Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

A Theoretical Studies of Imine-ene Reactions: Mechanism and Influencing Factors

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Supporting Material

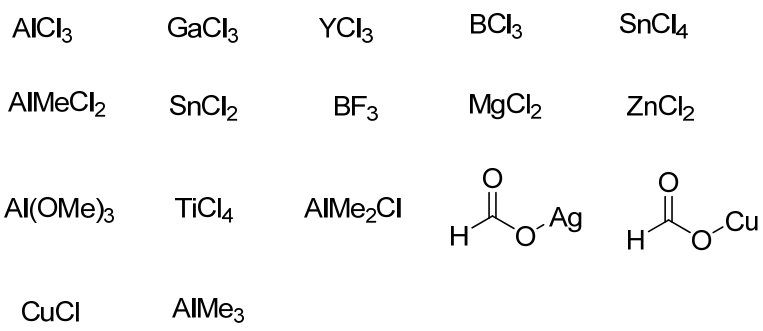


Chart S1: The selected Lewis acids

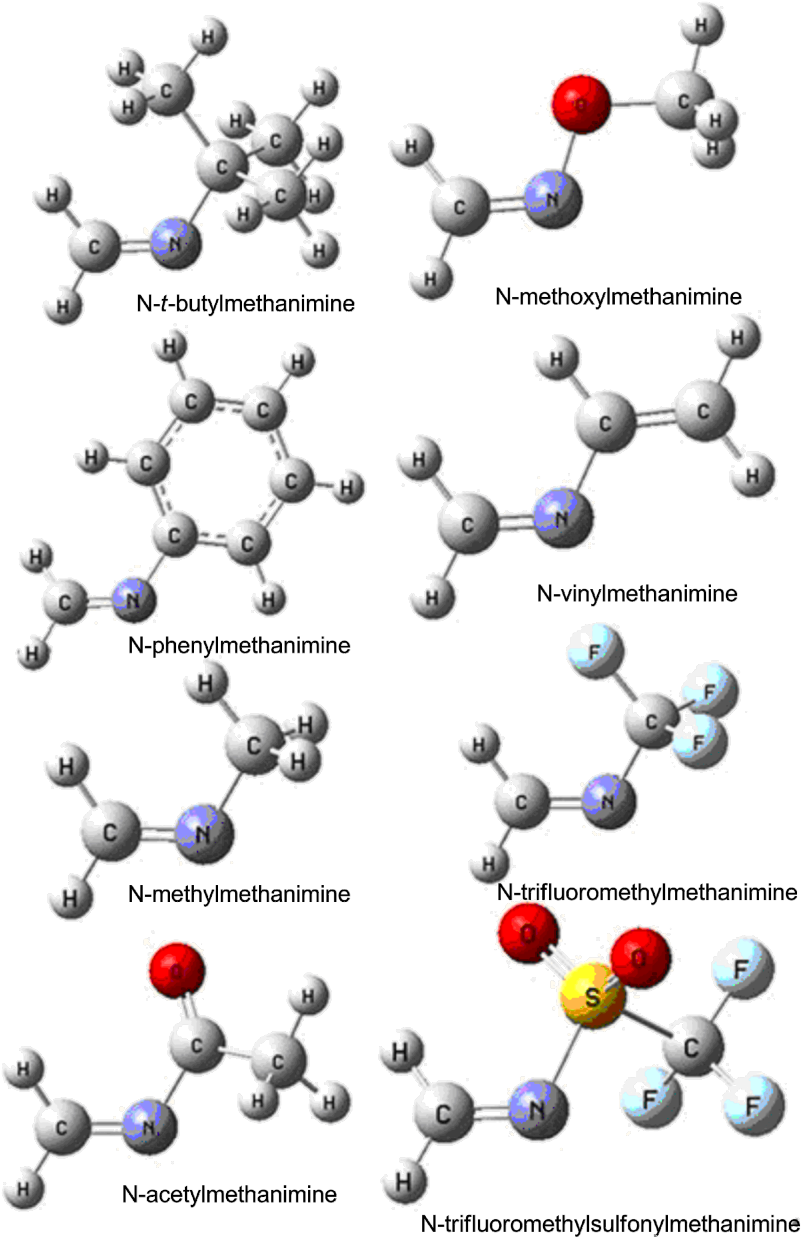


Chart S2: The selected Schiff base structures (substituent on nitrogen).

