

Supporting Information

Substituent Effect on the Himbert Intramolecular Arene/Allene Diels-Alder Reaction: NBO analysis and state specific dual Descriptors

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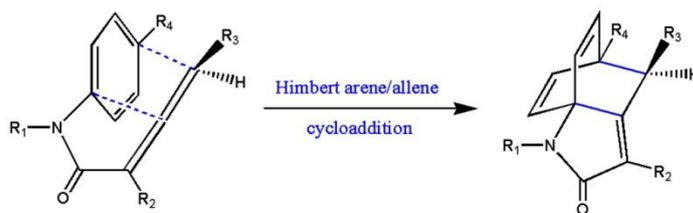
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Scheme S1. Himbert arene/allene [4+2] Cycloaddition

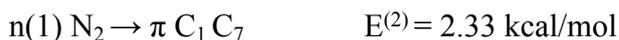


1. NBO analyses

➤ R1=CH₃

Inverse-electron demand reaction

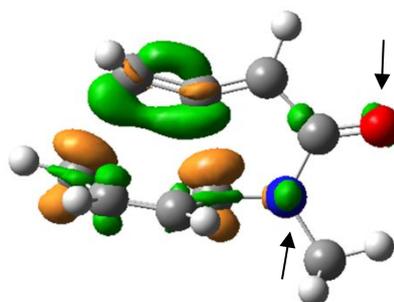
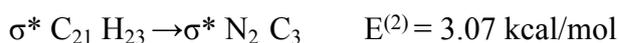
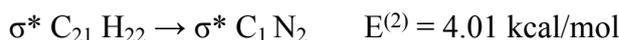
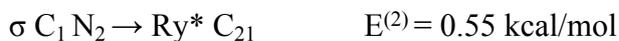
Diene



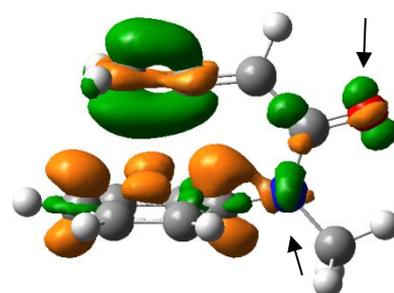
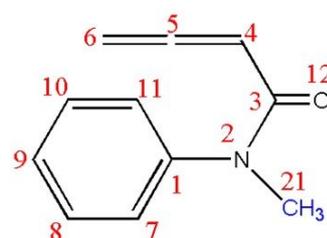
Dienophile



Substituent and core molecule interaction



SSDD_TS



SSDD_Reactant

➤ **R1= Si(Me)₃**

Normal-electron demand reaction

Diene

$$n(2) N_2 \rightarrow Ry^* C_1 \quad E^{(2)} = 2.55 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \pi^* C_1 C_7 \quad E^{(2)} = 10.76 \text{ kcal/mol}$$

Dienophile

$$\sigma C_4 C_5 \rightarrow \pi^* C_3 O_{12} \quad E^{(2)} = 19.11 \text{ kcal/mol}$$

$$\sigma C_4 H_{13} \rightarrow \sigma^* N_2 C_3 \quad E^{(2)} = 6.22 \text{ kcal/mol}$$

$$\sigma C_4 H_{13} \rightarrow \sigma^* C_3 O_{12} \quad E^{(2)} = 0.53 \text{ kcal/mol}$$

the nitrogen lone pair stabilizes the bonds constituting the chain connecting the diene to the dienophile in IMDA reaction

$$n(1) N_2 \rightarrow \pi^* C_3 O_{12} \quad E^{(2)} = 77.45 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow Ry^* C_3 \quad E^{(2)} = 1.45 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \sigma^* C_1 N_2 \quad E^{(2)} = 1.35 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \sigma^* C_3 C_4 \quad E^{(2)} = 6.86 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \sigma^* C_3 O_{12} \quad E^{(2)} = 2.28 \text{ kcal/mol}$$

$$n(2) O_{12} \rightarrow \sigma^* C_1 N_2 \quad E^{(2)} = 0.53 \text{ kcal/mol}$$

Si(Me)₃ as an electron-withdrawing groups (EWG)

$$\sigma C_1 N_2 \rightarrow n^*(2) Si_{21} \quad E^{(2)} = 20.26 \text{ kcal/mol}$$

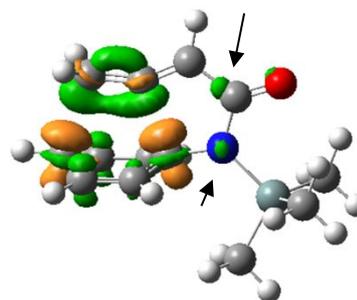
$$\sigma N_2 C_3 \rightarrow n^*(2) Si_{21} \quad E^{(2)} = 21.11 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow n^*(2) Si_{21} \quad E^{(2)} = 213.74 \text{ kcal/mol}$$

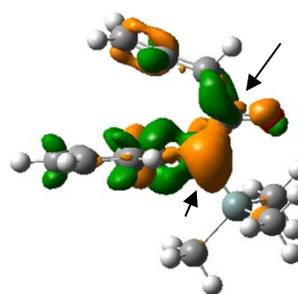
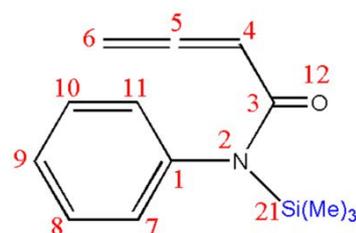
$$n(2) N_2 \rightarrow \sigma^* Si_{21} C_{26} \quad E^{(2)} = 6.54 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \sigma^* Si_{21} C_{30} \quad E^{(2)} = 7.61 \text{ kcal/mol}$$

$$n(2) N_2 \rightarrow \sigma^* Si_{21} C_{22} \quad E^{(2)} = 4.7 \text{ kcal/mol}$$



SSDD_TS



SSDD_Reactant

➤ **R1=CHO**

Normal-electron demand reaction

Diene



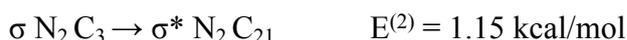
Dienophile



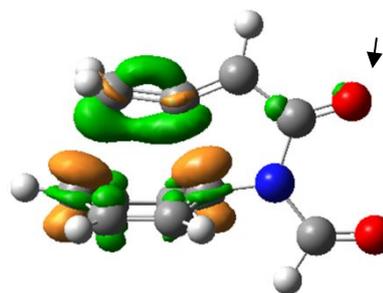
the oxygen O₁₂ lone pairs stabilizes the bonds constituting the chain connecting the diene to the dienophile in IMDA reaction



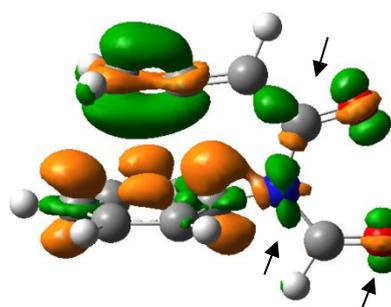
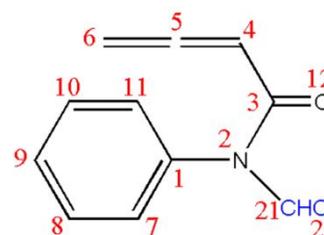
CHO as an electron-withdrawing groups (EWG)



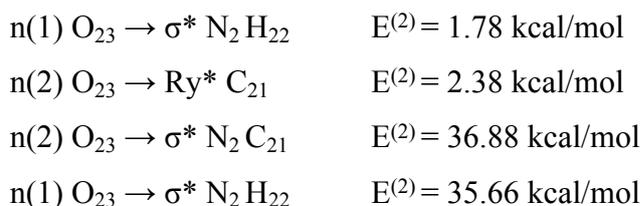
CHO stabilization



SSDD_TS



SSDD_Reactant



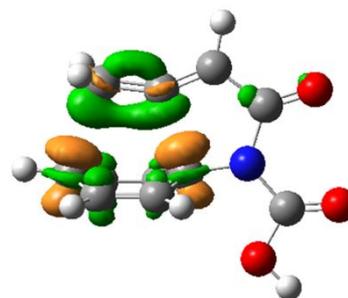
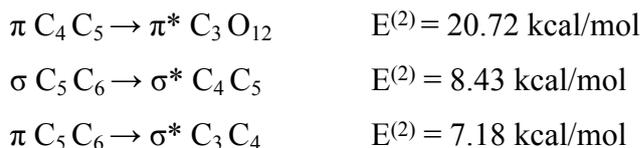
➤ **R1=COOH**

Normal-electron demand reaction

Diene

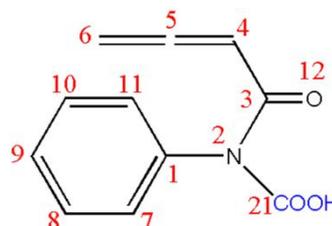
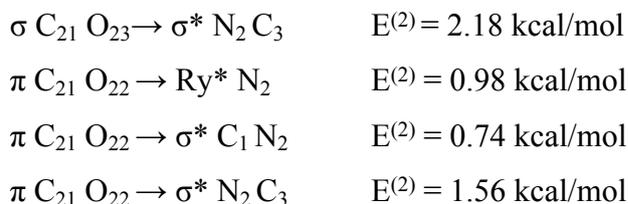


