.085
H_5-O_6	0.010
H_5-O_7	0.008
H_8-O_6	0.017
H_9-O_7	0.009

1f

	ρ(bcp)
C_1-C_2	0.090
H_5-O_6	0.011

1a

	ρ(bcp)
C_1-C_2	0.050
O_3-H_6	0.009
O_9-H_8	0.008

4b

	ρ(bcp)
C_1-C_2	0.051
O_3-H_6	0.009

4d

	ρ(bcp)
C_1-C_2	0.125
H_5-O_4	0.017
H_6-O_7	0.005

5a

	ρ(bcp)
C_1-C_2	0.165
H_6-O_4	0.012

5c
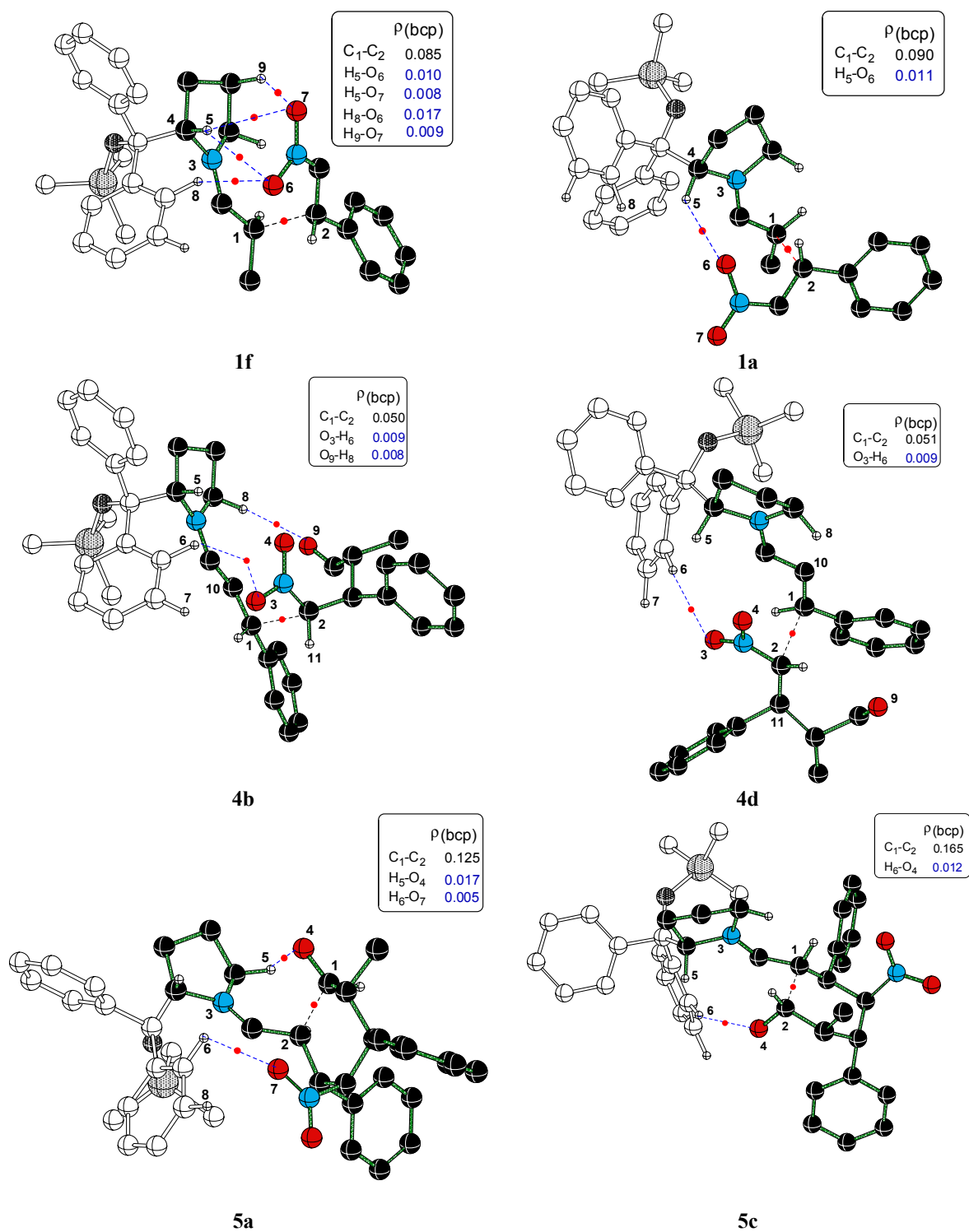
Figure S3. Key interactions detected using the AIM analysis and the electron densities at the

bond critical points (ρ(bcp)).

Table S4 Mulliken charge analysis (MCA) and Natural population analysis (NPA) on nitrogens

(N^*) on **TS-1f** and **TS-1a** involving in electrostatic interaction

	$-N^*O_2$	-Pyrrolidine N^*	Level of theory	
TS-1f	0.53	-0.21	I	MCA
	0.40	-0.40	II	
	0.44	-0.37	II	NPA
TS-1a	0.48	-0.32	I	MCA
	0.41	-0.38	II	
	0.44	-0.38	II	NPA

   I. ONIOM(B3LYP/6-31G*:AM1) II. B3LYP/6-31G*//ONIOM(B3LYP/6-31G*:AM1)

Table S5 Global Reactivity Descriptors (GRD) of nitrostyrene and cinnamaldehyde. Values are

given in a.u.

	Method	Nitrostyrene	Cinnamaldehyde
Absolute Electronegativity ($\chi = \frac{1}{2}(I^a+A^b)$)	I	0.1763	0.1589
	II	0.1847	0.1685
	III	0.1530	0.1229
Hardness ($\eta = \frac{1}{2}(I-A)$)	I	0.1409	0.1418
	II	0.1397	0.1401
	III	0.1241	0.1304
Electrophilicity index ($\omega = \mu^2/2\eta$)	I	0.0022	0.0017
	II	0.0024	0.0020
	III	0.0015	0.0010
LUMO Energy	III	0.0333	0.0595

  [a] *Ionization potential* [b] *Electron affinity*

   I. UB3LYP/6-31G* II. UB3LYP/6-311G** III. MP2/6-31G*//UB3LYP/6-311G**

Table S6 The optimized geometries and energetics of the lower energy TSs for the addition of

enamine to enal
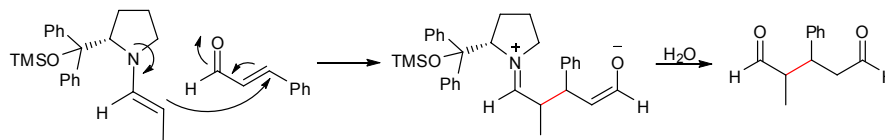
Enamine adding to the *re* face of enal	Enamine adding to the *si* face of enal
$\Delta E^{\ddagger a} = 29.2$	$\Delta E^{\ddagger} = 30.7$
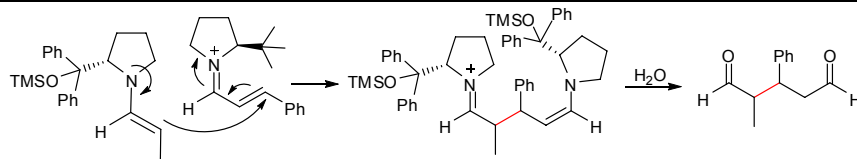
$\Delta E_{TS-R} = 14.8$ $\Delta E_{TS-P} = 7.9$	$\Delta E_{TS-R} = 13.7$ $\Delta E_{TS-P} = 6.0$

[a] *Absolute activation barriers with respect to isolated reactants in kcal/mol*
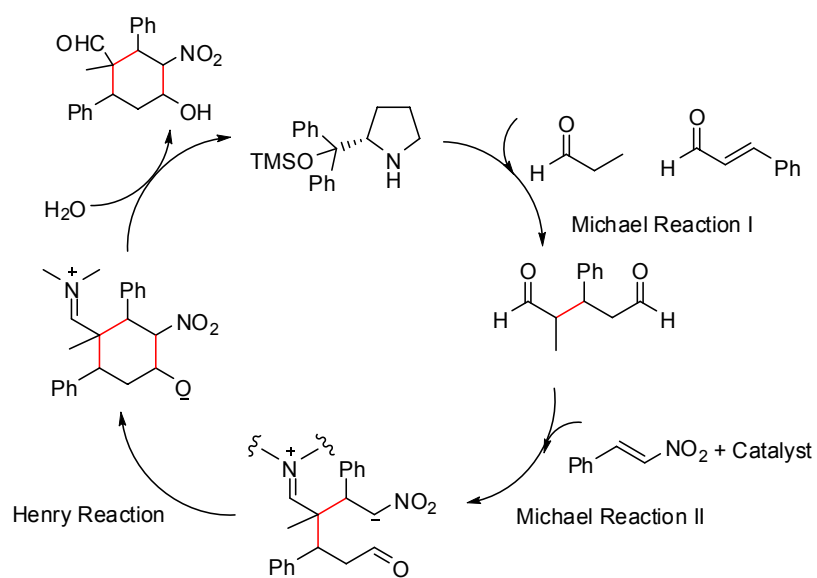
Pathway 1
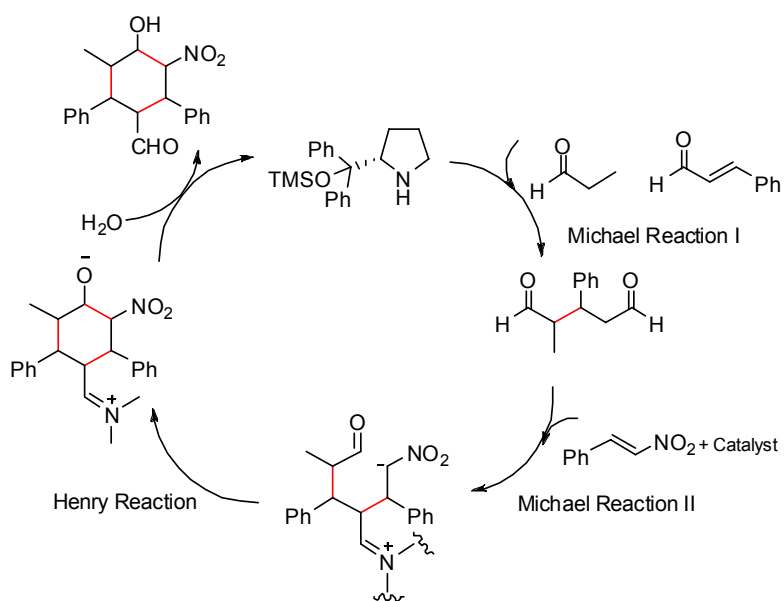
Pathway 2