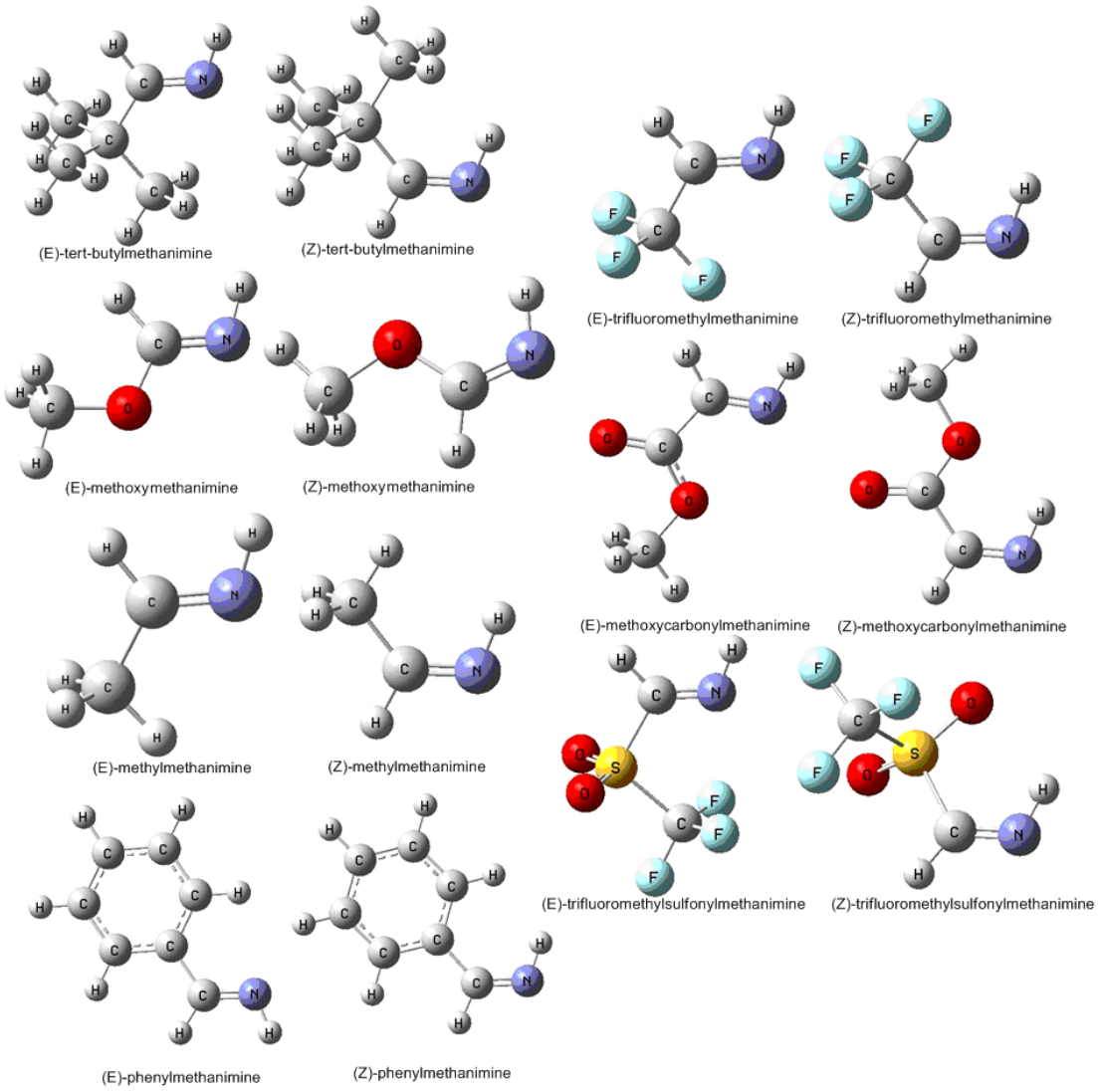
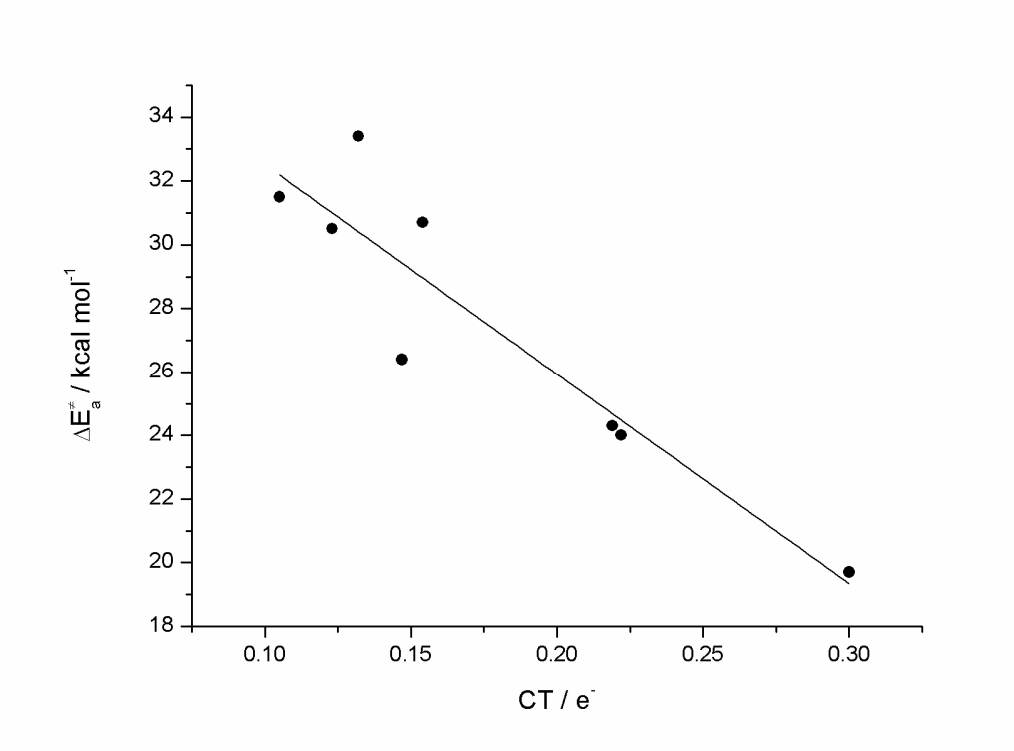
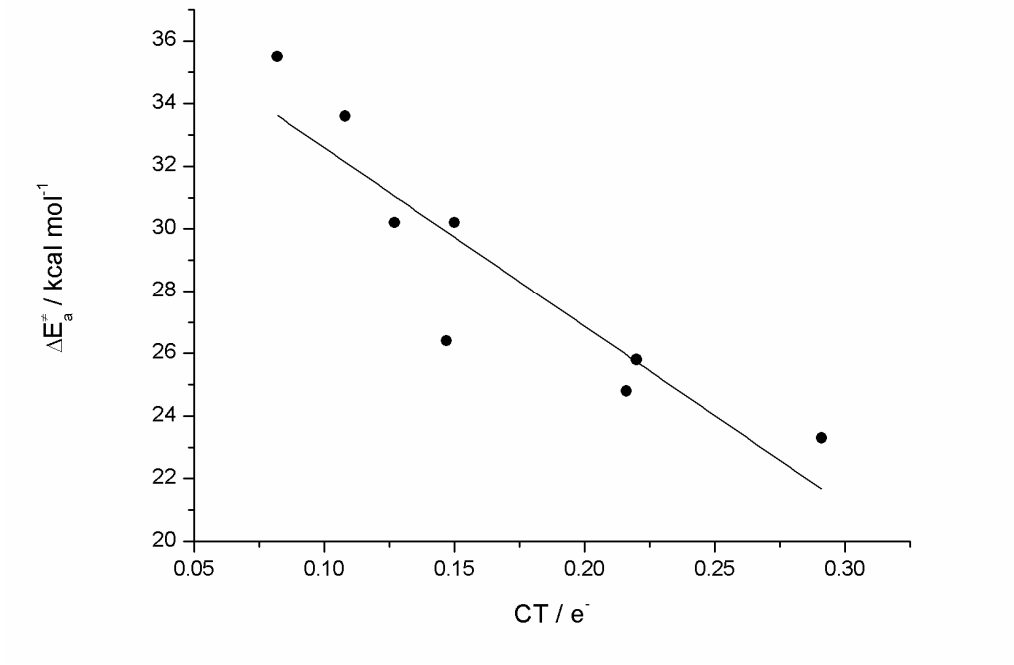