Dienophile



SSDD_TS

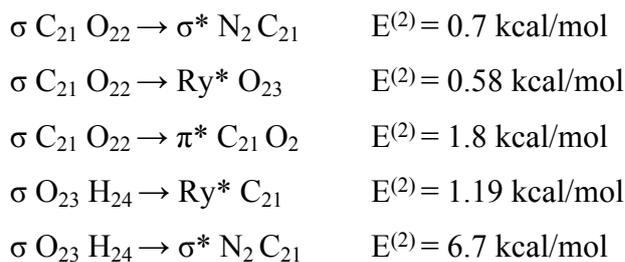
A weak stabilization by COOH of the bonds constituting the chain connecting the diene to the dienophile in IMDA reaction



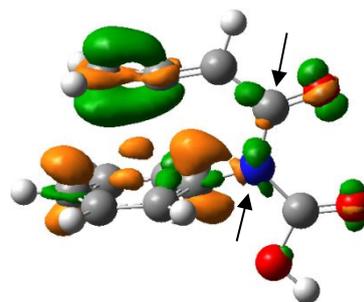
CHO as an electron-withdrawing groups (EWG)



COOH stabilization



σ O ₂₃ H ₂₄ → σ^* C ₂₁ O ₂₂	$E^{(2)} = 0.75$ kcal/mol
$n(1)$ O ₂₂ → Ry* C ₂₁	$E^{(2)} = 14.92$ kcal/mol
$n(2)$ O ₂₂ → σ^* C ₂₁ O ₂₃	$E^{(2)} = 40.11$ kcal/mol
$n(1)$ O ₂₃ → σ^* C ₂₁ O ₂₂	$E^{(2)} = 5.49$ kcal/mol
$n(2)$ O ₂₃ → π^* C ₂₁ O ₂₂	$E^{(2)} = 30.92$ kcal/mol
π^* C ₂₁ O ₂₂ → σ^* C ₂₁ O ₂₂	$E^{(2)} = 41.12$ kcal/mol



SSDD_Reactant

➤ **R1=SH**

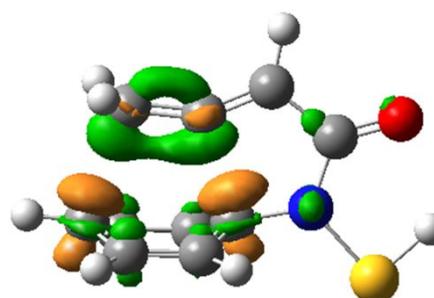
Inverse-electron demand reaction

Diene

π C ₁ C ₇ → σ^* N ₂ S ₂₁	$E^{(2)} = 1.01$ kcal/mol
σ C ₁ C ₇ → σ^* N ₂ S ₂₁	$E^{(2)} = 4.09$ kcal/mol

Dienophile

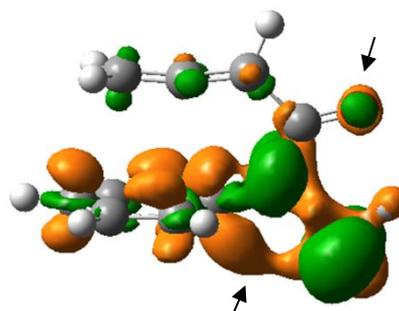
σ S ₂₁ H ₂₂ → σ^* C ₃ C ₄	$E^{(2)} = 0.56$ kcal/mol
σ C ₄ H ₁₃ → π^* C ₅ C ₆	$E^{(2)} = 12.13$ kcal/mol
$n(1)$ N ₂ → π^* C ₃ O ₁₂	$E^{(2)} = 80.43$ kcal/mol
π^* C ₃ O ₁₂ → π^* C ₄ C ₅	$E^{(2)} = 23.43$ kcal/mol



SSDD_TS

A weak stabilization by SH of the bonds constituting the chain connecting the diene to the dienophile in IMDA reaction

σ S ₂₁ H ₂₂ → σ^* C ₁ N ₂	$E^{(2)} = 2.16$ kcal/mol
$n(1)$ S ₂₁ → σ^* C ₁ N ₂	$E^{(2)} = 0.86$ kcal/mol
$n(1)$ S ₂₁ → σ^* N ₂ C ₃	$E^{(2)} = 2.37$ kcal/mol
$n(1)$ S ₂₁ → σ^* C ₃ O ₁₂	$E^{(2)} = 0.61$ kcal/mol
$n(2)$ S ₂₁ → π^* C ₃ O ₁₂	$E^{(2)} = 0.84$ kcal/mol

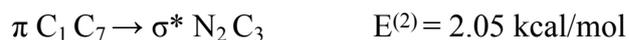


SSDD_Reactant

➤ **R1=NH2**

Inverse-electron demand reaction

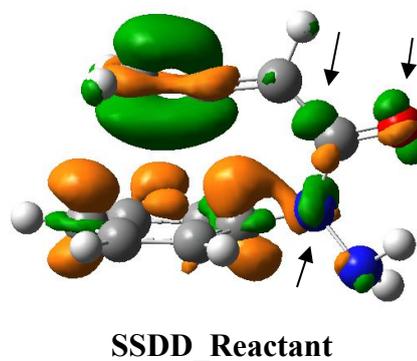
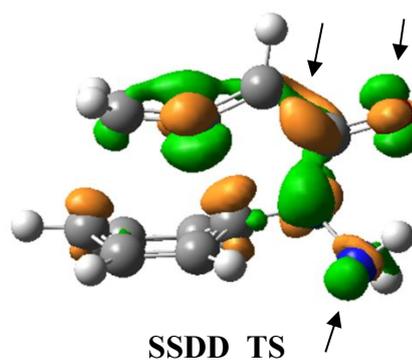
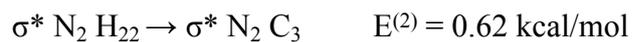
Diene



