

Computational Chemistry as a Powerful Tool in Development and Study of
Stereoselective Aminocatalytic Reactions

By
Simarpreet Singh

A Thesis Submitted to the Faculty of Graduate Studies of
The University of Manitoba
in partial fulfilment of the requirements for the Degree of

DOCTOR OF PHILOSOPHY

Department of Chemistry
University of Manitoba
Winnipeg, Manitoba

Copyright © 2023 by Simarpreet Singh

Abstract

The development and application of computational methods have revolutionized experimental chemistry, allowing calculations on real chemical systems without requiring in-depth mathematical understanding. Computational chemistry has become a valuable tool alongside experimental techniques in elucidating reaction mechanisms. In the field of aminocatalysis, these methods have facilitated a deeper understanding of selectivity, prediction of stereochemistry, and the design of novel catalysts to expand its scope.

Chapter 2 focuses on the aminocatalytic γ -amination reaction of enals with Diethyl azodicarboxylate. The observed stereochemistry of the product challenges existing mechanistic models, prompting a study that employs both experimental and computational methods to explore plausible downstream reaction pathways. Two mechanisms are proposed: one involving the formation of a downstream aminated dienamine intermediate and the other invoking a Michael addition pathway. However, the mechanistic investigations suggest that the aminated dienamine is not formed, necessitating further inquiry into the Michael addition mechanism for a comprehensive understanding of the reaction.

Chapter 3 examines the impact of aminocatalysts in promoting the dearomatization of several heteroaromatic aldehydes. The constructed hyperhomodesmotic equations indicate that the formation of an iminium ion reduces the energy cost for dearomatization compared to the parent aldehyde. The role of the catalyst and heteroatom of the aldehyde on the orbital coefficients at different positions of the trienamine intermediate is also explored.

In Chapter 4, the influence of substituents on a trienamine intermediate is investigated. Trienamine-mediated Diels-Alder reactions show reactivity at the terminal diene (3,6-scis diene)

over 1,4-scis diene. Various substituents are employed to assess their influence on the thermodynamics and HOMO energy of trienamine intermediates. Additionally, orbital coefficients are calculated to understand the impact of substituents on the pi-backbone.

Chapter 5 presents an investigation into the unprecedented dimerization of electron-deficient cyclic allenes. The study also explores the trapping of cyclic allenes with electron-rich dienes to gain insights into the observed selectivity. Computational data are utilized to develop a novel trapping method of allenes with enamines.

Overall, this dissertation showcases the application of computational chemistry in aminocatalytic reaction mechanism elucidation and method development, demonstrating its significance in advancing the understanding and manipulation of complex chemical processes.

Acknowledgements

There are so many people (and pets) that I am grateful for. It takes a village to raise a graduate student and that certainly was the case with me. First and foremost, I would like to extend my gratitude to my parents, Paramjit Kaur and Harpreet Singh for their immense support and encouragement throughout my graduate career. I also want to thank my sister, Simaranjeet Kaur, and brother-in-law, Prabhsimran Singh, for their support and taking me out for movie nights throughout my graduate studies.

I would also like to thank my academic mother, my supervisor, Dr. Rebecca Davis for letting me run with my ideas in the research group. I am extremely grateful for her mentorship and treating me as a colleague during my PhD. Due to her mentorship, I learned how to learn and was able to pick up a few things on studying reaction mechanisms. Thank you for having a compassionate mentoring style which is very rare in academia.

I would also like to thank the past and present members of the Davis group, especially Jorge Dourado who taught me almost all the lab techniques that I needed for my research. I also want to thank Guanyu Wang for his friendship during and after his time in Davis group. I also want to thank all the honours and summer students that I had the privilege of training because they helped me become a versatile teacher in the lab.

I would like to thank my advisory committee: Prof. Rebecca Davis, Prof. Frank Schweizer, Prof. John Sorenson and Prof. Francis Lin. Thank you for all the support, feedback, and helpful insights over the last few years.

I want to thank the staff in department office for their support throughout the past years. I also want to thank Dr. Kirk Marat and late Dr. Philip Hultin for their guidance with NMR and organic synthesis. I would also like to especially thank Dr. David Davidson for all the NMR

support, fun little projects, and great conversations. I also want to thank Dr. Mario Bieringer for his exceptional advice and amazing conversations throughout my graduate career.

I would like to thank all my friends, especially Prakshi, Sagar, Issiah, Ainsleigh, and other fellow graduate students who let me vent about graduate school and share a laugh about it.

I also want to thank Dr. Janitha Wanasundara from AAFC, Saskatoon who encouraged me to pursue further research after my undergraduate degree. I may not have enrolled in graduate school if it was not for my time in her research group. I am very thankful to Mr. Dale McKinnon, my high school chemistry teacher. His passion for teaching and chemistry led me to pursue an undergraduate degree in chemistry and eventually a PhD.

A big thank you to my dog, Lucy, and my cat, Ollie for their unconditional love and emotional support. Another big thank you to Wu Tang Clan whose music kept me going.

Last but not least, I would like to thank my wife, Rajveer Kaur, for always being there even if you did not understand some of the graduate school struggles. Your support made a huge difference in facing the hardships of graduate studies.

This thesis is dedicated to all the first-generation graduate students.

You are your ancestors' wildest dream. Keep going.

Table of Contents

Abstract	ii
Acknowledgements	iv
Table of Contents	vii
List of Tables	x
List of Figures	xii
List of Schemes.....	xv
List of Abbreviations.....	xviii
List of Published Work.....	xxi
Chapter 1 : Introduction	1
1.1 : Computational Chemistry	1
1.1.1 : Computational methods ^{2,4,7}	2
1.1.2 : Born-Oppenheimer Approximation	3
1.1.3 : Density Functional Theory ^{4,7}	3
1.2 : Asymmetric Synthesis	7
1.2.1 : Chirality.....	7
1.3 : Asymmetric synthetic methods	11
1.4 : Asymmetric Catalysis	12
1.5 : Organocatalysis.....	13
1.5.1 : Aminocatalysis	15
1.5.2 : Enamine Activation	17
1.5.3 : Dienamine activation	25
1.5.4 : Trienamine and Polynemamine activation.....	29
1.6 : References.....	37
Chapter 2 : Mechanistic Investigation of Aminocatalytic Remote Functionalization of α,β -Unsaturated Aldehydes	47
2.1 : Introduction.....	47
2.2 : Computational methods	51
2.3 : Results and Discussion	52
2.3.1 : Diels-Alder Cycloaddition between Dienamine and DEAD.....	52
2.3.2 : Plausible Mechanisms	56

2.3.3 : Aminated Dienamine.....	59
2.3.4 : Michael Addition pathway.....	64
2.4 : Conclusions.....	65
2.5 : References.....	66
Chapter 3 : Exploring the Role of Aminocatalysis in the Dearomatization and Regioselectivity of Heteroaromatic Aldehydes.	71
3.1 : Introduction.....	71
3.2 : Computational methods	73
3.3 : Results and Discussion	73
3.3.1 : Model System A	73
3.3.2 : Model system B.....	78
3.3.3 : Model System C	82
3.3.4 : Model System D	85
3.3.5 : Model system E.	89
3.3.6 : Fulvene systems.....	92
3.4 : Conclusions.....	93
3.5 : References.....	95
Chapter 4 : Exploring the Role of Substituents on Trienamine Backbone in Trienamine-Mediated Diels-Alder Reactions.	103
4.1 : Introduction.....	103
4.2 : Computational methods	108
4.3 : Results and Discussion	108
4.3.1 : Unsubstituted Trienamines	108
4.3.2 : β -Substituted Trienamines	111
4.3.3 : γ -Substituted Trienamines.....	116
4.3.4 : δ -Substituted Trienamines	121
4.3.5 : ϵ -Substituted Trienamines.....	125
4.4 : Conclusions.....	129
4.5 : References.....	131
Chapter 5 : Electron-deficient 1,2-cyclohexadienes: Mechanistic investigation of unprecedented dimerization.	137
5.1 : Introduction.....	137
5.2 : Generation of cyclic allenes.....	138
5.2.1 : Base mediated elimination.....	139

5.2.2 : Doering-Moore-Skattebøl rearrangement	140
5.2.3 : Fluoride mediated elimination	141
5.3 : Reactivity of 1,2-cyclohexadiene: Trapping and Dimerization	142
5.3.1 : Trapping of 1,2-cyclohexadienes <i>via</i> cycloaddition reactions	143
5.3.2 : Dimerization	146
5.4 : Polar Cyclic Allenes	147
5.5 : Mechanistic investigation of dimerization and trapping of electron deficient 1,2-cyclohexadienes.	149
5.6 : Computational study of observed experimental results: dimerization and selectivity of trapping reactions.	154
5.6.1 : Computational methods.....	154
5.6.2 : Investigation of dimerization.....	155
5.6.3 : Discussion of [2+2] dimerization of 5.45a	156
5.6.4 : Computational investigation of trapping reactions of 5.45a-d with furans.	157
5.6.5 : Investigation of trapping reactions of cyclic allenes with enamines	165
5.7 : Conclusions.....	169
5.8 : References.....	171
Chapter 6 : Conclusions and Future Work	176
Appendix.....	180
Supporting data.....	181
A1 : Experimental Data and Procedures	181
A2 : Supporting Data for Chapter 3	187
A.2.1 : Geometry Analysis of all Model systems.	187
A.2.2 : Charge Analysis and Fukui function Isosurfaces for all Model systems.....	195
A.2.3 Hyperhomodesmotic Equations and Orbital Coefficients for the <i>N</i> -Methyl systems	199
A3 : Dihedral angles of trienamine backbone for Chapter 4.....	203
A4 : Energies and Reaction Coordinates.....	210
A.4.1 : Energies and Reaction Coordinates for Chapter 2.....	210
A.4.2 : Energies and Reaction Coordinates for Chapter 3.....	289
A.4.3 : Energies and Reaction Coordinates for Chapter 4.....	400
A.4.4 : Energies and Reaction Coordinates for Chapter 5.....	450

List of Tables

Table 3.1: Hyperhomodesmotic equations used to assess the dearomatization of Model System A. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol	74
Table 3.2: Orbital coefficients of the HOMO of trienamines A12-A15	77
Table 3.3: Hyperhomodesmotic equations used to assess the dearomatization of Model System B. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.	79
Table 3.4:Orbital coefficients of the HOMO of Model System B.....	81
Table 3.5: Hyperhomodesmotic equations used to assess the dearomatization of Model System C. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol	82
Table 3.6: Orbital coefficients for the HOMO of trienamines C12-C15	84
Table 3.7: Hyperhomodesmotic equations used to assess the dearomatization of Model System D. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.	85
Table 3.8: Orbital coefficients for the HOMO of trienamines D12-D15	88
Table 3.9: Hyperhomodesmotic equations used to assess the dearomatization of Model System E. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.	89
Table 3.10: Orbital coefficients for the HOMO of trienamines E12-E15	91
Table 4.1:Relative energies and HOMO locations of unsubstituted trienamine system. Relative free energies are in kcal/mol.....	110
Table 4.2: Orbital coefficients of HOMOs of trienamine A1-A3	111
Table 4.3: Relative energies and HOMO locations of trienamines B1-B3 , C1-C3 , D1-D3 , and E1-E3 . All free enrgies are reported in kcal/mol.....	112
Table 4.4: Orbital coefficients of HOMOs of trienamine B1-B3	115
Table 4.5: Orbital coefficients of HOMOs of trienamine C1-C3	115
Table 4.6: Orbital coefficients of HOMOs of trienamine D1-D3	116
Table 4.7: Orbital coefficients of HOMOs of trienamine E1-E3	116

Table 4.8: Relative energies and HOMO locations of trienamines F1-F3 , G1-G3 . All free energies are reported in kcal/mol.....	118
Table 4.9: Relative energies and HOMO locations of trienamines H1 , H2 , I1 , and I2 . All free energies are reported in kcal/mol.....	119
Table 4.10: Orbital coefficients of HOMOs of trienamine F1-F3	120
Table 4.11: Orbital coefficients of HOMOs of trienamine G1-G3	121
Table 4.12: Orbital coefficients of HOMOs of trienamine H1 , H2 , I1 , and I2	121
Table 4.13: Relative energies and HOMO locations of trienamines J1 , J2 , K1 , K2 , L1 , L2 , M1 , and M2 . All free energies are reported in kcal/mol.....	123
Table 4.14: Orbital coefficients of HOMOs of trienamine J1 , J2 , K1 , and K2	124
Table 4.15: Orbital coefficients of HOMOs of trienamine L1 , L2 , M1 , and M2	125
Table 4.16: Relative energies and HOMO locations of trienamines N1 , N2 , O1 , O2 , P1 , P2 , Q1 , and Q2 . All free energies are reported in kcal/mol.	127
Table 4.17: Orbital coefficients of HOMOs of trienamine N1 , N2 , O1 , and O2	128
Table 4.18: Orbital coefficients of HOMOs of trienamine P1 , P2 , Q1 , and Q2	129
Table 5.1: Diels-Alder trapping of electron deficient 1,2-cyclohexadienes with furans	154
Table 5.2: Energies of trapping reactions with furan. All free energies reported in kcal/mol	160
Table 5.3: Energies of trapping reactions with 2,5-dimethylfuran. All free energies reported in kcal/mol.	161
Table 5.4: Energies of trapping reactions with DPIBF. All free energies reported in kcal/mol.	161
Table 5.5: Transition state energies of trapping allene 5.45d with various dienes. All free energies are reported in kcal/mol. The energy values are relative to allene 5.45d and diene.	164
Table 5.6: Hetero-Diels-Alder trapping of 2-keto aryl cyclohexadienes derived from 5.40a , 5.40b with electron-rich heterodienophiles	167

List of Figures

Figure 1.1: Differences in cis and trans isomers of butenedioic acid, commonly known as maleic acid (cis, left) and fumaric acid (trans, right).	7
Figure 1.2: Classes of stereoisomers.	9
Figure 1.3: Some examples of enantiomer pairs and their bioactivity.	10
Figure 1.4: a) Total synthesis of alkaloid (–)-allonorsecurinine starting from naturally occurring L-proline amino acid. b) Synthetic strategy using chiral auxiliaries to induce asymmetry in the final product and some selected examples of chiral auxiliaries.	12
Figure 1.5: Aminocatalytic activation modes. Enamine activation pathway (left) and Iminium-ion activation pathway (right).	16
Figure 1.6: Proposed early transition state models of HPESW reaction.	18
Figure 1.7: Illustration of proposed model for proline catalyzed intramolecular aldol reaction by Houk. Energies are in kcal/mol.	19
Figure 1.8: a) Transition states for proline catalyzed intermolecular reaction b) Houk-List model	20
Figure 1.9: Transition states for proline I catalyzed syn-selective Mannich reaction and computationally designed catalyst III for anti selective mannich reactions.	22
Figure 1.10: The two general models to induce chirality and predict stereoselectivity in Aminocatalysis: Hydrogen bond directed approach (left) and Steric shielding approach (right).	23
Figure 1.11: Relative free energies of enamine intermediates with Diarylprolinol silyl ether catalyst IV and b) Depiction of transition state structures for α -fluorination. Energies are in kcal/mol.	25
Figure 1.12: Vinylogous aminocatalytic activation modes (left). Reactivity of vinylogous aminocatalytic activation modes (right).	26
Figure 1.13: Relative energies of dienamine intermediates and their barriers for reactions with DEAD 1.14 . Energies are in kcal/mol.	28
Figure 1.14: Calculated conformations of trienamine and their rotational barriers. Energies are in kcal/mol.	30
Figure 1.15: Pathway comparison of Diels-Alder reaction between cyclic linear trienamine and olefinic oxindole (top), and cross-trienamine and olefinic oxindole (bottom). Energies are in kcal/mol.	33
Figure 1.16: Aminocatalytic higher-order formal [8+2] cycloaddition reaction between 1.43 and 1.45 , and its stepwise pathway. Potential [10+4] pathway (red) for cycloadduct 1.48 observed in silico. Energies are in kcal/mol.	35
Figure 2.1: Depiction of selectivity in dienamine intermediate by steric discrimination from aminocatalyst IV for γ -amination.	48

Figure 2.2: Christmann's proposed second dienamine.....	50
Figure 2.3: Computed energies of Dineamine A, B, and C. Free energies reported are in kcal/mol.	52
Figure 2.4: Experimental evidence of dienamines A and B by ^1H -NMR at 300MHz in CDCl_3 ...	53
Figure 2.5: Calculated barrier for Diels-Alder cycloaddition between Dienamine intermediate and DEAD . All energies are reported in kcal/mol.....	54
Figure 2.6: a) Reaction coordinate diagram of calculated barriers for mono-addition of DEAD and [4+2] cycloaddition to dienamine intermediate. B) The resulting iminium-ion intermediates after mono-addition of DEAD and [4+2] cycloaddition to dienamine intermediate. All energies are in kcal/mol.	55
Figure 2.7: Hydrolysis of cycloadduct leading to product with Z-configuration	56
Figure 2.8: Plausible pathways for dienamine mediated γ -amination reaction.	58
Figure 2.9:a) Formation of aminated dienamine intermediate D from the cycloadduct DA-INT . b) Conformers of aminated dienamine intermediate. Free energies are reported in kcal/mol.	60
Figure 2.10: Calculated Iminium ion intermediates resulting from protonation of aminated Dienamines D , E , and F	61
Figure 2.11: Resulting iminium ion intermediates upon protonation of Dienamines D, E, and F. Free energies are reported in kcal/mol. (C = grey, N = blue, O = red, F = green, Si = yellow, H = white).....	63
Figure 2.12: Stacked NMR segment of γ -amination reaction with deuterated enal. The signals on left (red) show the ethyl protons of DEAD, the signals on the right (green) show the ethyl protons of hydrazine moiety in the product.....	64
Figure 2.13: Michael addition intermediates.....	65
Figure 3.1: HOMO of trienamines A12-A15 for Model System A (isovalue 0.035).....	77
Figure 3.2: HOMO of trienamines B12-B15 (isovalue 0.035).....	81
Figure 3.3: HOMO of the trienamines C12-C15 for Model System C (isovalue (0.035).	84
Figure 3.4 HOMO of the trienamines D12-D15 for Model System D (isovalue 0.035):.	88
Figure 3.5:HOMO of the trienamines E12-E15 for Model System E (isovalue 0.035).	91
Figure 4.1:Conformations of trienamine intermediates and substituents studied in this report. .	108
Figure 4.2: Three dimensional stuctures of trienamines C1-C3	113
Figure 5.1: Cyclic strained reactive intermediates.....	137
Figure 5.2: Bending angle and strain energies for cyclic allenes.	138
Figure 5.3: Precursors for electron deficient 1,2-cyclohexadienes.....	150

Figure 5.4: DFT investigation of a) concerted allene dimerization and b) stepwise anionic addition pathways leading to formation of 5.46a . Reported values are Gibbs Free energies and are reported in kcal/mol.....	156
Figure 5.5: Transition state structure of [2+2] dimerization of 5.45a	157
Figure 5.6: a) Optimized transition state structures leading to the possible diastereomers and regioisomers for the addition of furan with allene 5.45d . The bond lengths are reported in Ångstroms. Reported values are Gibbs Free energies and are reported in kcal/mol. B) NCI figures (isovalue of 0.4) of TS1 and TS2 . Blue = strong attractive interactions, green = weak attractive interactions, red = strong repulsive interactions. C) LUMO coefficients (left) and its depiction (right) of allene 5.45d	159
Figure 5.7: Transition state structures for trapping of allene 5.45d with furan (left), 2,5-Dimethylfuran (center), and DPIBF (right) for endo approach (top) and exo approach (bottom).	163
Figure 5.8: a) LUMO of allene 5.45d . b) HOMOs of various furans.....	163
Figure 5.9: Transition state structures of trapping of allene 5.45d with isobenzofuran (left) and 2,5-Diphenylfuran (right) for endo approach (top) and exo approach (bottom).	165
Figure 5.10: Optimized transition state structure TS5 for the favoured diastereomer of the cycloaddition of 5.45a with 5.58a . b) NCI plot of TS5	168
Figure 5.11: Examination of reactivity of enamine 5.58a with allene 5.45a . Comparison of [4+2] pathway leading to 5.59a and stepwise pathway leading 5.60a . Energies are reported in kcal/mol.	169

List of Schemes

Scheme 1.1: Early examples of asymmetric organocatalysis. a) Hydrocyanation of benzaldehyde catalyzed by quinine. b) Hajos-Parrish-Eder-Sauer-Wiechert intramolecular aldol reaction catalyzed by L-proline.....	14
Scheme 1.2: First reports of modern aminocatalysis. a) Intramolecular aldol reaction catalyzed by L-proline (I) reported by List and coworkers. b) Diels-Alder reaction catalyzed by chiral imidazolidinone (II) reported by MacMillan and coworkers.	15
Scheme 1.3: Comparison of proline I catalyzed and computationally designed catalyst III for Mannich reaction.	22
Scheme 1.4: Aminocatalytic enantioselective α -functionalization of aldehydes via enamine activation reported by Jørgensen.	24
Scheme 1.5: Dienamine mediated enantioselective γ -amination of enals 1.13 catalyzed by IV , reported by Jørgensen.....	26
Scheme 1.6: Dienamine mediated intramolecular [4+2] cycloaddition catalyzed by V	29
Scheme 1.7: Trienamine mediated enantioselective Diels-Alder reactions of 2,4-Dienals 1.18 with olefinic oxindoles 1.20 and cyanoacetates 1.22 , reported by Jørgensen and Chen.	30
Scheme 1.8: Cross-trienamine activation mode in aminocatalysis promoted by γ' -deprotonation.	31
Scheme 1.9: Cross-trienamine mediated enantioselective Diels-Alder reactions reported by Jørgensen.	32
Scheme 1.10: Enantioselective formal [10+4] cycloaddition catalyzed by aminocatalyst, reported by Jørgensen.	36
Scheme 2.1: Dienamine mediated γ -amination of α,β -unsaturated aldehydes reported by Jørgensen.	48
Scheme 2.2: Dienamine mediated γ -alkylation of α,β -unsaturated aldehydes reported by Christmann.....	49
Scheme 2.3: Proposed reaction.	63
Scheme 3.1: Model systems studied in this work (X=O, NH, and S).....	72
Scheme 3.2: Energy differences between linear trienamines and (hetero)fulvene systems for all Model Systems (X = CH ₂ or NH; relative free energies in kcal/mol calculated at the M06-2X/6-31+G(d,p) level of theory).....	93
Scheme 4.1: Dienamine mediated γ -amination of α,β -unsaturated aldehydes.	104
Scheme 4.2: General trienamine mediated Diels-Alder reaction.	105
Scheme 4.3: Trienamine mediated enantioselective Diels-Alder reactions reported by Jørgensen and Chen.	106