Chart S3: The selected Schiff base structures (substituent on carbon)



(a)



(b)

Chart S4: Plot of the activation barriers ($\Delta E_a^{\neq}$) vs. the charge transfer (CT) of the reactions between propene and the C-substituted imines. R^2 =0.83 for (a) and R^2=0.80 for (b)

Table S1: The comparison of the basis sets

	6-31G*				LanL2DZ			
	ΔE_{rxn} / kcal mol^{-1}	ΔG_{rxn} / kcal mol^{-1}	$\Delta E_a^{\neq}$ / kcal mol^{-1}	$\Delta G_a^{\neq}$ / kcal mol^{-1}	ΔE_{rxn} / kcal mol^{-1}	ΔG_{rxn} / kcal mol^{-1}	$\Delta E_a^{\neq}$ / kcal mol^{-1}	$\Delta G_a^{\neq}$ / kcal mol^{-1}
$AlCl_3$	-23.2	-7.4	17.1	30.3	-23.7	-7.8	16.5	30.0
BCl_3	-23.8	-7.7	17.4	31.2	-23.9	-7.7	17.6	31.5
$AlMe_3$	-21.1	-5.4	24.3	37.5	-22.7	-7.0	22.6	35.4

Table S2: The comparison of the solvent effect

		vacuum	cyclohexane	dichloromethane	water
		$\Delta G_a^{\neq}$ / kcal mol^{-1}	$\Delta G_a^{\neq}$ / kcal mol^{-1}	$\Delta G_a^{\neq}$ / kcal mol^{-1}	$\Delta G_a^{\neq}$ / kcal mol^{-1}
Concerted	TS-barrier	38.2	37.9	38.3	37.8
	product	-3.4	-3.4	-3.1	-3.5
Stepwise	TS1	77.1	77.2	77.2	76.8
	INT1	50.7	51.1	51.5	49.0
	INT2	51.1	51.5	52.2	51.9
	TS2	67.9	67.6	68.3	67.8
	product	57.8	56.9	58.4	58.0

The evolution of the IRC as a function of the reaction coordinates has also been performed, and the results are given in Figure S1. The reaction can be described by the relative and interdependent distances of N4-H5 and C6-H5. The two distances decreases and increases respectively as a function of *s*. Bond formation and breaking occur in the range from -0.5 to +0.5 amu$^{1/2}$ bohr. The path from the reactant ($s < 0$) to the TS ($s = 0$) is characterized by the changes in the distances between N4-H5 and C6-H5. The distance change of C1-C11 is independent of the distance of N4-H5 or C6-H5, and it begins at -0.5 amu$^{1/2}$ bohr and is nearly linear with *s* during the whole process. It is noteworthy that the breaking and forming of the C9-C11, C1-N4 and C6-C9 π bonds start at s = -0.5 amu$^{1/2}$ bohr simultaneously, and so do the breaking and forming of the C6-H5 and N4-H5 σ bonds. The path after the TS ($s > 0$) follows the completion of the H migration as the bond length of C6-H5 increases and N4-H5 decreases. The C1 and C11 get closer, followed by the σ-bond formation and finally the amine product is generated.

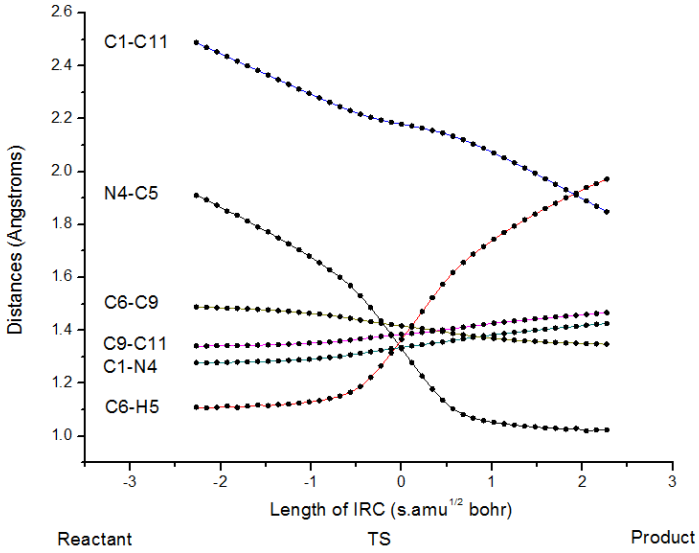


Figure S1 The evolution of the IRC for the concerted mechanism (without a Lewis acid)