Figure S4. Alternative mechanism if the first step involves reaction between enal and enamine

Table S7 Relative energies of iminium conformers formed between α,β-unsaturated aldehyde

(**C**) and the catalyst calculated at the B3LYP/6-31G* in kcal/mol

Z,s-trans,E	Z,s-trans,Z	E,s-trans,E	E,s-cis,Z
1.52	6.12	0.00	6.66

Table S8 Computed activation barriers ($\Delta E^{\ddagger}$) at the B3LYP/6-31G*//ONIOM(B3LYP/6-

31G*:AM1) level for the intramolecular cyclization [a]

Total Energy of PRC in a.u	Transition state	$\Delta E^{\ddagger}$ in kcal/mol		Relative $\Delta E^{\ddagger}$ at the B3LYP/6-31+G** level in kcal/mol
		Absolute	Relative	
-2251.764704	**TS-5a**	21.43	0.00	0.0
-2251.747337	**TS-5b**	22.44	11.90	11.1
-2251.751410	**TS-5c**	22.25	9.15	9.6
-2251.748843	**TS-5d**	22.11	10.63	11.0

[a] Absolute barriers are with respect to the corresponding pre-reacting complexes while the relative barriers are with respect to **TS-5a**.

Ref. 19) **Gaussian 03**, Revision C.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table S9 The computed relative energy ($\Delta E^{\ddagger}$) at the B3LYP/6-31+G*//ONIOM2(B3LYP/6-31G*:AM1) and B3LYP/6-31+G*//ONIOM2(B3LYP/6-31G*:AM1) levels for the addition of enamines to (*E*)-nitrostyrene
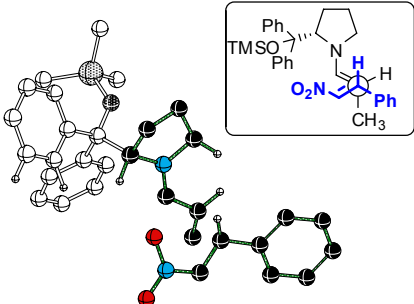
Enamine	Transition state	Relative Energy $\Delta E^{\ddagger}$ in kcal/mol	
		B3LYP/6-31+G*	B3LYP/6-31+G**
(*E*)-*anti*	**TS-1a**	2.6	2.8
	TS-1b	6.8	7.0
	TS-1d	6.1	6.3
	TS-1f	0.0	0.0
(*Z*)-*anti*	**TS-2a**	6.0	6.1
	TS-2f	6.7	6.9
(*E*)-*syn*	**TS-3a**	6.5	6.5
	TS-3c	8.8	8.9
	TS-3e	9.0	9.0
	TS-3f	8.5	8.6
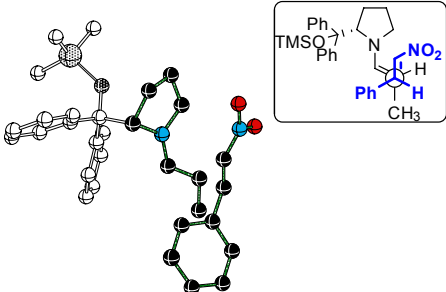
Table S10 The computed relative energy ($\Delta E^{\ddagger}$) at the B3LYP/6-31+G*//ONIOM2(B3LYP/6-31G*:AM1) and B3LYP/6-31+G**//ONIOM2(B3LYP/6-31G*:AM1) levels for the addition of nitroalkane anion to the iminium derived from the enal (**C**)

Transition state	Relative Energy $\Delta E^{\ddagger}$ in kcal/mol	
	B3LYP/6-31+G*	B3LYP/6-31+G**
TS-4b	0.0	0.0
TS-4c	2.5	2.6
TS-4d	0.9	1.0
TS-4e	3.5	3.3
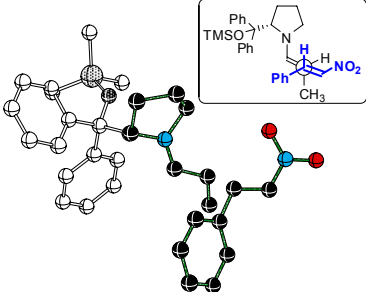
ONIOM2(B3LYP/6-31G*:AM1) optimized geometries and Cartesian coordinates for the transition states for **(I)** the Michael addition between (*E*)-nitrostyrene and different conformers of enamine **(II)** the Michael addition between iminium and nitroalkane **(III)** Intramolecular cyclization. Electronic energies in the gas phase (in a.u) at the ONIOM2(B3LYP/6-31G*:AM1). Single point energies calculated in the gas phase using the B3LYP/6-31G*//ONIOM2(B3LYP/6-31G*:AM1) are given in parenthesis
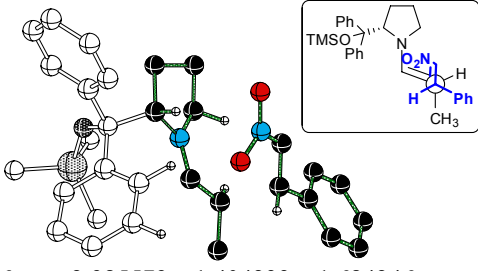
I. Michael addition between (*E*)-nitrostyrene and different conformers of enamine
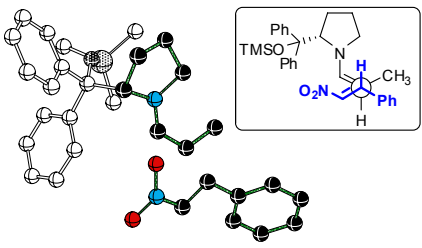
1a

Et = -843.463951(-1828.732300)

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6	-0.751563	0.099851	-2.452566
6	-0.258619	-1.350680	-2.591114
6	0.861391	-1.450381	-1.545901
1	-0.430707	1.416623	-0.713399
1	-0.068619	0.789187	-2.960626
1	-1.758040	0.242441	-2.858307
1	-1.071064	-2.044328	-2.339884
1	0.096210	-1.590852	-3.596983
1	0.930383	-2.438244	-1.075691
1	1.838978	-1.213759	-1.979149
6	-2.033420	0.053753	-0.204996
8	-2.343355	-1.272649	-0.515501
14	-3.594943	-2.358512	0.195692
6	-4.864547	-1.511622	1.164360
1	-5.732907	-1.199120	0.538227
1	-4.459953	-0.586829	1.644377
1	-5.263314	-2.156018	1.982793
6	-4.275954	-3.135807	-1.295061
1	-4.329462	-4.245580	-1.204935
1	-3.632914	-2.906990	-2.179390
1	-5.303022	-2.773199	-1.531671
6	-2.674568	-3.559089	1.192464
1	-3.241486	-4.509134	1.331236
1	-2.437065	-3.162612	2.207593
1	-1.703595	-3.820979	0.709412
6	-3.026859	1.033816	-0.828830
6	-2.779026	2.415074	-0.787713
6	-3.654376	3.311912	-1.396860
6	-4.788558	2.846482	-2.062149
6	-5.037293	1.476758	-2.119449
6	-4.158967	0.579394	-1.513213
1	-1.887629	2.806701	-0.269877

1	-3.443125	4.391180	-1.355094
1	-5.478364	3.555808	-2.542005
1	-5.924496	1.098560	-2.648268
1	-4.356653	-0.503633	-1.584105
6	-1.897436	0.253174	1.298159
6	-1.117624	-0.646781	2.043095
6	-0.953602	-0.488927	3.417634
6	-1.576159	0.567677	4.081004
6	-2.379758	1.447680	3.359851
6	-2.547277	1.285993	1.983821
1	-3.215271	1.985086	1.456783
1	-2.888867	2.276560	3.874429
1	-1.438697	0.700826	5.163982
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6	1.302450	-0.062351	0.456916
6	2.612296	-0.550207	0.717107
1	0.896790	0.712405	1.099706
1	2.854824	-1.496076	0.233485
6	3.796224	0.643252	-0.339921
6	3.852370	1.947758	0.214463
1	3.191165	0.594403	-1.241729
1	4.656080	2.342292	0.816383
6	5.063782	-0.142741	-0.442788
6	6.115630	-0.019878	0.480812
6	7.283099	-0.769821	0.340730
6	7.426193	-1.661725	-0.723595
6	6.390182	-1.796535	-1.649468
6	5.223739	-1.047048	-1.505246
1	6.025343	0.671813	1.312523
1	8.084781	-0.653807	1.065152
1	8.337071	-2.243954	-0.831781
1	6.491544	-2.482031	-2.486748
1	4.424332	-1.151860	-2.236443
7	2.771749	2.781428	0.092892
8	1.736019	2.333467	-0.511798
8	2.803925	3.934820	0.578495
6	3.091615	-0.449244	2.153796
1	2.957980	0.568664	2.537104
1	2.545653	-1.133544	2.815441
1	4.154399	-0.699755	2.224873