Scheme 4.4: HOMO-raising strategy through substitution on 2,4-dienals for Diels–Alder reactions with nitroalkenes reported by Chen. a) No reaction is observed with unsubstituted dienal and nitroalkenes via trienamine intermediate. b) Dienals with substituents at γ - and δ -carbons to enhance HOMO of trienamine for Diels-Alder reaction with nitroalkenes.	107
Scheme 4.5: Trienamine mediated [4+2] cycloaddition reaction between γ -substituted 2,4-dienals and vinylquinolines reported by Wang et al.	117
Scheme 4.6: Trienamine mediated Diels-Alder reaction between δ -substituted 2,4-dienals and 5-nitro-2,3-dihydro-4-pyridones, reported by Ishikawa et al.	122
Scheme 4.7: Trienamine mediated Diels-Alder reaction between ϵ -substituted 2,4-Dienals and Coumarin-3-carboxylic acids, reported by Albrecht et al.	126
Scheme 5.1: Common methods to generate 1,2-cyclohexadiene	139
Scheme 5.2: Generation of 1,2-cyclohexadiene via base elimination and trapping with DPIBF.	139
Scheme 5.3: Comparison of generation of cyclohexyne and 1,2-cyclohexadiene with different 1-chlorocyclohexenes	140
Scheme 5.4: a) Allene synthesis via Doering-Moore-Skattebøl reaction. b) Generation of 1,2-cyclohexadiene via Doering-Moore-Skattebøl reaction.....	141
Scheme 5.5: Generation of 1,2-cyclohexadiene via fluoride mediated elimination.....	142
Scheme 5.6: Common reactions of 1,2-cyclohexadiene intermediate.....	143
Scheme 5.7: Trapping of 1,2-cyclohexadiene via [4+2] cycloaddition reaction.....	144
Scheme 5.8: Trapping of in-situ generated 1,2-cyclohexadiene via intramolecular [4+2] cycloaddition reaction.	144
Scheme 5.9: Generation and trapping of acyloxy 1,2-cyclohexadienes with styrenes.	145
Scheme 5.10: a) [3+2] cycloaddition of 1,2-cyclohexadiene and nitrones by Garg. b) [3+2] cycloaddition of 1,2-cyclohexadiene and 1,3-dipoles by West.	146
Scheme 5.11: Dimer, trimer, and tetramer products of 1,2-cyclohexadiene.....	147
Scheme 5.12: Generation and trapping of 1-oxa-2,3-cyclohexadiene with furans and styrenes.	148
Scheme 5.13: Generation and trapping of ester-substituted 1,2-cyclohexadienes.	149
Scheme 5.14: a) Synthesis of 2-aroyle enol triflate allene precursors. b) Synthesis of 2-cyano enol triflate allene precursor.....	150
Scheme 5.15: Unexpected dimerization of 2-aroyle 1,2-cyclohexadienes.	151
Scheme 5.16: Possible mechanisms for the formation of 5.46a	152
Scheme 5.17: Generation of electron deficient 1,2-cyclohexadienes and trapping reactions with furans.....	153

Scheme 5.18: [2+2] dimerization of 5.45a . Reported values are Gibbs Free energies and are reported in kcal/mol.	157

List of Abbreviations

APTC	Asymmetric Phase <i>Transfer</i> Catalyst
Ar	Aryl
B3LYP	Becke, 3-parameter, Lee-Yang-Parr
BA	Benzoic Acid
Boc	tertiary-Butoxycarbonyl
cat	catalytic
CH ₃ CN	Acetonitrile
DCE	Dichloroethane
DCM	Dichloromethane
DEAD	Diethyl Azodicarboxylate
DFT	Density Functional Theory
DMS	Doering-Moore-Skattebol
DMSO	Dimethyl Sulfoxide
DPIBF	Diphenylisobenzofuran
dr	Diastereomeric Ratio
DZ	Double-Zeta
ee	Enantiomeric Excess
Et	Ethyl
H-bond	Hydrogen bond
HCN	Hydrogen Cyanide
HF	Hartree-Fock
HOMO	Highest Occupied Molecular Orbital

HPESW	Hajos-Parrish-Eder-Sauer-Wiechart
IEFPCM	Integral Equation Formalism Polarizable Continuum Model
<i>i</i> -Pr	<i>iso</i> -Propyl
KOt-Bu	Potassium <i>tert</i> -butoxide
LUMO	Lowest Unoccupied Molecular Orbital
M06	Minnesota 2006 Functional
Me	Methyl
MeOH	Methanol
MO	Molecular Orbital
mp	Melting Point
MP2	Møller–Plesset perturbation level 2
NFSI	N-Fluorobenzenesulfonimide
NHC	N-Heterocyclic Carbene
NMR	Nuclear Magnetic Resonance
OFBA	<i>ortho</i> -fluorobenzoic acid
PES	Potential Energy Surface
Ph	Phenyl
p-MeO-BA	<i>para</i> -Methoxybenzoic acid
PMP	<i>para</i> -Methoxyphenyl
pTS	<i>para</i> -Toluenesulfonyl
QM	Quantum Mechanics/Mechanical
QZ	Quadruple-Zeta
rt	Room Temperature

SOMO	Singly Occupied Molecular Orbital
TBAF	Tetra-n-butylammonium fluoride
tBu	tertiary-Butyl
TES	Triethylsilyl
Tf ₂ O	Trifluoromethanesulfonic anhydride
THF	Tetrahydrofuran
TMS	Trimethylsilyl
TS	Transition State
TZ	Triple-Zeta
UV	Ultraviolet
UV-Vis	Ultraviolet Visible

List of Published Work

1. Dourado, J.; Singh, S.; Davis, R. L. Exploring the Role of Aminocatalysis in the Dearomatization and Regioselectivity of Heteroaromatic Aldehydes. *Journal of Organic Chemistry* **2021**, 86 (17), 11673–11682.

The work presented in the journal article is a co-first author paper by J. Dourado and S. Singh. Both authors contributed equally to the project and the manuscript. This publication is included in the dissertation as Chapter 3.

2. Wang, B.; Constantin, M. G.; Singh, S.; Zhou, Y.; Davis, R. L.; West, F. G. Generation and Trapping of Electron-Deficient 1,2-Cyclohexadienes. Unexpected Hetero-Diels-Alder Reactivity. *Organic and Biomolecular Chemistry* **2021**, 19 (2), 399–405

This work was done in collaboration with West group in University of Alberta. The experimental work was performed by West group, and I performed the computational investigation. Parts of the experimental data are presented for context in this dissertation in Chapter 5

Chapter 1 : Introduction

1.1: Computational Chemistry

Over the past decades, computational chemistry has emerged as a powerful aid for experimental chemists. The significant advances in the development of hardware with the associated software have resulted in immense progress in accuracy and speed of computational methods. The advancement in software packages such as Gaussian have allowed computational chemistry to be applied without a deep understanding of its theoretical aspects. Now, computational chemistry is routinely used by experimental chemists to explain chemical phenomena that are not well understood. One of the main goals of computational chemistry is to generate robust models of chemical systems that may have some predictive ability. The accuracy of experimental investigations of chemical systems are limited by the resolution of probe being employed, whereas computational investigations of chemical systems are performed by creating models which are limited only by the accuracy of approximations used in the quantum mechanical methods. The significant improvements of computational methods have made it possible to not only explain difficult chemical phenomena but also the ability to make predictions.¹⁻⁴

For an organic chemist, computational chemistry has become crucial to investigate reaction mechanisms which can lead to development of novel reactions and prevent side products. One of the most attractive characteristics is that computational chemistry allows the exploration of various aspects of a potential energy surface (PES) and study systems that are difficult to observe experimentally such as transition state structures and short-lived intermediates. The examination of PES provides crucial information such as geometric, thermal, and electronic properties of the molecular structures of local minima and transition states.⁵ Such properties are used to generate the energy profiles of chemical reactions, examine dipole moments, electronic charge distribution,

orbital composition, vibrational frequencies, and predict molecular spectra of novel asymmetric remote functionalization reactions.⁶

1.1.1: Computational methods^{2,4,7}

In this thesis, the computational models are derived from quantum mechanical (QM) methods. There are various quantum mechanical methods that have been developed and are employed by chemists to perform computations regarding structural and electronic features of molecules. The resulting answers, depending on the method, range from approximate to extremely accurate. The basis of quantum mechanical methods is the Schrödinger equation (eq 1):

$$\hat{H}\Psi = E\Psi \quad (1)$$

Where $\hat{H}$ is the Hamiltonian operator, Ψ is the wavefunction consisting of complete mathematical description of the system and E is the scalar quantity corresponding to the total energy of the Ψ obtained as an eigenvalue. The resultant eigenfunction Ψ is the wavefunction which contains all the essential information of an atom or molecule such as the spatial coordinates of the electrons and nuclei. The Hamiltonian accounts for the total energy of a molecule by potential and kinetic energy contributions: the kinetic energy of the electrons and nuclei, and the potential energy due to the attractive and repulsive interactions between electrons and nuclei. However, the exact solutions of the Schrödinger equation are limited for one electron systems such as the hydrogen atom or one-electron ions. In order to solve the equation for many-electron system, approximations must be used.

1.1.2: Born-Oppenheimer Approximation

One of the first approximations is the Born-Oppenheimer approximation⁸ which simplifies the Schrödinger equation by separating into one part that depicts the electronic structure around fixed nuclei and another describing the nuclei motion. This approximation allows the wavefunction to be only a function of electron coordinates while the solution depends on nuclear coordinate parameters. Thus, by solving the Schrödinger equation with Born-Oppenheimer approximation, the electronic energies for various positions of the nuclei can be calculated to result in potential energy surface which can be utilized further to elucidate structural and electronic properties.⁷

The Schrödinger equation is simplified by the Born-Oppenheimer approximation, however the exact solution only exists for one-electron molecules (rather than one-electron atoms). Therefore, an approximate solution is found by utilizing the variational principle. It states that the energy of a wavefunction generated as a linear combination of orthonormal functions is greater than or equal to the lowest energy of the system i.e., the energy of any approximate trial wavefunction is higher than the energy of the exact wavefunction. The computational methods used to find an approximate solution for Schrödinger equation employ the variational principle.

1.1.3: Density Functional Theory^{4,7}

The use of a specific method depends largely on the complexity of the system and computational cost. When starting a computational investigation, a balance between speed and accuracy is determined. The computational work presented in this thesis utilizes Density Functional Theory (DFT) which has gained significant popularity amongst the experimental chemists. Initially developed by Hohenburg, Kohn and Sham in 1960s, this method determines the energy of a molecule from the electron density function (electron distribution) instead of relying

on the correct wavefunction. By utilizing variational principle, Hohenburg, Kohn, and Sham determined that the energy functional adopts its minimum value, the ground state electron density which fully specifies all molecular properties such as the electronic energy and molecular potential energy surface.

Density functional theory is an exact theory meaning that no approximations can be made in order to solve for the electron density. However, the exact electron density functional is unknown because the theory includes an exchange-correlation functional term, which is unknown. Therefore, applying the density functional theory is accompanied by an estimate of the exchange-correlation functional term which results in a range of density functionals each with their own advantages and disadvantages offering a combination of accuracy and computational cost. Since there are various different functionals, choosing a functional relies on literature precedent for certain class of molecules, benchmarking with available experimental data, speed, and computational cost. However, it is important to be consistent with the functional throughout the investigation because results using the B3LYP functional cannot be directly compared M06-2X functional.

The density functionals employed for most of the calculations in this thesis are Becke, three-parameter, Lee-Yang-Parr (B3LYP) and Minnesota 2006 (M06) hybrid functionals (specifically M06-2X). These functionals are classified as hybrid functionals which incorporate a fragment of exact exchange from Hartree-Fock (HF) theory with local density functional when approximating exchange-correlation energy.

The one-electron atomic orbitals in the hydrogen wavefunction are described by mathematical functions known as basis functions. A set of these basis functions is called a basis set. The accuracy of atomic orbital descriptions can be further improved by using a linear

combination of sets of basis functions. For instance, when two sets of functions to describe each atomic orbital are called double zeta (DZ) basis sets. Similarly, basis sets with three and four functions are called triple zeta (TZ) and quadruple zeta (QZ) basis sets respectively. The number of basis functions increases as the number of atoms increase, therefore, the choosing a DZ, TZ, or QZ basis set may depend on factors such as number of atoms, speed, and computational cost.

The core orbitals do not play a crucial role in formation of molecules compared to valence orbitals, hence, approximations in basis functions to represent the valence orbitals separately from the core orbitals are made. The resulting basis sets are known as split valence basis sets. The most commonly used split valence basis sets are known as Pople basis sets which use the notation of X-YZg. The number of primitive gaussian functions which describe the core atomic orbitals is represented by X, whereas Y and Z indicate that the valence orbitals are composed of two basis functions each. Some examples of these basis sets include 3-21g, 6-31g, 6-311g.

The accuracy of Pople basis sets can be adding polarization and diffuse functions. Polarization functions describe the higher angular momentum functions to improve the description of bonds since the orbitals are not purely *s* or *p* orbitals in a molecule. For example, *p* functions can be added to *s* orbitals and *d* functions can be added to *p* orbitals. Addition of polarization function to Pople basis sets is noted as a the type of functions, for example, the notation 6-31g(d) adds *d* functions on all atoms with *p* valence orbitals. Similarly, 6-31g(d,p) implies addition of *d* functions on all atoms with *p* valence orbitals and *p* functions to all atoms with *s* valence orbitals. The notation (*d*) and (*d,p*) are used interchangeably with asterisk. Hence, 6-31g(d) and 6-31g(d,p) are also denoted as 6-31g* and 6-31g**. Diffuse functions, denoted as +, are used for atoms to correctly describe when electron density is far from the nuclei such as anions or lone pairs. The + notation describes that one *s*-type and one *p*-type diffuse function is added to the standard basis set

on all non-hydrogen atoms. Hence, the double-zeta split valence basis set with polarization and diffuse basis function would be denoted as 6-31+g(d,p). The work presented in this thesis is mostly concerned with p-block of first three-rows of the periodic table, therefore, the double zeta split valence and triple split valence basis sets with polarization and diffuse basis functions were utilized. The exact functional and basis set used for calculations is described at the beginning of every chapter.

Most chemical reactions are performed in a solvent medium which needs to be taken account of when performing computational investigation. While calculations can be performed in gas phase, the solvent properties such as the dielectric constant play a crucial role in a reaction. Such properties result in interactions between the reactants and the solvent which gives rise to energy being associated with those interactions. Hence, solvation models are necessary to approximate the 'real-world' scenario. The solvation models employed in this thesis are the integral equation formalism polarizable continuum model (IEFPCM) which places the solute molecule in a cavity described by Van der Waals surface simulating a continuum medium of solvent molecules; and solvation model based on density (SMD) which is based on the electron density of the solute.

The significant development in computational methods have decreased calculation time and increased accuracy of results. This progress has proved to be notably beneficial in modelling organic reactions to investigate the reaction pathway, study the driving forces behind reactivity, and the origin of selectivity. The transition state structure of a chemical reaction cannot be directly observed with any experimental techniques, however, various possible transition state structures and their relative energies can be calculated using computational chemistry. This provides a method to compare the energies and visualize the transition state structure which gives rise to the

observed product. This allows chemists to develop methodology of novel organic reactions with a more rational approach.

1.2: Asymmetric Synthesis

1.2.1: Chirality

Stereochemistry is the study of stereoisomers, also known as spatial isomers, are type of isomers for molecules with the same connectivity that differ in spatial arrangement of atoms. The differences in spatial arrangement might seem unimportant but stereoisomers have different chemical, physical, and biological properties.⁹ The *cis* and *trans* isomers of butenedioic acid, shown in Figure 1.1, demonstrate this difference in properties. The *cis* isomer commonly known as maleic acid and *trans* isomer which is commonly known as fumaric acid not only have different melting points¹⁰ but different biological properties. Fumaric acid is an important metabolite in plants and animals¹¹, whereas, maleic acid is toxic to tissues.¹²

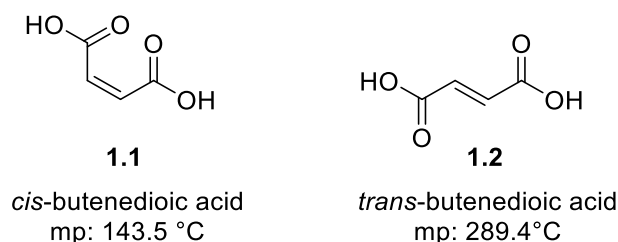
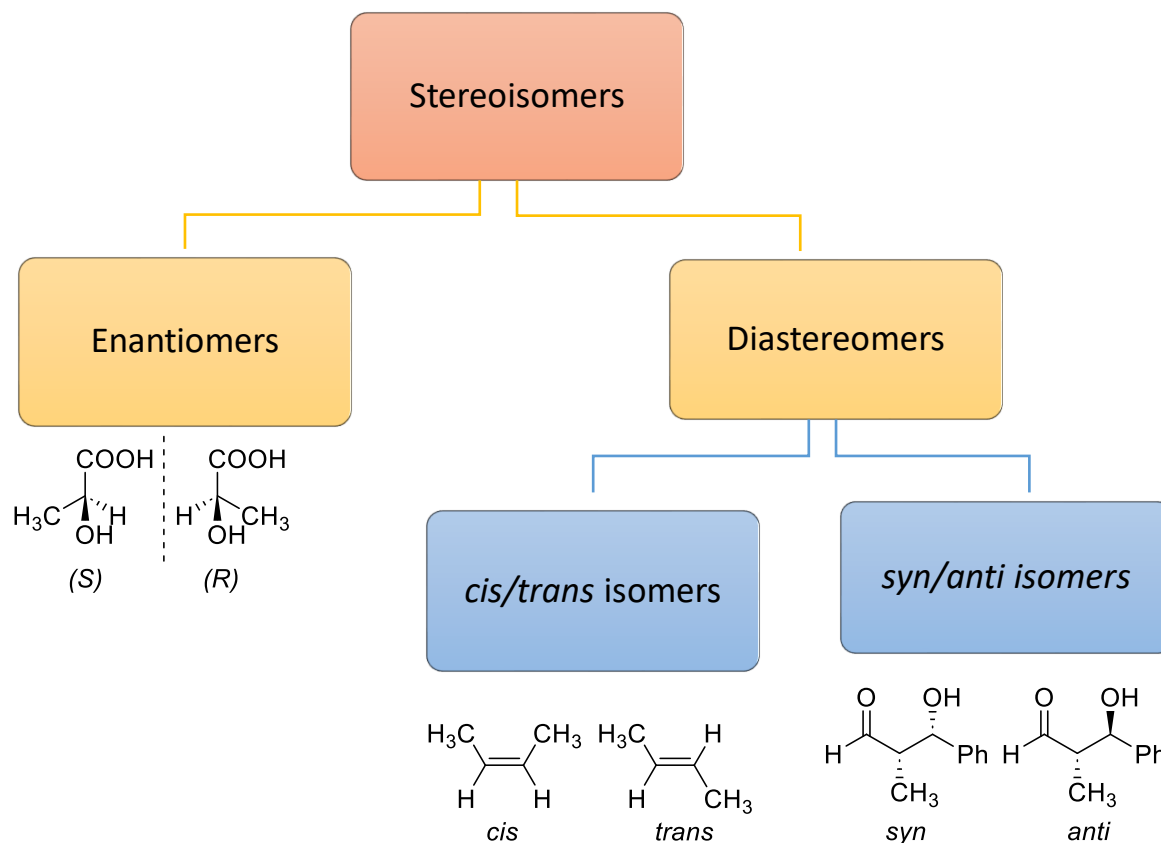


Figure 1.1: Differences in *cis* and *trans* isomers of butenedioic acid, commonly known as maleic acid (*cis*, left) and fumaric acid (*trans*, right).

There are two types of stereoisomers, enantiomers and diastereomers (Figure 1.2). When two stereoisomers are non-superimposable mirror images of each other, they are called enantiomers and the rest of stereoisomers are called diastereomers (Figure 1.2). A molecule that is non-superimposable with its mirror image is called a chiral molecule and this property is called chirality. This property results in molecules being optically active, the ability to rotate plane-

polarized light. Enantiomers, a pair of chiral molecules which differ in structure only in the left- and right-handedness of their orientation, *i.e.* non-superimposable mirror images of each other rotate the plane of polarized light in opposite directions by equal amount. Enantiomers have identical physical and chemical properties, except the ability to rotate polarized light in opposite directions. The isomer that rotates the plane to the left is called the *levo* isomer and is represented as (-), whereas the isomer that rotates the plane to the right is called the *dextro* isomer and is represented as (+). A mixture that contains equal amounts of a pair of enantiomers (50:50) is referred to as a racemic mixture. If a mixture contains higher amount of one enantiomer over another, it is referred to enantiomerically enriched. Furthermore, if only one enantiomer is present in the sample, it is called enantiomerically pure.⁹



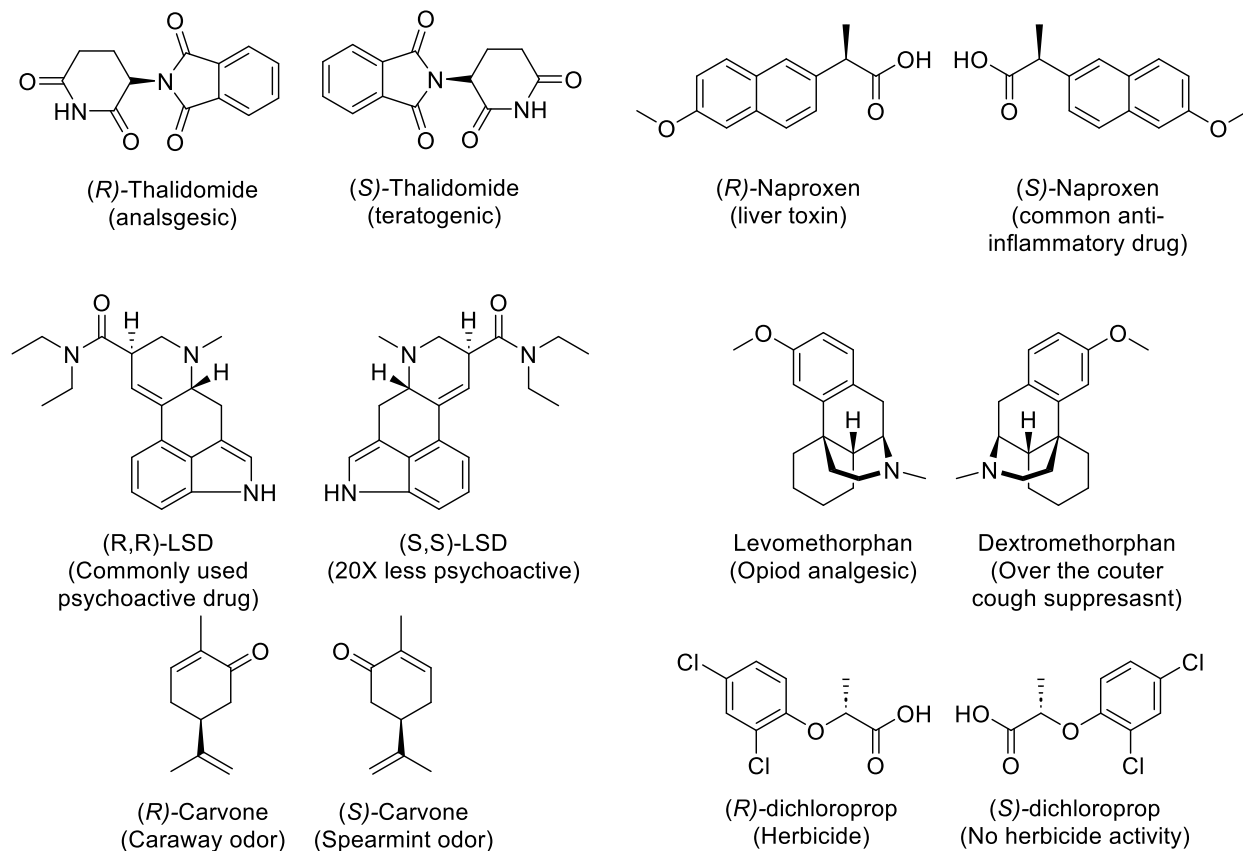


Figure 1.3: Some examples of enantiomer pairs and their bioactivity.