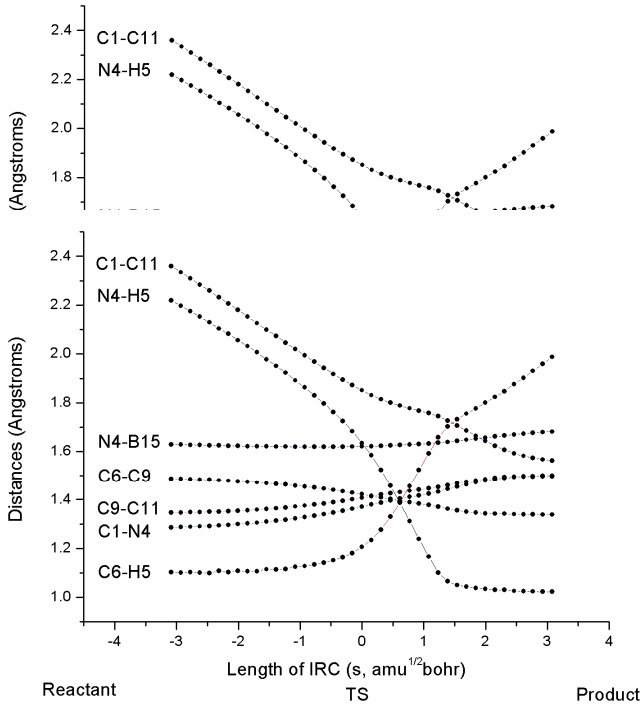


Figure S2 [illegible] promoter)

Concerted:

Lewis acid present:

Propene

E(RB+HF-LYP) = -117.9140126 a.u.

Sum of electronic and thermal Free Energies= -117.859187 a.u.

C	-1.23465200	0.16290700	-0.00000700
H	-1.81134400	-0.15060800	0.87955000
H	-1.18143200	1.25582100	-0.00022800
H	-1.81150300	-0.15093300	-0.87936800
C	0.13379000	-0.45551700	0.00001500
H	0.16478300	-1.54580000	-0.00001300
C	1.28280100	0.22064500	0.00003000
H	2.24397700	-0.28497600	-0.00015300
H	1.30388400	1.30828300	-0.00002000

Imine-$AlCl_3$

E(RB+HF-LYP) = -141.744565072 a.u.

Sum of electronic and thermal Free Energies= -141.731585 a.u.

C	-2.16547900	-0.00076500	1.65506600
H	-2.74931500	-0.00097600	0.73594000
H	-2.67619200	-0.00093000	2.61764100
N	-0.89261500	-0.00031400	1.56560700
H	-0.39213700	-0.00009700	2.45555900
Al	0.21107700	-0.00001800	-0.13728600
Cl	1.33495600	-1.83218400	0.08582700
Cl	-1.35618100	-0.00011000	-1.63752200
Cl	1.33386100	1.83282500	0.08616100

TS-H-$AlCl_3$

E(RB+HF-LYP) = -259.632329752 a.u.

Sum of electronic and thermal Free Energies= -259.543021 a.u.

C	1.42944600	-1.40406100	-0.79078100
H	1.20829100	-1.91218100	0.14537300
H	1.60429200	-2.10162200	-1.61103300
N	0.54704600	-0.37294600	-1.07138200
H	1.44976900	0.96407500	-0.48715600
C	2.49574100	1.41597600	-0.13333400
H	2.32794300	2.19830300	0.60318200
H	2.89125200	1.78805900	-1.08183500
C	3.02919000	0.17929800	0.32758600
H	3.01255200	-0.03453300	1.39486200
C	3.14019900	-0.90070400	-0.57703100
H	3.62224700	-1.80735500	-0.21625600
H	3.43567700	-0.63708700	-1.59287000
H	0.48444000	-0.15665400	-2.06356000
Al	-1.00961800	0.03181900	0.02955900
Cl	-2.59949400	-1.37185200	-0.43725700
Cl	-0.14337500	-0.25281400	2.03339900
Cl	-1.45173100	2.10424900	-0.47460800

Pro-$AlCl_3$

E(RB+HF-LYP) = -259.696344734 a.u.

Sum of electronic and thermal Free Energies= -259.603187 a.u.

C	1.48630200	-1.17961000	-0.05740700
H	1.32286000	-1.27595800	1.01929300
H	1.03991700	-2.04962100	-0.54370500
N	0.70834100	0.02163600	-0.50338400
H	1.19073000	0.86041500	-0.16399400
C	4.06048500	1.22380000	-0.29019200
H	4.48995000	2.05042100	0.26741000
H	4.03672400	1.32762700	-1.37300700
C	3.61283900	0.12385000	0.31966000
H	3.66622200	0.05844200	1.40698600
C	2.98297700	-1.05202500	-0.38029400
H	3.46755500	-1.98567600	-0.06749300
H	3.12303700	-0.96934300	-1.46566700
H	0.74961800	0.08993900	-1.52317300
Al	-1.24686100	0.09370400	0.04552700
Cl	-2.04461100	-1.66550600	-0.93887500
Cl	-1.12651400	0.00440400	2.20753100
Cl	-1.81072300	2.00392800	-0.80838600

Imine-BF_3

E(RB+HF-LYP) = -419.213406522 a.u.

Sum of electronic and thermal Free Energies= -419.186812 a.u.