NImag = 1

Imag. Freq = -344

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6	0.609484	1.816900	-1.403829
6	0.520423	2.947851	-0.359012
6	-0.411728	2.406611	0.741424
1	-0.094267	-0.274469	-1.199870
1	-0.204182	1.926444	-2.126523
1	1.565020	1.829694	-1.936299
1	1.511209	3.165605	0.054999
1	0.109964	3.857322	-0.800349
1	0.046892	2.452557	1.736682
1	-1.368084	2.932780	0.772309
6	1.701619	-0.121586	-0.024950
8	2.539402	0.945405	0.293416
14	4.334568	1.068437	0.250010
6	5.112079	-0.285844	1.164328
1	6.067996	0.033110	1.642745
1	5.346109	-1.159589	0.511723
1	4.444392	-0.655500	1.979573
6	4.901811	1.159576	-1.464702
1	5.173581	2.199839	-1.761012
1	4.104825	0.816941	-2.169396
1	5.796959	0.520617	-1.649023
6	4.527174	2.650832	1.111482
1	3.527350	3.115748	1.294349
1	5.126364	3.383433	0.522437
1	5.023339	2.536591	2.102808
6	2.297275	-1.065759	-1.065637
6	2.113074	-0.868274	-2.439383
6	2.666019	-1.751049	-3.367640
6	3.415299	-2.844834	-2.939114
6	3.611189	-3.049415	-1.573804
6	3.057759	-2.168571	-0.646678
1	1.528734	-0.014766	-2.816282
1	2.507234	-1.578617	-4.442910
1	3.849385	-3.540927	-3.671861
1	4.202734	-3.908706	-1.224120
1	3.222765	-2.347129	0.428991
6	1.347979	-0.911362	1.229620
6	1.617709	-0.393977	2.500811
6	1.284690	-1.121529	3.644130
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6	0.719677	-2.160312	1.121722
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6	-2.756320	0.649176	1.501679
1	-1.425526	-0.872788	0.716007
1	-2.735945	1.686138	1.831990
6	-3.448333	-0.276232	2.490285
1	-2.970504	-0.225575	3.475826
1	-4.497273	0.010985	2.619242
1	-3.430130	-1.318919	2.156392
6	-3.891211	0.897187	0.029439
6	-3.318129	1.661708	-1.039389
1	-3.046462	1.246899	-1.998443
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6	-3.715204	-1.344744	-1.152968
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1	-7.317492	-2.271559	-0.085736
1	-5.980868	-3.868725	-1.449272
1	-3.668402	-3.257717	-2.136386
1	-2.706987	-1.086587	-1.468627

NImag =1
Imag. Freq. = -215

1d

Et = -843.460768 (-1828.727039)

7	0.518699	-0.600429	-0.601268
6	-0.615381	0.260770	-1.032580
6	-0.874920	-0.198077	-2.507998
6	0.263113	-1.181098	-2.847620
6	0.640780	-1.774992	-1.489286
1	-0.269306	1.299472	-0.974837
1	-0.912158	0.658421	-3.186647
1	-1.843730	-0.708693	-2.567837
1	-0.045995	-1.947568	-3.563020
1	1.127415	-0.656634	-3.269338
1	-0.092656	-2.530596	-1.170596
1	1.645787	-2.198654	-1.449191
6	-1.932630	0.160762	-0.188549
8	-2.326430	-1.175244	-0.275783
14	-3.577517	-2.106821	0.634583
6	-4.703547	-1.073388	1.598353
1	-5.059484	-1.592453	2.519577
1	-5.608673	-0.779701	1.016714
1	-4.207367	-0.128061	1.928452
6	-4.428873	-2.983016	-0.702360
1	-4.508862	-4.077317	-0.502574
1	-3.872762	-2.866649	-1.664232
1	-5.462945	-2.602438	-0.871150
6	-2.626231	-3.241840	1.672378
1	-3.173341	-4.195099	1.862476
1	-2.378661	-2.799564	2.665629
1	-1.658664	-3.511552	1.184478
6	-2.905389	1.092703	-0.909758
6	-2.574807	2.440652	-1.119879
6	-3.435996	3.284961	-1.817177
6	-4.640927	2.797388	-2.323495
6	-4.974284	1.458411	-2.130941
6	-4.109818	0.613683	-1.435231
1	-1.631139	2.849080	-0.725670
1	-3.161576	4.339507	-1.969790
1	-5.320361	3.464841	-2.873492
1	-5.918858	1.061538	-2.532010
1	-4.377157	-0.449262	-1.308387
6	-1.690725	0.582621	1.252717
6	-0.958581	-0.264060	2.101714
6	-0.699195	0.092446	3.423509
6	-1.179091	1.299344	3.930781
6	-1.937619	2.131177	3.110320
6	-2.199625	1.771702	1.787540
1	-2.835619	2.439365	1.185779
1	-2.341208	3.075571	3.505831
1	-0.969495	1.585901	4.971900
1	-0.115930	-0.584535	4.066247
1	-0.610743	-1.245230	1.736872
6	1.331179	-0.296394	0.402604
6	2.538574	-0.971224	0.740017
1	1.094536	0.640106	0.908253
1	2.573836	-2.010851	0.416331
6	3.829324	-0.354682	-0.470250
1	3.255094	-0.541419	-1.377729
6	3.043678	-0.772531	2.157803
1	3.012242	0.278797	2.465386
1	2.452535	-1.353475	2.875655
1	4.080932	-1.119662	2.226685
6	4.960712	-1.218130	-0.368957
1	5.886485	-0.982873	0.132251
6	4.056548	1.111175	-0.245975
6	3.368882	2.043380	-1.039434
6	3.545159	3.415716	-0.862192
6	4.415883	3.887640	0.121191
6	5.109478	2.974276	0.916898
6	4.932525	1.602441	0.735114
1	2.701554	1.683811	-1.820267
1	3.009217	4.115468	-1.498329
1	4.557906	4.955585	0.261506
1	5.795733	3.329469	1.681014
1	5.484225	0.908041	1.360940
7	4.879527	-2.506771	-0.844607
8	3.781415	-2.912777	-1.349249
8	5.883475	-3.250440	-0.770649

NImag =1
Imag. Freq = -249

1f
Et = -843.473496 (-1828.740296)

6	2.985579	1.404233	1.684246
6	2.140274	0.352374	1.297808
6	1.436838	-0.338990	2.290903
6	1.549468	0.039365	3.630032
6	2.375557	1.098490	3.999425
6	3.097957	1.779929	3.019898
6	2.137280	-0.075027	-0.160964
8	2.358366	0.972452	-1.058874
14	1.830365	2.679560	-1.195927
6	0.714628	3.292904	0.087646
6	0.888681	-0.879975	-0.604059
6	1.103867	-1.476344	-2.020676
6	-0.307069	-1.580024	-2.609531
6	-0.966833	-0.296146	-2.108778
7	-0.407474	-0.132509	-0.747028
1	1.615926	-2.440411	-1.960610
6	3.323135	-1.038818	-0.311996
6	3.363995	-2.212374	0.452000
6	4.439723	-3.089904	0.332498
6	5.485699	-2.802462	-0.544800
6	5.450952	-1.633479	-1.302870
6	4.374199	-0.753764	-1.188847
6	3.401292	3.583027	-1.190252
6	1.047363	2.722613	-2.831127
1	0.695829	-1.682668	0.120580
1	2.548234	-2.442307	1.156103
1	4.461386	-4.010612	0.933979
1	6.334391	-3.495545	-0.636245
1	6.273809	-1.400787	-1.994306
1	4.349133	0.167641	-1.791283
1	0.782324	-1.195488	2.045053
1	0.982157	-0.513321	4.394550
1	2.464518	1.390343	5.055842
1	3.765312	2.607501	3.301582
1	3.575104	1.931193	0.914204
1	4.256084	2.875276	-1.319899
1	3.463763	4.327829	-2.017440
1	3.571640	4.133428	-0.236116

1	1.435424	3.559013	-3.458295
1	1.251643	1.774993	-3.386274
1	-0.059073	2.841637	-2.771270
1	-0.309735	2.854561	0.015748
1	1.097699	3.061933	1.111218
1	0.598158	4.401229	0.025355
1	-0.679209	0.572358	-2.722555
1	-2.052481	-0.352814	-2.070226
1	1.726357	-0.797063	-2.620168
1	-0.822246	-2.448464	-2.188129
1	-0.313388	-1.649240	-3.701294
6	-1.030403	0.472327	0.255408
6	-2.370799	0.932570	0.246162
1	-0.466545	0.530947	1.182331
1	-2.789246	1.154474	-0.733053
6	-3.470432	-0.713478	0.654521
6	-2.921709	-1.892547	0.093161
1	-3.291622	-2.391397	-0.790594
1	-3.292157	-0.619389	1.722740
7	-1.776153	-2.424351	0.620526
8	-1.261255	-1.857350	1.638887
8	-1.232735	-3.426100	0.081018
6	-4.843325	-0.317244	0.224836
6	-5.239553	-0.336893	-1.123177
6	-6.534971	0.015910	-1.495381
6	-7.464546	0.403163	-0.526615
6	-7.085479	0.433162	0.815467
6	-5.787025	0.079811	1.185459
1	-4.527008	-0.634314	-1.888942
1	-6.819946	-0.009739	-2.543904
1	-5.502654	0.092910	2.234551
1	-7.800466	0.729482	1.578336
1	-8.474302	0.679654	-0.817212
6	-2.751803	1.938335	1.317086
1	-2.389300	2.946311	1.075910
1	-3.839164	2.000895	1.425319
1	-2.330314	1.657654	2.289755