One of the most famous examples that demonstrated the importance of chirality is of thalidomide.^{15,16} This drug was commercialized as a racemic mixture in the 1950s and prescribes to treat morning sickness in pregnant people. It was observed that people prescribed thalidomide had newborns with severe birth defects. It was later discovered that R-enantiomer had the desirable analgesic properties whereas, the S-enantiomer has teratogenic properties. This understanding of importance of chirality led to government agencies tightening regulations around pharmaceutical drugs resulting in rigorous testing of both enantiomers. Hence, the development of methods to selectively synthesize one stereoisomer over another to result in enantiomerically pure compounds is crucial in synthetic organic chemistry.

1.3: Asymmetric synthetic methods

There have been three main strategies developed for achieving stereoselectivity in organic synthesis,¹⁷ 1) chiral auxiliaries, 2) chiral pool synthesis and 3) asymmetric catalysis. The chiral pool strategy utilizes cheap, readily available enantiomerically pure natural products to induce chirality and as the building blocks for the target molecule (Figure 1.4a).^{18–20} The chiral compounds employed are incorporated in the final product. Some examples of chiral pool are amino acids, sugars, and terpenes which naturally occur as single enantiomers. The example shown in Figure 1.4a utilizes the naturally occurring amino acid for the total synthesis of alkaloid (–)-allonorsecurinine.

Chiral auxiliaries are a class of chiral molecules that are enantiomerically pure, usually derived from chiral pool, that are attached to the pro-chiral starting material (Figure 1.4b).^{21,22} Upon completion of the reaction, the chiral auxiliary is removed resulting in enantiomerically pure compound as the final product. It is important to note that stoichiometric amount of the chiral auxiliary must be used for a reaction, however, it is possible to recover them. The final approach is asymmetric catalysis which is the main focus of work presented in this thesis. These compounds are used in sub-stoichiometric amounts to induce chirality and achieve highly stereoselective transformations.

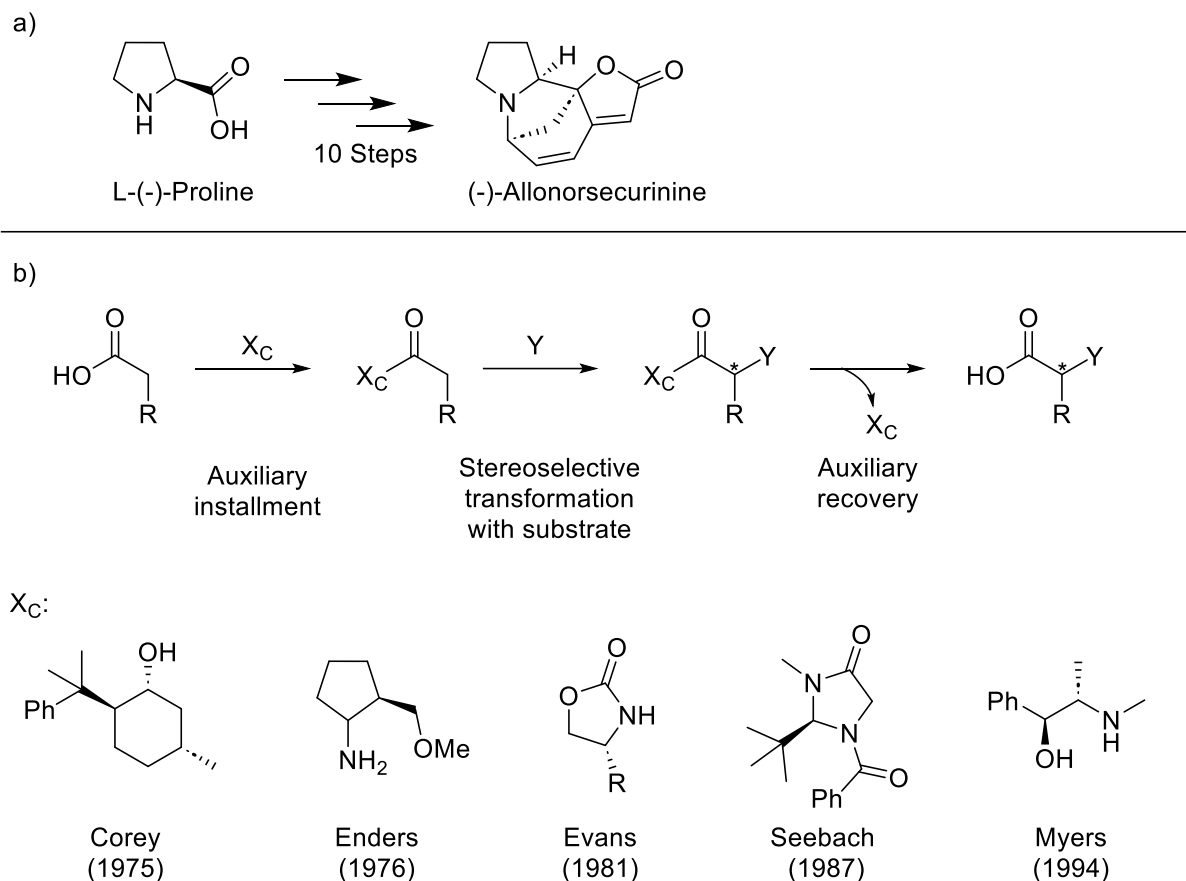


Figure 1.4: a) Total synthesis of alkaloid (-)-allonorsecurinine starting from naturally occurring L-proline amino acid. b) Synthetic strategy using chiral auxiliaries to induce asymmetry in the final product and some selected examples of chiral auxiliaries.

1.4: Asymmetric Catalysis

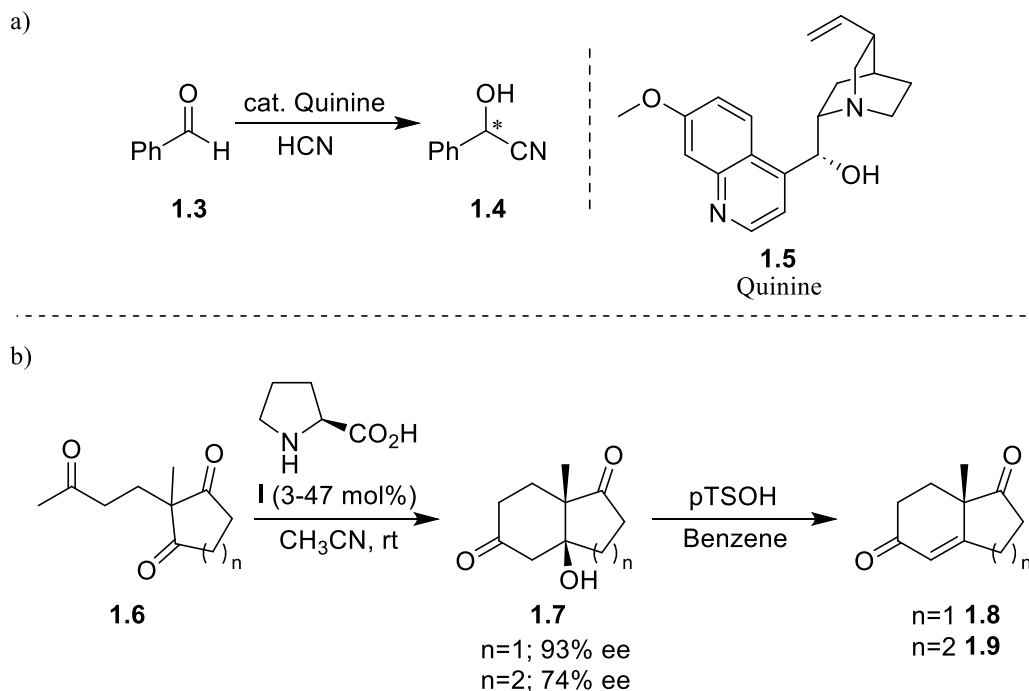
There are three classes of asymmetric catalysis,^{23–26} 1) biocatalysis, 2) metal catalysis, and 3) organocatalysis. Biocatalysis mainly utilizes enzymatic processes to perform highly regio-, chemo-, and stereoselective transformations. Since enzymes are very substrate specific, this method is limited to certain substrates and reactions.^{27,28}

Metal catalysis utilizes transition metals coordinated to chiral ligands to induce asymmetry.^{29,30} The 2001 Nobel Prize in Chemistry was awarded to Knowles, Noyori, and Sharpless who had made significant contributions to asymmetric catalysis.³¹ Transition metal

catalysis is highly effective and widely used in industrial scale synthesis due to sub-stoichiometric catalyst loading. However, the highly effectiveness of this method comes with some disadvantages such as the toxicity of metal residue leftover in pharmaceutical drugs, highly expensive equipment needed to handle the transition metal complexes sensitive to air and moisture.³²

1.5: Organocatalysis

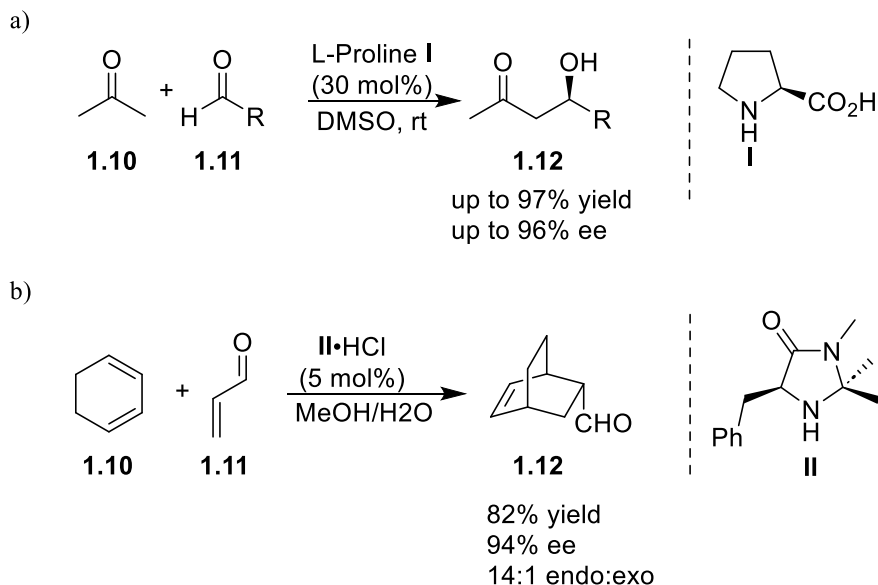
Organocatalysis, the main focus of this dissertation, has emerged as an important synthetic tool, comparable with biocatalysis and metal catalysis. This method has gained popularity because of its relatively low cost, mild reaction condition, wide scope of applicability, while resulting in highly stereoselective transformations. Organocatalysis employs small chiral organic molecules that are largely derived from naturally occurring amino acids and other natural compounds. These catalysts are also attractive because of their stability towards air and moisture making them easier to handle without utilizing any expensive equipment for inert environment.³³⁻³⁵ The impact of this field has been recognized by Royal Swedish Academy of Sciences by awarding the 2021 Nobel Prize in Chemistry to the founders of this field, Benjamin List and David MacMillan.³⁶



Scheme 1.1: Early examples of asymmetric organocatalysis. a) Hydrocyanation of benzaldehyde catalyzed by quinine. b) Hajos-Parrish-Eder-Sauer-Wiechert intramolecular aldol reaction catalyzed by L-proline.

For over a century, small organic molecules have been used as catalysts. One of the earliest examples from 1912 of an asymmetric reaction employing an organocatalyst is of hydrocyanation of benzaldehyde **1.3**, reported by Bredig and Fiske, catalyzed by alkaloids quinine and quinidine (Scheme 1.1a).³⁷ Later in the century, Hajos-Parrish-Eder-Sauer-Wiechert (HPESW) reaction, reported by two independent groups in 1970s, which is an enantioselective intramolecular aldol reaction catalyzed by L-proline **I** (Scheme 1.1b).^{38,39} This report was significant since it demonstrated the use of proline, a small chiral secondary amine, did not only catalyze the aldol reaction but also performed it stereoselectively. This report also made it possible to synthesize Wieland-Miescher ketone **1.9**, a key scaffold for total synthesis, in a stereoselective fashion.⁴⁰ Despite these initial reports, the field of organocatalysis was not explored further until 2000 when two independent works reported by List *et al.*, L-proline **I** catalyzed enantioselective aldol reaction

(Scheme 1.2a),⁴¹ and MacMillan *et al.* performed enantioselective Diel-Alder reaction catalyzed by chiral imidazolidinone **II** (Scheme 1.2b).⁴²



*Scheme 1.2: First reports of modern aminocatalysis. a) Intramolecular aldol reaction catalyzed by L-proline (**I**) reported by List and coworkers. b) Diels-Alder reaction catalyzed by chiral imidazolidinone (**II**) reported by MacMillan and coworkers.*

Since the seminal works by List and MacMillan, the field of organocatalysis grew significantly and has become one of the most powerful strategies for asymmetric synthesis in last two decades. There are four main classes of organocatalysis³⁷, 1) aminocatalysis, 2) hydrogen bond (H-bond) catalysis, 3) N-heterocyclic carbene (NHC) catalysis, and 4) asymmetric phase-transfer catalysis (APTC). This dissertation mainly focuses on aminocatalysis, thus the discussion for other types of organocatalysis is beyond the scope of work presented here.

1.5.1: Aminocatalysis

Amongst different classes of asymmetric organocatalysis, aminocatalyst is one the most widely used method. This method uses small chiral primary or secondary amines to activate carbonyl compounds. A chiral secondary amine condenses with carbonyl compounds which results

in a positively charged iminium-ion intermediate. The positive charge results in redistribution of the electron density towards the nitrogen centre which lowers the Lowest Unoccupied Molecular Orbital (LUMO) of the system making the β -carbon more electrophilic, according to the vinylogy principle. This allows nucleophilic addition at β -carbon in a stereoselective fashion (Figure 1.5, right). The LUMO-lowering strategy by aminocatalysis has become a general strategy for enantioselective β -functionalization of carbonyl compounds.^{43,44}

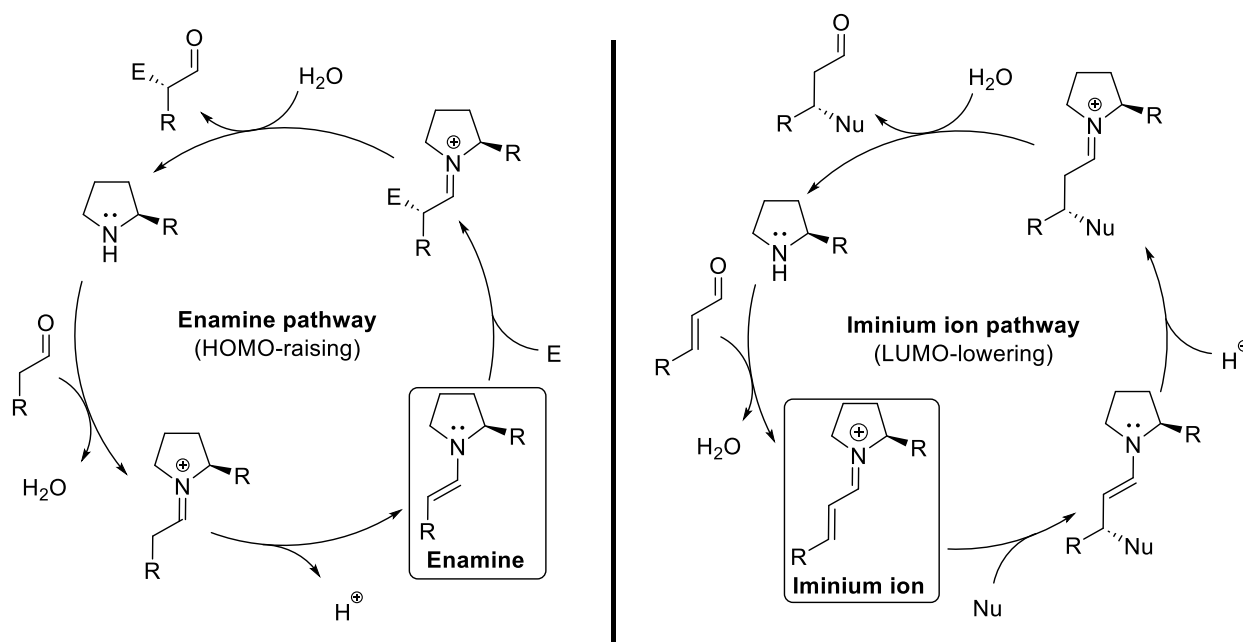


Figure 1.5: Aminocatalytic activation modes. Enamine activation pathway (left) and Iminium-ion activation pathway (right)

The lowered LUMO makes the proton at α -position more acidic making it prone to deprotonation. This results in the formation of reactive enamine intermediate which is equivalent of the nucleophilic enolate where the Highest Occupied Molecular Orbital (HOMO) energy is raised. This allows enamine intermediate to be reactive towards electrophiles and perform enantioselective α -functionalization of the carbonyl compounds (Figure 1.5, left). The HOMO-raising strategy has become a general method for enantioselective α -functionalization for

aldehydes and ketones.^{44–46} The nucleophilic enamine intermediate may also undergo one-electron oxidation, photochemically or by utilizing one-electron oxidants, to form a radical cation by Singly Occupied Molecular Orbital (SOMO) activation, however, it is not discussed in this dissertation.

The development of aminocatalytic systems has allowed for stereoselective, chemoselective, and efficient reactions to create novel molecules which has enormously expanded the chemical space. In relation to the work presented in this thesis, computational chemistry has proved to be a valuable tool for modelling catalytic processes to gain an understanding of their mechanisms. A complex catalytic mechanism contains various elementary steps, short-lived intermediates, unknown active species, and competing processes that might be similar in thermodynamics. Therefore, by gaining a deeper understanding of the catalytic cycles, the knowledge gained can ultimately aid to design novel catalysts and catalytic methods. The mechanistic investigations performed computationally have not only helped explain the experimental results but have also allowed to develop novel catalysts and new models to predict selectivity in the field of aminocatalysis.

1.5.2: Enamine Activation

The report of HPESW reaction was very significant, however, the mechanism remained debateable with a number of different mechanisms and models being proposed for the C-C bond formation. Hajos initially proposed a mechanism which suggests activation of one of the carbonyl groups as a carbinolamine intermediate, according to H_2^{18}O labelled kinetic studies (Figure 1.6).^{38,47} Later kinetic studies by Agami suggested an enamine mechanism⁴⁸ by one proline molecule with the side chain carbonyl and another proline molecule is involved in proton-transfer

(Figure 1.6).⁴⁹ This mechanism with two proline molecules was widely accepted for HPESW reaction.

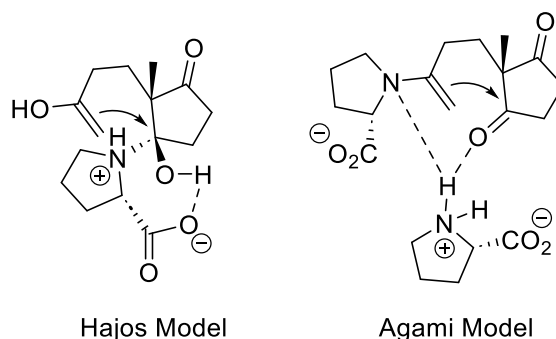


Figure 1.6: Proposed early transition state models of HPESW reaction.

In 2001, Houk led a computational investigation for intramolecular aldol reaction using diketones to understand the origin of stereoselectivity and proposed a similar mechanism as Agami, invoking an enamine intermediate, but with one molecule of proline.⁵⁰ The study performed using B3LYP/6-31g(d) level of theory determined that four transition states, two chair-like and two boat-like, were possible. The chair transition states were determined to be favourable. Further examination of transition state structure revealed that the *anti* orientation of enamine with respect to the carboxylic acid resulted in the observed stereochemistry. The *syn* and *anti* orientation of enamine with respect to the carboxylic acid provided a model to understand the preference of *anti* product. The *syn* TS leading to the major product showed preference by 1.0 kcal/mol relative to *syn* TS due to the enamine of *anti* TS being more planar. The intramolecular hydrogen bond in *syn* TS distorts the pyrrolidine ring. After applying the same model for HPESW reaction, the *anti* TS showed preference by 3.4 kcal/mol relative to *syn* TS. In another investigation by Houk and Hanessian in 2004, the *anti* TS showed preference of 2.2 kcal/mol relative to *anti* TS at B3LYP/6-311+G(2df,p) level of theory which was consistent with experimental *anti-syn* TS difference of 2.1 kcal/mol.⁵¹

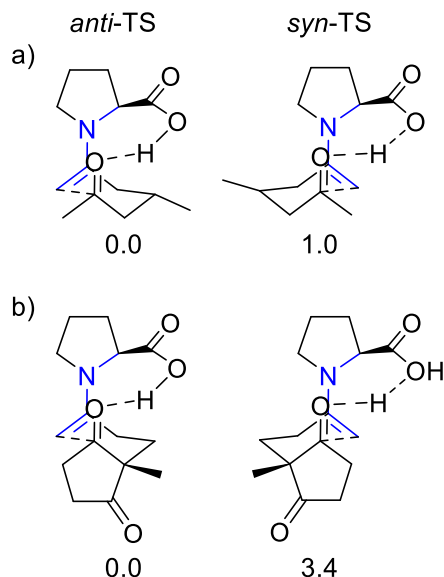


Figure 1.7: Illustration of proposed model for proline catalyzed intramolecular aldol reaction by Houk. Energies are in kcal/mol

The computational study of proline catalyzed intramolecular aldol reaction led to further investigation of HPESW reaction. This kinetic and computational study provided more evidence of only one proline molecule being utilized to catalyze the aldol reaction.⁵² The DFT study was performed with B3LYP/6-31g(d) level of theory. It was proposed that the proline acts as a bifunctional catalyst. The nucleophilic pyrrolidine portion condenses with the carbonyl moiety of the substrate and after subsequent deprotonation of the α -proton the reactive enamine intermediate is formed. The carboxylic acid part of the proline induced enamine intermediate acts to direct the electrophilic carbonyl carbon to the enamine *via* hydrogen bonding. The hydrogen bond pre-configures the side chain enamine and cyclic ketone in a highly ordered transition state. This highly ordered transition state was calculated to be more thermodynamically preferred than other transition states from previous models. Further examination of the transition state suggested that the approach from *re* face of the enamine had a stabilizing CH-O interaction resulting in the observed selectivity.