C	2.07375600	0.04085300	-0.00006000
H	1.99364500	1.12492200	0.00054300
H	3.05241000	-0.43639600	-0.00052500
N	0.99170200	-0.62431800	-0.00042500
H	1.06567100	-1.64096000	-0.00111200
B	-0.54558800	0.04802900	0.00001000
F	-1.11263900	-0.43346200	-1.15041600
F	-1.11095900	-0.43215300	1.15188200
F	-0.30620700	1.40310400	-0.00097900

TS-H-BF_3

E(RB+HF-LYP) = -537.094380727 a.u.

Sum of electronic and thermal Free Energies= -536.991836 a.u.

C	0.67117100	-1.42663600	-0.25127800
H	0.38908500	-1.70268300	0.76013000
H	0.95546700	-2.27163500	-0.87710400
N	-0.18178200	-0.51456300	-0.81601400
H	0.63059900	0.89150800	-0.63984100
C	1.62837500	1.49748800	-0.33555200
H	1.34679500	2.45629000	0.09354200

H	2.12953000	1.58294200	-1.30280000
C	2.12870100	0.49949200	0.54494700
H	1.95895100	0.61300700	1.61368800
C	2.38407900	-0.78675200	0.03604200
H	2.80637000	-1.53074100	0.70796000
H	2.79805100	-0.83127900	-0.97094800
H	-0.30550200	-0.59355700	-1.82048400
B	-1.40926700	0.07260900	0.06513500
F	-1.77055900	1.26509200	-0.53310900
F	-0.83469600	0.25129500	1.32996300
F	-2.42413300	-0.85822100	0.07618100

Pro-BF_3

E(RB+HF-LYP) = -537.165689841 a.u.

Sum of electronic and thermal Free Energies= -537.058944 a.u.

C	0.54937800	-1.09164500	0.05456600
H	0.35452500	-1.15352000	1.12795400
H	0.06568800	-1.94758300	-0.41983000
N	-0.16757900	0.12257700	-0.41941400
H	0.30538300	0.95745800	-0.06669000
C	3.27840600	1.15395700	-0.16101700
H	3.74676100	1.96047000	0.39490000
H	3.28865700	1.24058500	-1.24553700
C	2.74172100	0.09745400	0.45297500
H	2.76133200	0.04916100	1.54252200
C	2.05563900	-1.04919400	-0.24250700
H	2.48534200	-2.00301700	0.08985100
H	2.22110200	-0.98855600	-1.32592000
H	-0.13231000	0.18234900	-1.43775400
B	-1.78040200	0.18306900	0.03771700
F	-2.22598000	1.36689500	-0.49866800
F	-1.74672600	0.15935800	1.41332400
F	-2.33532500	-0.94116000	-0.52979800

Lewis acid absent:

Imine

E(RB+HF-LYP) = -94.6309726057 a.u.

Sum of electronic and thermal Free Energies= -94.612903 a.u.

C	-0.58645700	0.02863400	-0.00014400
H	-1.24468800	-0.84498800	0.00010200
H	-1.09191000	1.00409800	0.00020400
N	0.67038200	-0.15384200	0.00004400
H	1.16266700	0.74598000	0.00025000

TS-endo

E(RB+HF-LYP) = -212.499071487 a.u.

Sum of electronic and thermal Free Energies= -212.407580 a.u.

C	-1.48895500	0.40865300	0.04544800
H	-1.81293700	0.99635600	-0.81152200
H	-1.72634900	0.82865600	1.01944200
N	-1.36805700	-0.92231500	-0.03052500
H	-0.12640100	-1.22120800	0.18115700
C	1.24719900	-1.00810300	0.24077700
H	1.78847500	-1.82042200	-0.24063100
H	1.29417600	-1.03687900	1.33154900
C	1.23305300	0.25937400	-0.38118700
H	1.48810300	0.30143600	-1.44160200
C	0.53697200	1.32921800	0.15333500
H	0.46028200	2.26319900	-0.39581000
H	0.45212200	1.42107600	1.23239200
H	-1.41068300	-1.21086500	-1.01154300

TS-exo

E(RB+HF-LYP) = -212.502979988 a.u.

Sum of electronic and thermal Free Energies= -212.411230 a.u.

C	-1.44227900	0.39850700	-0.20931200
H	-1.44267800	0.77643400	-1.22935600
H	-1.95788400	1.02502800	0.51711300
N	-1.35930500	-0.92451000	-0.04908200
H	-0.06843300	-1.23493900	-0.14073200
C	1.25733800	-1.01979400	0.10716700
H	1.85383800	-1.72754700	-0.46618900
H	1.27782100	-1.21247300	1.18139700
C	1.24096700	0.33328300	-0.31130700
H	1.56044700	0.55193700	-1.33109500
C	0.47217700	1.28512200	0.33661400
H	0.41337500	2.29960300	-0.04808100
H	0.29092700	1.18688900	1.40451300
H	-1.58149500	-1.17607500	0.91703600

Pro

E(RB+HF-LYP) = -212.574643701 a.u.

Sum of electronic and thermal Free Energies= -212.477463 a.u.

C	1.35214300	-0.43172400	-0.17231600
H	1.42305000	-0.70574800	-1.23308900
H	2.15705600	-0.97273800	0.33891700
N	1.62187800	1.00000800	-0.05585500
H	0.85030700	1.52221200	-0.46704600
C	-2.03205400	0.57015900	0.11717800
H	-2.84280400	0.97058900	-0.48471600
H	-1.96143200	0.93181800	1.14077400
C	-1.17687700	-0.33440700	-0.36413500
H	-1.29059900	-0.66807400	-1.39732100
C	-0.01097100	-0.91651500	0.38489700
H	-0.04291200	-2.01401500	0.32376100

H	-0.07987400	-0.65301900	1.44858000
H	1.64061900	1.26383900	0.92738800

Stepwise:

Lewis acid present:

TS-1-BF_3

E(UB+HF-LYP) = -537.029040142 a.u.

Sum of electronic and thermal Free Energies= -536.932828 a.u.