Dienophile

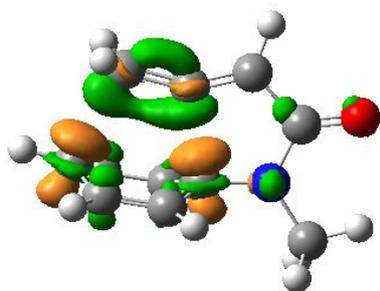


NH₂ interaction with the molecular core

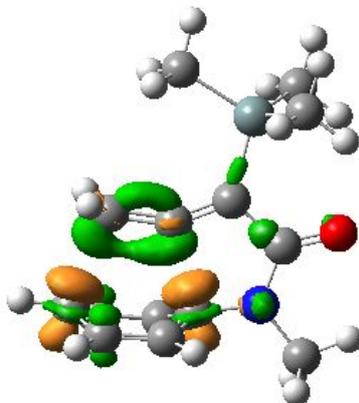


2. SSDD calculation for R2 substituent

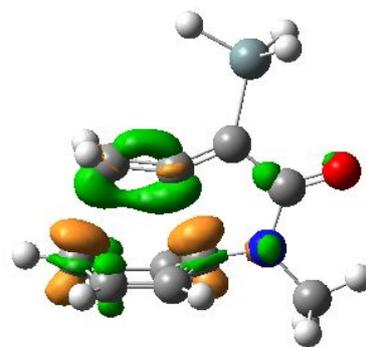
$R_2=H$



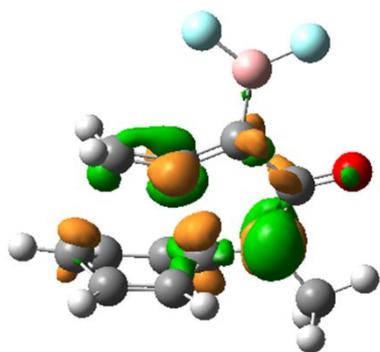
$R_2=SiMe_3$



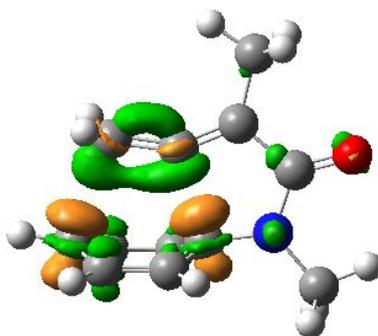
$R_2=SiH_3$



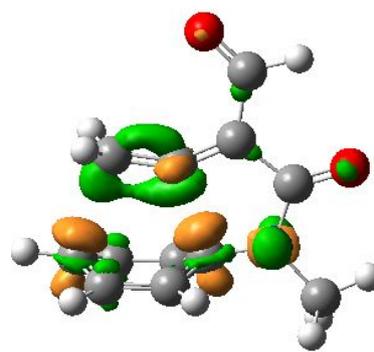
$R_2=BF_2$



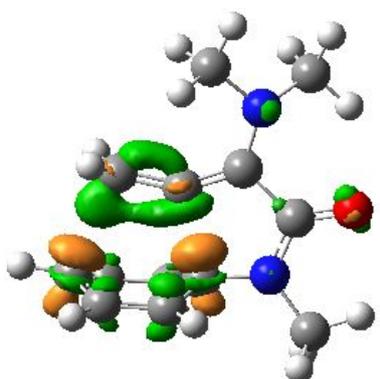
$R_2=CH_3$



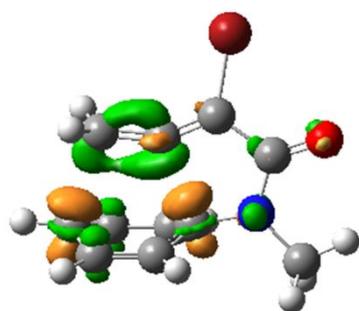
$R_2=CHO$



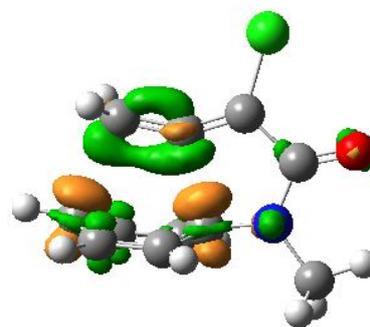
$R_2=NMe_2$



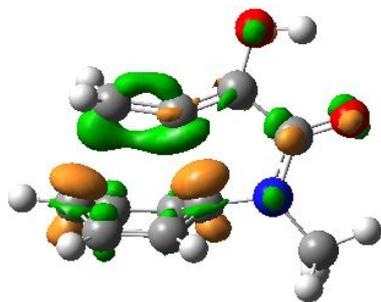
$R_2=Br$



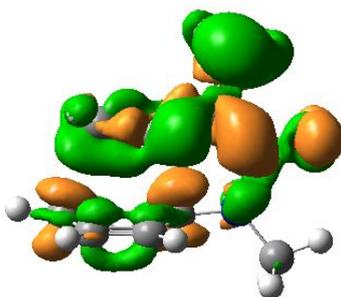
$R_2=Cl$



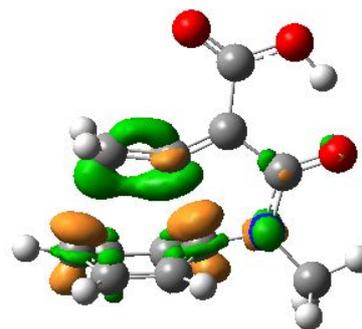
$R_2=OH$



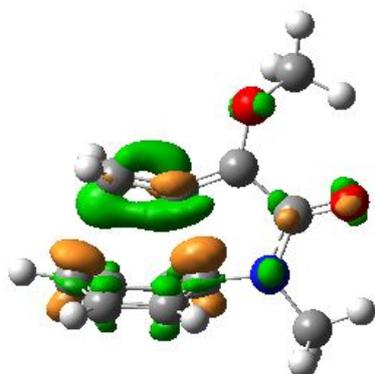
$R_2=NH_2$



$R_2=COOH$



$R_2=OCH_3$



3. Geometric structures

R1 Substituent

TS_R1--CH₃

E(RM062X) = -555.51498170 a.u.

Imaginary Freq = 1

C	-0.04025100	-0.58197400	-0.00006400
N	1.38561700	-0.59319000	-0.00015600
C	2.01870900	0.64067200	-0.00002700
C	1.01420500	1.74063900	-0.00005200
C	-0.27566800	1.43367700	-0.00010600
C	-1.59971400	1.81081900	0.00008600
C	-0.74584500	-0.85558800	1.23152600
C	-2.08825700	-0.62803600	1.22777600
C	-2.66981500	-0.16373400	0.00006800
C	-2.08837300	-0.62800600	-1.22770200
C	-0.74596400	-0.85555300	-1.23159000
O	3.23221100	0.79152800	0.00008900
H	1.39590000	2.75749400	-0.00005400
H	-2.04887900	2.18028400	-0.91646800
H	-2.04853600	2.18022300	0.91683400
H	-0.18280100	-1.07321700	2.13323100

H	-2.68176300	-0.66448700	2.13596900
H	-3.72066000	0.11298000	0.00012500
H	-2.68197300	-0.66444900	-2.13583500
H	-0.18300200	-1.07314600	-2.13335600
C	2.14520800	-1.83112800	0.00003200
H	1.92342300	-2.43343400	-0.88883000
H	3.20190300	-1.56001100	-0.00035100
H	1.92397500	-2.43285400	0.88942400

TS_R1--CHO

E(RM062X)= -629.52534284 a.u.

Imaginary Freq = 1

C	0.17967200	-0.48476000	0.00009600
N	-1.24645100	-0.30486000	0.00005000
C	-1.69498300	1.05468600	0.00008000
C	-0.52594400	1.96886500	-0.00033800
C	0.70103900	1.46364500	-0.00052400
C	2.06352400	1.65049300	-0.00080800
C	0.83016300	-0.86453300	-1.23220300
C	2.19169500	-0.84334700	-1.22747800
C	2.83865500	-0.48073700	0.00022800
C	2.19160800	-0.84233800	1.22819600
C	0.83009100	-0.86345000	1.23280300
O	-2.85453100	1.39577400	0.00036100
H	-0.74357900	3.03291600	-0.00056300
H	2.56199900	1.94636200	0.91667800
H	2.56170600	1.94534000	-0.91878400
H	0.23890100	-0.99691100	-2.13210800
H	2.77212500	-0.97403800	-2.13512800
H	3.91866000	-0.36327800	0.00021100
H	2.77198600	-0.97241000	2.13596800
H	0.23867600	-0.99520700	2.13269500
C	-2.08942300	-1.42385600	-0.00008500
H	-1.49067100	-2.35587700	-0.00007500
O	-3.29562200	-1.41338400	-0.00024200

TS_R1--C1

E(RM062X)= -975.76522605 a.u.

Imaginary Freq = 1

C	0.16441300	-0.45656700	0.10031900
N	-1.23461100	-0.19008500	0.23075700
C	-1.67764800	1.12983700	0.03922900
C	-0.49279100	2.02856300	0.00363900
C	0.72414800	1.49938300	-0.00999700
C	2.09131400	1.64385300	-0.07618400
C	0.70986300	-0.87057200	-1.17192200
C	2.06707800	-0.86536200	-1.26827100
C	2.80746300	-0.47318100	-0.10044200
C	2.25537600	-0.81142600	1.18201600
C	0.89873900	-0.81751800	1.28901800
O	-2.83958300	1.46105400	-0.06162600

H	-0.69269100	3.09562500	-0.03626900
H	2.63993100	1.94048300	0.81218900
H	2.54681200	1.92993200	-1.01918700
H	0.04982300	-1.03012700	-2.01749400
H	2.57832900	-1.02627500	-2.21198000
H	3.88594300	-0.37187700	-0.18570300
H	2.90348000	-0.92982700	2.04446400
H	0.36809400	-0.92859900	2.22797500
Cl	-2.36520700	-1.47524900	-0.03886600

TS_R1--COOH

E(RM062X) = -704.76684597 a.u.

Imaginary Freq = 1

C	0.25731800	-0.34620600	0.00003700
N	-1.13387200	0.02965600	-0.00007500
C	-1.39359500	1.44061400	0.00011200
C	-0.11473400	2.18905100	-0.00116900
C	1.03717000	1.53253100	-0.00153500
C	2.41143800	1.54225100	-0.00073300
C	0.85731400	-0.79421900	-1.23228700
C	2.21062300	-0.94201200	-1.22756000
C	2.89826500	-0.66509800	0.00049400
C	2.21040800	-0.94035800	1.22880200
C	0.85712500	-0.79251600	1.23307800
O	-2.49382900	1.93988100	0.00109400
H	-0.19631000	3.27210100	-0.00136000
H	2.94250000	1.77354900	0.91699500
H	2.94362300	1.77246600	-0.91809300
H	0.25264800	-0.86011800	-2.12991400
H	2.76991900	-1.14071700	-2.13614000
H	3.98447800	-0.68741600	0.00061800
H	2.76955800	-1.13790700	2.13772400
H	0.25231300	-0.85722700	2.13069200
C	-2.16046700	-0.91584500	-0.00015400
O	-3.34687800	-0.69580200	-0.00046400
O	-1.63443900	-2.17280400	0.00006500
H	-2.40563600	-2.76168100	-0.00007100

TS_R1--H

E(RM062X) = -516.22221549 a.u.

Imaginary Freq = 1

C	-0.01654800	-0.80300200	-0.00522800
N	-1.41552700	-1.06309900	-0.01466500
C	-2.28481400	0.01485200	-0.00239900
C	-1.50794500	1.28764100	-0.00382500
C	-0.18297200	1.22917300	-0.00150500
C	1.04663800	1.85105400	0.00050800
C	0.73514800	-0.92714900	-1.23354500
C	2.00479000	-0.43696200	-1.22303900
C	2.47272500	0.13783500	0.00760700
C	1.99324100	-0.44025800	1.23225700
C	0.72348600	-0.93048500	1.22994800

O	-3.50050900	-0.08362400	0.00814300
H	-2.07412300	2.21451600	-0.00378200
H	1.40840900	2.30735600	0.91675800
H	1.41385400	2.30302300	-0.91569500
H	0.22943800	-1.25560600	-2.13544200
H	2.59927300	-0.35543200	-2.12759700
H	3.44776300	0.61763800	0.01294500
H	2.57990300	-0.36234700	2.14222300
H	0.21030900	-1.26066300	2.12710000
H	-1.80455400	-1.99398900	0.01632200

TS_R1--NH₂

E(RM062X) = -571.53126964 a.u.