Since the HPSEW reaction, the first proline catalyzed aldol reaction reported by List and coworkers is one of the most well-studied reactions in aminocatalysis. The authors initially proposed the observed stereoselectivity by invoking Zimmerman-Traxler type transition state. However, Houk and List performed an extensive computational investigation using B3LYP/6-31g(d)//CPCM(DMSO) to gain insights about the observed stereoselectivity.⁵³ Unlike the HPSEW reaction, the electrophile for an intermolecular reaction can approach at different dihedral angle with respect to the enamine pi-bond. The examination of the transition states showed that the transition state with dihedral angle of $+60^\circ$ (carbonyl group and C=C bond enamine) was the preferred approach of the electrophile (Figure 1.8a). This preference is due to stabilization due to the increased hydrogen bonding interaction between carboxylic acid of the proline and electrophile resulting in the observed facial selectivity. This study led to one of the most generally applied stereochemical models, the Houk-List model (Figure 1.8b),⁵⁴ for predicting stereoselectivity of proline catalyzed reactions, with X=Y electrophiles, such as Mannich reaction,⁵⁵ aminoxylation,⁵⁶ α -amination,⁵⁷ and Michael addition.⁵⁸

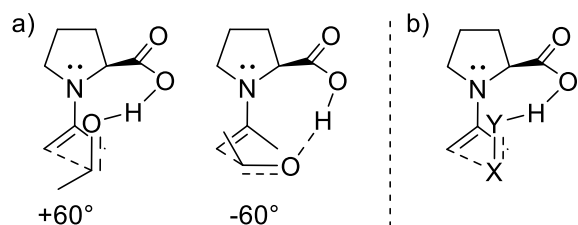


Figure 1.8: a) Transition states for proline catalyzed intermolecular reaction b) Houk-List model

Following the development of Houk-List model, computational studies were then also used to design new catalysts to achieve desired stereoselectivity. One of the earliest examples of this is a collaborative report by Houk (computational) and Barbas (experimental) groups to develop stereoselective Mannich reaction with *anti*-diastereoselectivity.⁵⁹ The proline catalyzed Mannich

reactions result in *syn*-diastereoselectivity (Scheme 1.3). The computational studies were performed with HF/6-31g(d) level of theory. By calculating the transition states of proline catalyzed Mannich reactions, the authors determined that the *s-trans* conformation of (*E*)-enamine results in *syn*-diastereoselectivity. The *s-trans* conformation dominates due to the steric interaction between the enamine and the carboxylic acid substituent of proline. Therefore, it was determined that the selectivity for *anti*-product is a result of a nucleophilic attack of *s-cis* conformation of the enamine intermediate (Figure 1.9). Hence, in order to shift the equilibrium, it was determined that a catalyst with substituents at 3- and 5-position of the pyrrolidine ring would be adequate. The methyl substituent at 5-position was deemed to sterically fix the conformation of enamine to *s-cis* and the carboxylic acid substituent at 3-position controlled the facial selectivity. The substituents at 3- and 5-positions were required to be in *trans* configuration in order to avoid steric interactions between the electrophile and the methyl substituent at 5-position. Computationally, the catalyst **III** was predicted to result in 95:5 *anti:syn* diastereomeric ratio (dr) and 98% enantiomeric excess (ee). These computational predictions were then experimentally verified which were consistent. Experimentally, the Mannich reaction with new catalyst resulted in 94:6 *anti:syn* dr and 99% ee (Scheme 1.3).

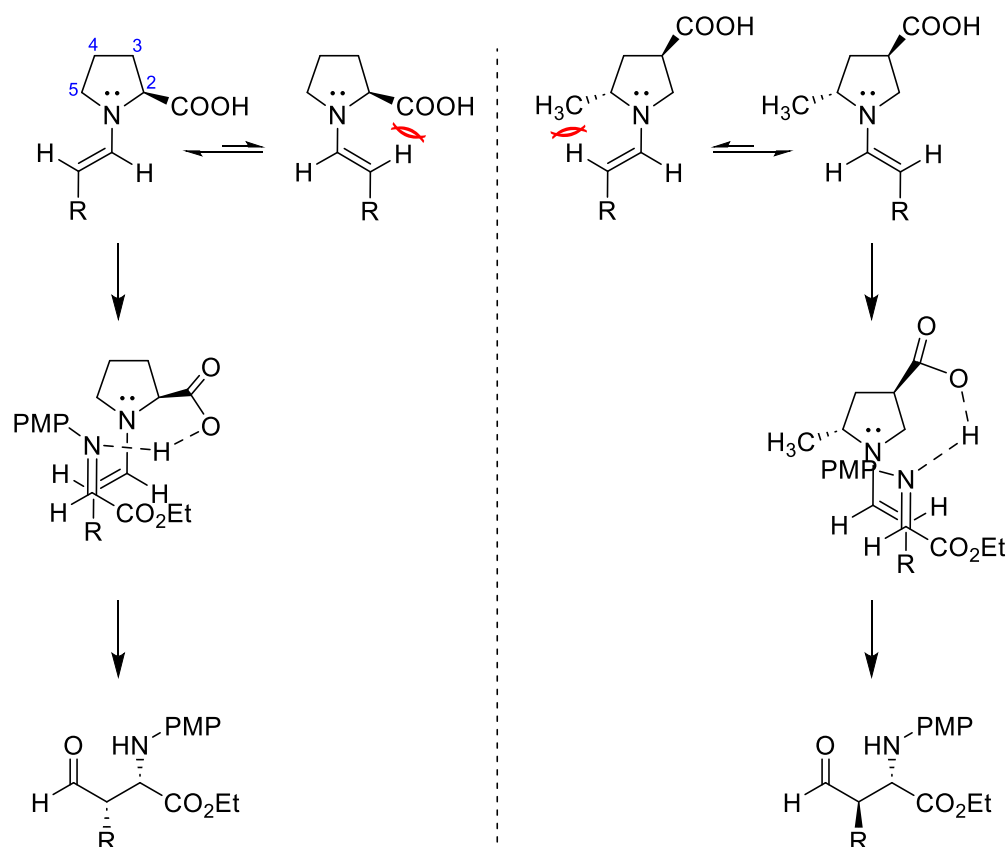
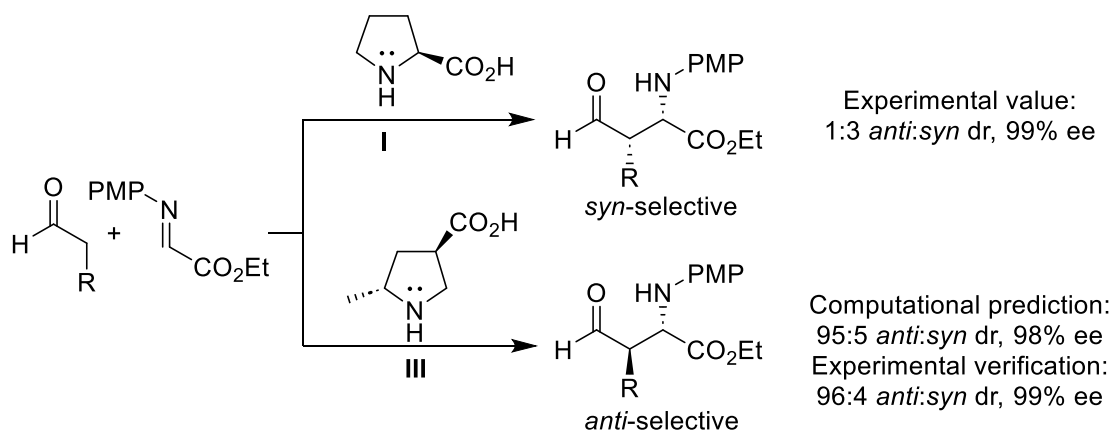


Figure 1.9: Transition states for proline **I** catalyzed *syn*-selective Mannich reaction and computationally designed catalyst **III** for *anti* selective mannich reactions.



Scheme 1.3: Comparison of proline **I** catalyzed and computationally designed catalyst **III** for Mannich reaction.

The asymmetry in aminocatalytic reactions is induced using two different approaches, 1) hydrogen-bond (H-bond) directed approach, and 2) steric-bias approach (Figure 1.10). The chiral

aminocatalysts possess substituents which direct the approach of substrates towards the reactive intermediates. If the catalyst contains an H-bond donor, as is the case for L-proline, the H-bonding interaction will direct the electrophile from the same face as the H-bond moiety preferentially. Due to its H-bonding abilities, L-proline has been extensively exploited for stereoselective functionalization of carbonyl compounds. Furthermore, this has led to the design and development of proline derived H-bonding bifunctional catalysts with thiourea, and squareamide moieties.

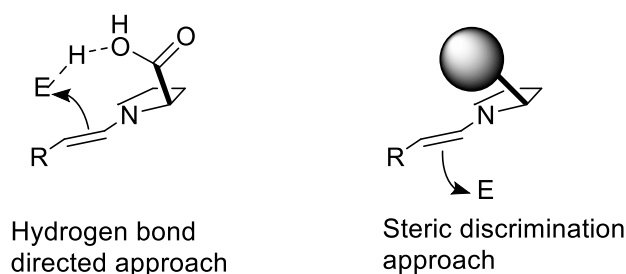
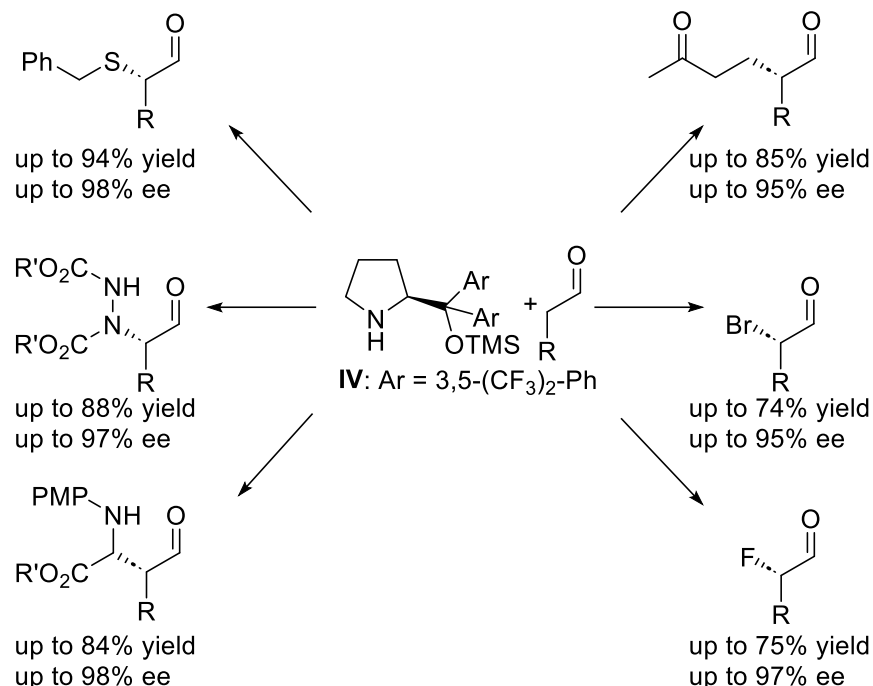


Figure 1.10: The two general models to induce chirality and predict stereoselectivity in Aminocatalysis: Hydrogen bond directed approach (left) and Steric shielding approach (right).

The steric-bias approach which is more widely used in aminocatalysts utilizes steric hinderance of a bulky group to direct the approach of substrates to the reactive intermediates. This approach to induce chirality has led to various other imidazolidnone aminocatalysts by MacMillan^{42,60,61} and diarylprolinol silyl ether aminocatalysts^{62–64} by Hayashi and Jørgensen which are two of the most utilized and studied aminocatalysts. An example of a scope of various types of enamine mediated α -functionalizations of carbonyl compounds is shown in Scheme 1.4, reported by Jørgensen, showcasing the robustness and generalization of the aminocatalyst.⁶⁵



Scheme 1.4: Aminocatalytic enantioselective α -functionalization of aldehydes via enamine activation reported by Jørgensen.

Following the development of enamine mediated reactions using the diarylprolinol-silyl ether catalyst, computational investigations were performed to understand the origin of stereoselectivity.⁶⁶ A DFT study of possible enamine intermediates for α -fluorination was performed using B3LYP/6-31g(d) level of theory. It was determined that out of four possible enamine configurations, the two *E*-enamine intermediates were energetically favoured and were similar in energy. While examining the α -fluorination reaction performed with *N*-fluorobenzenesulfonimide (NFSI) revealed that in addition to the steric shielding by catalyst, the configuration of enamine intermediate was a crucial factor. The study revealed that *E-s-trans* conformation resulted in a transition state which was favoured over transition state resulting from *E-s-cis* conformation by 2.4 kcal/mol (Figure 1.11). This difference in two transition state structure was a result of unfavourable steric interactions between the bulky *tert*-butyl group of enamine and the diaryl catalyst bulk and between the aryl ring of the NFSI.

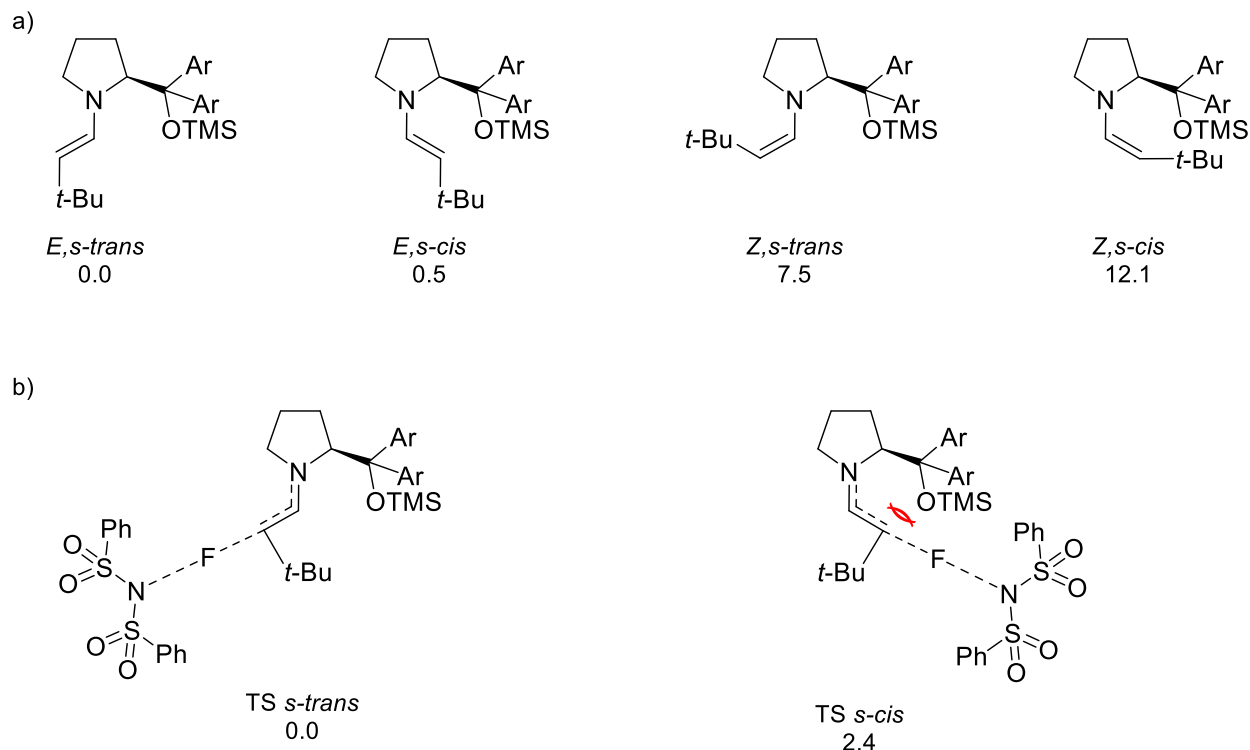


Figure 1.11: Relative free energies of enamine intermediates with Diarylprolinol silyl ether catalyst **IV** and b) Depiction of transition state structures for α -fluorination. Energies are in kcal/mol.

1.5.3: Dienamine activation

The diarylprolinol silyl ether aminocatalysts allowed to expand the scope of organocatalysis by extending enamine activation. The vinylogy principle reported in 1934, states the propagation of electronic effects through a conjugated π -system.⁶⁷ Therefore, by utilizing poly-unsaturated carbonyl compounds, the enamine activation mode has been extended to poly-enamine activation allowing for stereoselective functionalization at more distal positions of the carbonyl compound (Figure 1.12). This has allowed the development of remote functionalization methods with a range of substrates.^{68–70}

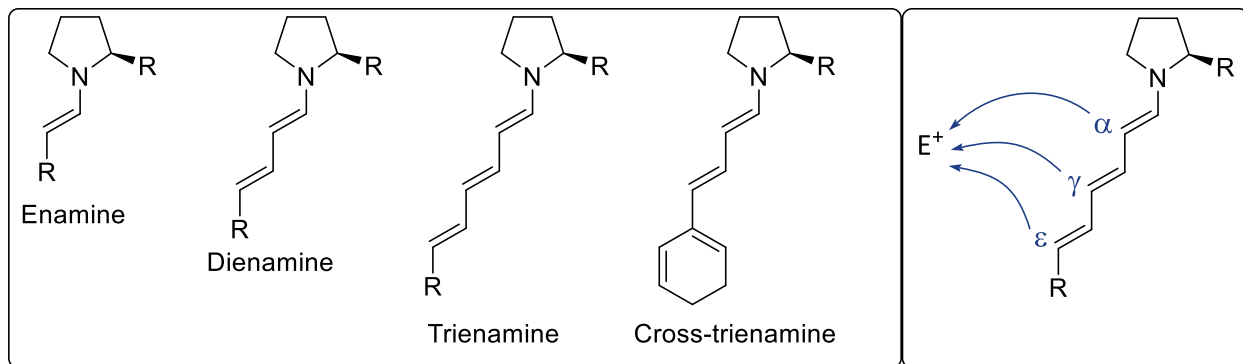
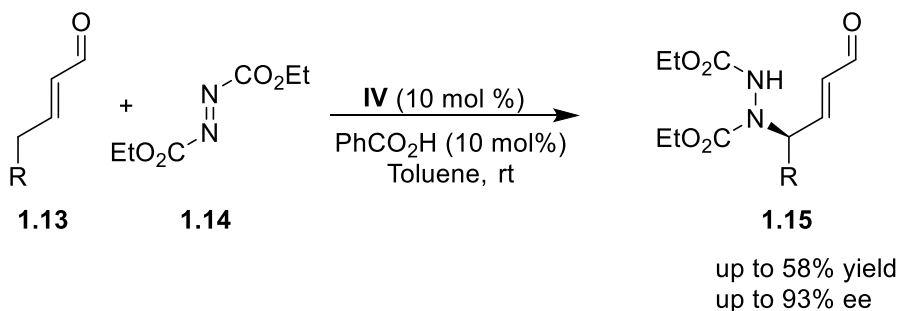


Figure 1.12: Vinylogous aminocatalytic activation modes (left). Reactivity of vinylogous aminocatalytic activation modes (right)

By using an aminocatalyst with α,β -unsaturated carbonyl compounds, dienamine activation can be achieved.⁷¹ The first example of dienamine mediated reaction was reported by Jørgensen in 2006.⁷² This work was extremely significant in the field of aminocatalysis since it demonstrated induction of chirality at a remote position. The authors reported an enantioselective γ -amination of α,β -unsaturated aldehydes **1.13** with diethyl azodicarboxylate (DEAD) **1.14** by utilizing diarylprolinol silyl ether catalyst **IV** (Scheme 1.5).



Scheme 1.5: Dienamine mediated enantioselective γ -amination of enals **1.13** catalyzed by **IV**, reported by Jørgensen.

Interestingly, the observed stereochemistry of the product was opposite of expected stereochemistry. A DFT investigation performed with B3LYP/6-31g(d)/CPCM(toluene)//B3LYP/6-31g(d) level of theory determined that *E,s-trans* conformation of dienamines were energetically favoured than *E,s-cis* dienamines with *E,s-trans,E* being

favoured by 1.4 kcal/mol relative to *E,s-trans,Z* (Figure 1.13). The barrier of addition of DEAD for *E,s-trans,Z* dienamine, resulting in *S*-enantiomer was calculated to be 13.0 kcal/mol while the barrier was 15.7 kcal/mol for *E,s-trans,Z* dienamine. The higher energy *E-s-cis* dienamines are electron-rich dienes and are arranged to take part in [4+2] cycloaddition with DEAD **1.14**. The [4+2] cycloaddition transition state energy for *E,s-cis,Z* dienamine and DEAD **1.14** was calculated to be 12.3 kcal/mol, resulting in *S*-enantiomer upon hydrolysis of cycloadduct. The cycloaddition barrier was only 6.7 kcal/mol for *E,s-cis,E* dienamine, resulting in *R*-enantiomer upon hydrolysis of cycloadduct. The cycloadducts were also found to be thermodynamically favoured significantly when compared to iminium ion intermediates resulting from mono-addition of DEAD **1.14**. Therefore, the authors concluded that the γ -amination proceeds *via* [4+2] cycloaddition between *E,s-cis,E* dienamine and DEAD **1.14**, resulting in the observed *R*-enantiomer upon hydrolysis of the cycloadduct. This computational investigation explained the observed enantioselectivity, however, it does not rationalize the observed *E*-configuration of the α,β -double bond. The [4+2] cycloaddition reaction pathway result in intermediates with *Z*-double bond. The work presented in chapter 2 of this dissertation is related to a detailed mechanistic study to answer this anomaly by utilizing experimental and computational methods.