C	0.23159500	1.16720100	-1.11756800
H	0.66454100	0.23845400	-1.46706100
H	0.62021800	2.11167600	-1.48808300
N	-0.92997300	1.09534100	-0.54283100
H	2.77464100	-0.80253000	-1.50103000
C	2.62497200	-1.14221700	-0.46392300
H	3.37768300	-1.90854500	-0.26479200
H	1.63179700	-1.61092000	-0.42335300
C	2.73256800	-0.01504000	0.51751100
H	3.46661200	-0.10041300	1.32178700
C	1.74536200	1.05128000	0.67929800
H	2.05381100	2.09171900	0.55376200
H	0.91790200	0.90012800	1.37674900
H	-1.38677100	1.97256200	-0.30646600
B	-1.51870200	-0.27360300	0.12206000
F	-1.24673300	-0.12197900	1.47590000
F	-2.85798300	-0.30610200	-0.16407100
F	-0.78685000	-1.30068000	-0.45670800

INT-1-BF_3

E(UB+HF-LYP) = -537.062469645 a.u.

Sum of electronic and thermal Free Energies= -536.966123 a.u.

C	-0.60884500	-0.74086800	-0.79120300
H	-0.65854100	0.25058200	-1.24503100
H	-0.94161300	-1.50190300	-1.50680900
N	0.75800000	-0.96274200	-0.41329100
H	-4.22599800	1.12399800	-0.67336100
C	-3.31625300	1.03488500	-0.07000700
H	-3.51835000	1.55205100	0.88388000
H	-2.52193100	1.60551200	-0.56546500
C	-2.93859100	-0.39138800	0.14916000
H	-3.72561300	-1.12483600	0.30097600
C	-1.52643400	-0.78974800	0.47601200
H	-1.49363400	-1.80169900	0.89360900
H	-1.07881400	-0.11621000	1.21959700
H	1.02044800	-1.93542000	-0.24333700
B	1.77757500	0.22943800	0.06127000
F	1.43509400	0.37376700	1.39782700
F	3.03856100	-0.26388800	-0.14096000
F	1.44755800	1.31930300	-0.70810600

INT-1'-BF_3

E(UB3LYP) = -537.062635593 a.u.

Sum of electronic and thermal Free Energies= -536.962762 a.u.

C	0.66084000	-1.02558600	0.22828200
H	0.57599000	-0.78537900	1.29009900
H	0.14795700	-1.97497800	0.06036600
N	-0.13341900	0.00620000	-0.49240500
H	2.24269700	2.06582000	0.86325400
C	2.56492600	1.47714300	0.00350700
H	2.76056500	2.04182600	-0.91049100
H	0.31745000	0.91947300	-0.38537100
C	2.97935900	0.08670100	0.14284700
H	4.02902100	-0.11627600	0.36531600
C	2.12682000	-1.10359100	-0.21677100
H	2.56699400	-2.00451900	0.22627100
H	2.15096300	-1.27711600	-1.30959600
H	-0.14946200	-0.19360700	-1.49334800
B	-1.72196900	0.12613600	0.03090800
F	-2.25479300	1.10868900	-0.76865700
F	-2.24619100	-1.12811400	-0.18688900
F	-1.62013500	0.46861200	1.35983500

TS-2-BF_3

E(UB3LYP) = -537.041835482 a.u.

Sum of electronic and thermal Free Energies= -536.945629 a.u.

C	0.78226400	-1.23291200	0.11861700
H	0.55160400	-1.14584200	1.18249400
H	0.47744800	-2.22994000	-0.21943500
N	-0.05059300	-0.23537900	-0.56352900
H	1.37095300	2.07439600	0.84664900
C	1.70861400	1.52775900	-0.04174800
H	1.90264800	2.21058700	-0.87828600
H	0.63868100	0.87149500	-0.36843400
C	2.66863500	0.42583000	0.16776700
H	3.71131900	0.65337100	0.38257100
C	2.28152700	-0.99329100	-0.13855800
H	2.86839300	-1.69864200	0.46099600
H	2.51149600	-1.23817900	-1.19278000
H	-0.02992000	-0.33820500	-1.58032900
B	-1.55857800	0.07800600	0.03842800
F	-2.02901900	1.11518100	-0.73097900
F	-2.24178300	-1.10728400	-0.13136000
F	-1.34051300	0.40702100	1.36041200

Lewis acid absent:

TS-1

E(UB3LYP) = -212.434380615 a.u.

Sum of electronic and thermal Free Energies= -212.349222 a.u.

C	-1.33189600	-0.62197900	-0.07306700
H	-0.81614500	-1.12145700	0.74860700
H	-0.96813300	-0.87722100	-1.07555900
N	-2.49305300	-0.09107400	0.17658400
H	1.40702900	-1.45615400	-0.66989600
C	1.97506800	-0.81677900	0.01754300
H	3.03645900	-0.92082500	-0.22543000
H	1.83187400	-1.24319600	1.02504400
C	1.54200500	0.61437900	-0.05421700
H	2.31985100	1.37801700	0.02117300
C	0.15412900	1.08348600	0.02453400
H	-0.25532300	1.62830200	-0.82849300
H	-0.21804500	1.46592500	0.97797800
H	-2.92203000	0.22948400	-0.69826800

INT-1

E(UB+HF-LYP) = -212.478846582 a.u.

Sum of electronic and thermal Free Energies= -212.391235 a.u.