NImag = 1
Imag. Freq = -339

2a
Et = -843.457219 (-1828.729118)

7	-0.191496	0.658726	-0.962853
6	1.062637	-0.129154	-1.234420
6	1.450617	0.338523	-2.662960
6	0.851760	1.743602	-2.792624
6	-0.478604	1.616498	-2.053991
1	0.764333	-1.182565	-1.251491
1	0.988003	-0.336602	-3.391242
1	2.532370	0.327741	-2.831768
1	1.493487	2.477880	-2.288139
1	0.717805	2.062036	-3.830265
1	-0.839333	2.563897	-1.651501
1	-1.253303	1.197778	-2.708612
6	2.212026	0.033613	-0.200505
8	2.500779	1.388278	-0.021973
14	1.939896	2.661383	1.111213
6	3.414688	3.087252	2.075847
1	3.573488	4.189805	2.127935
1	4.329654	2.646553	1.610877
1	3.363810	2.712087	3.124176
6	1.517786	4.024902	-0.008110
1	2.249631	4.091024	-0.848175
1	1.528631	5.008675	0.516964
1	0.507003	3.901857	-0.461672
6	0.544555	2.229801	2.177575
1	0.729686	1.278167	2.732326
1	-0.406479	2.097350	1.607687
1	0.357817	3.021524	2.941687
6	3.456636	-0.607935	-0.827176
6	3.456940	-1.977234	-1.123438
6	4.585759	-2.574632	-1.680698
6	5.725033	-1.813603	-1.943384
6	5.730186	-0.451690	-1.646926
6	4.601116	0.150904	-1.091915
1	2.566707	-2.589332	-0.906816
1	4.576136	-3.650517	-1.909658
1	6.615758	-2.287562	-2.380441
1	6.626540	0.152494	-1.849226
1	4.608290	1.227337	-0.860251
6	1.975513	-0.733245	1.095251
6	2.699731	-0.354794	2.236411
6	2.587139	-1.064913	3.428489
6	1.755918	-2.182687	3.500049

6	1.053154	-2.586523	2.367211
6	1.170015	-1.876137	1.170835
1	0.614728	-2.263193	0.296619
1	0.400900	-3.474640	2.399144
1	1.664516	-2.746215	4.439852
1	3.163641	-0.748204	4.310020
1	3.379403	0.512481	2.179356
6	-1.058948	0.265300	-0.035146
6	-2.397963	0.674617	0.234988
1	-0.659581	-0.495393	0.628226
1	-2.636110	0.468100	1.276641
6	-2.972033	2.006943	-0.227463
1	-2.351308	2.851099	0.101078
1	-3.086240	2.073275	-1.313952
1	-3.965206	2.146300	0.205354
6	-3.545097	-0.796637	-0.505097
6	-3.232028	-2.059292	0.063133
1	-3.194915	-0.672337	-1.526876
1	-3.804077	-2.539102	0.843169
6	-4.932796	-0.297198	-0.272726
6	-5.522915	-0.315855	1.002186
6	-6.827889	0.135204	1.191743
6	-7.570788	0.616581	0.110610
6	-6.995661	0.645216	-1.160462
6	-5.687365	0.197927	-1.347035
1	-4.953168	-0.684664	1.851202
1	-7.266669	0.111214	2.185789
1	-8.588306	0.967505	0.259489
1	-7.564887	1.015408	-2.009099
1	-5.246719	0.217932	-2.341004
7	-2.076351	-2.700808	-0.279414
8	-1.304749	-2.130004	-1.128959
8	-1.770326	-3.794036	0.253431

NImag = 1
Imag. Freq = -352

2f	**Et= -843.464365 (-1828.727663)**

7	0.566909	-0.098763	0.710578
6	-0.662538	-0.818218	0.234510
6	-0.842110	-1.880610	1.348299
6	-0.361092	-1.173911	2.624416
6	0.840877	-0.352247	2.150331
1	-0.375637	-1.280134	-0.719071
1	-0.196264	-2.730730	1.106293
1	-1.876283	-2.226877	1.437077
1	-1.144275	-0.507253	3.008424
1	-0.085328	-1.871567	3.419910
1	0.949345	0.594518	2.685518
1	1.768517	-0.918502	2.239326
6	-1.926809	0.064322	-0.007346
8	-2.534947	0.227661	1.240073
14	-4.272820	0.347058	1.680066
6	-5.118608	1.646912	0.746828
1	-5.588122	1.259885	-0.188078
1	-4.407363	2.453405	0.446112
1	-5.926409	2.128209	1.346696
6	-5.072532	-1.265869	1.499219
1	-6.078364	-1.188475	1.024151
1	-5.209990	-1.778262	2.479920
1	-4.459649	-1.945690	0.857477
6	-4.083826	0.807584	3.425779
1	-4.603452	0.096813	4.109032
1	-4.481735	1.826192	3.639640
1	-3.003037	0.807933	3.709036
6	-2.826369	-0.631438	-1.025476
6	-2.818710	-2.020580	-1.199236
6	-3.648151	-2.624858	-2.145150
6	-4.500373	-1.852555	-2.931136
6	-4.518508	-0.467893	-2.766582
6	-3.688456	0.136084	-1.824843
1	-2.150328	-2.665593	-0.606962
1	-3.619029	-3.717702	-2.271759
1	-5.150608	-2.330188	-3.678485
1	-5.184850	0.152287	-3.384131
1	-3.710153	1.232998	-1.714935
6	-1.500897	1.419192	-0.558800
6	-1.467012	2.548908	0.265272
6	-1.078870	3.786679	-0.249020
6	-0.713821	3.906490	-1.588474
6	-0.732365	2.781230	-2.413774
6	-1.121871	1.544819	-1.903336

1	-1.139297	0.659889	-2.560378
1	-0.441345	2.868438	-3.471153
1	-0.410888	4.882788	-1.994071
1	-1.061265	4.668808	0.407852
1	-1.740819	2.457869	1.328114
6	1.377696	0.506400	-0.143802
6	2.714332	0.963003	0.043273
1	0.988626	0.548743	-1.156383
1	2.991589	1.624867	-0.776719
6	3.792880	-0.615803	-0.572535
1	3.514018	-0.478199	-1.613264
6	3.320808	-1.850784	-0.054348
1	3.722269	-2.375160	0.799435
7	2.202087	-2.423604	-0.594062
8	1.635465	-1.851279	-1.585381
8	1.744497	-3.490171	-0.099312
6	5.191663	-0.185883	-0.280800
6	5.878706	-0.557074	0.887070
6	7.191105	-0.142615	1.107944
6	7.845870	0.657454	0.168948
6	7.175651	1.038802	-0.994472
6	5.863160	0.622196	-1.212921
1	5.385835	-1.177636	1.629396
1	7.704709	-0.447330	2.015916
1	8.869261	0.978521	0.342059
1	7.675903	1.656448	-1.735517
1	5.349697	0.916587	-2.125514
6	3.253717	1.463135	1.375916
1	2.619052	2.253220	1.796580
1	3.351328	0.674131	2.126235
1	4.249436	1.887584	1.228110

NImag = 1

Imag. Freq = -316

3a   **Et = -843.4636643 (-1828.729916)**

7	0.211717	1.596533	-0.575812
6	-0.321192	0.769873	0.550165
6	-0.664937	1.894965	1.552312
6	-1.274415	3.002524	0.677303
6	-0.458727	2.923571	-0.624940
1	0.486074	0.142729	0.936984
1	0.276708	2.261385	1.971805
1	-1.301133	1.579752	2.383535
1	-2.333828	2.799493	0.478084
1	-1.189260	3.986828	1.142300
1	-1.087076	2.991461	-1.520270
1	0.331923	3.679613	-0.669987
6	-1.497791	-0.199074	0.136757
8	-2.360144	0.549513	-0.669541
14	-4.014926	0.216520	-1.305480
6	-4.574678	-1.494977	-1.146149
1	-3.721878	-2.213768	-1.200575
1	-5.286707	-1.772004	-1.959340
1	-5.095881	-1.681076	-0.177926
6	-5.091606	1.369909	-0.415492
1	-5.475370	0.936206	0.537441
1	-5.976936	1.669065	-1.023969
1	-4.541854	2.305208	-0.151722
6	-3.842745	0.704154	-3.043952
1	-2.869729	1.226846	-3.209550
1	-4.649222	1.404541	-3.363742
1	-3.870759	-0.169160	-3.735867
6	-2.222784	-0.695980	1.385393
6	-3.097596	0.181066	2.050604
6	-3.778731	-0.208233	3.200395
6	-3.615435	-1.497220	3.707199
6	-2.783784	-2.390468	3.037594
6	-2.103821	-1.997940	1.882818
1	-3.256741	1.196620	1.647687
1	-4.447227	0.503671	3.706950
1	-4.144650	-1.806118	4.620234
1	-2.662629	-3.417439	3.413573
1	-1.496557	-2.758205	1.369271
6	-0.857395	-1.349849	-0.635812
6	-1.221772	-1.629712	-1.957305
6	-0.638414	-2.685277	-2.657798
6	0.334243	-3.476313	-2.050886
6	0.729627	-3.192464	-0.743745