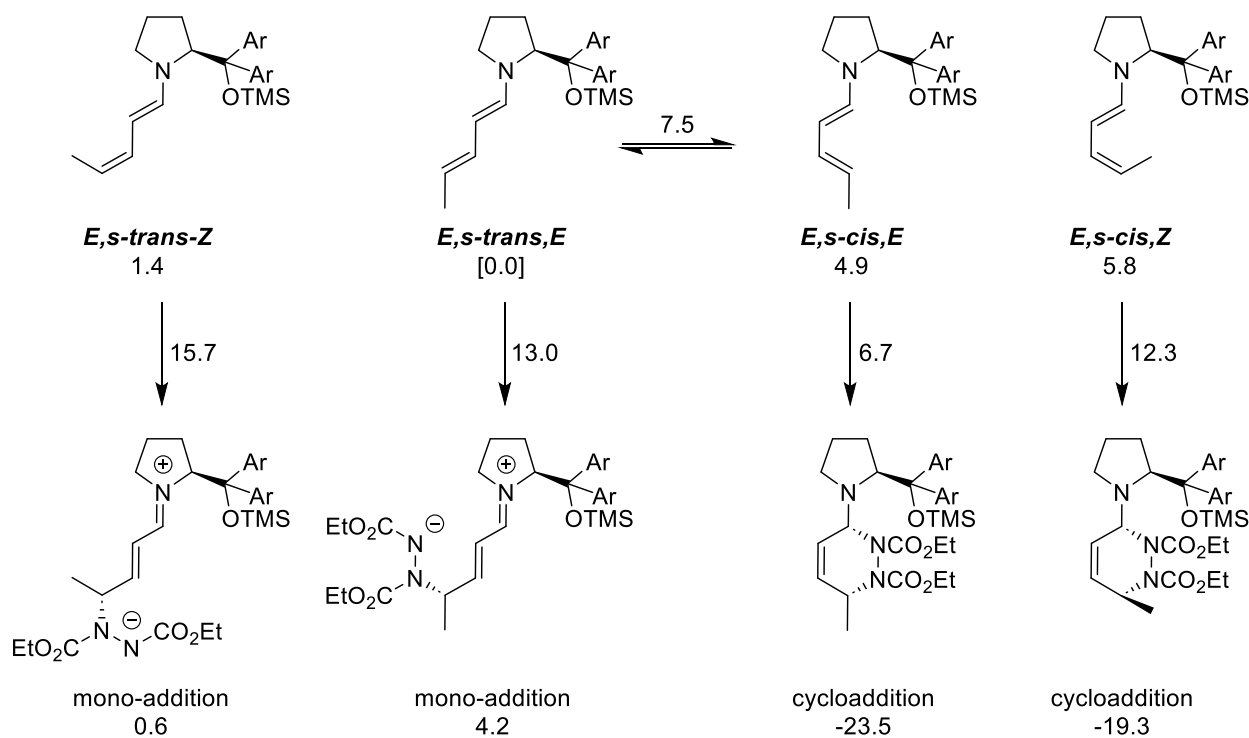
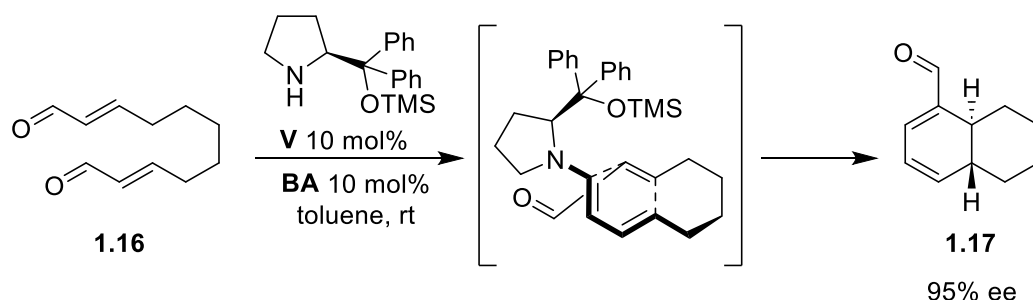


Figure 1.13: Relative energies of dienamine intermediates and their barriers for reactions with DEAD **1.14**. Energies are in kcal/mol.

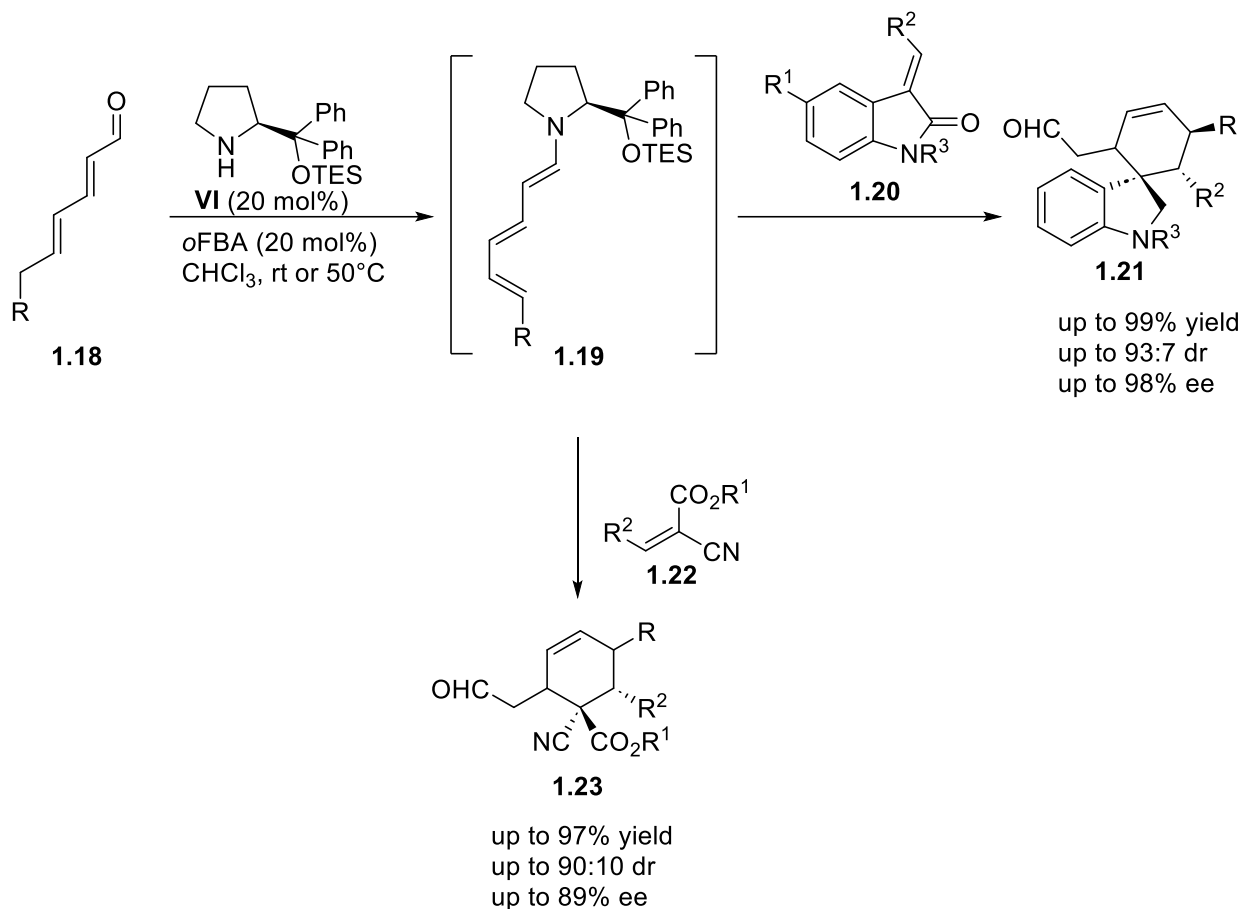
Using the electron rich nature of dienamine, Christmann reported dienamine mediated intramolecular Diels-Alder of α,β -unsaturated carbonyl compounds **1.16** to make bicyclic compounds **1.17** with great enantioselectivity (Scheme 1.6).⁷³ This report was investigated using DFT methods by Gil Santos in 2012 to determine the origin of selectivity.⁷⁴ It was found that the enantioselectivity was dictated by the combination of *E,s-cis-E* conformation of the dienamine and steric bulk of the catalyst during the cyclization step. The experimental report by Christmann and computational work by Santos helped expand the use of electron rich dienamine for Diels-Alder type reactions.



Scheme 1.6: Dienamine mediated intramolecular [4+2] cycloaddition catalyzed by V

1.5.4: Trienamine and Polynemamine activation

The enamine and dienamine activation have been further extended to trienamine by using poly-unsaturated carbonyl compounds. The first example of trienamine activation was reported by Jørgensen and Chen in 2011.⁷⁵ They reported Diels-Alder reactions between 2,4-dienals **1.18** with 3-olefinic oxindoles **1.20** and cyanoacetates **1.22** with excellent selectivity, driven by diarylprolinol silyl ether (Scheme 1.7). This report was significant as it demonstrated the ability to induce enantioselectivity in more distal positions. By using B3LYP/6-31G(d) level of theory, authors studied the observed β,ϵ -reactivity. The linear all-*trans* trienamine conformer **1.25** was determined to be the lowest in energy (Figure 1.14). The authors determined that barrier for rotation of α - β bond of all-*trans* trienamine to result in **1.26** was 1.8 kcal/mol higher than the barrier for rotation of γ - δ bond to result in **1.24**. Furthermore, the HOMO of **1.24** is located higher in 2.17 eV energy than the corresponding HOMO of **1.26**, set up to favourably interact with LUMO of dienophile. The difference in HOMO energy level combined with low rotational barrier around γ - δ bond explained the observed β,ϵ -reactivity. This initial report demonstrated the ability of aminocatalyst to induce chirality at a distal position. Following the initial report of trienamine activation, there have been various reports^{76,77} utilizing linear trienamine intermediate along with cross-trienamines⁷⁸ and tetraenamines.⁷⁹



Scheme 1.7: Trienamine mediated enantioselective Diels-Alder reactions of 2,4-Dienals **1.18** with olefinic oxindoles **1.20** and cyanoacetates **1.22**, reported by Jørgensen and Chen.

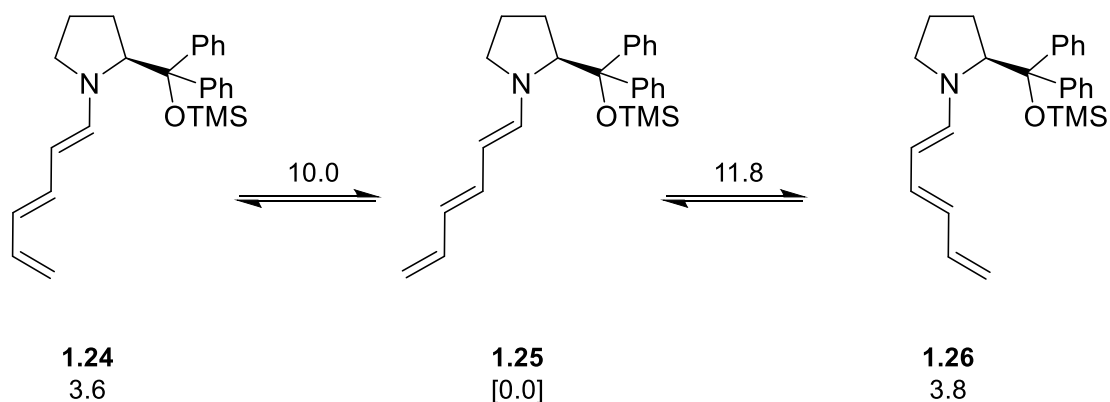
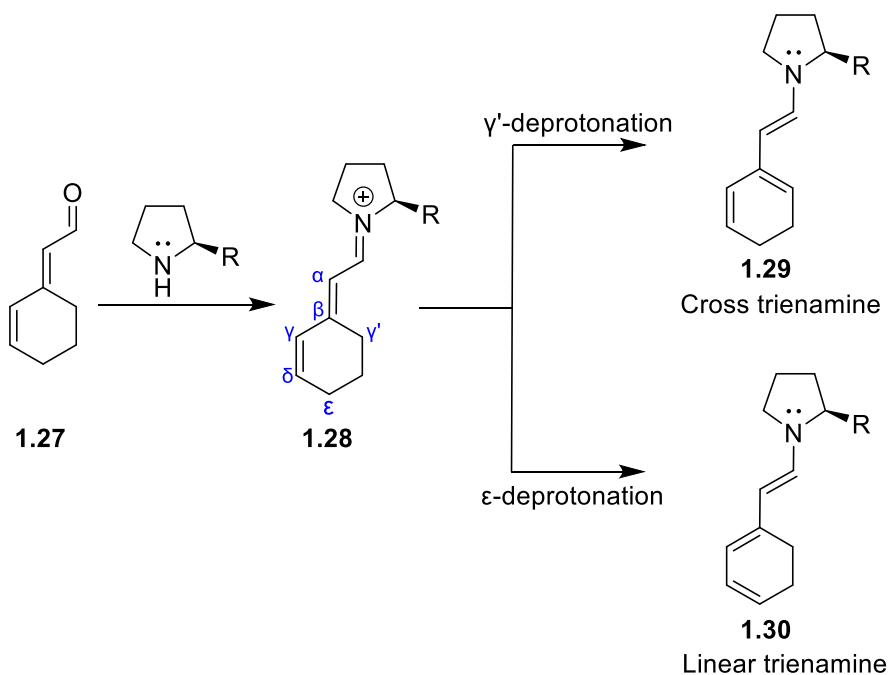


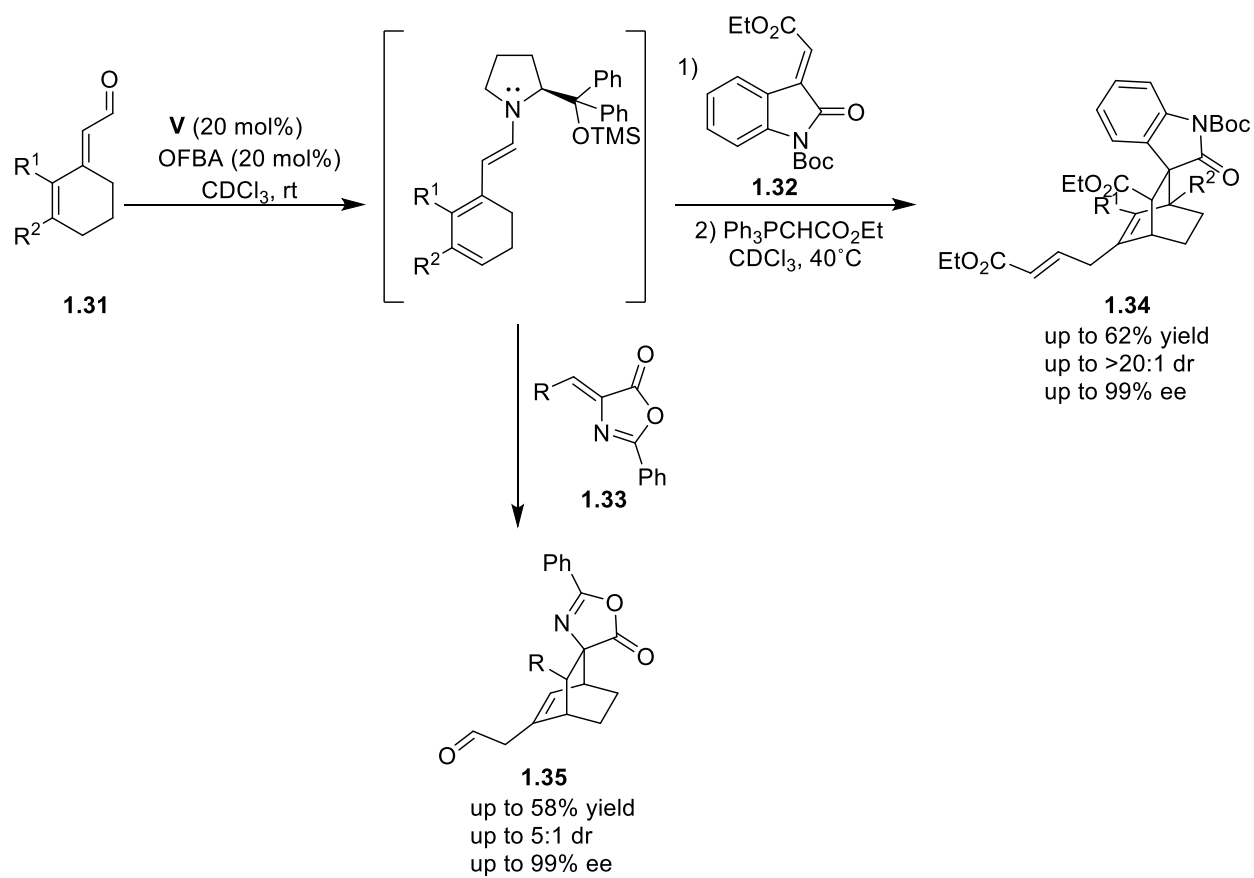
Figure 1.14: Calculated conformations of trienamine and their rotational barriers. Energies are in kcal/mol.

The first example of utilizing the cross-trienamine intermediate was reported by Jorgenson. When an aminocatalyst condenses with cyclic 2,4-dienals **1.27**, the resulting intermediate can be either a cross-trienamine **1.29** or linear-trienamine **1.30** (Scheme 1.8).



Scheme 1.8: Cross-trienamine activation mode in aminocatalysis promoted by γ' -deprotonation.

By exploiting this feature, Jørgensen demonstrated a [4+2] cycloaddition reaction between cyclic 2,4-dienals and olefinic oxindoles or azalactones to result in complex polycyclic compounds.⁷⁸ Interestingly, the computational investigation suggests that linear trienamine intermediate **1.36** is thermodynamically favoured by 4.2 kcal/mol relative to the cross trienamine **1.38** which was also confirmed by NMR studies. The study further determined that the thermodynamic preference of [4+2] cycloadduct **1.41** utilizing cross-trienamine intermediate was determined to be favoured by 8.8 kcal/mol relative to the cycloadduct **1.39** *via* linear trienamine intermediate (Figure 1.15). This thermodynamic preference was found to be a result of formation of a conjugated π -system which is not formed for cycloadduct with linear trienamine suggesting that the reaction is thermodynamically driven.



Scheme 1.9: Cross-trienamine mediated enantioselective Diels-Alder reactions reported by Jørgensen.

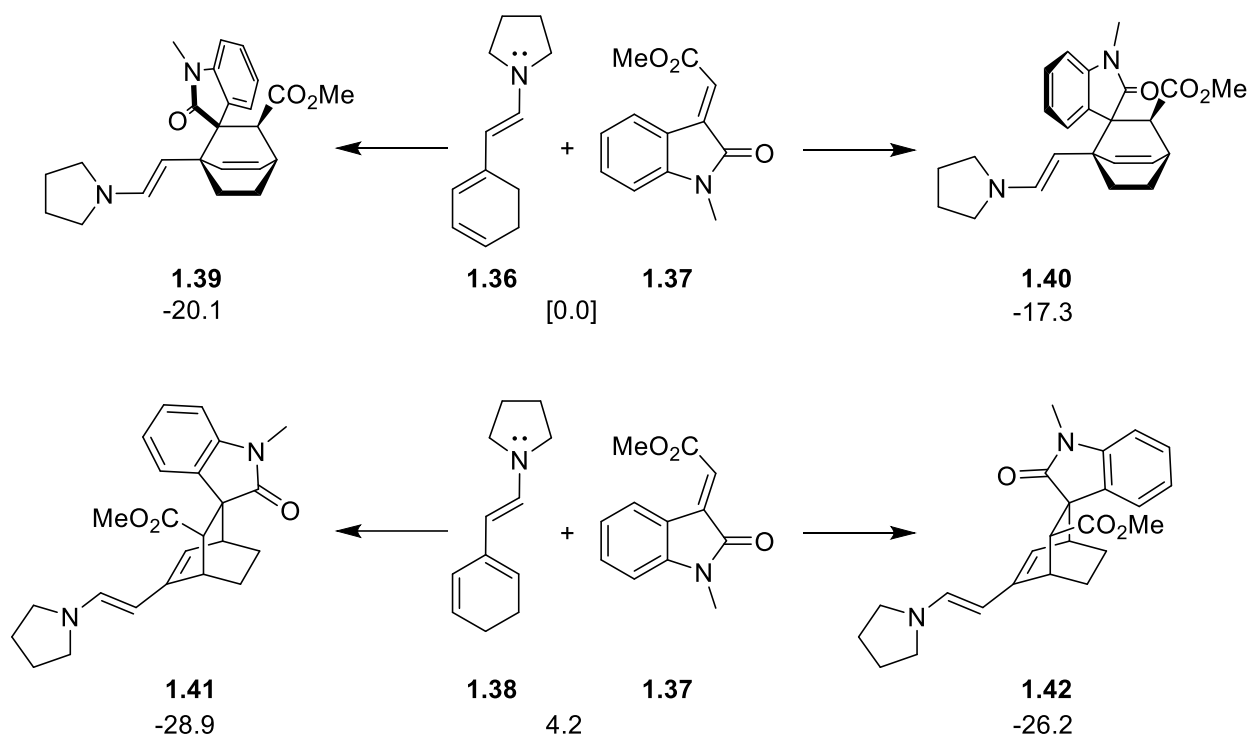


Figure 1.15: Pathway comparison of Diels-Alder reaction between cyclic linear trienamine and olefinic oxindole (top), and cross-trienamine and olefinic oxindole (bottom). Energies are in kcal/mol.

By using cyclic substrates with extended conjugation, resulting in extended enamine, aminocatalysis has allowed the development of enantioselective higher-order cycloadditions beyond [4+2] cycloadditions resulting in complex polycyclic compounds. In 2018, Jørgensen reported highly stereoselective [8+2] cycloadditions between indene-2-carbaldehydes **1.43** and nitroolefins **1.45** using a C_2 -symmetric aminocatalyst **VII**.⁸⁰ The condensation of catalyst with indene-2-carbaldehydes allowed the first report of catalytic formation of electron rich amino isobenzofulvene intermediate **1.44** (Figure 1.16). The authors performed a DFT study using ω B97XD/6-31+g(d,p)//SMD(chloroform) level of theory to understand the origin of stereoselectivity. It was determined that the reaction proceeds *via* stepwise pathway and the barriers were determined to be 13.7 kcal/mol and 10.1 kcal/mol for **TS1** and **TS2**, respectively. The authors also concluded that transition states for concerted cycloaddition pathways were not

located, however, a zwitterionic intermediate **1.46** resulting from Michael addition of the amino isobenzofulvene to the nitroolefin was found for various stereochemical approaches. It was also determined that the observed stereoselectivity was dictated by (i) the kinetics of the initial Michael addition step and (ii) the electrostatic interactions between nitro group of nitroolefin and *ipso* carbon of amino isobenzofulvene intermediate. The electrostatic interactions between the oxygen atom of the nitro group and *ipso* carbon of amino isobenzofulvene following the first addition step suggested the possibility of a [10+4] cycloaddition pathway. The [10+4] cycloadduct **1.48** was found while optimizing the zwitterionic intermediate, however, it was not observed experimentally, suggesting the likelihood of post-TS bifurcation.