C	1.14816700	-0.29053000	0.34264500
H	0.82109300	-1.34336900	0.25753200
H	1.20763100	-0.10306300	1.43102100
N	2.44664800	-0.11811400	-0.26434400
H	-2.09632500	-1.49104400	0.28700900
C	-2.25918900	-0.49575700	-0.16436300
H	-3.28623500	-0.20921400	0.08859200
H	-2.20314000	-0.63747900	-1.25098000
C	-1.26895200	0.51802000	0.30654600
H	-1.46678000	1.03153000	1.24572700
C	0.09428900	0.64543800	-0.29389800
H	0.46891200	1.67214500	-0.19295200
H	0.06320900	0.42529400	-1.36909800
H	3.07921400	-0.78102700	0.20797700

INT-1'

E(UB+HF-LYP) = -212.469998671 a.u.

Sum of electronic and thermal Free Energies= -212.379968 a.u.

C	1.19495100	0.38130800	0.38392700
H	1.00420700	0.26540700	1.46611500
H	2.07138400	1.03403000	0.28800300
N	1.49956500	-0.87263400	-0.31316500
H	0.70417300	-1.50390800	-0.22520200
C	-1.64078800	-0.93630900	0.08472000
H	-1.71672900	-1.48110300	1.02616800
H	-1.92579400	-1.49157600	-0.81105100
C	-1.35726700	0.49153700	0.04296800
H	-2.20620900	1.18021800	0.04331700
C	-0.00758300	1.09464900	-0.25488500
H	-0.01715100	2.14310400	0.06875000
H	0.16939100	1.11104100	-1.34488600
H	2.28389400	-1.33588700	0.14056100

TS-2

E(UB+HF-LYP) = -212.451612471 a.u.

Sum of electronic and thermal Free Energies= -212.363812 a.u.

C	1.25945800	0.27229800	0.29195200
H	1.25191900	0.26331100	1.39338400
H	2.23174100	0.68518800	-0.01707100
N	1.11040700	-1.05792200	-0.31031800
H	-0.12904500	-1.23102800	-0.24841000
C	-1.39829600	-0.85944800	0.05315700
H	-1.67484400	-1.35080800	0.99385300
H	-1.99819000	-1.25359800	-0.77734000
C	-1.21660500	0.60688200	0.09927800
H	-2.07953500	1.27019800	0.15561600
C	0.13284000	1.19176400	-0.21117400
H	0.24130300	2.19306200	0.22252800
H	0.25343000	1.31376000	-1.30284400
H	1.46599200	-1.75360500	0.35322800

Functional groups on N

Imine-CF_3

E(RB+HF-LYP) = -431.665583044 a.u.

Sum of electronic and thermal Free Energies= -431.648666 a.u.

C	1.97371200	-0.01888300	-0.00010000
H	2.93020400	-0.54132800	0.00023600
H	1.98926900	1.07475000	0.00022400
N	0.91164600	-0.71427200	-0.00011300
C	-0.34107100	-0.03526300	-0.00000200
F	-0.26929900	1.32048700	-0.00017100
F	-1.03754500	-0.39417500	-1.08941300
F	-1.03724800	-0.39393900	1.08968800

TS-CF_3

E(RB+HF-LYP) = -549.541939434 a.u.

Sum of electronic and thermal Free Energies= -549.449823 a.u.

C	-0.53119800	-1.28604000	-0.61095500
H	-1.07919700	-1.70774600	-1.45148300
H	-0.10396700	-2.03899400	0.05291300
N	0.20534900	-0.18876400	-0.90719300
C	1.26517500	0.07705100	-0.02820000
H	-0.78051900	0.94632000	-0.69489000
C	-1.75909800	1.44777700	-0.09493100

H	-2.16619100	2.28256600	-0.66303000
H	-1.26940300	1.75471700	0.83089200
C	-2.52375500	0.25001400	-0.04615000
H	-3.31251700	0.10836400	-0.78535000
C	-2.01093000	-0.88256900	0.59390100
H	-2.59904500	-1.79739900	0.59045300
H	-1.41735600	-0.73161900	1.49138400
F	0.88862800	0.18596800	1.29457000
F	2.21778300	-0.88724500	-0.05040000
F	1.85465400	1.24213600	-0.34445100

Pro-CF_3

E(RB+HF-LYP) = -549.614079897 a.u.

Sum of electronic and thermal Free Energies= -549.517503 a.u.

C	0.51437700	1.41624800	-0.36575500
H	0.93341300	1.94494300	-1.22896600
H	-0.11327100	2.13227300	0.17045800
N	-0.36324200	0.36509500	-0.89220000
C	-1.34123500	-0.15734700	-0.04236300
H	0.16085800	-0.39289100	-1.32010900
C	2.54152200	-1.37331400	-0.00183700
H	3.20182200	-2.03166600	-0.55903800
H	1.86137200	-1.84267600	0.70511800
C	2.56912400	-0.04784500	-0.16175700
H	3.26132300	0.38549200	-0.88548900
C	1.65783900	0.91655000	0.54947400
H	2.22619800	1.79366600	0.88565000
H	1.22699300	0.44416700	1.43648000
F	-0.86422200	-0.79569600	1.08033100
F	-2.15635900	0.81358400	0.41465400
F	-2.07561600	-1.07507800	-0.69779300

Imine-CH_3

E(RB+HF-LYP) = -133.945975551 a.u.

Sum of electronic and thermal Free Energies= -133.902388 a.u.

C	1.18206100	0.18277800	-0.00001200
H	2.16310500	-0.29664100	0.00015800
H	1.16866600	1.28448400	-0.00007100
N	0.13962000	-0.53719200	-0.00003500
C	-1.14749700	0.13522400	-0.00001900
H	-1.71662000	-0.18473800	0.88018000
H	-1.08214800	1.23573200	-0.00102200
H	-1.71773000	-0.18650100	-0.87881300

TS-CH_3

E(RB+HF-LYP) = -251.812094164 a.u.

Sum of electronic and thermal Free Energies= -251.695116 a.u.