Imaginary Freq = 1

C	0.05225400	-0.59941500	0.11094800
N	-1.37300800	-0.60604900	0.23556100
C	-2.01384300	0.61524400	0.06507700
C	-1.02955200	1.72373400	0.01594700
C	0.26221900	1.41930300	-0.02781800
C	1.57925000	1.80797700	-0.12339000
C	0.66494000	-0.94612400	-1.14889200
C	1.99991800	-0.70229100	-1.25457900
C	2.66306000	-0.15215900	-0.10481600
C	2.18026800	-0.54389900	1.18943100
C	0.84516100	-0.78452700	1.30315000
O	-3.22702300	0.70974000	-0.07519700
H	-1.41764300	2.73729400	-0.02996400
H	2.08199600	2.22172400	0.74504000
H	1.96103600	2.14391200	-1.08251200
H	0.04097000	-1.26029300	-1.97775700
H	2.53011300	-0.79987500	-2.19678000
H	3.70745700	0.13242500	-0.20062500
H	2.83842500	-0.51770500	2.05219700
H	0.34589000	-0.95170700	2.25152500
N	-2.07882100	-1.78629300	-0.12839900
H	-2.40803400	-2.21624900	0.73686400
H	-2.92327500	-1.44810200	-0.59689300

TS_R1--OCH₃

E(RM062X) = -630.65452623 a.u.

Imaginary Freq = 1

C	0.17736500	-0.46050000	-0.04952900
N	-1.21963600	-0.16578200	-0.16611600
C	-1.57364400	1.19412500	-0.02399400
C	-0.36534700	2.04821100	-0.12765700
C	0.82783800	1.46492300	-0.10012500
C	2.20110900	1.55663600	-0.08106200
C	0.86949600	-0.93026300	-1.22611200
C	2.22758600	-0.97994000	-1.15227000
C	2.82628000	-0.58306400	0.09144000
C	2.09701800	-0.86195200	1.29787300
C	0.73829600	-0.81140800	1.23428500

O	-2.71718600	1.57188700	0.13990200
H	-0.51509000	3.12362700	-0.16732600
H	2.69051500	1.89839200	0.82584200
H	2.73954000	1.75854500	-1.00151100
H	0.31145200	-1.07549900	-2.14441100
H	2.84718500	-1.18408700	-2.01983300
H	3.91017900	-0.52844500	0.14701600
H	2.62385100	-0.98340200	2.23911400
H	0.09087100	-0.89160600	2.09971000
O	-2.05546200	-1.05336100	0.55030100
C	-3.04124300	-1.60780700	-0.32495400
H	-3.61424300	-2.29768100	0.29945600
H	-3.69814500	-0.82449900	-0.71213200
H	-2.57599900	-2.15683500	-1.15210500

TS_R1--SH

E(RM062X)= -914.37410935 a.u.

Imaginary Freq = 1

C	0.17449200	-0.46008900	-0.00128400
N	-1.22673200	-0.19807300	-0.00263700
C	-1.63866300	1.12210300	-0.00055500
C	-0.45919100	2.02550000	-0.00076400
C	0.75578400	1.49252600	-0.00089300
C	2.12611600	1.62736400	0.00123400
C	0.81779700	-0.85101800	-1.23459700
C	2.17870100	-0.85366000	-1.22775600
C	2.82842200	-0.49114300	0.00145100
C	2.17615700	-0.85405100	1.22921600
C	0.81527300	-0.85131800	1.23326300
O	-2.81681200	1.46250000	0.00127000
H	-0.65631200	3.09350100	-0.00038400
H	2.62938600	1.91685500	0.91856900
H	2.63255700	1.91699400	-0.91430700
H	0.22135600	-0.98011300	-2.13109700
H	2.75959400	-0.99591800	-2.13349400
H	3.91102500	-0.39783400	0.00259900
H	2.75521600	-0.99674100	2.13606100
H	0.21697400	-0.98088000	2.12845400
S	-2.41184400	-1.48528200	0.00014400
H	-3.40799200	-0.56212500	0.00371500

TS_R1--SiH₃

E(RM062X)= -806.90535916 a.u.

Imaginary Freq = 1

C	-0.17354200	-0.45634800	-0.00002100
N	1.22989800	-0.17738800	-0.00009500
C	1.57081300	1.17526900	-0.00001900
C	0.37174600	2.04967500	-0.00003400
C	-0.82546600	1.47840100	-0.00000300
C	-2.19930400	1.57282800	-0.00004600
C	-0.81468500	-0.85936200	1.23127600
C	-2.17498800	-0.90070700	1.22723100

C	-2.83730300	-0.55530000	0.00005100
C	-2.17504900	-0.90076100	-1.22714800
C	-0.81474900	-0.85942000	-1.23126100
O	2.73624700	1.54888900	0.00006200
H	0.53698800	3.12311900	-0.00006500
H	-2.71063700	1.85194100	-0.91613600
H	-2.71067300	1.85205800	0.91598700
H	-0.21976300	-0.96806600	2.13205700
H	-2.74909100	-1.05838300	2.13481000
H	-3.92242300	-0.49729000	0.00007200
H	-2.74919200	-1.05849000	-2.13469200
H	-0.21986500	-0.96818700	-2.13206100
Si	2.56896100	-1.34325200	-0.00000200
H	3.40610500	-1.20803900	-1.21439100
H	3.40576700	-1.20825600	1.21465200
H	1.90322200	-2.66992700	-0.00020100

TS_R1--SiMe₃

E(RM062X) = -924.84917377 a.u.

Imaginary Freq = 1

C	0.70810200	-0.25474800	0.00009300
N	-0.59375000	0.34073500	0.00003200
C	-0.59455900	1.73454100	0.00010400
C	0.78246800	2.29579100	-0.00033900
C	1.81112100	1.46033500	-0.00072000
C	3.16743900	1.22203700	-0.00075000
C	1.23828900	-0.79966800	-1.23065600
C	2.54775300	-1.17092300	-1.22667200
C	3.27396500	-0.99600300	0.00027800
C	2.54790000	-1.16981400	1.22747100
C	1.23843900	-0.79858600	1.23126000
O	-1.61980500	2.40662000	0.00037500
H	0.87472300	3.37819300	-0.00050500
H	3.73154500	1.36974200	0.91501400
H	3.73120400	1.36869100	-0.91689800
H	0.63759400	-0.75648500	-2.13311200
H	3.06712100	-1.46073100	-2.13478900
H	4.34068300	-1.20377800	0.00031600
H	3.06735800	-1.45881300	2.13579400
H	0.63780100	-0.75466300	2.13371600
Si	-2.16949000	-0.54199200	-0.00006000
C	-3.12889200	-0.09239400	1.55583000
H	-3.27689500	0.98919800	1.60463400
H	-4.11190300	-0.57700100	1.56207200
H	-2.59596800	-0.40762700	2.45930800
C	-3.12880100	-0.09211400	-1.55592300
H	-4.11166700	-0.57700800	-1.56248400
H	-3.27712600	0.98945100	-1.60437400
H	-2.59565300	-0.40686400	-2.45943800
C	-1.73820600	-2.37824200	-0.00016500
H	-1.16023900	-2.66722500	-0.88337200
H	-1.15992600	-2.66720000	0.88284900
H	-2.66121200	-2.96936200	0.00001200

R2 Substituent

TS_R2--BF₂

E(RM062X) = -779.55133039 a.u.

Imaginary Freq = 1

C	-1.18226000	0.69610200	0.00001600
N	-0.17126200	1.69912800	0.00002600
C	1.14952200	1.27381000	-0.00001200
C	1.23108600	-0.22672900	-0.00000400
C	0.07231200	-0.89568400	0.00000000
C	-0.59151600	-2.09838700	-0.00000100
C	-1.87320700	0.39173600	-1.23181100
C	-2.66820100	-0.71448200	-1.22756600
C	-2.76157300	-1.45064600	0.00000000
C	-2.66820400	-0.71449700	1.22757500
C	-1.87321000	0.39172100	1.23183600
O	2.10464000	2.03471600	-0.00004800
H	-0.63998400	-2.67674000	0.91688400
H	-0.63998700	-2.67673700	-0.91688700
H	-1.62431000	0.94041900	-2.13419600
H	-3.11464600	-1.10610300	-2.13619800
H	-3.31230300	-2.38723600	-0.00000600
H	-3.11465100	-1.10612900	2.13620200
H	-1.62431400	0.94039300	2.13422800
C	-0.50201300	3.11470700	-0.00001900
H	-1.08298800	3.38541400	0.88920200
H	0.43944500	3.66540700	0.00004100
H	-1.08285500	3.38539900	-0.88933200
B	2.58621100	-0.98435800	0.00000300
F	2.60065500	-2.31576300	-0.00008400
F	3.75832800	-0.37532900	0.00010100

TS_R2--Br

E(RM062X) = -3129.09557764 a.u.