6	0.146313	-2.136174	-0.047118
1	0.486622	-1.925353	0.979922
1	1.510305	-3.799120	-0.260899
1	0.792906	-4.311928	-2.599004
1	-0.947198	-2.887975	-3.694049
1	-1.971566	-0.999390	-2.464583
6	1.158183	1.298695	-1.457728
6	2.114751	0.263576	-1.377705
1	1.284406	2.047880	-2.233255
1	1.842116	-0.600321	-0.772304
6	2.868835	-0.079837	-2.648142
1	3.794659	-0.617616	-2.420099
1	2.276651	-0.721190	-3.313331
1	3.132328	0.826090	-3.207065
6	3.536155	1.036129	-0.125312
6	2.992720	1.868324	0.876974
1	2.860549	1.590549	1.911800
1	4.005522	1.581533	-0.939656
6	4.277099	-0.181541	0.312814
6	3.784587	-1.035669	1.314189
6	4.510447	-2.151237	1.725839
6	5.744757	-2.443472	1.139638
6	6.244279	-1.609672	0.139267
6	5.515431	-0.492447	-0.271138
1	2.821874	-0.823386	1.773539
1	4.112626	-2.794975	2.505799
1	6.310003	-3.313953	1.460575
1	7.204264	-1.824989	-0.322155
1	5.917363	0.160762	-1.041460
7	2.541820	3.124539	0.553587
8	2.631127	3.509456	-0.653769
8	2.022002	3.850727	1.442979

NImag = 1
Imag. Freq = -319

3c
Et= -843.457674 (1828.724104)

7	0.583789	-1.252193	0.037509
6	-0.285918	-0.331109	-0.760041
6	-0.325632	-1.129595	-2.083165
6	-0.450500	-2.604975	-1.650876
6	0.238695	-2.660001	-0.264598
1	0.233173	0.623232	-0.895991
1	0.633943	-0.961151	-2.584985
1	-1.106445	-0.811078	-2.777950
1	-1.505301	-2.883488	-1.552439
1	0.011709	-3.289916	-2.366921
1	-0.441333	-3.048174	0.504634
1	1.154572	-3.257652	-0.257789
6	-1.671597	-0.021703	-0.081117
8	-2.218043	-1.260233	0.280695
14	-3.862232	-1.717151	0.866991
6	-4.930120	-0.346153	1.357884
1	-4.337842	0.520092	1.740783
1	-5.635230	-0.642677	2.170207
1	-5.548281	0.033049	0.510455
6	-4.581654	-2.694031	-0.481040
1	-5.143176	-2.059320	-1.205900
1	-5.289331	-3.467606	-0.101034
1	-3.788376	-3.227315	-1.057152
6	-3.454578	-2.795638	2.270418
1	-2.360810	-3.019909	2.286239
1	-3.990412	-3.771752	2.216681
1	-3.711038	-2.332050	3.251039
6	-2.565814	0.692245	-1.090736
6	-3.199805	-0.071229	-2.086791
6	-4.013313	0.522618	-3.046891
6	-4.222976	1.901548	-3.028629
6	-3.625820	2.667377	-2.031480
6	-2.813209	2.068309	-1.066202
1	-3.059599	-1.165927	-2.100884
1	-4.489764	-0.097742	-3.820061
1	-4.856163	2.376730	-3.791735
1	-3.790051	3.755126	-1.998581
1	-2.389344	2.717306	-0.284926
6	-1.372957	0.844370	1.138917
6	-1.756053	0.444187	2.424012

6	-1.488781	1.239703	3.537285
6	-0.818239	2.451466	3.386513
6	-0.401903	2.849152	2.116636
6	-0.666705	2.050664	1.004682
1	-0.294372	2.385946	0.016609
1	0.147387	3.794296	1.983522
1	-0.612211	3.084935	4.261316
1	-1.807680	0.905251	4.535258
1	-2.266548	-0.521839	2.570775
6	1.584316	-0.934473	0.851577
6	2.194853	0.331475	1.019094
1	2.070456	-1.798523	1.303944
1	1.565225	1.182352	0.762697
6	3.022533	0.537288	2.271962
1	3.675530	1.408327	2.144144
1	2.386301	0.731357	3.143799
1	3.651130	-0.331406	2.498201
6	3.354519	0.525454	-0.526423
6	3.720270	1.894610	-0.595175
1	4.671758	2.306108	-0.296828
1	2.591906	0.258379	-1.255894
6	4.442473	-0.495361	-0.427612
6	5.623726	-0.281514	0.301152
6	6.612423	-1.263292	0.367829
6	6.444242	-2.481712	-0.292490
6	5.277319	-2.708987	-1.023998
6	4.289969	-1.726241	-1.086774
1	5.773968	0.659891	0.820167
1	7.519095	-1.072936	0.935876
1	7.217050	-3.243698	-0.242147
1	5.138914	-3.648300	-1.553270
1	3.390464	-1.903795	-1.672828
7	2.788412	2.836256	-0.971506
8	1.600915	2.461821	-1.243575
8	3.129375	4.038265	-1.034928

NImag = 1

Imag. Freq = -352

3e Et = -843.458384(-1828.724264)

6	-1.297302	-0.528344	1.406076
6	-1.535756	-1.868722	1.728779
6	-1.233179	-2.373281	2.993017
6	-0.672257	-1.544010	3.961283
6	-0.400857	-0.212936	3.646570
6	-0.701173	0.289177	2.381303
1	-0.445224	1.343511	2.162855
1	0.060852	0.449647	4.394578
1	-0.439445	-1.936161	4.961682
1	-1.438417	-3.429317	3.221524
1	-1.959282	-2.550649	0.973269
6	1.601490	-0.938247	-0.308152
6	2.159406	-0.557311	0.929869
1	2.097245	-1.737457	-0.859956
1	1.553485	0.117353	1.533767
6	2.885998	-1.625669	1.725692
1	3.581125	-1.174098	2.442146
1	2.180992	-2.238394	2.300993
1	3.465298	-2.294039	1.079168
6	3.493253	0.822438	0.478445
6	2.948040	1.900862	-0.262640
1	3.201914	2.126372	-1.287217
1	3.595273	1.034637	1.542132
6	4.680067	0.138932	-0.117186
6	5.806222	-0.133863	0.674162
6	6.932177	-0.756756	0.134074
6	6.952402	-1.124884	-1.211277
6	5.838421	-0.861808	-2.012445
6	4.715913	-0.239035	-1.469932
1	5.803645	0.159520	1.720815
1	7.794371	-0.951552	0.766130
1	7.827282	-1.611302	-1.633535
1	5.844650	-1.142634	-3.062461
1	3.856343	-0.035161	-2.104005
7	2.020828	2.746412	0.291908
8	1.596190	2.516835	1.468815
8	1.573949	3.698774	-0.396972

7	0.684555	-0.285850	-1.012836
6	-0.344874	0.700601	-0.545129
6	-0.499668	1.534547	-1.836218
6	-0.456653	0.501061	-2.977177
6	0.445686	-0.630145	-2.437977
1	0.076388	1.313642	0.254787
1	0.356922	2.212997	-1.880343
1	-1.395018	2.160815	-1.852463
1	-1.459934	0.108234	-3.177284
1	-0.070419	0.923139	-3.908892
1	-0.047874	-1.608191	-2.502230
1	1.410254	-0.691813	-2.950275
6	-1.650842	0.031353	0.030077
8	-2.001286	-0.983272	-0.869530
14	-3.495071	-1.977124	-1.047764
6	-4.661223	-1.875458	0.328906
1	-4.178698	-1.445908	1.240428
1	-5.058286	-2.878457	0.612989
1	-5.539471	-1.229977	0.092288
6	-4.236463	-1.442033	-2.613512
1	-4.978619	-0.622425	-2.468709
1	-4.763925	-2.278336	-3.129377
1	-3.458098	-1.060101	-3.316391
6	-2.799057	-3.645651	-1.222253
1	-1.690235	-3.595870	-1.343249
1	-3.204468	-4.176353	-2.114881
1	-3.006074	-4.287289	-0.334690
6	-2.748928	1.086981	0.124809
6	-3.443889	1.447214	-1.042862
6	-4.446485	2.412035	-1.020269
6	-4.785983	3.038787	0.178666
6	-4.121778	2.677610	1.347476
6	-3.118673	1.706291	1.322947
1	-3.191535	0.952020	-1.996413
1	-4.967569	2.681402	-1.950661
1	-5.570413	3.808992	0.199362
1	-4.383638	3.159413	2.301503
1	-2.641116	1.442498	2.278588