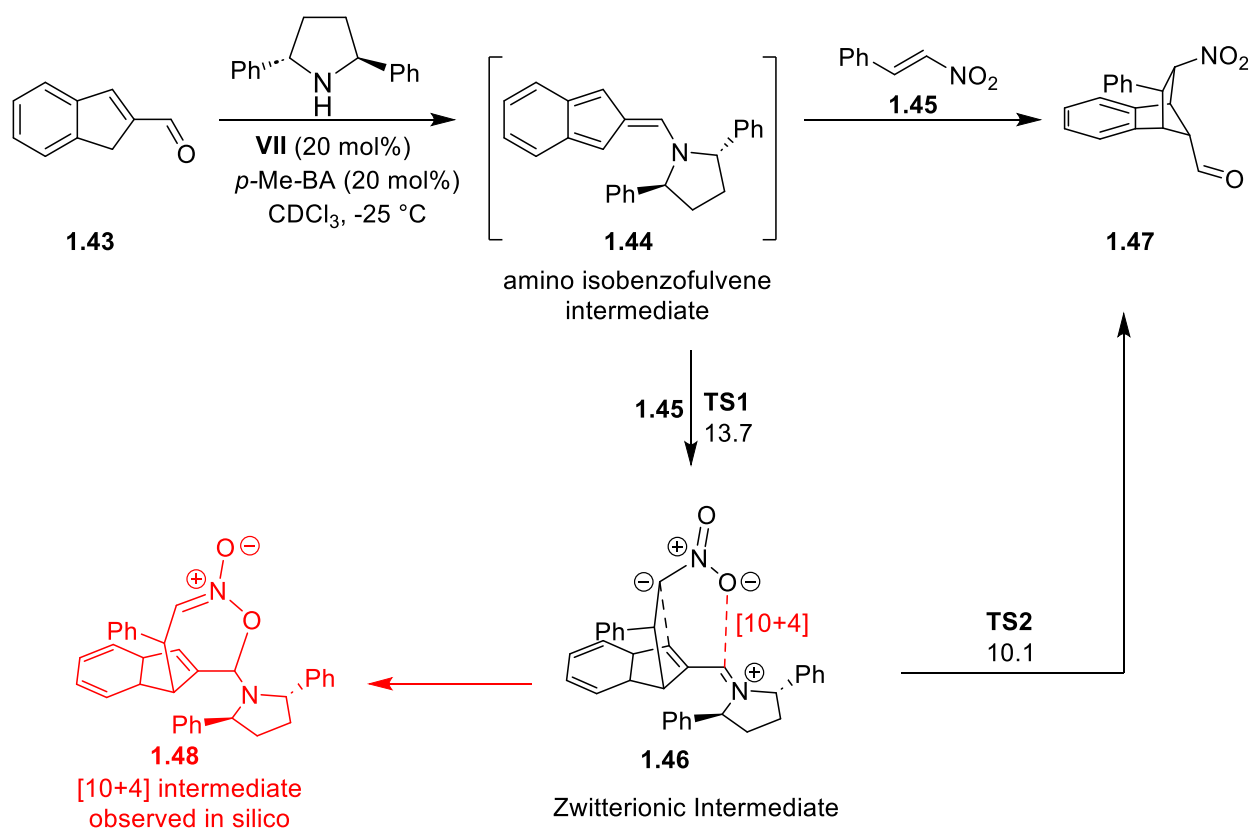
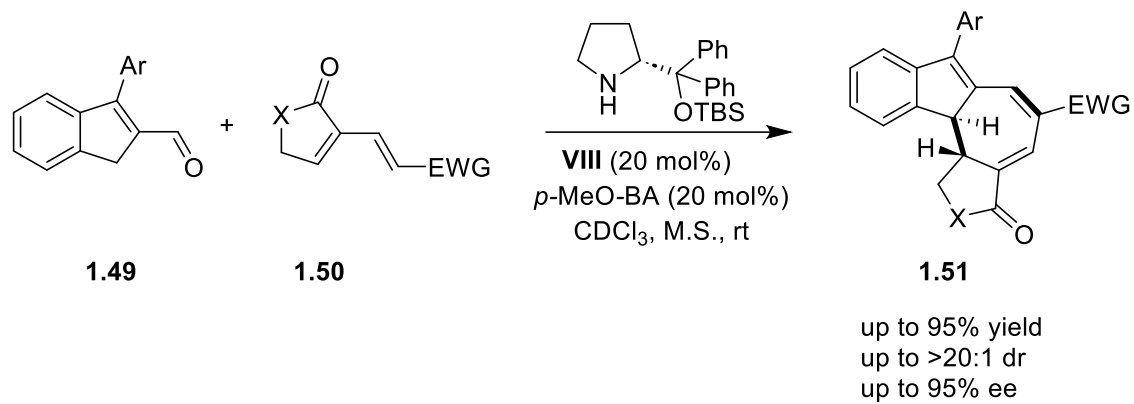


Figure 1.16: Aminocatalytic higher-order formal [8+2] cycloaddition reaction between **1.43** and **1.45**, and its stepwise pathway. Potential [10+4] pathway (red) for cycloadduct **1.48** observed in silico. Energies are in kcal/mol.

The computational insights gathered from the study of amino isobenzofulvene from [8+2] cycloaddition, Jørgensen reported the first stereoselective [10+4] cycloaddition amino isobenzofulvenes and electron deficient all-carbon dienes (Figure 9).⁸¹ Similar to [8+2] cycloaddition, the reaction was determined to proceed in a stepwise fashion. As predicted from [8+2] cycloaddition report, the [10+4] cycloadduct resulted from the initial Michael addition step which formed a zwitterionic intermediate. This was followed by ring closure at the *ipso* carbon of amino isobenzofulvene.



Scheme 1.10: Enantioselective formal [10+4] cycloaddition catalyzed by aminocatalyst, reported by Jørgensen.

1.6: References

- (1) Young, D. C. *Computational Chemistry a Practical Guide for Applying Techniques to Real-World Problems*; Wiley: New York, 2001.
- (2) Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*, 2nd ed.; Wiley: Chichester, West Sussex, England ;, 2004.
- (3) Bachrach, S. M. *Computational Organic Chemistry*; John Wiley & Sons, 2014.
- (4) Koch, Wolfram.; Holthausen, M. C. *A Chemist's Guide to Density Functional Theory*; Wiley-VCH, 2001.
- (5) Cheng, G.-J.; Zhang, X.; Chung, L. W.; Xu, L.; Wu, Y.-D. Computational Organic Chemistry: Bridging Theory and Experiment in Establishing the Mechanisms of Chemical Reactions. *J. Am. Chem. Soc.* **2015**, *137* (5), 1706–1725. <https://doi.org/10.1021/ja5112749>.
- (6) Lodewyk, M. W.; Siebert, M. R.; Tantillo, D. J. Computational Prediction of ¹H and ¹³C Chemical Shifts: A Useful Tool for Natural Product, Mechanistic, and Synthetic Organic Chemistry. *Chem. Rev.* **2012**, *112* (3), 1839–1862. <https://doi.org/10.1021/cr200106v>.
- (7) Cooksy, A. *Physical Chemistry: Quantum Chemistry and Molecular Interactions*; Pearson Higher Ed, 2013.
- (8) Born, M.; Oppenheimer, R. Zur Quantentheorie Der Molekeln. *Ann. Phys.* **1927**, *389* (20), 457–484. <https://doi.org/10.1002/andp.19273892002>.
- (9) Smith, M. B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*; John Wiley & Sons, 2020.
- (10) Physical Constants of Organic Compounds. In *CRC Handbook of Chemistry and Physics*; Haynes, W. M., Lide, D. R., Bruno, T. J., Eds.; CRC Press, 2016.

- (11) Araújo, W. L.; Nunes-Nesi, A.; Fernie, A. R. Fumarate: Multiple Functions of a Simple Metabolite. *Phytochemistry* **2011**, *72* (9), 838–843. <https://doi.org/10.1016/j.phytochem.2011.02.028>.
- (12) Final Report on the Safety Assessment of Maleic Acid¹. *Int. J. Toxicol.* **2007**, *26* (2_suppl), 125–130. <https://doi.org/10.1080/10915810701351251>.
- (13) Leffingwell, J. C. Chirality & Bioactivity I.: Pharmacology. **2003**, *3* (1).
- (14) Bou-Abdallah, F.; Sprague, S. E.; Smith, B. M.; Giffune, T. R. Binding Thermodynamics of Diclofenac and Naproxen with Human and Bovine Serum Albumins: A Calorimetric and Spectroscopic Study. *J. Chem. Thermodyn.* **2016**, *103*, 299–309. <https://doi.org/10.1016/j.jct.2016.08.020>.
- (15) Miller, M. T. Thalidomide Embryopathy: A Model for the Study of Congenital Incomitant Horizontal Strabismus. *Trans. Am. Ophthalmol. Soc.* **1991**, *89*, 623–674.
- (16) Vargesson, N. Thalidomide-Induced Teratogenesis: History and Mechanisms. *Birth Defects Res. Part C Embryo Today Rev.* **2015**, *105* (2), 140–156. <https://doi.org/10.1002/BDRC.21096>.
- (17) Krupadanam, G. D. *Fundamentals of Asymmetric Synthesis*; Universities Press, 2014.
- (18) Chida, N.; Sato, T. 2.8 Chiral Pool Synthesis: Chiral Pool Syntheses Starting from Carbohydrates. In *Comprehensive Chirality*; Carreira, E. M., Yamamoto, H., Eds.; Elsevier: Amsterdam, 2012; pp 207–239. <https://doi.org/10.1016/B978-0-08-095167-6.00203-2>.
- (19) Paek, S.-M.; Jeong, M.; Jo, J.; Heo, Y. M.; Han, Y. T.; Yun, H. Recent Advances in Substrate-Controlled Asymmetric Induction Derived from Chiral Pool α -Amino Acids for Natural Product Synthesis. *Molecules* **2016**, *21* (7), 951. <https://doi.org/10.3390/molecules21070951>.

- (20) Li, F.-Z.; Li, S.; Zhang, P.-P.; Huang, Z.-H.; Zhang, W.-B.; Gong, J.; Yang, Z. A Chiral Pool Approach for Asymmetric Syntheses of (–)-Antrocin, (+)-Asperolide C, and (–)-*Trans*-Ozic Acid. *Chem. Commun.* **2016**, 52 (84), 12426–12429. <https://doi.org/10.1039/C6CC06794H>.
- (21) Diaz-Muñoz, G.; Miranda, I. L.; Sartori, S. K.; de Rezende, D. C.; Alves Nogueira Diaz, M. Use of Chiral Auxiliaries in the Asymmetric Synthesis of Biologically Active Compounds: A Review. *Chirality* **2019**, 31 (10), 776–812. <https://doi.org/10.1002/chir.23103>.
- (22) Heravi, M. M.; Zadsirjan, V.; Farajpour, B. Applications of Oxazolidinones as Chiral Auxiliaries in the Asymmetric Alkylation Reaction Applied to Total Synthesis. *RSC Adv.* **2016**, 6 (36), 30498–30551. <https://doi.org/10.1039/C6RA00653A>.
- (23) Walsh, P. J.; Kozlowski, M. C. *Fundamentals of Asymmetric Catalysis*; University Science Books, 2009.
- (24) Mikami, K.; Lautens, M. *New Frontiers in Asymmetric Catalysis*; John Wiley & Sons, 2007.
- (25) Trost, B. M. Asymmetric Catalysis: An Enabling Science. *Proc. Natl. Acad. Sci.* **2004**, 101 (15), 5348–5355. <https://doi.org/10.1073/PNAS.0306715101>.
- (26) Jacobsen, E. N.; Pfaltz, A.; Yamamoto, H. *Comprehensive Asymmetric Catalysis: Supplement 1*; Springer Science & Business Media, 2003; Vol. 1.
- (27) Zagrebelsky, S. N. Directed Evolution as an Approach to the Design of Efficient Biocatalysts. *Russ. Chem. Rev.* **2005**, 74 (3), 285. <https://doi.org/10.1070/RC2005v074n03ABEH000899>.
- (28) Reetz, M. T.; Brunner, B.; Schneider, T.; Schulz, F.; Clouthier, C. M.; Kayser, M. M. Directed Evolution as a Method to Create Enantioselective Cyclohexanone Monooxygenases for Catalysis in Baeyer-Villiger Reactions. *Angew. Chem. Int. Ed Engl.* **2004**, 43 (31), 4075–4078. <https://doi.org/10.1002/anie.200460272>.

- (29) Leenders, S. H. A. M.; Gramage-Doria, R.; Bruin, B. de; Reek, J. N. H. Transition Metal Catalysis in Confined Spaces. *Chem. Soc. Rev.* **2014**, 44 (2), 433–448. <https://doi.org/10.1039/C4CS00192C>.
- (30) Steinborn, D. *Fundamentals of Organometallic Catalysis*; John Wiley & Sons, 2011.
- (31) *The Nobel Prize in Chemistry 2001*. NobelPrize.org. <https://www.nobelprize.org/prizes/chemistry/2001/summary/> (accessed 2023-04-28).
- (32) Cantillo, D.; Kappe, C. O. Immobilized Transition Metals as Catalysts for Cross-Couplings in Continuous Flow—A Critical Assessment of the Reaction Mechanism and Metal Leaching. *ChemCatChem* **2014**, 6 (12), 3286–3305. <https://doi.org/10.1002/cctc.201402483>.
- (33) Dalko, P. I.; Moisan, L. In the Golden Age of Organocatalysis. *Angew. Chem. Int. Ed.* **2004**, 43 (39), 5138–5175. <https://doi.org/10.1002/anie.200400650>.
- (34) Gaunt, M. J.; Johansson, C. C. C.; McNally, A.; Vo, N. T. Enantioselective Organocatalysis. *Drug Discov. Today* **2007**, 12 (1–2), 8–27. <https://doi.org/10.1016/j.drudis.2006.11.004>.
- (35) List, B. Introduction: Organocatalysis. **2007**. <https://doi.org/10.1021/CR078412E>.
- (36) *The Nobel Prize in Chemistry 2021*. NobelPrize.org. <https://www.nobelprize.org/prizes/chemistry/2021/summary/> (accessed 2023-04-28).
- (37) Berkessel, A.; Gröger, H. *Asymmetric Organocatalysis: From Biomimetic Concepts to Applications in Asymmetric Synthesis*; John Wiley & Sons, 2006.
- (38) Hajos, Z. G.; Parrish, D. R. Asymmetric Synthesis of Bicyclic Intermediates of Natural Product Chemistry. *J. Org. Chem.* **1974**, 39 (12), 1615–1621. <https://doi.org/10.1021/jo00925a003>.

- (39) Eder, U.; Sauer, G.; Wiechert, R. New Type of Asymmetric Cyclization to Optically Active Steroid CD Partial Structures. *Angew. Chem. Int. Ed. Engl.* **1971**, *10* (7), 496–497. <https://doi.org/10.1002/anie.197104961>.
- (40) Danishefsky, S. J.; Masters, J. J.; Young, W. B.; Link, J. T.; Snyder, L. B.; Magee, T. V.; Jung, D. K.; Isaacs, R. C. A.; Bornmann, W. G.; Alaimo, C. A.; Coburn, C. A.; Di Grandi, M. J. Total Synthesis of Baccatin III and Taxol. *J. Am. Chem. Soc.* **1996**, *118* (12), 2843–2859. <https://doi.org/10.1021/ja952692a>.
- (41) List, B.; Lerner, R. A.; Barbas, C. F. Proline-Catalyzed Direct Asymmetric Aldol Reactions. *J. Am. Chem. Soc.* **2000**, *122* (10), 2395–2396. <https://doi.org/10.1021/ja994280y>.
- (42) Ahrendt, K. A.; Borths, C. J.; MacMillan, D. W. C. New Strategies for Organic Catalysis: The First Highly Enantioselective Organocatalytic Diels–Alder Reaction. *J. Am. Chem. Soc.* **2000**, *122* (17), 4243–4244. <https://doi.org/10.1021/JA000092S>.
- (43) Anniina Erkkilä; Inkeri Majander, and; Pihko*, P. M. Iminium Catalysis. *Chem. Rev.* **2007**, *107* (12), 5416–5470. <https://doi.org/10.1021/CR068388P>.
- (44) List, B. The Ying and Yang of Asymmetric Aminocatalysis. *Chem. Commun.* **2006**, No. 8, 819–824. <https://doi.org/10.1039/b514296m>.
- (45) Melchiorre, P.; Marigo, M.; Carlone, A.; Bartoli, G. Asymmetric Aminocatalysis—Gold Rush in Organic Chemistry. *Angew. Chem. Int. Ed.* **2008**, *47* (33), 6138–6171. <https://doi.org/10.1002/anie.200705523>.
- (46) Nielsen, M.; Worgull, D.; Zweifel, T.; Gschwend, B.; Bertelsen, S.; Jørgensen, K. A. Mechanisms in Aminocatalysis. *Chem Commun* **2011**, *47* (2), 632–649. <https://doi.org/10.1039/C0CC02417A>.

- (47) Jung, M. E. A Review of Annulation. *Tetrahedron* **1976**, 32 (1), 3–31.
[https://doi.org/10.1016/0040-4020\(76\)80016-6](https://doi.org/10.1016/0040-4020(76)80016-6).
- (48) Brown, K. L.; Damm, L.; Dunitz, J. D.; Eschenmoser, A.; Hobi, R.; Kratky, C. Structural Studies of Crystalline Enamines. *Helv. Chim. Acta* **1978**, 61 (8), 3108–3135.
- (49) Puchot, C.; Agami, C.; Samuel, O.; Dunach, E.; Zhao, S.; Kagan, H. B. Nonlinear Effects in Asymmetric Synthesis. Examples in Asymmetric Oxidations and Aldolization Reactions. *J. Am. Chem. Soc.* **1986**, 108 (9), 2353–2357. <https://doi.org/10.1021/ja00269a036>.
- (50) Bahmanyar, S.; Houk, K. N. The Origin of Stereoselectivity in Proline-Catalyzed Intramolecular Aldol Reactions. *J. Am. Chem. Soc.* **2001**, 123 (51), 12911–12912.
<https://doi.org/10.1021/ja011714s>.
- (51) Cheong, P. H. Y.; Houk, K. N.; Warrier, J. S.; Hanessian, S. Catalysis of the Hajos-Parrish-Eder-Sauer-Wiechert Reaction by Cis- and Trans-4,5-Methanoproline: Sensitivity of Proline Catalysis to Pyrrolidine Ring Conformation. *Adv. Synth. Catal.* **2004**, 346 (9–10), 1111–1115. <https://doi.org/10.1002/adsc.200404127>.
- (52) Clemente, F. R.; Houk, K. N. Computational Evidence for the Enamine Mechanism of Intramolecular Aldol Reactions Catalyzed by Proline. *Angew. Chem. - Int. Ed.* **2004**, 43 (43), 5766–5768. <https://doi.org/10.1002/anie.200460916>.
- (53) Hoang, L.; Bahmanyar, S.; Houk, K. N.; List, B. Kinetic and Stereochemical Evidence for the Involvement of Only One Proline Molecule in the Transition States of Proline-Catalyzed Intra- and Intermolecular Aldol Reactions. *J. Am. Chem. Soc.* **2003**, 125 (1), 16–17.
<https://doi.org/10.1021/ja028634o>.

- (54) Bahmanyar, S.; Houk, K. N.; Martin, H. J.; List, B. Quantum Mechanical Predictions of the Stereoselectivities of Proline-Catalyzed Asymmetric Intermolecular Aldol Reactions. *J. Am. Chem. Soc.* **2003**, *125* (9), 2475–2479. <https://doi.org/10.1021/ja028812d>.
- (55) Notz, W.; Tanaka, F.; Watanabe, S. I.; Chowdari, N. S.; Turner, J. M.; Thayumanavan, R.; Barbas, C. F. The Direct Organocatalytic Asymmetric Mannich Reaction: Unmodified Aldehydes as Nucleophiles. *J. Org. Chem.* **2003**, *68* (25), 9624–9634. <https://doi.org/10.1021/jo0347359>.
- (56) Hayashi, Y.; Yamaguchi, J.; Hibino, K.; Shoji, M. Direct Proline Catalyzed Asymmetric α -Aminooxylation of Aldehydes. *Tetrahedron Lett.* **2003**, *44* (45), 8293–8296. <https://doi.org/10.1016/j.tetlet.2003.09.057>.
- (57) Bøgevig, A.; Juhl, K.; Kumaragurubaran, N.; Zhuang, W.; Jørgensen, K. A. Direct Organocatalytic Asymmetric α -Amination of Aldehydes - A Simple Approach to Optically Active α -Amino Aldehydes, α -Amino Alcohols, and α -Amino Acids. *Angew. Chem. - Int. Ed.* **2002**, *41* (10), 1790–1793. [https://doi.org/10.1002/1521-3773\(20020517\)41:10<1790::AID-ANIE1790>3.0.CO;2-Y](https://doi.org/10.1002/1521-3773(20020517)41:10<1790::AID-ANIE1790>3.0.CO;2-Y).
- (58) List, B.; Pojarliev, P.; Martin, H. J. Efficient Proline-Catalyzed Michael Additions of Unmodified Ketones to Nitro Olefins. *Org. Lett.* **2001**, *3* (16), 2423–2425. <https://doi.org/10.1021/ol015799d>.
- (59) Mitsumori, S.; Zhang, H.; Cheong, P. H.-Y.; Houk, K. N.; Fujie, T.; Barbas, C. F. Direct Asymmetric Anti-Mannich-Type Reactions Catalyzed by a Designed Amino Acid. *J. Am. Chem. Soc.* **2006**, *128* (4), 1040–1041. <https://doi.org/10.1021/JA056984F>.

- (60) Austin, J. F.; MacMillan, D. W. C. Enantioselective Organocatalytic Indole Alkylations. Design of a New and Highly Effective Chiral Amine for Iminium Catalysis. *J. Am. Chem. Soc.* **2002**, *124* (7), 1172–1173. <https://doi.org/10.1021/JA017255C>.
- (61) Northrup, A. B.; Macmillan, D. W. C. The First General Enantioselective Catalytic Diels-Alder Reaction with Simple α,β -Unsaturated Ketones. *J. Am. Chem. Soc.* **2002**, *124* (11), 2458–2460. <https://doi.org/10.1021/ja017641u>.
- (62) Hayashi, Y.; Gotoh, H.; Hayashi, T.; Shoji, M. Diphenylprolinol Silyl Ethers as Efficient Organocatalysts for the Asymmetric Michael Reaction of Aldehydes and Nitroalkenes. *Angew. Chem. Int. Ed.* **2005**, *44* (27), 4212–4215. <https://doi.org/10.1002/anie.200500599>.
- (63) Hiroaki Gotoh; Hayato Ishikawa, A.; Hayashi, Y. Diphenylprolinol Silyl Ether as Catalyst of an Asymmetric, Catalytic, and Direct Michael Reaction of Nitroalkanes with α,β -Unsaturated Aldehydes. *Org. Lett.* **2007**, *9* (25), 5307–5309. <https://doi.org/10.1021/OL702545Z>.
- (64) Donslund, B. S.; Johansen, T. K.; Poulsen, P. H.; Halskov, K. S.; Jørgensen, K. A. The Diarylprolinol Silyl Ethers: Ten Years After. *Angew. Chem. - Int. Ed.* **2015**, *54* (47), 13860–13874. <https://doi.org/10.1002/anie.201503920>.
- (65) Franzén, J.; Marigo, M.; Fielenbach, D.; Wabnitz, T. C.; Kjærsgaard, A.; Jørgensen, K. A. A General Organocatalyst for Direct α -Functionalization of Aldehydes: Stereoselective C-C, C-N, C-F, C-Br, and C-S Bond-Forming Reactions. Scope and Mechanistic Insights. *J. Am. Chem. Soc.* **2005**, *127* (51), 18296–18304. <https://doi.org/10.1021/ja056120u>.
- (66) Dinér, P.; Kjærsgaard, A.; Lie, M. A.; Jørgensen, K. A. On the Origin of the Stereoselectivity in Organocatalysed Reactions with Trimethylsilyl-Protected Diarylprolinol. *Chem. - Eur. J.* **2007**, *14* (1), 122–127. <https://doi.org/10.1002/chem.200701244>.