Imaginary Freq = 1

C	-1.48933800	0.64481200	0.00007300
N	-0.55415100	1.72248800	0.00017800
C	0.78868900	1.39172500	0.00004000
C	0.93924200	-0.10227400	0.00001500
C	-0.12212800	-0.88381600	-0.00001700
C	-0.71414700	-2.12443400	-0.00009300
C	-2.14997100	0.28642400	-1.23206900
C	-2.85763000	-0.87730700	-1.22824900
C	-2.89383400	-1.61934200	-0.00006200
C	-2.85761400	-0.87746700	1.22821700
C	-2.14997500	0.28627300	1.23217100
O	1.70034100	2.19933100	-0.00004800

H	-0.72485100	-2.70643800	0.91663900
H	-0.72478700	-2.70633300	-0.91689400
H	-1.93985700	0.84986300	-2.13515600
H	-3.26815500	-1.30388800	-2.13793700
H	-3.37692400	-2.59253700	-0.00013600
H	-3.26814600	-1.30419000	2.13783800
H	-1.93979800	0.84953500	2.13534900
C	-0.98605000	3.11111900	-0.00004800
H	-1.58530500	3.33760700	0.88919000
H	-0.08798100	3.72985200	0.00042400
H	-1.58433900	3.33763600	-0.88993000
Br	2.73522900	-0.75878400	-0.00000300

TS_R1--CH₃

E(RM062X) = -594.81901292 a.u.

Imaginary Freq = 1

C	0.39316500	-0.76665400	-0.00026700
N	-0.97740200	-1.16074500	-0.00058300
C	-1.91326000	-0.14252800	-0.00010600
C	-1.25344400	1.20162200	-0.00005500
C	0.07609100	1.22666500	-0.00004800
C	1.24617200	1.95340800	0.00014100
C	1.14566500	-0.84654100	-1.23173500
C	2.38215700	-0.27594300	-1.22763400
C	2.82656500	0.31661700	0.00029700
C	2.38172300	-0.27623300	1.22792600
C	1.14523600	-0.84683400	1.23145400
O	-3.12471800	-0.32115300	0.00020200
H	1.59072400	2.42189200	0.91711100
H	1.59100600	2.42190700	-0.91671500
H	0.65831000	-1.20094600	-2.13412500
H	2.96328800	-0.15396100	-2.13642000
H	3.76673900	0.86138800	0.00052700
H	2.96253600	-0.15447700	2.13694800
H	0.65759100	-1.20145800	2.13359800
C	-1.37742800	-2.55686100	0.00011900
H	-1.00250800	-3.07679100	0.88956700
H	-2.46808700	-2.57957800	-0.00032800
H	-1.00170300	-3.07779100	-0.88838800
C	-2.16185700	2.40230600	0.00001600
H	-2.81733000	2.38518700	-0.87725100
H	-2.81813200	2.38444400	0.87666000
H	-1.58757200	3.33048200	0.00064200

TS_R2--CHO

E(RM062X) = -668.81878469 a.u.

Imaginary Freq = 1

C	-0.74953100	0.80139200	0.00016700
N	0.44723700	1.58153500	0.00031600
C	1.64403000	0.88909400	0.00015300
C	1.40007600	-0.58655400	0.00004800
C	0.13523100	-1.01049200	-0.00017500

C	-0.74003200	-2.06490100	-0.00035000
C	-1.48924500	0.64841500	-1.23163900
C	-2.49375500	-0.27236300	-1.22702400
C	-2.74236800	-0.97160000	-0.00004500
C	-2.49362700	-0.27281800	1.22716100
C	-1.48912500	0.64795700	1.23199500
O	2.74892700	1.41584700	0.00005000
H	-0.89826500	-2.62218400	0.91734300
H	-0.89827000	-2.62179800	-0.91827900
H	-1.13232400	1.13220600	-2.13480800
H	-3.01001800	-0.56331400	-2.13645100
H	-3.47581800	-1.77287000	-0.00016300
H	-3.00980500	-0.56410500	2.13653100
H	-1.13207700	1.13140600	2.13528900
C	0.41489100	3.03509100	-0.00025300
H	-0.09747400	3.41885600	0.88917200
H	1.44923700	3.38120900	-0.00103100
H	-0.09855100	3.41799300	-0.88940400
C	2.56767300	-1.50727500	-0.00000100
H	3.54466100	-0.98742500	0.00010800
O	2.48141600	-2.72039600	-0.00014400

TS_R2--C1

E(RM062X) = -1015.10599433 a.u.
Imaginary Freq = 1

C	-0.80610800	0.78270000	-0.00017500
N	0.40687100	1.53499400	-0.00047600
C	1.58969700	0.81925700	-0.00001400
C	1.28478800	-0.65255800	-0.00010400
C	0.03237100	-1.07281200	-0.00021100
C	-0.89544100	-2.08645300	-0.00018300
C	-1.54656600	0.64504600	-1.23215900
C	-2.57599900	-0.24699800	-1.22805100
C	-2.84226100	-0.93832700	0.00032300
C	-2.57542200	-0.24698800	1.22855300
C	-1.54601400	0.64507500	1.23215800
O	2.70172500	1.31546300	0.00025500
H	-1.08561000	-2.63558200	0.91709900
H	-1.08585000	-2.63534800	-0.91755600
H	-1.17430200	1.11686000	-2.13546100
H	-3.09691900	-0.52793600	-2.13790800
H	-3.59792700	-1.71891200	0.00047700
H	-3.09598400	-0.52792600	2.13862000
H	-1.17330800	1.11674600	2.13534400
C	0.40707300	2.98901200	0.00001700
H	-0.09482300	3.38318600	0.89099800
H	1.44863300	3.31226700	-0.00278300
H	-0.09987400	3.38331100	-0.88797500
C1	2.67278600	-1.72688500	-0.00003000

TS_R2--COOH

E(RM062X) = -744.05822787 a.u.
Imaginary Freq = 1

C	-1.10753600	0.73881800	-0.00001000
N	-0.00872000	1.65677700	-0.00004700
C	1.24244400	1.10532800	0.00002200
C	1.19803300	-0.38447700	-0.00000700
C	-0.00523900	-0.95645300	-0.00005000
C	-0.75039600	-2.10424600	-0.00008300
C	-1.82137800	0.50348200	-1.23239500
C	-2.71062900	-0.52940100	-1.22692300
C	-2.87925400	-1.25007900	0.00004000
C	-2.71052100	-0.52944100	1.22701200
C	-1.82126900	0.50344100	1.23243300
O	2.28699100	1.77149000	0.00007600
H	-0.84587400	-2.67409200	0.91823200
H	-0.84592700	-2.67398700	-0.91845800
H	-1.52202100	1.02324300	-2.13639400
H	-3.18819500	-0.87921600	-2.13659600
H	-3.51192600	-2.13291400	0.00005300
H	-3.18801100	-0.87927800	2.13671600
H	-1.52184400	1.02319000	2.13641600
C	-0.21386800	3.09849500	-0.00001900
H	-0.76985100	3.41201600	0.88993300
H	0.76790900	3.57235200	-0.00085300
H	-0.77130500	3.41175500	-0.88914200
C	2.46822900	-1.20803700	-0.00000200
O	2.45113800	-2.41868300	0.00004200
O	3.60460600	-0.50170400	-0.00007300
H	3.38450600	0.46609400	-0.00003500

TS_R2--H

E(RM062X) = -555.51498170 a.u.
Imaginary Freq = 1

C	-0.04025100	-0.58197400	-0.00006400
N	1.38561700	-0.59319000	-0.00015600
C	2.01870900	0.64067200	-0.00002700
C	1.01420500	1.74063900	-0.00005200
C	-0.27566800	1.43367700	-0.00010600
C	-1.59971400	1.81081900	0.00008600
C	-0.74584500	-0.85558800	1.23152600
C	-2.08825700	-0.62803600	1.22777600
C	-2.66981500	-0.16373400	0.00006800
C	-2.08837300	-0.62800600	-1.22770200
C	-0.74596400	-0.85555300	-1.23159000
O	3.23221100	0.79152800	0.00008900
H	1.39590000	2.75749400	-0.00005400
H	-2.04887900	2.18028400	-0.91646800
H	-2.04853600	2.18022300	0.91683400
H	-0.18280100	-1.07321700	2.13323100
H	-2.68176300	-0.66448700	2.13596900
H	-3.72066000	0.11298000	0.00012500
H	-2.68197300	-0.66444900	-2.13583500
H	-0.18300200	-1.07314600	-2.13335600
C	2.14520800	-1.83112800	0.00003200

H	1.92342300	-2.43343400	-0.88883000
H	3.20190300	-1.56001100	-0.00035100
H	1.92397500	-2.43285400	0.88942400

TS_R2--NH₂

E(RM062X) = -610.86728475 a.u.