NImag = 1

Imag. Freq = -302

3f Et = -843.4565765 (-1828.723583)			1	-4.024689	1.173879	-3.960077

				1	-3.844479	3.642430	-3.596189
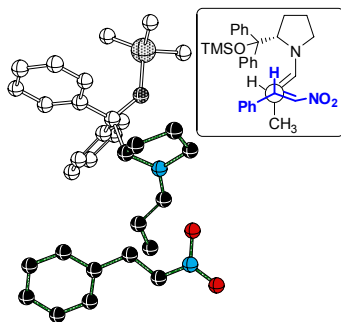
7	0.223621	-1.630908	0.038938
6	-0.341855	-0.485253	-0.723181
6	-0.489595	-1.159467	-2.107565
6	-1.021770	-2.567803	-1.786813
6	-0.388471	-2.903585	-0.415530
1	0.397617	0.319705	-0.759301
1	0.519919	-1.240705	-2.524856
1	-1.099977	-0.605444	-2.825278
1	-2.115094	-2.552024	-1.708809
1	-0.744267	-3.298139	-2.550589
1	-1.143193	-3.233542	0.308495
1	0.407905	-3.646646	-0.489688
6	-1.637554	0.127354	-0.070932
8	-2.515264	-0.938818	0.143095
14	-4.248847	-0.979847	0.641976
6	-4.905647	0.575964	1.285063
1	-4.124448	1.158367	1.830544
1	-5.743075	0.403316	2.002056
1	-5.298766	1.235982	0.476637
6	-5.135447	-1.536253	-0.836503
1	-5.422953	-0.686245	-1.498532
1	-6.069823	-2.088743	-0.581238
1	-4.500735	-2.224747	-1.444537
6	-4.225082	-2.276667	1.909454
1	-3.242036	-2.807499	1.905253
1	-5.013659	-3.045874	1.737465
1	-4.377555	-1.871862	2.936610
6	-2.251243	1.149003	-1.023186
6	-2.939441	0.683065	-2.156809
6	-3.502439	1.565507	-3.074542
6	-3.408906	2.941775	-2.869127
6	-2.770678	3.417568	-1.726861
6	-2.208156	2.530297	-0.807134
1	-3.054743	-0.403876	-2.312399

| 1	-4.024689	1.173879	-3.960077
1	-3.844479	3.642430	-3.596189
1	-2.712603	4.500249	-1.539181
1	-1.758396	2.956210	0.102396
6	-1.179590	0.759510	1.241235
6	-1.671976	0.312202	2.472083
6	-1.234735	0.876414	3.670104
6	-0.283151	1.893784	3.659389
6	0.237152	2.332166	2.441876
6	-0.200160	1.765160	1.246555
1	0.236416	2.120852	0.298954
1	1.002116	3.122857	2.422172
1	0.061566	2.342099	4.602448
1	-1.640731	0.510540	4.624888
1	-2.405905	-0.510919	2.501890
6	1.327400	-1.645369	0.777778
6	2.225053	-0.587453	1.065409
1	1.583772	-2.633926	1.145000
1	1.820492	0.419499	0.963622
6	3.116507	-0.778849	2.277602
1	3.891808	-0.007331	2.311654
1	2.551697	-0.718222	3.216565
1	3.614556	-1.754643	2.245593
6	3.474338	-0.549272	-0.529781
6	4.374665	-1.637627	-0.506961
1	5.410337	-1.591842	-0.208041
1	2.667800	-0.669991	-1.248180
6	4.023964	0.837289	-0.484327
6	3.353506	1.863454	-1.170727
6	3.833937	3.171972	-1.166698
6	4.999463	3.486383	-0.465804
6	5.677012	2.479841	0.224794
6	5.195369	1.171165	0.216853
1	2.450955	1.625076	-1.730378
1	3.301845	3.944060	-1.716155
1	5.378157	4.504632	-0.460632
1	6.587733	2.712393	0.770193
1	5.739479	0.401304	0.755279
7	3.918175	-2.904301	-0.780263
8	2.674913	-3.051290	-1.032387
8	4.709027	-3.873712	-0.760249

NImag = 1
Imag. Freq = -333

II. Michael addition between iminium and nitroalkane anion

4b (NImag = 1, Imag. Freq = -178
Et = -1266.465070 (-2251.733881)

6	-3.529060	0.751523	-2.366243
6	-3.705659	-0.659176	-1.854633
6	-4.103323	-0.642047	-0.343766
6	-4.806478	-1.276106	-2.750267
1	-2.767600	-1.197077	-1.990018
6	-3.009847	-0.326315	0.675047
1	-4.823344	0.181352	-0.224431
6	-4.845280	-1.908766	0.101601
6	-1.793790	1.600356	0.605895
1	-3.397041	-0.116652	1.665763
7	-1.853821	-1.084873	0.772613
6	-0.835655	1.520297	-0.422148
6	-2.845893	2.635820	0.666830
1	-1.480605	1.220858	1.575991
6	0.265888	0.680813	-0.280478
1	-4.970215	-2.324696	-2.491512
1	-5.763400	-0.751236	-2.636894
1	-4.511832	-1.222638	-3.804111
6	-6.170593	-1.823127	0.546491
6	-6.863360	-2.958808	0.972216
6	-6.237402	-4.204538	0.956884
6	-4.914677	-4.303066	0.516986
6	-4.222728	-3.168236	0.095766
1	-6.667753	-0.855218	0.562065
1	-7.891053	-2.866883	1.314578
1	-6.772662	-5.091212	1.286150
1	-4.416503	-5.269144	0.504451
1	-3.191140	-3.253881	-0.231867
8	-1.345248	-1.605036	-0.262074
8	-1.222155	-1.077171	1.864042
6	-3.507190	2.852649	1.891092
6	-4.483214	3.836922	2.021031
6	-4.824750	4.632209	0.924527
6	-4.177660	4.432988	-0.296745
6	-3.198754	3.448757	-0.426785
1	-3.239863	2.242098	2.750405
1	-4.974126	3.986849	2.978882
1	-5.585195	5.402230	1.021976
1	-4.432648	5.049996	-1.154367

1	-2.711727	3.313233	-1.386917
1	0.434803	0.231119	0.695611
7	1.162060	0.362224	-1.220731
6	2.196098	-0.699654	-1.016012
6	2.712632	-0.956449	-2.455662
6	1.522124	-0.602313	-3.351295
6	0.922599	0.622276	-2.656100
1	3.563519	-0.292764	-2.664175
1	3.058796	-1.987883	-2.573253
1	1.808293	-0.395832	-4.386795
1	0.789794	-1.417393	-3.354865
1	1.430864	1.548715	-2.961463
1	-0.148503	0.729838	-2.840212
1	1.673800	-1.589151	-0.636396
6	3.380837	-0.386925	-0.066357
8	4.055667	0.757022	-0.496839
14	3.804563	2.520916	-0.278074
6	3.538072	3.125269	-1.966546
1	3.719518	2.308802	-2.706872
1	2.497694	3.492016	-2.126637
1	4.227317	3.962351	-2.225997
6	2.469055	3.018639	0.832155
1	1.457457	2.812478	0.407075
1	2.528019	2.482715	1.810442
1	2.511381	4.111379	1.054596
6	5.419019	3.039996	0.364717
1	5.816439	3.938551	-0.161531
1	5.382508	3.280973	1.452281
1	6.168485	2.222033	0.233708
6	4.359273	-1.558469	-0.236811
6	5.631667	-1.358929	-0.781332
6	6.511644	-2.432522	-0.920202
6	6.128555	-3.710993	-0.518470
6	4.861118	-3.914039	0.027990
6	3.980539	-2.843775	0.171406
1	5.936420	-0.349373	-1.099217
1	7.511185	-2.266095	-1.347575
1	6.822997	-4.556305	-0.628580
1	4.555039	-4.919727	0.351327
1	2.988297	-3.009008	0.620373
6	3.020757	-0.357785	1.410298
6	1.923718	-1.043290	1.942728
6	1.679327	-1.032455	3.317597
6	2.543608	-0.365839	4.182709
6	3.657883	0.295680	3.665709
6	3.893825	0.296891	2.293910
1	1.213933	-1.600540	1.305712
1	0.784146	-1.548006	3.701287
1	2.351581	-0.363554	5.265282
1	4.354884	0.813100	4.340978
1	4.781003	0.812786	1.888612
1	-1.005742	2.027170	-1.363074
1	-4.375372	1.433842	-2.121634
8	-2.603385	1.157776	-3.040341

**4c** (NImag = 1, Imag. Freq = -156)
Et= -1266.458611(-2251.727244)
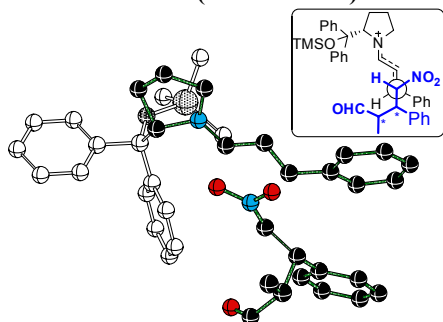
6	-3.362686	-3.823801	-0.510222
6	-4.073593	-2.708948	-1.252344
6	-3.750861	-1.252893	-0.759316
6	-3.854030	-2.948345	-2.765300
1	-5.146441	-2.876199	-1.062004
6	-2.289161	-0.898715	-0.836092
1	-4.275122	-0.588971	-1.455342
6	-4.364907	-1.048446	0.626845
6	-1.849165	1.370970	-0.098210
6	-0.722398	1.732369	-0.846700
6	-3.134373	2.065338	-0.271786
1	-1.691603	0.905239	0.870475
6	0.492444	1.085345	-0.635482
1	-4.406139	-2.207981	-3.349366
1	-2.800370	-2.867368	-3.042642
1	-4.207902	-3.947618	-3.047550
6	-5.703267	-0.638520	0.715665
6	-6.332343	-0.474164	1.949405
6	-5.627371	-0.711977	3.130537
6	-4.295331	-1.121436	3.059474
6	-3.672063	-1.293933	1.821127
1	-6.255546	-0.429248	-0.198046
1	-7.369501	-0.150493	1.986863
1	-6.111291	-0.582091	4.095107
1	-3.736676	-1.317432	3.971428
1	-2.645871	-1.642978	1.789225
6	-3.916512	2.379372	0.853227
6	-5.092633	3.114276	0.721360
6	-5.521345	3.528662	-0.541367
6	-4.768384	3.196892	-1.671289
6	-3.583846	2.475514	-1.542099
1	-3.594528	2.046314	1.836305
1	-5.678236	3.355712	1.604256
1	-6.441146	4.098243	-0.646127
1	-5.108016	3.497863	-2.658940
1	-3.024111	2.179831	-2.423416
1	0.552597	0.404128	0.211224
7	1.628423	1.255073	-1.316304
6	2.782880	0.308370	-1.280483
6	3.795930	1.019839	-2.201115