- (67) Fuson, R. C. The Principle of Vinylogy. *Chem. Rev.* **1935**, 16 (1), 1–27.
<https://doi.org/10.1021/cr60053a001>.
- (68) Jurberg, I. D.; Chatterjee, I.; Tannert, R.; Melchiorre, P. When Asymmetric Aminocatalysis Meets the Vinylogy Principle. *Chem. Commun.* **2013**, 49 (43), 4869.
<https://doi.org/10.1039/c3cc41270a>.
- (69) Jiang, H.; Albrecht, L.; Jørgensen, K. A. Aminocatalytic Remote Functionalization Strategies. *Chem. Sci.* **2013**, 4 (6), 2287. <https://doi.org/10.1039/c3sc50405k>.
- (70) Arceo, E.; Melchiorre, P. Extending the Aminocatalytic HOMO-Raising Activation Strategy: Where Is the Limit? *Angew. Chem. Int. Ed.* **2012**, 51 (22), 5290–5292.
<https://doi.org/10.1002/anie.201201347>.
- (71) Ramachary, D. B.; Reddy, Y. V. Dienamine Catalysis: An Emerging Technology in Organic Synthesis. *Eur. J. Org. Chem.* **2012**, 2012 (5), 865–887.
<https://doi.org/10.1002/ejoc.201101157>.
- (72) Bertelsen, S.; Marigo, M.; Brandes, S.; Dinér, P.; Jørgensen, K. A. Dienamine Catalysis: Organocatalytic Asymmetric γ -Amination of α,β -Unsaturated Aldehydes. *J. Am. Chem. Soc.* **2006**, 128 (39), 12973–12980. <https://doi.org/10.1021/ja064637f>.
- (73) De Figueiredo, R. M.; Fröhlich, R.; Christmann, M. Amine-Catalyzed Cyclizations of Tethered α,β -Unsaturated Carbonyl Compounds. *Angew. Chem. - Int. Ed.* **2008**, 47 (8), 1450–1453. <https://doi.org/10.1002/anie.200704688>.
- (74) Duarte, F. J. S.; Santos, A. G. Enantioselective Organocatalytic Intramolecular Diels-Alder Reactions: A Computational Study. *J. Org. Chem.* **2012**, 77 (7), 3252–3261.
<https://doi.org/10.1021/jo300005e>.

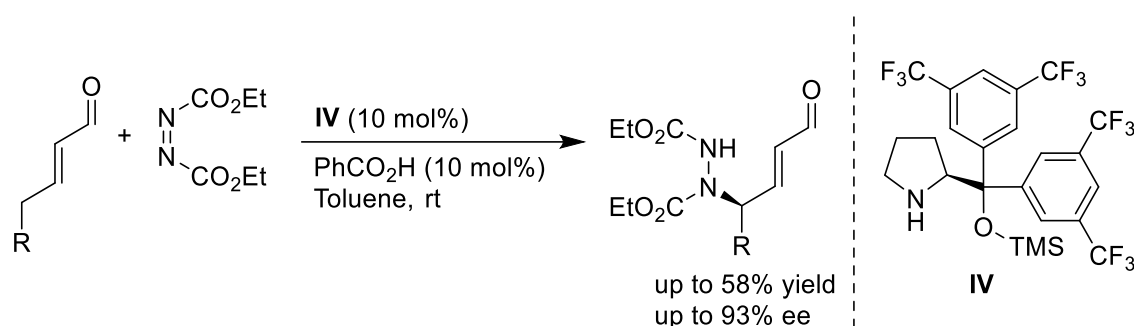
- (75) Jia, Z. J.; Jiang, H.; Li, J. L.; Gschwend, B.; Li, Q. Z.; Yin, X.; Grouleff, J.; Chen, Y. C.; Jørgensen, K. A. Trienamines in Asymmetric Organocatalysis: Diels-Alder and Tandem Reactions. *J. Am. Chem. Soc.* **2011**, *133* (13), 5053–5061. <https://doi.org/10.1021/ja1112194>.
- (76) Albrecht, L.; Cruz Acosta, F.; Fraile, A.; Albrecht, A.; Christensen, J.; Jørgensen, K. A. Enantioselective H-Bond-Directing Approach for Trienamine-Mediated Reactions in Asymmetric Synthesis. *Angew. Chem. Int. Ed.* **2012**, *51* (36), 9088–9092. <https://doi.org/10.1002/anie.201204790>.
- (77) Kumar, I.; Ramaraju, P.; Mir, N. A. Asymmetric Trienamine Catalysis: New Opportunities in Amine Catalysis. *Org. Biomol. Chem.* **2013**, *11* (5), 709–716. <https://doi.org/10.1039/c2ob26681d>.
- (78) Halskov, K. S.; Johansen, T. K.; Davis, R. L.; Steurer, M.; Jensen, F.; Jørgensen, K. A. Cross-Trienamines in Asymmetric Organocatalysis. *J. Am. Chem. Soc.* **2012**, *134* (31), 12943–12946. <https://doi.org/10.1021/ja3068269>.
- (79) Stiller, J.; Poulsen, P. H.; Cruz, D. C.; Dourado, J.; Davis, R. L.; Jørgensen, K. A. Organocatalytic [4+2] Addition Reactions via Tetraenamine Intermediate. *Chem. Sci.* **2014**, *5* (5), 2052–2056. <https://doi.org/10.1039/c4sc00081a>.
- (80) [ASAP] Organocatalytic Higher-Order [8+2] Cycloaddition for the Assembly of Atropoenantiomeric 3-Arylindolizines. *Org. Lett.* <https://doi.org/10.1021/acs.orglett.1c03220>.
- (81) Donslund, B. S.; Jessen, N. I.; Bertuzzi, G.; Giardinetti, M.; Palazzo, T. A.; Christensen, M. L.; Jørgensen, K. A. Catalytic Enantioselective [10+4] Cycloadditions. *Angew. Chem. - Int. Ed.* **2018**, *57* (40), 13182–13186. <https://doi.org/10.1002/anie.201807830>.

Chapter 2 : Mechanistic Investigation of Aminocatalytic Remote Functionalization of α,β -Unsaturated Aldehydes

2.1: Introduction

Since the proline catalyzed aldol reaction reported by List *et al.* in 2000, aminocatalysis has become one of the most efficient and widely studied strategies for stereoselective functionalization of carbonyl compounds.^{1,2} There now exist transition state models which are utilized to rationalize experimental results and predict stereochemical outcomes for enamine facilitated reactions, aiding in reaction development.³⁻⁶ These models are widely accepted which explain the regio- and stereochemical outcomes for most enamine mediated reactions. See section 1.5.2 in Chapter 1 for details.

More recently, the enamine activation mode has been extended to dienamines, trienamines, and even tetraenamines by using polyunsaturated carbonyl compounds which has allowed for stereoselective functionalization at more distant positions.⁷⁻¹³ However, efforts to understand the mechanism of these extended activation modes have been limited. Additionally, this understanding has mostly relied on analogy of models that are well established for enamine reactions.



Scheme 2.1: Dienamine mediated γ -amination of α,β -unsaturated aldehydes reported by Jørgensen.

The first remote functionalization, with the aid of dienamine activation, was reported by Jørgensen *et al.* where the authors successfully performed γ -amination of α,β -unsaturated aldehydes (Scheme 2.1).⁷ In this work, the authors detail the reaction of enals with diethyl azodicarboxylate (DEAD) yielding remotely functionalized aldehydes. The γ -amination reaction provides high enantioselectivity, however, the observed stereochemistry is determined to be opposite of that expected. The steric shielding from the catalyst would interfere with electrophile to be added from the back, instead, the observed stereochemistry is in the same face as the catalyst (Figure 2.1).

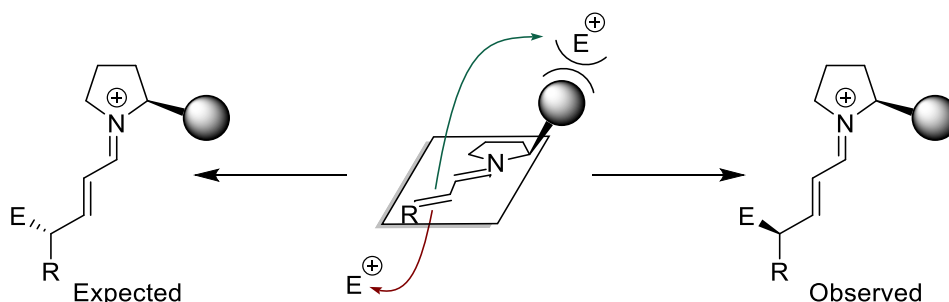
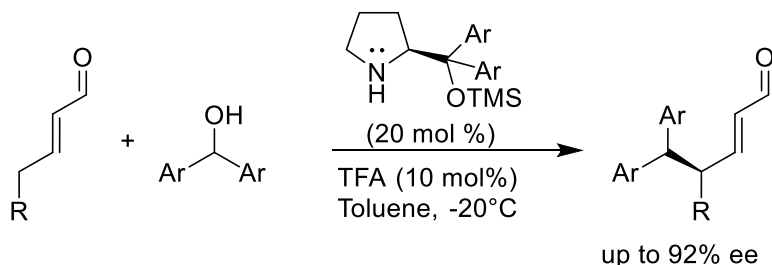


Figure 2.1: Depiction of selectivity in dienamine intermediate by steric discrimination from aminocatalyst **IV** for γ -amination.

The proposed mechanism by Jørgensen *et al.* suggests that reaction proceeds *via* Diels-Alder type pathway between the dienamine intermediate and DEAD. In the report, the Diels-Alder pathway was shown to be more favoured than mono addition of DEAD at γ -position of the

dienamine. The authors suggested that the resulting cycloadduct undergoes hydrolysis to give the γ -aminated product and release the catalyst. It was also stated that the configuration of the double bond in the product was determined to be *E*. However, no explanation was provided about how the hydrolysis of the cycloadduct leads to the *R*-enantiomer with *E*-configuration of the double bond.

In 2011, Christmann reported γ -alkylation reaction, with high *E:Z* selectivity, between enals and stabilized carbocations using diaryl alcohols (Scheme 2.2).¹⁰ The authors noted that the stereochemical configuration of the remote stereocenter in the product was not expected. The general stereochemical models for enamine reactions would invoke a steric-shielding model, and the diaryl electrophile should add on the ‘back-side’ which is opposite of the steric bulk of catalyst. This was determined to be completely opposite to what was observed.



Scheme 2.2: Dienamine mediated γ -alkylation of α,β -unsaturated aldehydes reported by Christmann.

To explain the observed stereochemistry, Christmann proposed that the iminium ion produced after the electrophilic attack can interconvert between *E* and *Z* isomers *via* a sequence of deprotonation/protonation.¹⁴ This sequence suggests that a second dienamine intermediate which is alkylated at gamma position may be plausible. The authors proposed this second dienamine intermediate to explain the *E/Z* selectivity of gamma alkylation where the *E/Z* ratio of the second dienamine intermediate is dictated by thermodynamics. It was further proposed that the protonation of the alkylated dienamine intermediate would be the stereodetermining intermediate and not the initial electrophilic attack (Figure 2.2).

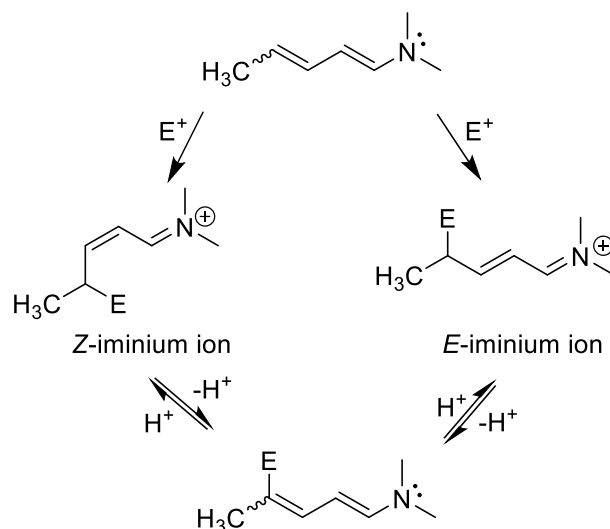


Figure 2.2: Christmann's proposed second dienamine

The mechanistic investigations of the γ -alkylation reaction by Gschwind found that the stereochemical outcome of the reaction depended heavily on the induced conformation of the reactive dienamine intermediate.¹⁵ While these conformations are well understood for more simple enamine systems, the additional complexity of a second, conformationally flexible *pi*-backbone cannot be ignored. The authors explored the *E/Z* ratios, relative to terminal double bond, of the dienamine intermediate by NMR and computational studies. The report suggests that the terminal double bond shows a kinetic preference for the *Z*-isomer during the formation of dienamine, which slowly isomerizes to thermodynamically preferred *E*-isomer with *E:Z* ratio of 1:2. With the steric shielding model, the *E*-isomer leads to the *S*-enantiomer and *Z*-isomer leads to the *R*-enantiomer, the *E:Z* ratio of 1:2 which does not correlate to the experimental *ee* values of up to 92%. Hence, by NMR and computational studies, it was observed that the barrier for reaction between *Z*-dienamine and the electrophile was lower than that with *E*-dienamine. Additionally, in the case of *Z*-dienamines, there were favourable CH- π interactions observed with the electrophile. In summary, the authors proposed that the kinetic preference of *Z*-dienamine, lower activation barrier for attack on electrophile from nucleophilic dienamine, and the favourable non-covalent

interactions with the electrophile are responsible for the high *ee* favouring the R-enantiomer. The authors did not perform an extensive study on the γ -amination report, however, it was suggested that the Diels-Alder pathway requires a downstream isomerization of the product.

In aminocatalytic reactions with diarylprolinol ether catalysts, the enantioselectivity is rationalized by simple steric shielding model which states that the bulky group of the catalyst hinders the approach of the catalyst from one face which promotes reactivity from the other face. However, mechanistic studies on enamine mediated reactions reported by Blackmond suggest the interaction of enamine intermediate and electrophile, relating to kinetic preference, alone may not provide the whole picture.⁴ The authors note that the enantioselectivity in aminocatalytic reactions must be rationalized by the thermodynamic stability and of the intermediates formed after interactions between enamine and the electrophile termed ‘downstream intermediates’.

Herein, an extensive mechanistic study to gain insights about the principles of origin of selectivity for dienamine mediated γ -amination is reported. The results of this work will not only aid in understanding the pathway but also benefit chemists in designing and expanding the scope of novel asymmetric remote functionalization reactions.

2.2: Computational methods

All structures were optimized using B3LYP^{16,17} with the double- ζ split valence 6-31G(d) basis set.^{18,19} Solvation with toluene was performed using the Integration Equation Formalism Polarizable Continuum Model (IEFPCM) model²⁰ and vibrational analysis verified that each structure was either a minimum or transition state. All optimizations were performed in Gaussian 09.e01.²¹ Single point energies were calculated using M06-2X²² functional and the triple zeta for valence electrons plus polarization function (TZVP) basis set²³ using the IEFPCM solvation model with toluene. All 3D figures were generated using CYLview^{20,24}

2.3: Results and Discussion

2.3.1: Diels-Alder Cycloaddition between Dienamine and DEAD

We started our investigation by studying the different conformations of the dienamine intermediate in order to examine its thermodynamic preference. It was determined that the *E,s-trans,E* dienamine (**A**) and *E,s-trans,Z* dienamine (**B**) were similar in energy, however, the *E,s-cis,E* dienamine (**C**) is disfavoured by 2.0 kcal/mol relative to **A** (Figure 2.3). Experimentally, only the peaks of dienamines **A** and **B** were observed as evidenced by E:Z ratio to be 1:1. (Figure 2.4) gschwend and Jørgensen reference In order for the reaction to proceed through a Diels-Alder type pathway, as proposed by Jorgenson, the formation of thermodynamically disfavoured *E,s-cis,E* dienamine (**C**) configuration is crucial.

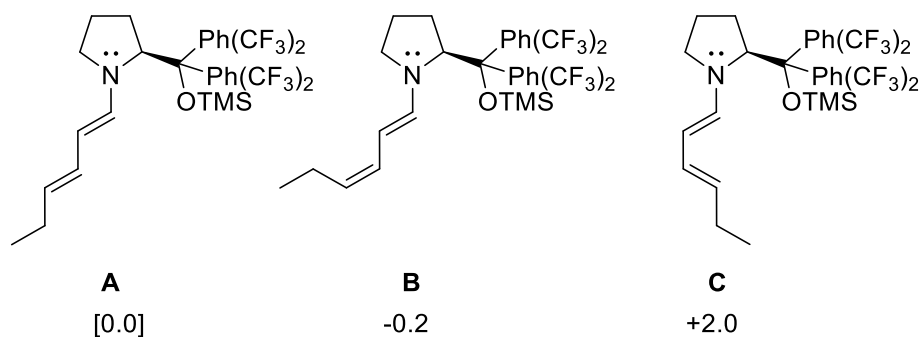


Figure 2.3: Computed energies of Dineamine A, B, and C. Free energies reported are in kcal/mol.

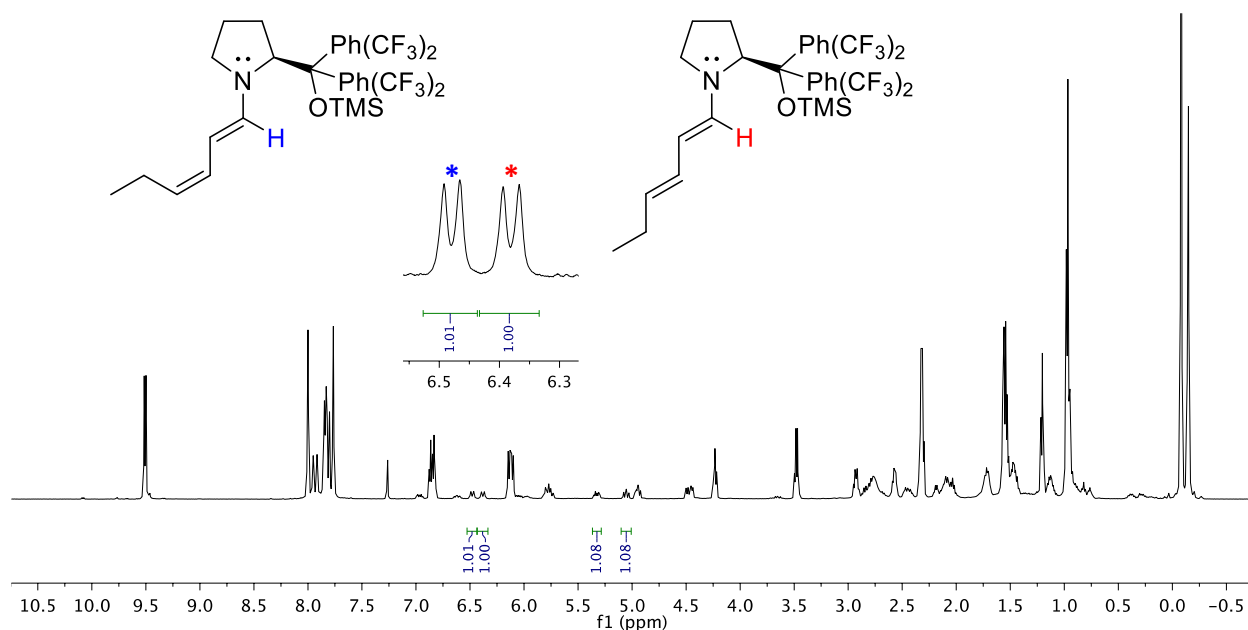


Figure 2.4: Experimental evidence of dienamines **A** and **B** by $^1\text{H-NMR}$ at 300MHz in CDCl_3 .

We then investigated the barrier for addition of electrophile to the dienamine intermediate. The barrier for [4+2] addition between dienamine **C** and DEAD (**DA-TS**) was calculated to be +23.7 kcal/mol relative to dienamine **A** and **DEAD**. The resulting Diels-Alder cycloadduct, **DA-INT**, was found to be thermodynamically favoured by 31.6 kcal/mol relative to **A** and **DEAD**. (Figure 2.5) In comparison, the barriers for mono-addition of **DEAD** to the γ -carbon of the dienamines were determined to be disfavoured by 5-13 kcal/mol relative to **DA-TS**. The resulting mono-addition intermediates were found to be endergonic by 6-14 kcal/mol. This suggests that the reaction proceeds through the kinetically favoured cycloaddition pathway to result in the notably thermodynamically favoured cycloadduct **DA-INT**.

The kinetic preference for cycloaddition suggests that the E/Z dilemma of the dienamine intermediate is not an important factor during the addition of DEAD. Since, the dienamine **C** is too sterically hindered for DEAD to be approached from the same face as the catalyst bulk, the formation of cycloadduct **DA-INT** obeys the steric shielding model resulting in high

enantioselectivity. Due to the nature of [4+2] pathway, the dienophile **DEAD** reacts at *ipso* and γ -carbon resulting in high regioselectivity for the amination reaction at the γ -position.

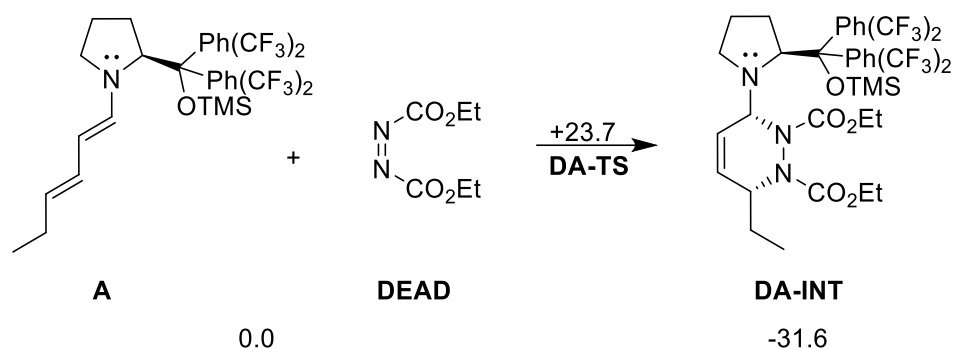
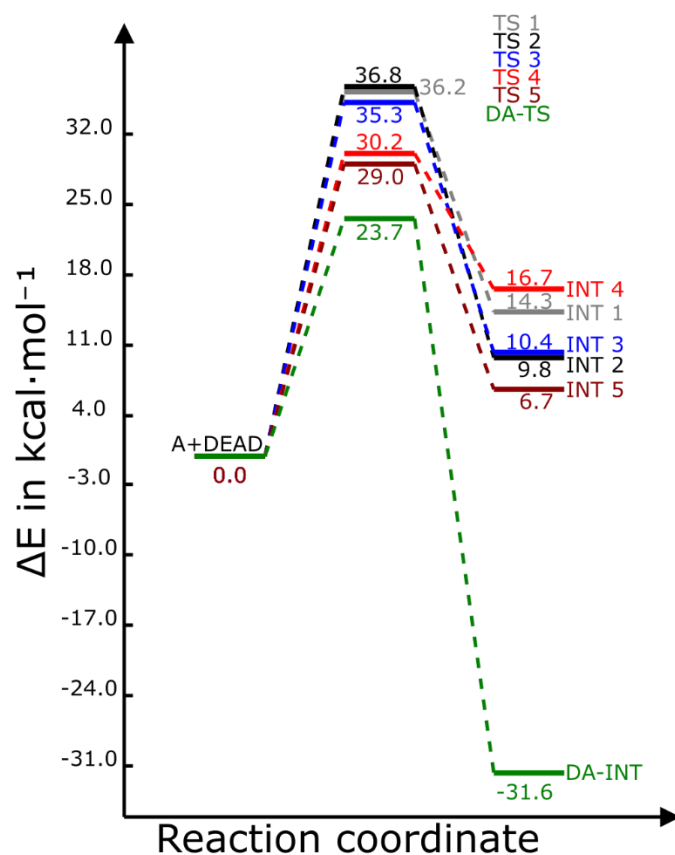


Figure 2.5: Calculated barrier for Diels-Alder cycloaddition between Dienamine intermediate and **DEAD**. All energies are reported in kcal/mol.

a)



b)

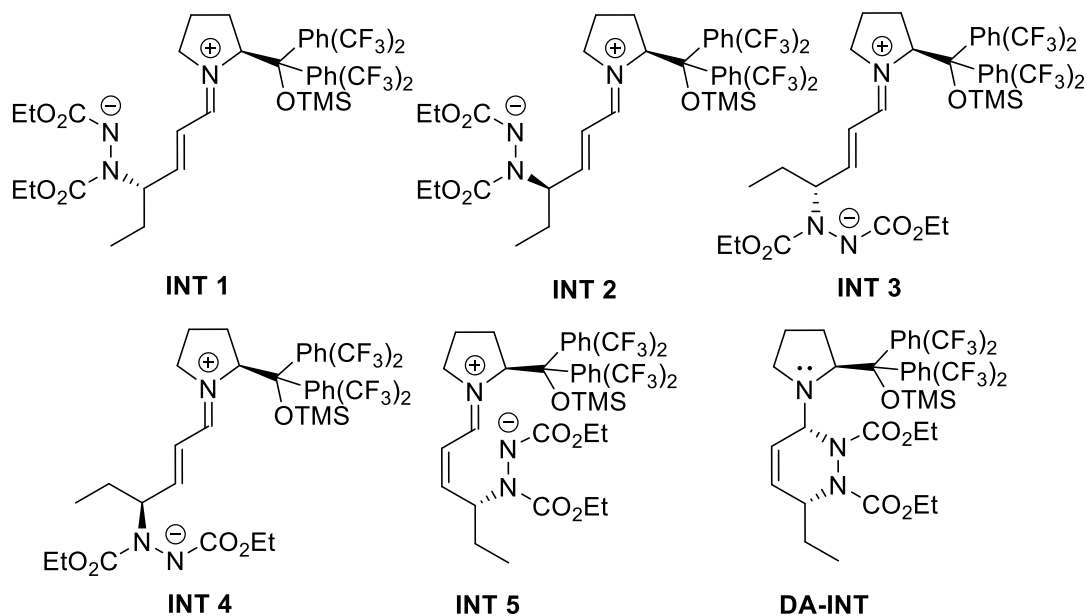


Figure 2.6: a) Reaction coordinate diagram of calculated barriers for mono-addition of DEAD and [4+2] cycloaddition to dienamine intermediate. B) The resulting iminium-ion intermediates

after mono-addition of DEAD and [4+2] cycloaddition to dienamine intermediate. All energies are in kcal/mol.