Imaginary Freq = 1

C	-0.36957400	-0.74189200	0.01489300
N	1.01032700	-1.12134700	0.02590200
C	1.92001400	-0.09279300	0.00793000
C	1.22855700	1.23625300	0.01425200
C	-0.10612300	1.23582200	-0.01792300
C	-1.27975900	1.95515300	-0.03463900
C	-1.12114700	-0.82766900	1.24605300
C	-2.37627300	-0.29806900	1.22965800
C	-2.84423800	0.24573000	-0.00959800
C	-2.36914400	-0.34135700	-1.22640700
C	-1.11374600	-0.87061100	-1.21743900
O	3.13934100	-0.22456500	-0.02929900
H	-1.65547600	2.38491200	-0.96058900
H	-1.65705400	2.42075200	0.87296100
H	-0.62165500	-1.14274600	2.15622500
H	-2.95926800	-0.17345600	2.13682400
H	-3.80062000	0.76117200	-0.02154900
H	-2.94781900	-0.25038600	-2.14036700
H	-0.61092700	-1.21845600	-2.11387900
C	1.43055200	-2.51148100	-0.00129200
H	1.06488400	-3.01884000	-0.90163800
H	2.52132300	-2.52202300	0.00197700
H	1.05722000	-3.05163400	0.87596500
N	2.09160200	2.32353000	0.08838400
H	3.03538300	2.07462100	-0.18660500
H	1.75105900	3.18279100	-0.31786700

TS_R2--NMe₂

E(RM062X) = -689.43818062 a.u.

Imaginary Freq = 1

C	-1.18084700	0.67249000	0.02598900
N	-0.18430000	1.69531700	0.00845600
C	1.12352400	1.28047700	-0.12251900
C	1.21009500	-0.22508300	-0.06032100
C	0.05007800	-0.88698100	0.07264000
C	-0.60837800	-2.09510600	0.15069200
C	-1.85082000	0.34950200	-1.21509700
C	-2.67588100	-0.73541200	-1.19969000
C	-2.83623300	-1.41694800	0.04669100
C	-2.73790400	-0.65179600	1.25432400
C	-1.91798800	0.43588400	1.24579700
O	2.06858500	2.04822600	-0.25749700
H	-0.75501000	-2.57660900	1.11303100
H	-0.67513000	-2.75603400	-0.70932300
H	-1.55830500	0.85905200	-2.12733300

H	-3.10012700	-1.14892500	-2.10935700
H	-3.40523400	-2.34244200	0.06491200
H	-3.21481500	-1.00405700	2.16386900
H	-1.67776000	1.00554400	2.13739500
C	-0.54056800	3.10104000	-0.07993700
H	0.38841000	3.67201400	-0.09723600
H	-1.11199400	3.31247000	-0.99191100
H	-1.14318300	3.40321800	0.78346900
N	2.48403700	-0.79786900	-0.20462400
C	3.52241400	-0.36747500	0.73424600
H	3.41554600	-0.84881400	1.72152100
H	4.50199100	-0.63780900	0.32741700
H	3.48415900	0.71385800	0.84841100
C	2.53217100	-2.21726700	-0.50361500
H	3.55815100	-2.48002700	-0.77895200
H	2.22888700	-2.85789900	0.34220400
H	1.87960100	-2.44143200	-1.35017400

TS_R2--OCH₃

E(RM062X) = -670.00411671 a.u.

Imaginary Freq = 1

C	-0.83270900	0.73357600	0.06398100
N	0.38362400	1.48544800	0.06421300
C	1.54690000	0.77140000	-0.13540300
C	1.24979100	-0.69884200	-0.21006400
C	-0.01977000	-1.08877700	-0.11754700
C	-0.93636000	-2.11120300	-0.14642500
C	-1.63207800	0.71017400	-1.13981900
C	-2.68252400	-0.15790800	-1.15759500
C	-2.92156200	-0.92596900	0.02645500
C	-2.57516300	-0.34411900	1.28859100
C	-1.52599100	0.52528400	1.31387300
O	2.65877400	1.27677800	-0.23109500
H	-1.12112500	-2.70363800	0.74455300
H	-1.18546700	-2.59372300	-1.08705000
H	-1.28624700	1.23924300	-2.02170900
H	-3.24672600	-0.35833000	-2.06303900
H	-3.69111900	-1.69244000	0.00231700
H	-3.06182200	-0.68239700	2.19813000
H	-1.10383400	0.91894700	2.23259000
C	0.38717600	2.93697400	0.12941900
H	1.42849200	3.26008100	0.09831800
H	-0.15333100	3.37532100	-0.71794800
H	-0.07922600	3.28770800	1.05665700
O	2.27206400	-1.57458300	-0.45287600
C	3.35417600	-1.56779900	0.48945200
H	3.00352000	-1.87928500	1.48223800
H	4.07301300	-2.30098500	0.11909600
H	3.82049700	-0.58294300	0.54861700

TS_R2--OH

E(RM062X) = -630.73469482 a.u.

Imaginary Freq = 1

C	-0.35417800	-0.75058900	-0.00000500
N	1.03613700	-1.10241500	-0.00001900
C	1.90640400	-0.04919300	-0.00000900
C	1.19014700	1.25856700	-0.00001000
C	-0.13776300	1.26060900	-0.00003800
C	-1.33420600	1.93790600	-0.00003400
C	-1.09873700	-0.86526300	1.23214400
C	-2.35875600	-0.34818700	1.22806600
C	-2.83167100	0.22108900	0.00001700
C	-2.35879600	-0.34823500	-1.22802600
C	-1.09877700	-0.86531100	-1.23212600
O	3.13545800	-0.11414600	-0.00001300
H	-1.70592900	2.38808400	-0.91681900
H	-1.70593200	2.38808800	0.91674800
H	-0.59547800	-1.19406500	2.13540300
H	-2.94213800	-0.24907200	2.13799600
H	-3.79584500	0.72180900	0.00002300
H	-2.94220700	-0.24915300	-2.13794300
H	-0.59554600	-1.19414600	-2.13538800
C	1.49342300	-2.48215000	0.00001900
H	1.13733700	-3.01400400	-0.88921500
H	2.58417800	-2.46562100	0.00011600
H	1.13717400	-3.01400500	0.88918500
O	2.00937600	2.34197600	0.00002000
H	2.91021900	1.96089500	-0.00001900

TS_R2--SiH₃

E(RM062X) = -846.18326153 a.u.

Imaginary Freq = 1

C	-0.90223300	0.74773700	-0.00003100
N	0.25713600	1.57727200	-0.00006700
C	1.48175400	0.93558500	-0.00001100
C	1.32727600	-0.55326100	-0.00002000
C	0.08749200	-1.03730600	-0.00001800
C	-0.78471400	-2.10518300	0.00003200
C	-1.63300700	0.55871600	-1.23186900
C	-2.59116800	-0.40826600	-1.22769400
C	-2.78685400	-1.12820900	0.00003300
C	-2.59113500	-0.40821600	1.22772500
C	-1.63297100	0.55876200	1.23183700
O	2.56216500	1.51448500	0.00004400
H	-0.92809700	-2.67010800	0.91585100
H	-0.92813400	-2.67017700	-0.91573800
H	-1.30388300	1.06508500	-2.13339400
H	-3.09687400	-0.72347700	-2.13496200
H	-3.47941100	-1.96557800	0.00005900
H	-3.09681900	-0.72338200	2.13502100
H	-1.30381400	1.06516200	2.13333400
C	0.16430800	3.02802500	0.00000700
H	-0.36446500	3.39006400	0.88922900

H	1.18292600	3.41793300	0.00000000
H	-0.36450500	3.39013500	-0.88916100
Si	2.90094000	-1.58635900	-0.00000500
H	3.71940400	-1.31712100	-1.20918200
H	3.71909400	-1.31754900	1.20948100
H	2.50164800	-3.01904800	-0.00030200

TS_ R2--SiMe₃

E(RM062X) = -964.12305938 a.u.

Imaginary Freq = 1

C	-1.80157400	0.58779100	-0.00002300
N	-0.94934400	1.72909200	-0.00005400
C	0.41340600	1.49150200	-0.00003500
C	0.72858200	0.02546300	-0.00004500
C	-0.31202000	-0.80574500	-0.00002300
C	-0.82506000	-2.08716000	-0.00000300
C	-2.44189700	0.18796100	-1.23151000
C	-3.06418400	-1.02287300	-1.22767000
C	-3.03237500	-1.76819600	0.00002900
C	-3.06414200	-1.02284000	1.22770800
C	-2.44185400	0.18799300	1.23149600
O	1.25520000	2.38538200	-0.00000700
H	-0.79470600	-2.66982700	0.91541500
H	-0.79473800	-2.66984100	-0.91541400
H	-2.27986400	0.76992600	-2.13298900
H	-3.45090500	-1.47617600	-2.13503900
H	-3.43833600	-2.77627200	0.00004900
H	-3.45083400	-1.47611900	2.13510300
H	-2.27978900	0.76997900	2.13295700
C	-1.48159400	3.08141500	-0.00001000
H	-0.63162600	3.76482600	-0.00011300
H	-2.09664800	3.26415700	-0.88883600
H	-2.09644400	3.26419700	0.88895200
Si	2.55965700	-0.49216300	0.00000900
C	3.38858300	0.19747700	1.55184600
H	4.45896500	-0.03764800	1.56467600
H	3.27428500	1.28456100	1.58199600
H	2.94475000	-0.21788200	2.46303700
C	3.38880000	0.19750500	-1.55170800
H	3.27415200	1.28454500	-1.58206000
H	4.45926400	-0.03726800	-1.56415800
H	2.94539900	-0.21816700	-2.46296800
C	2.65669300	-2.38138600	-0.00006000
H	2.17694100	-2.81368400	0.88402600
H	2.17687400	-2.81359800	-0.88415200
H	3.70369100	-2.70558200	-0.00011800

R3 Substituent

TS_ R3--OCH₃

E(RM062X) = -670.00276258 a.u.