6	2.911254	1.606655	-3.307775
6	1.629107	2.030836	-2.573749
1	4.308869	1.811822	-1.639219
1	4.555520	0.326497	-2.575753
1	3.381110	2.441546	-3.835092
1	2.675690	0.834152	-4.047366
1	1.614230	3.102362	-2.337998
1	0.725978	1.782622	-3.142499
1	2.455739	-0.629052	-1.757404
6	3.407423	-0.058098	0.085938
8	3.897983	1.071491	0.740638
14	3.171772	2.428768	1.662160
6	3.237683	3.857358	0.552611
1	4.094079	3.766826	-0.158071
1	2.313315	3.960999	-0.062203
1	3.372458	4.813593	1.110444
6	1.500471	2.133335	2.286911
1	0.710133	2.418729	1.552655
1	1.345735	1.055552	2.538217
1	1.305195	2.715844	3.218588
6	4.366540	2.580615	3.015387
1	5.234690	1.899222	2.839667
1	4.773058	3.614102	3.109658
1	3.926844	2.305234	4.001744
6	4.631681	-0.923290	-0.253454
6	5.928011	-0.476315	0.018972
6	7.025773	-1.280244	-0.289416
6	6.837527	-2.532843	-0.870975
6	5.545150	-2.984441	-1.139976
6	4.445908	-2.186254	-0.830335
1	6.078527	0.512168	0.480888
1	8.042213	-0.922031	-0.070264
1	7.703707	-3.165117	-1.113973
1	5.390458	-3.974556	-1.593276
1	3.427080	-2.557045	-1.026395
6	2.521742	-0.925883	0.968445
6	1.450582	-1.679499	0.471853
6	0.712066	-2.506743	1.320310
6	1.052385	-2.615247	2.667433
6	2.136102	-1.892106	3.165596
6	2.866890	-1.058924	2.322280
1	1.150770	-1.629893	-0.591188
1	-0.147572	-3.071158	0.917292
1	0.472654	-3.272897	3.331604
1	2.421331	-1.984466	4.223850
1	3.738217	-0.509092	2.713524
1	-0.840895	2.405444	-1.687791
1	-3.764059	-4.836350	-0.753315
8	-2.424319	-3.719147	0.252393
1	-1.591342	-1.385367	-0.169960
7	-1.713845	-0.642965	-2.056674
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8	-2.391297	-0.199666	-3.024106

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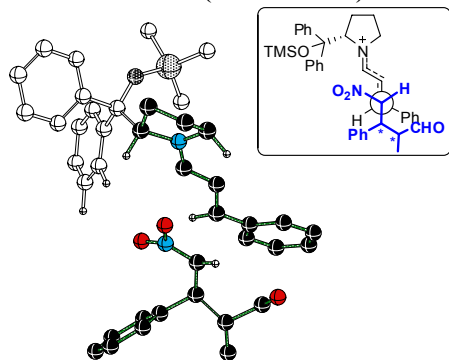
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6	4.127085	4.589272	-0.622087
6	4.338115	5.033242	0.685173
6	4.454974	4.099947	1.715205
6	4.115861	0.779033	-0.169190
6	5.409963	0.394981	-0.981584
1	5.389184	0.960792	-1.920126
6	2.884618	0.316625	-0.933366
7	1.700854	1.023762	-0.842066
8	1.394979	1.614583	0.228840
8	0.867642	0.894682	-1.783589
6	5.422067	-1.071956	-1.368028
8	5.148835	-1.492973	-2.473659
6	1.865169	-1.417080	0.183073
6	2.944408	-2.386164	0.448734
6	3.632437	-2.322871	1.674953
6	4.626851	-3.248871	1.991002
6	4.957104	-4.256641	1.083603
6	4.285715	-4.329534	-0.141293
6	3.292544	-3.406817	-0.455595
6	0.724966	-1.762945	-0.563577
6	-0.397356	-0.936958	-0.554535
7	-1.510934	-1.068524	-1.287141
6	-2.556166	0.001404	-1.341499
6	-3.396611	-0.404277	-2.579664
6	-2.404984	-1.146841	-3.479883
6	-1.563836	-1.939609	-2.476199
6	-3.471928	0.182933	-0.104129
6	-2.793333	0.816612	1.099677
6	-1.663671	1.635225	0.996504
6	-1.119975	2.241169	2.131208
6	-1.715792	2.066242	3.377882
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6	-4.558758	1.174990	-0.543745
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6	-6.874309	1.700683	-1.018331
6	-6.520548	3.012373	-1.329701
6	-5.185383	3.407912	-1.244981
6	-4.208295	2.495847	-0.851437
6	-3.729401	-3.801764	-0.153248
6	-2.094830	-2.463969	1.973307
1	1.730745	-0.661812	0.955718
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1	5.138421	-3.185555	2.947757
1	5.731850	-4.978995	1.325725
1	4.546279	-5.102305	-0.859158
1	2.807971	-3.455898	-1.425603
1	-0.408519	-0.119326	0.161522
1	-4.211760	-1.072406	-2.268123
1	-3.847780	0.471510	-3.055789
1	-2.891539	-1.790783	-4.218460
1	-1.765573	-0.435022	-4.013504
1	-2.033005	-2.901514	-2.222923
1	-0.550035	-2.131428	-2.836137
1	-2.036255	0.950887	-1.530023
1	-4.136622	-3.403977	-1.114190
1	-2.719751	-4.221422	-0.369595
1	-4.382400	-4.651953	0.153008
1	-1.985277	-1.539689	2.590991
1	-1.994122	-3.333921	2.664867
1	-1.221951	-2.497941	1.278227
1	-5.891340	-1.951716	1.965964
1	-5.483727	-3.669153	2.299378
1	-4.769408	-2.364318	3.305594
1	-6.180223	-0.252329	-0.380793
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1	-1.158068	1.820788	0.031735
1	-0.204346	2.845268	2.021719
1	-1.289214	2.549310	4.268662
1	-3.348098	1.144176	4.464688
1	-4.305622	0.045126	2.447097
1	0.746437	-2.647678	-1.191122
1	3.015124	-0.106039	-1.921594
1	4.171852	0.254423	0.796098
1	3.861550	2.894228	-1.915754
1	4.029578	5.307215	-1.432493
1	4.408196	6.096727	0.897927
1	4.615488	4.432113	2.737808
1	4.446408	2.014250	2.247560
6	6.699944	0.707724	-0.205619
1	5.722627	-1.770152	-0.557462
1	7.583677	0.455455	-0.802859
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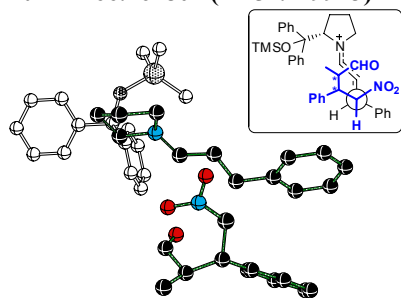
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6	-3.808792	-1.934656	-0.851757
6	-2.824949	-4.144123	-1.736004
1	-3.381474	-3.701141	0.282677
6	-3.191465	-0.686617	-1.491713
1	-4.501741	-2.313135	-1.620701
6	-4.724593	-1.537158	0.312408
6	-2.213031	0.897114	-0.162156
6	-0.995663	1.220104	-0.791339
6	-3.309203	1.889673	-0.124917
1	-2.173449	0.192019	0.662253
6	0.133467	0.424469	-0.620933
1	-3.828486	-4.479419	-2.019796
1	-2.351929	-3.672264	-2.600946
1	-2.242105	-5.035867	-1.475206
6	-6.041779	-1.147615	0.031936
6	-6.924177	-0.792761	1.052675
6	-6.504980	-0.832403	2.383109
6	-5.197376	-1.221703	2.677073
6	-4.312438	-1.566161	1.652507
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1	-7.940685	-0.495777	0.807804
1	-7.192266	-0.568283	3.182648
1	-4.860209	-1.260478	3.710107
1	-3.292885	-1.852928	1.889501
6	-4.074119	2.046059	1.042140
6	-5.071715	3.017353	1.117249
6	-5.333544	3.841439	0.021862
6	-4.593596	3.682166	-1.153352
6	-3.591136	2.718453	-1.227627
1	-3.884122	1.400159	1.893858
1	-5.648131	3.125290	2.032171
1	-6.113697	4.596001	0.078470
1	-4.802270	4.308335	-2.017021
1	-3.043822	2.574580	-2.154758
1	0.118776	-0.323322	0.168494
7	1.271653	0.515622	-1.320546
6	2.437020	-0.388867	-1.088994
6	3.223791	-0.294175	-2.425392
6	2.166824	0.105093	-3.458954
6	1.287757	1.088782	-2.684318
1	3.995460	0.484173	-2.343211
1	3.728385	-1.237956	-2.653889
1	2.595595	0.545991	-4.363820
1	1.557085	-0.758534	-3.746481
1	1.714646	2.101818	-2.678391
1	0.263846	1.119218	-3.062399
1	2.049825	-1.408465	-0.953432
6	3.365936	-0.061699	0.110191
8	3.876496	1.231708	-0.014152
14	3.277568	2.868999	0.419958
6	3.277288	3.746480	-1.166199
1	3.730089	3.110734	-1.965237
1	2.249535	4.019059	-1.500899
1	3.870937	4.689341	-1.122615
6	1.673106	2.955105	1.243915
1	0.830374	2.643192	0.580511
1	1.638356	2.297334	2.145733
1	1.447815	3.992934	1.587059
6	4.601998	3.479958	1.499741
1	5.505038	2.828228	1.415013
1	4.917858	4.515540	1.234265
1	4.302212	3.489999	2.573108
6	4.561443	-1.015518	-0.025077
6	5.842696	-0.525527	-0.297649
6	6.920832	-1.403513	-0.410766
6	6.728908	-2.775252	-0.254939
6	5.453066	-3.268546	0.018656
6	4.374507	-2.394151	0.135605
1	5.996426	0.558057	-0.422449
1	7.925105	-1.008793	-0.623409
1	7.579422	-3.466269	-0.344855
1	5.296286	-4.349546	0.146424
1	3.374059	-2.790632	0.368160
6	2.757904	-0.340243	1.475793
6	1.738312	-1.274846	1.681606
6	1.253187	-1.528199	2.965963
6	1.801108	-0.876631	4.068169
6	2.841891	0.032946	3.879476
6	3.315209	0.295255	2.596934
1	1.290534	-1.838195	0.846534
1	0.424201	-2.242194	3.091873
1	1.419940	-1.080371	5.079111
1	3.293603	0.541487	4.743873
1	4.144363	1.009195	2.452177
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1	-0.683715	-3.439181	-0.496811
8	-1.257469	-2.123732	0.917806
7	-2.107842	-0.758506	-2.340120
8	-1.176358	-1.598111	-2.118973
8	-1.939517	0.157316	-3.183727
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III. Intramolecular cyclization