C	0.56986900	-1.16697700	-0.48693300
H	0.10553200	-1.61396900	-1.36232500
H	0.95758200	-1.86758700	0.25402100
N	1.11652300	0.03876900	-0.62490100
C	2.03670800	0.44524400	0.44048000
H	2.05100200	1.53681500	0.51386200
H	1.77773500	0.03900800	1.43140800
H	3.05272400	0.11522800	0.19647600
H	0.11721400	0.88900600	-0.60487300
C	-1.05182100	1.39502100	-0.07303400
H	-1.42900100	2.20219200	-0.69879900
H	-0.66454700	1.73910600	0.88834100
C	-1.73581900	0.15627100	-0.09334300
H	-2.40991700	-0.03864900	-0.92850900
C	-1.28874100	-0.93136100	0.63877300
H	-1.77748100	-1.89716400	0.54485800
H	-0.77767900	-0.76456100	1.58418200

Pro-CH_3

E(RB+HF-LYP) = -251.881736493 a.u.

Sum of electronic and thermal Free Energies= -251.758803 a.u.

C	-0.68373700	1.10397800	-0.18529500
H	-0.43531600	1.74890600	-1.03891900
H	-1.39700800	1.66554600	0.43116400
N	-1.36782900	-0.07711400	-0.69801100
C	-2.00095400	-0.91152600	0.31673300
H	-2.49885000	-1.75573400	-0.17092800
H	-1.32655000	-1.32298000	1.08862900
H	-2.77306000	-0.32891700	0.83297300
H	-0.70929300	-0.63596100	-1.23546600
C	2.14815300	-1.02911100	-0.02907000
H	2.92040000	-1.44086400	-0.67255900
H	1.77549200	-1.67813000	0.76047800
C	1.69137000	0.21537600	-0.18382600
H	2.09878900	0.82824800	-0.99038800
C	0.60824800	0.85516300	0.63912700
H	0.95772100	1.82436300	1.02238400
H	0.38399300	0.23204400	1.51268700

Imine-Ph

E(RB+HF-LYP) = -325.687864991 a.u.

Sum of electronic and thermal Free Energies= -325.596789 a.u.

C	2.78681400	0.23438800	0.30358900
H	3.84690400	0.02901800	0.14863200
H	2.53170700	1.05710500	0.98560300
N	1.92636000	-0.48559500	-0.29617300
C	0.55006900	-0.20288000	-0.14716100
C	-0.33014800	-1.28985700	-0.03201100

C	0.03159900	1.10226400	-0.16168400
C	-1.69776500	-1.07265300	0.11515700
H	0.08165600	-2.29393200	-0.04878200
C	-1.34179800	1.31139900	-0.03635100
H	0.70274200	1.94376100	-0.30625200
C	-2.20977700	0.22822100	0.11281700
H	-2.36854300	-1.92075400	0.21942600
H	-1.73442100	2.32414100	-0.06140400
H	-3.27854100	0.39453300	0.20984600

TS-Ph

E(RB+HF-LYP) = -443.555926865 a.u.

Sum of electronic and thermal Free Energies= -443.390367 a.u.

C	-1.49071000	-1.30577400	-0.58331800
H	-2.27186800	-1.62605400	-1.27027500
H	-1.05815000	-2.11215000	0.00973000
N	-0.71557600	-0.28759800	-0.99723700
H	-1.48342500	0.86611200	-0.66990900
C	-2.26594500	1.54454400	0.11685200
H	-2.66635400	2.41982300	-0.39297700
H	-1.54120900	1.79617300	0.89498900
C	-3.15397400	0.47156200	0.38631600
H	-4.09757200	0.42965700	-0.15805600
C	-2.67097000	-0.70753500	0.95072200
H	-3.34606100	-1.54667100	1.10021500
H	-1.86907900	-0.63941800	1.68315900
C	0.58385600	-0.14427700	-0.46517100
C	1.39090500	-1.23786800	-0.09335400
C	1.14439900	1.14629000	-0.38250300
C	2.69206600	-1.04002100	0.36833100
H	1.01618700	-2.25035300	-0.20480800
C	2.44301600	1.33539400	0.08073700
H	0.54779700	1.99884700	-0.69176200
C	3.22675500	0.24481600	0.46731000
H	3.29480900	-1.90225500	0.64138100
H	2.84669300	2.34276600	0.13804200
H	4.24087000	0.39391900	0.82540300

Pro-Ph

E(RB+HF-LYP) = -443.630554898 a.u.

Sum of electronic and thermal Free Energies= -443.460022 a.u.

C	1.33880200	-1.19186600	-0.06137200
H	1.19563200	-1.52062900	0.98383700
H	1.01611200	-2.02367200	-0.69944500
N	0.55463100	-0.01258000	-0.37606100
H	1.03818100	0.85427200	-0.17681200
C	3.88341300	1.32625800	0.11910400
H	4.26203600	2.08182200	0.80126900
H	3.94588400	1.55203900	-0.94314400
C	3.38360200	0.16929800	0.55881300
H	3.34326400	-0.01674500	1.63346100
C	2.83208600	-0.92408700	-0.31672800
H	3.37665000	-1.85873200	-0.12859600
H	2.97694200	-0.66813500	-1.37247000
C	-0.82003800	0.03818800	-0.16399700
C	-1.59406700	-1.11803800	0.04867700
C	-1.47800300	1.28542100	-0.19445600
C	-2.97680700	-1.02026300	0.21359200
H	-1.12082900	-2.09308900	0.08554200
C	-2.85477400	1.36832600	-0.02325000
H	-0.89386000	2.18808500	-0.35982300
C	-3.62074800	0.21580800	0.18119500
H	-3.55249800	-1.92799400	0.37513000
H	-3.33474300	2.34312500	-0.04972100
H	-4.69598800	0.28344800	0.31372700