Imaginary Freq = 1

C	-0.67820500	-0.69169800	0.04864100
N	-2.01804100	-0.18194800	0.15015800
C	-2.17704500	1.17075400	-0.08301200
C	-0.84904000	1.75061600	-0.42232400
C	0.17508300	0.90134000	-0.40920200
C	1.55706700	0.88517600	-0.56410600
C	-0.35727600	-1.51252800	-1.11663600
C	0.93997100	-1.91640300	-1.22983000
C	1.83488700	-1.63108500	-0.15525300
C	1.29844100	-1.46449200	1.15707100
C	0.00348000	-1.05556700	1.28332400
O	-3.24069700	1.77309200	-0.03312000
H	-0.78797700	2.80111400	-0.68731800
H	2.03463400	0.69060500	-1.51919700
H	-1.08848300	-1.62126400	-1.91040100
H	1.30824200	-2.39937400	-2.13062300
H	2.88085200	-1.90417700	-0.26308600
H	1.93441500	-1.60751400	2.02577300
H	-0.45933200	-0.82909500	2.23757100
C	-3.13893500	-1.03675400	0.49010400
H	-3.01251700	-1.48478000	1.48260400
H	-4.03317900	-0.41171200	0.48656700
H	-3.25493800	-1.84575500	-0.24066100
O	2.30367000	1.48460700	0.40008300
C	3.70691600	1.28433500	0.28822400
H	4.17217200	1.88169600	1.07315300
H	3.95716200	0.22513400	0.42701300
H	4.07940400	1.61500400	-0.69020100

TS_ R3--SiH₃

E(RM062X) = -846.18398298 a.u.

Imaginary Freq = 1

C	-0.71103800	-0.74807200	0.06899800
N	-2.00463500	-0.15008000	0.15869000
C	-2.07301400	1.20395900	-0.13442700
C	-0.72627600	1.69816100	-0.52216300
C	0.28230000	0.82925500	-0.51159000
C	1.63471300	0.61945400	-0.72649100
C	-0.41186700	-1.60217100	-1.06670900
C	0.87824600	-2.01736600	-1.18845500
C	1.79707800	-1.62138500	-0.15940400
C	1.28493600	-1.47078900	1.17265800
C	-0.00032600	-1.04436900	1.29921100
O	-3.09661400	1.87059800	-0.08655600
H	-0.63239800	2.73722300	-0.82096600
H	1.93551400	0.42242100	-1.75508800
H	-1.15805600	-1.73978200	-1.84218300
H	1.23884400	-2.52936300	-2.07507300
H	2.84921700	-1.85951900	-0.28628400
H	1.94298800	-1.58431100	2.02801500
H	-0.44687600	-0.77682200	2.25101300

C	-3.17351200	-0.89386300	0.59148000
H	-3.04469700	-1.28876600	1.60632800
H	-4.01620500	-0.20101900	0.57838100
H	-3.38148500	-1.73303800	-0.08242700
Si	2.92577000	1.42613300	0.36141900
H	4.22965200	0.72132000	0.21609100
H	3.13932300	2.85151400	-0.01753600
H	2.50131500	1.38318000	1.78284600

R4 Substituent

TS_R4--OCH₃

E(RM062X) = -670.00863266 a.u.

Imaginary Freq = 1

C	0.60942000	-0.55602900	0.00002600
N	2.03167300	-0.65521300	0.00006400
C	2.73787800	0.53901900	0.00001500
C	1.80031700	1.69652600	-0.00000700
C	0.49512700	1.46326800	-0.00001000
C	-0.80961000	1.90162500	-0.00003200
C	-0.11236500	-0.78663600	1.23192400
C	-1.43939400	-0.48663900	1.22959600
C	-1.99162600	0.01633400	-0.00001400
C	-1.43936700	-0.48668200	-1.22959500
C	-0.11233500	-0.78667400	-1.23188500
O	3.95818300	0.61607300	-0.00000700
H	2.23965100	2.68972000	-0.00000400
H	-1.25147700	2.28284400	-0.91521100
H	-1.25152600	2.28287000	0.91511200
H	0.43696500	-1.02523100	2.13669900
H	-2.04331600	-0.47162600	2.13133200
H	-2.04327500	-0.47171500	-2.13134100
H	0.43701300	-1.02529600	-2.13664100
C	2.71580500	-1.93620200	-0.00003000
H	2.45938200	-2.52424300	-0.88920700
H	3.78685100	-1.72882300	0.00004900
H	2.45927200	-2.52439500	0.88901000
O	-3.28777900	0.50018300	-0.00003500
C	-4.30084100	-0.50505100	0.00001500
H	-4.23718100	-1.14209200	0.89177000
H	-5.25815900	0.01942100	0.00000200
H	-4.23719600	-1.14216300	-0.89169100

TS_R4-SiH₃

E(RM062X) = -846.17662179 a.u.

Imaginary Freq = 1

C	0.67413200	-0.58037200	0.00114400
N	2.10110200	-0.55302800	0.00149300
C	2.69460700	0.69971000	-0.00009000

C	1.64537500	1.75517000	0.00168300
C	0.37325000	1.37485600	0.00224700
C	-0.95831200	1.74097000	-0.00053300
C	-0.02028300	-0.90303700	1.23051400
C	-1.37035200	-0.73992700	1.22551400
C	-2.00385600	-0.31082400	-0.00018000
C	-1.36914800	-0.73972900	-1.22533600
C	-0.01911600	-0.90279000	-1.22895100
O	3.90169400	0.89307200	-0.00234800
H	1.97261900	2.79021400	0.00137100
H	-1.41173700	2.09750500	-0.92001000
H	-1.41557200	2.09918500	0.91639600
H	0.55030500	-1.09805900	2.13281700
H	-1.94617500	-0.80917900	2.14473800
H	-1.94400600	-0.80877500	-2.14517200
H	0.55239400	-1.09786600	-2.13066400
C	2.89498700	-1.76878900	-0.00083600
H	2.69144900	-2.37509400	-0.89128600
H	3.94332100	-1.46676900	-0.00014300
H	2.69102100	-2.37842600	0.88719700
Si	-3.84395400	0.09845700	-0.00101600
H	-4.17811400	0.88895200	-1.21453000
H	-4.67984100	-1.13359800	-0.00154000
H	-4.17926900	0.88871400	1.21233500

TS_Himbert arene/ethylene cycloaddition

E(RM062X) = -517.45028795 a.u.

Imaginary Freq = 1

C	0.01695600	-0.85410900	0.00821100
N	-1.38215600	-1.10894500	-0.14347400
C	-2.24601700	-0.03832700	0.00354100
C	-0.13647300	1.11364900	-0.68780300
C	1.07957800	1.75180800	-0.35925300
C	0.97885900	-1.27672400	-0.98185800
C	2.21488200	-0.71578200	-0.87919000
C	2.42156600	0.22234000	0.20209100
C	1.76114000	-0.09049100	1.44667200
C	0.52587200	-0.64687200	1.34717200
O	-3.45363200	-0.14700400	0.11048200
H	1.13138000	2.35309100	0.54500300
H	1.69480300	2.12628500	-1.17186400
H	-0.12943300	-0.80358100	2.19914200
H	0.66166900	-1.87197500	-1.83357700
H	2.97541200	-0.85068400	-1.64275900
H	3.38338500	0.72793300	0.25348200
H	2.18187100	0.23466800	2.39417400
C	-1.47033600	1.29234200	0.00120800
H	-1.34158600	1.62309700	1.03987400

H	-2.10347700	2.03675300	-0.49503100
H	-1.77891100	-2.03484500	-0.03397400
H	-0.24713400	0.85090500	-1.73874600

TS_Himbert arene/allene cycloaddition

E(RM062X) = -516.22221549 a.u.

Imaginary Freq = 1

C	-0.01654800	-0.80300200	-0.00522800
N	-1.41552700	-1.06309900	-0.01466500
C	-2.28481400	0.01485200	-0.00239900
C	-1.50794500	1.28764100	-0.00382500
C	-0.18297200	1.22917300	-0.00150500
C	1.04663800	1.85105400	0.00050800
C	0.73514800	-0.92714900	-1.23354500
C	2.00479000	-0.43696200	-1.22303900
C	2.47272500	0.13783500	0.00760700
C	1.99324100	-0.44025800	1.23225700
C	0.72348600	-0.93048500	1.22994800
O	-3.50050900	-0.08362400	0.00814300
H	-2.07412300	2.21451600	-0.00378200
H	1.40840900	2.30735600	0.91675800
H	1.41385400	2.30302300	-0.91569500
H	0.22943800	-1.25560600	-2.13544200
H	2.59927300	-0.35543200	-2.12759700
H	3.44776300	0.61763800	0.01294500
H	2.57990300	-0.36234700	2.14222300
H	0.21030900	-1.26066300	2.12710000
H	-1.80455400	-1.99398900	0.01632200

TS_Cyclopentadiene/cis-dimethylmaleate (endo)

E(RM062X) = -728.22710826 a.u.