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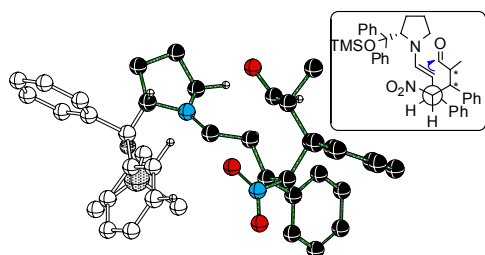
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6	-2.707413	2.516762	0.269841
1	-1.383456	1.152197	1.131789
6	0.034140	0.173178	-0.764716
6	-2.780775	3.220076	1.469933
6	-3.399342	4.456272	1.540495
6	-3.961407	5.018070	0.405655
6	-3.895863	4.331365	-0.793730
6	-3.274374	3.093318	-0.861636
1	-2.348300	2.797618	2.360439
1	-3.438294	4.979581	2.479188
1	-4.441216	5.978994	0.455926
1	-4.326336	4.756356	-1.682951
1	-3.233911	2.585974	-1.806599
1	0.043615	-0.525689	0.042719
7	1.111904	0.222874	-1.465928
6	2.257253	-0.725850	-1.310821
6	3.005614	-0.587743	-2.656100
6	2.009330	0.065258	-3.608239
6	1.267541	1.023916	-2.698197
1	3.864832	0.056116	-2.530292
1	3.362155	-1.548938	-2.999357
1	2.498076	0.574394	-4.430725
1	1.295826	-0.645516	-4.001583
1	1.863257	1.896758	-2.463588
1	0.308732	1.293800	-3.089191
1	1.840005	-1.717816	-1.236696
6	3.194614	-0.451953	-0.084605
8	3.516108	0.908643	-0.122467
14	3.395557	2.419441	0.548400
6	3.747384	3.623271	-0.858763
1	2.971517	3.630368	-1.616978
1	3.830248	4.637298	-0.474128
1	4.686619	3.386134	-1.352276
6	1.700630	2.766906	1.292405
1	1.430844	2.042730	2.055124
1	1.705722	3.747786	1.763481
1	0.916092	2.778308	0.541976
6	4.727694	2.717510	1.858097
1	5.673998	2.254527	1.589752
1	4.908184	3.786836	1.944646
1	4.450355	2.361130	2.844523
6	4.488482	-1.271596	-0.299901
6	5.708917	-0.653608	-0.527373
6	6.860212	-1.404889	-0.721022
6	6.807604	-2.785525	-0.699088
6	5.591726	-3.413400	-0.474188
6	4.447831	-2.664285	-0.270390
1	5.764521	0.415682	-0.560639
1	7.796200	-0.903361	-0.892468
1	7.698986	-3.367210	-0.851261
1	5.534640	-4.486939	-0.448731
1	3.523435	-3.175242	-0.072135
6	2.641970	-0.873624	1.294897
6	1.584999	-1.750593	1.488313
6	1.178421	-2.121321	2.766181
6	1.844182	-1.644336	3.875551
6	2.937889	-0.807641	3.697983
6	3.331763	-0.438622	2.427951
1	1.051162	-2.176163	0.661958
1	0.330312	-2.770901	2.874289
1	1.528621	-1.927060	4.863465
1	3.490329	-0.451885	4.549474
1	4.206994	0.167765	2.311178
1	-1.008810	1.814517	-1.517430
6	-3.823685	-0.579557	-0.633735
1	-4.332364	0.266560	-1.089306
6	-4.925649	-1.521050	-0.150161
6	-4.671378	-2.839344	0.219232
6	-5.689772	-3.655474	0.682118
6	-6.984012	-3.172034	0.785480
6	-7.251174	-1.864235	0.420514
6	-6.229462	-1.050393	-0.042333
1	-3.676536	-3.236958	0.142034
1	-5.470408	-4.670884	0.960615
1	-7.773675	-3.808145	1.143578
1	-8.251863	-1.476315	0.491521
1	-6.452991	-0.036486	-0.327265
6	-2.884141	-1.149088	-1.717652
6	-1.988662	-0.066517	-2.353094
1	-2.645861	0.751909	-2.696156
8	-1.109525	-0.473472	-3.171796
1	-2.236245	-1.909758	-1.304429
6	-3.680781	-1.769414	-2.874450
1	-4.373854	-1.046150	-3.300333
1	-2.991257	-2.068597	-3.651064
1	-4.256565	-2.631602	-2.560924
1	-3.868191	0.508176	1.213628
7	-2.509346	-0.959062	1.492953
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8	-2.855830	-0.951036	2.628764

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[a] Optimization done at HF/6-31G* level of theory
[b] Energy reported at HF/6-31G* level of theory

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6	3.911592	-0.636738	0.716076
6	3.487027	-0.359396	3.248586
1	3.220253	-2.140792	2.113376
6	2.999040	-0.183196	-0.437865
1	4.544997	0.211612	0.993830
6	4.820926	-1.773680	0.255813
6	1.931350	0.919556	-0.121623
6	1.102804	0.514930	1.130051
6	2.464220	2.347071	-0.055964
1	1.276230	0.891150	-0.999507
6	-0.273444	0.145357	0.801015
1	4.565600	-0.465749	3.414054
1	3.262589	0.714591	3.238484
1	2.975581	-0.789329	4.118421
6	6.206425	-1.603194	0.161851
6	7.029472	-2.655004	-0.246716
6	6.474407	-3.891340	-0.577528
6	5.091326	-4.069879	-0.492778
6	4.270248	-3.022635	-0.075794
1	6.642703	-0.636272	0.398039
1	8.104296	-2.504268	-0.310804
1	7.113734	-4.709930	-0.898481
1	4.649954	-5.030458	-0.747026
1	3.194144	-3.163590	0.013012
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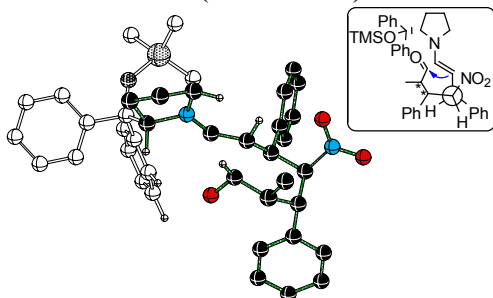
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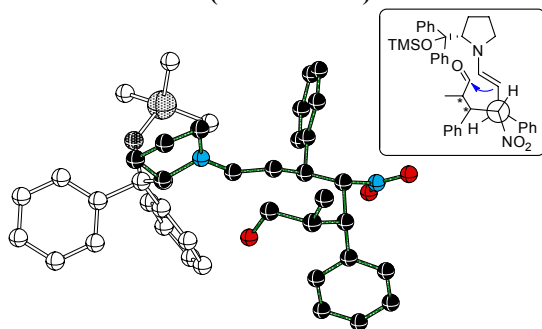
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