Imaginary Freq = 1

C	2.15770200	0.21974700	1.12274600
C	1.45061500	-0.96930900	1.39312400
C	1.48019600	-1.78078900	0.26131300
C	2.69365200	0.14620000	-0.14130400
C	2.60268500	-1.27021200	-0.60349100
H	2.18314100	1.09417400	1.76618600
H	0.85277400	-1.16401200	2.27553300
H	1.16267700	-2.82046900	0.27237700
H	0.09194400	-1.72842800	-1.69087700
H	0.99100100	0.44607700	-2.24231100
H	3.27331000	0.92050300	-0.63306400
C	-0.01628800	-0.94210800	-0.94025500
C	0.42987400	0.31260800	-1.32259000
C	0.09767500	1.56217200	-0.65100400
O	0.43849800	2.66828500	-1.01364900

C	-1.25800300	-1.15190300	-0.11487200
O	-1.35063000	-1.72975000	0.94044600
O	-0.63731300	1.35691200	0.47383800
O	-2.31803800	-0.67041000	-0.78467300
C	-3.55350200	-0.76782800	-0.08594700
C	-0.92318200	2.53061300	1.21685200
H	2.49164600	-1.41578700	-1.68148900
H	3.52564000	-1.79033000	-0.29586500
H	-3.50612200	-0.19414100	0.84628100
H	-4.31116100	-0.35096500	-0.75050300
H	-3.78826300	-1.80837400	0.15794200
H	0.00222300	3.00607800	1.56192000
H	-1.47208400	3.25595300	0.60844700
H	-1.52539400	2.21428600	2.07030500

TS_Cyclopentadiene/cis-dimethylmaleate (exo)

E(RM062X) = -728.22586474 a.u.

Imaginary Freq = 1

C	2.84944700	-1.37172500	-0.26991800
C	3.23804300	-0.02516000	-0.37331600
C	2.40697700	0.74250200	0.42020000
C	0.44975000	0.46489400	-1.10920300
C	0.19836700	-0.86985200	-0.81522600
C	1.71292700	-1.45524100	0.53696600
C	1.64569300	-0.17245900	1.31461700
C	-1.03196900	-1.29426500	-0.05821500
O	-1.10137900	-1.69930400	1.07655000
C	-0.23872100	1.62360100	-0.54903500
O	-0.06930900	2.77052100	-0.90528700
O	-2.09443200	-1.21381600	-0.87684100
O	-1.11170200	1.29193800	0.43846200
C	-1.80726100	2.38865700	1.01427200
C	-3.33989100	-1.52401000	-0.26182400
H	3.27906800	-2.19204900	-0.83703600
H	4.00396700	0.35997700	-1.03903800
H	2.46477400	1.81929300	0.54573900
H	1.06823500	0.72014800	-1.96280500
H	0.45604500	-1.58681300	-1.59373000
H	1.29454200	-2.38190500	0.91830500
H	0.64909200	0.15074400	1.61974100
H	2.24095000	-0.32092800	2.23226400
H	-2.40831000	2.90596200	0.26011600
H	-2.44930600	1.96828700	1.78985100
H	-1.10893000	3.11061200	1.44940800
H	-3.34519300	-2.54791500	0.12406200
H	-3.53185800	-0.83778400	0.57005400
H	-4.09867400	-1.40398400	-1.03591800

TS_Cyclopentadiene/trans-dimethylmaleate

E(RM062X) = -728.24185245 a.u.
Imaginary Freq = 1

C	0.20877500	2.13484200	1.12312100
C	1.35794000	1.99329700	0.33843200
C	0.98340800	1.55746600	-0.93135100
C	0.48372200	-0.56761900	-0.42198800
C	-0.64526700	-0.41976400	0.37427000
C	-0.90535400	1.80278200	0.35397500
C	-0.47967700	1.83201100	-1.08210100
H	0.19849500	2.34069300	2.18828000
H	2.37739700	2.06051500	0.70571400
H	1.66523700	1.43225400	-1.76759900
H	0.37403700	-0.83845300	-1.46955300
H	-0.54358000	-0.51929300	1.45112800
H	-1.93525600	1.92727100	0.67858200
C	-1.97229600	-0.69339000	-0.19407200
O	-2.24214900	-0.77237900	-1.37530700
C	1.76793500	-0.86000400	0.22489200
O	1.98180100	-0.83098300	1.41796500
O	-2.89698300	-0.82909200	0.77821800
O	2.72503800	-1.13205100	-0.68886900
C	4.01276200	-1.37540300	-0.13939500
C	-4.21542400	-1.09283600	0.31486600
H	-1.03250700	1.17181200	-1.75479600
H	-0.59610300	2.86594000	-1.44819200
H	3.98842500	-2.21867000	0.55767500
H	4.66770900	-1.59875200	-0.98257800
H	4.37694100	-0.49551100	0.40230500
H	-4.83918200	-1.17702300	1.20559800
H	-4.57437400	-0.28043200	-0.32510600
H	-4.24805000	-2.02259800	-0.26142600

TS_7-(methoxymethyl)cyclopentadiene/chloroacrylonitrile (syn)

E(RM062X) = -978.17233543 a.u.
Imaginary Freq = 1

C	0.27242000	-1.89978200	-0.74974300
C	-0.19198900	-2.00742000	0.57792700
C	-0.62878400	-0.75070500	1.00981900
C	1.11144400	0.13220000	1.55765400
C	1.85437600	0.43293500	0.42207300
C	0.04255100	-0.62139100	-1.19794600
C	-0.86338500	0.07243500	-0.23586100
H	0.81354200	-2.66988600	-1.28916700
H	-0.08697600	-2.88565300	1.20725300
H	-1.24125300	-0.60607500	1.89702800
H	1.48439300	-0.65952200	2.20099200

H	0.31508600	-0.22501400	-2.17130500
H	-0.65780300	1.14237800	-0.11789800
H	0.64566500	0.96366100	2.08303900
C	2.87999900	-0.41134600	-0.06381700
N	3.71537700	-1.13200600	-0.44390800
Cl	1.83760800	2.06228000	-0.24572600
C	-2.32289500	-0.04629000	-0.67536500
H	-2.46660100	0.46044300	-1.64808700
H	-2.59325400	-1.10969300	-0.81399300
O	-3.11862000	0.55114500	0.31215100
C	-4.47884400	0.51701100	-0.02019500
H	-4.68006400	1.04742700	-0.96596300
H	-4.84763000	-0.51700200	-0.12506500
H	-5.03248000	1.00918500	0.78337200

TS_7-(methoxymethyl)cyclopentadiene/chloroacrylonitrile (anti)

E(RM062X) = -978.16516928 a.u.

Imaginary Freq = 1

C	0.30487700	2.33872000	0.33093200
C	0.86664000	1.97200000	-0.90390200
C	0.22351200	0.84519300	-1.36537500
C	-0.64056800	1.37665600	0.70573700
H	0.65228600	3.15263500	0.95954200
H	1.72882800	2.44003200	-1.36591300
H	0.44311100	0.30943500	-2.28472500
H	-1.34539500	1.53482200	1.52078600
C	0.58402200	-0.07565400	1.50153000
H	-0.19811800	-0.70991600	1.91519700
H	1.05736000	0.58198700	2.22445900
C	1.38839300	-0.60201300	0.49875400
C	2.68181700	-0.08269000	0.24172900
N	3.73824900	0.37117100	0.04581100
Cl	1.10955400	-2.20428100	-0.18409300
C	-1.02193200	0.64958400	-0.56730200
H	-1.74500300	1.33871100	-1.05044300
C	-1.74541300	-0.69349000	-0.56974800
H	-1.50839800	-1.22368900	-1.50049800
H	-1.42060300	-1.34230500	0.25829500
O	-3.14532000	-0.55683900	-0.54677200
C	-3.65649500	-0.15929500	0.69436900
H	-4.73760800	-0.32246600	0.67732700
H	-3.22563100	-0.75166400	1.52097400
H	-3.47755700	0.90765000	0.90773900

TS_Cyclopentadiene/ethylene

E(RM062X) = -272.56035381 a.u.

Imaginary Freq = 1

C	0.58629200	-1.26422500	0.70184500
C	0.58629200	-1.26422500	-0.70184500
C	0.58629200	0.05088700	-1.15135900
C	-1.54204400	0.60265300	-0.68883000
C	-1.54204400	0.60265300	0.68883000
C	0.58629200	0.05088700	1.15135900
C	1.02780300	0.90305300	0.00000000
H	0.46914100	-2.14252600	1.32934100
H	0.46914100	-2.14252600	-1.32934100
H	0.70207700	0.34836000	-2.18994700
H	-1.98756100	-0.21758100	-1.24363100
H	-1.98756100	-0.21758100	1.24363100
H	0.70207700	0.34836000	2.18994700
H	0.67172200	1.93686400	0.00000000
H	2.13171200	0.92399100	0.00000000
H	-1.45202600	1.53626500	-1.24010700
H	-1.45202600	1.53626500	1.24010700