In order to obtain the observed product, the cycloadduct **DA-INT** must undergo ring opening and hydrolysis. Our calculations indicate that the protonation of the nitrogen of **DEAD** attached at the *ipso* carbon results in a barrierless ring opening of the cycloadduct leading to **INT 6**. However, the hydrolysis of **INT 6** would not result in observed product with *E* configuration of the double bond (Figure 2.7). Therefore, the downstream reaction following the ring opening of **DA-INT** must go through an intermediate which allows rotation around the α,β -bond in order to generate the observed product.

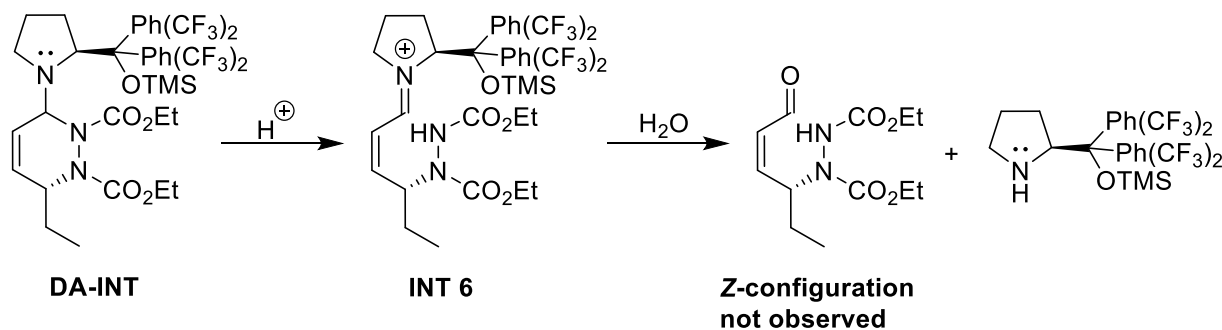


Figure 2.7: Hydrolysis of cycloadduct leading to product with *Z*-configuration

2.3.2: Plausible Mechanisms

The conversion of the *Z* to *E* double bond could occur *via* 2 pathways: 1) formation of aminated dienamine intermediate which examines the second dienamine intermediate proposed by Christmann¹⁰ (Figure 2.8, left, green) or 2) reversible Michael addition at the β -carbon of **INT 6**. (Figure 2.8, right, blue). For the mechanism involving aminated dienamine downstream intermediate, we propose that deprotonation at the γ -carbon of **INT 6** leads to aminated dienamine intermediate. The favoured conformation dictated by thermodynamics would then get protonated

that may lead to the productive iminium ion conformer. Upon hydrolysis, this would result in the observed product with *E*-configuration of the double bond and (*R*)-stereocenter.

For the Michael addition pathway, we propose a nucleophilic addition of a water molecule to the β -carbon of **INT 6**, resulting in an enamine intermediate that has free rotation around the α - β bond. Upon rotation and elimination of water, the resulting iminium ion conformer would lead to the observed product. Therefore, we examined both plausible mechanisms with computational and experimental methods.

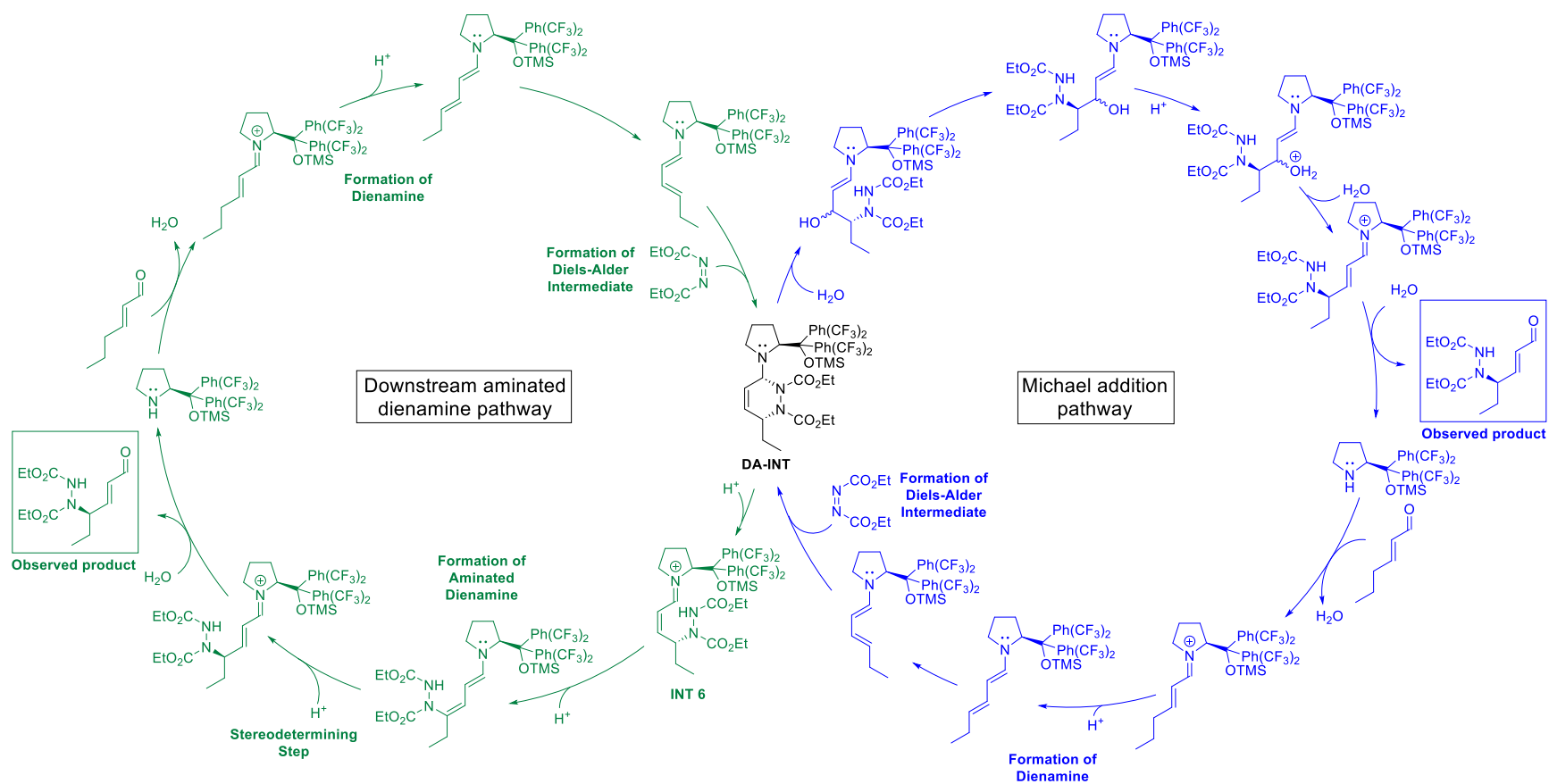


Figure 2.8: Plausible pathways for dienamine mediated γ -amination reaction.

2.3.3: Aminated Dienamine

Upon ring opening of the cycloadduct **DA-INT**, the iminium ion intermediate **INT 6** can undergo deprotonation at the γ -carbon to result in the aminated dienamine intermediate **D** (Figure 2.9a). The formation of dienamine **D** is important since rotation around the α,β -bond allows for a downstream intermediate with *E*-configuration to result in the observed product. Therefore, we started by calculating different configurations of aminated dienamine intermediate were also calculated (Figure 2.9). It was determined that dienamine **D** was thermodynamically disfavoured relative to **E** and **F** by 7.0 and 5.1 kcal/mol, respectively. This suggests that, upon rotation around the α,β -bond, the thermodynamic preference of dienamines **E** and **F** could be the driving force that promotes *E*-configuration of the double bond in the observed product.

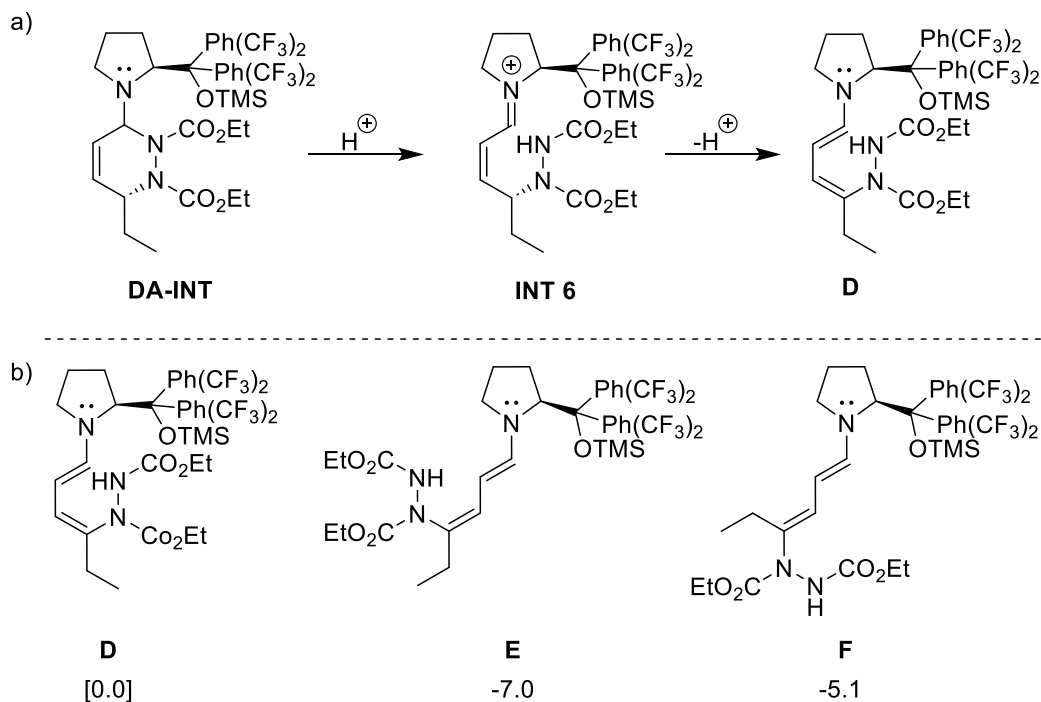


Figure 2.9:a) Formation of aminated dienamine intermediate **D** from the cycloadduct **DA-INT**. b) Conformers of aminated dienamine intermediate. Free energies are reported in kcal/mol.

In the downstream second dienamine pathway, the formation of aminated dienamine **E** is an important step. The protonation of aminated dienamines **E** and **F** would result in iminium ion intermediates with *E*-configuration of the double bond which, upon hydrolysis, would lead to observed product. The protonation at the γ -carbon can take place from both faces of dienamine **E** and **F** resulting in iminium ion intermediates with *S*- and *R*- stereochemistry. Upon protonation, dienamine **E** would result in iminium intermediates **INT 7** and **INT 8**, and dienamine **F** results in **INT 9** and **INT 10** (Figure 2.10). It was determined that intermediates **INT 7** and **INT 8**, resulting from dienamine **E**, were thermodynamically favoured than intermediates **INT 9** and **INT 10**, resulting from Dienamine **F**, which were similar in energy as **INT 6** (Figure 2.10). The iminium ion intermediate **INT 7** and **INT 8** were determined to 1.1 and 2.6 kcal/mol, respectively, more thermodynamically favoured relative to **INT 6**.

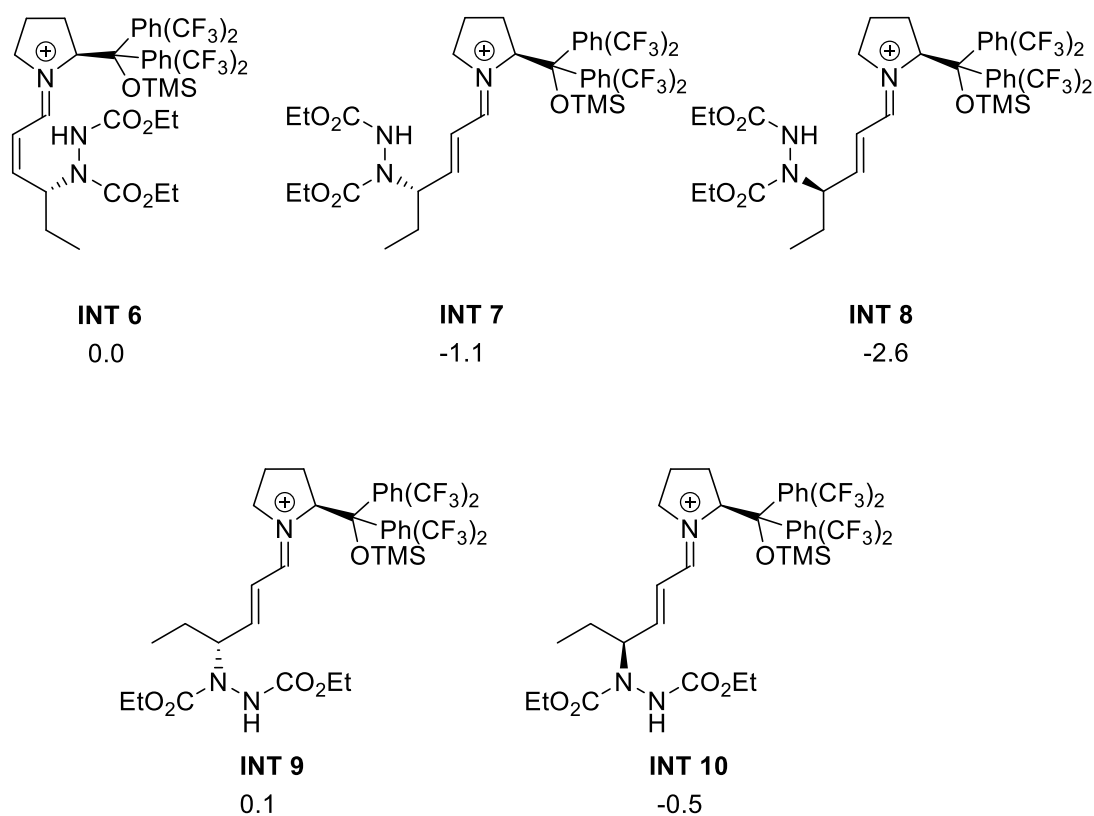


Figure 2.10: Calculated Iminium ion intermediates resulting from protonation of aminated Dienamines **D**, **E**, and **F**.

The thermodynamically favoured intermediates (**INT 7** and **INT 8**) result in the *E*-configuration around the double bond with *S*- and *R*-stereocenters at the γ -carbon. In order to determine the thermodynamically favoured conformers of **INT 7** and **INT 8**, a conformational analysis was performed. It was determined that the iminium ion intermediate (**INT 11**) leading to the expected product with (*S*)-stereocenter and *E*-configuration around the double bond was determined to be thermodynamically favourable by 6.6 kcal/mol, relative to **INT 6**. The iminium ion intermediate leading to the observed product with (*R*)-stereocenter and *E*-configuration, **INT 12**, was determined to be 3.0 kcal/mol higher in energy than **INT 11** (Figure 2.11). This suggests that the γ -amination reaction may undergo another pathway from the cycloadduct **DA-INT**.

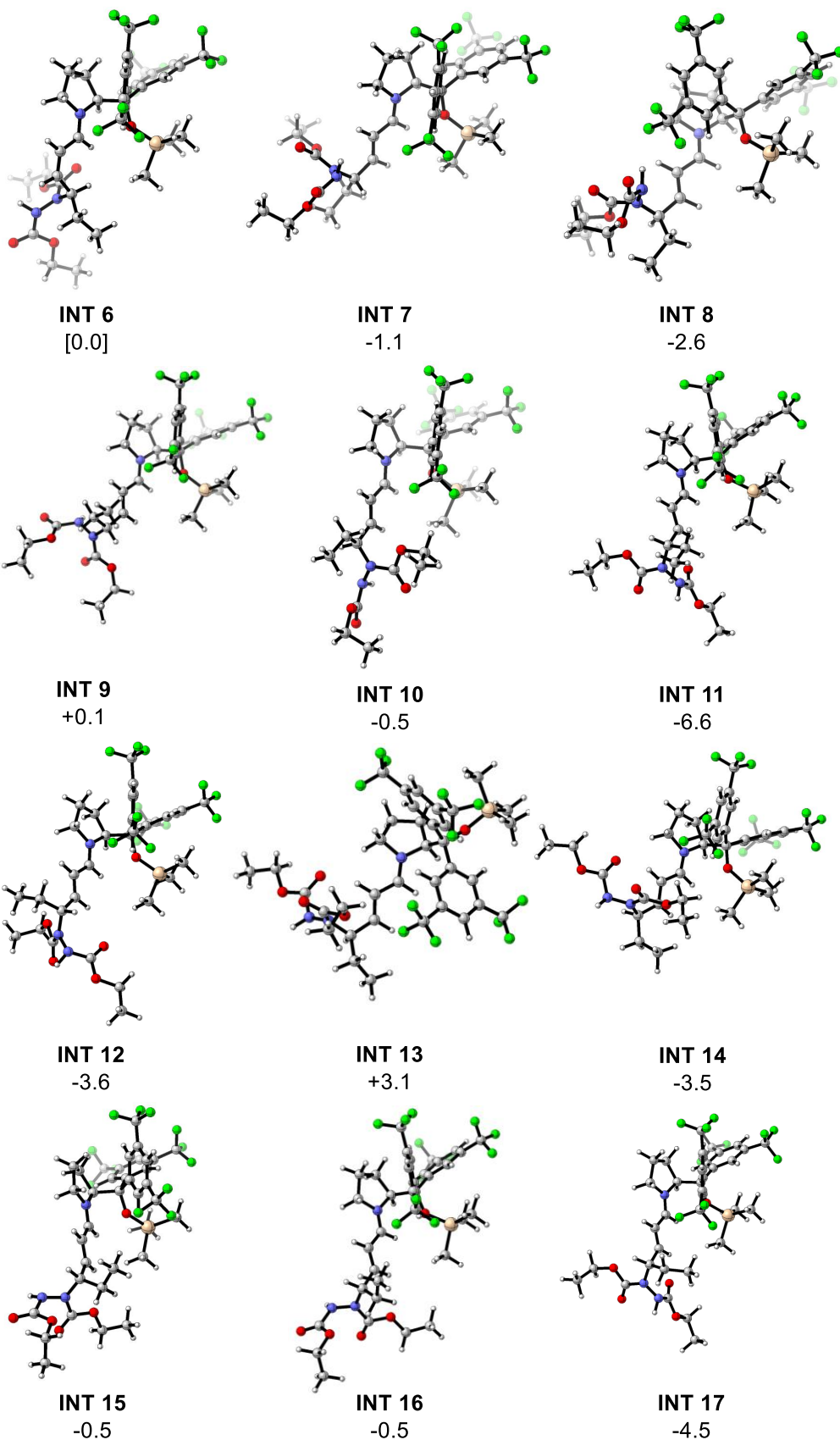
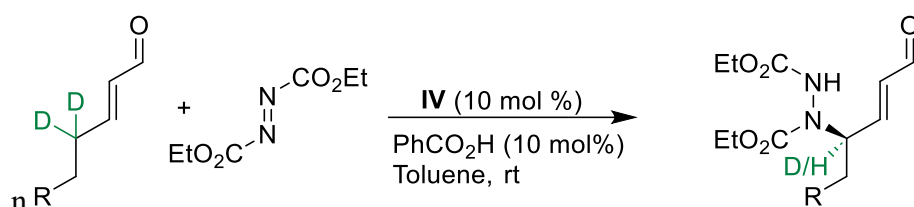


Figure 2.11: Resulting iminium ion intermediates upon protonation of Dienamines D, E, and F. Free energies are reported in kcal/mol. (C = grey, N = blue, O = red, F = green, Si = yellow, H = white).

We further investigated this mechanism by experimental methods. We proposed that if the reaction does form γ -aminated dienamine, evidence for the presence or absence of the second dienamine can be gathered by deuterium labelling the gamma position. Hence, if the amination reaction is performed with γ -deuterated aldehyde and the product shows evidence of γ -proton, it would provide evidence of the aminated dienamine intermediate (Scheme 2.3).



Scheme 2.3: Proposed reaction.

Hence, the reaction was performed with 5-phenyl-2-pentenal-4,4-*d*₂ while mimicking the conditions reported by Jørgensen et al. After carefully monitoring the reaction with NMR, there was no product observed containing protons at gamma position. In the reaction with non-deuterated aldehyde, the gamma proton of the product appears at 5.16-5.15 ppm⁷, however, as the reaction was monitored over time, this signal was not present in the reaction with deuterated aldehyde (Figure 2.12). The consumption of starting material and formation of product was evident, but no gamma-proton was observed as we hypothesized. Therefore, this study suggests that the formation of aminated dienamine is very unlikely.

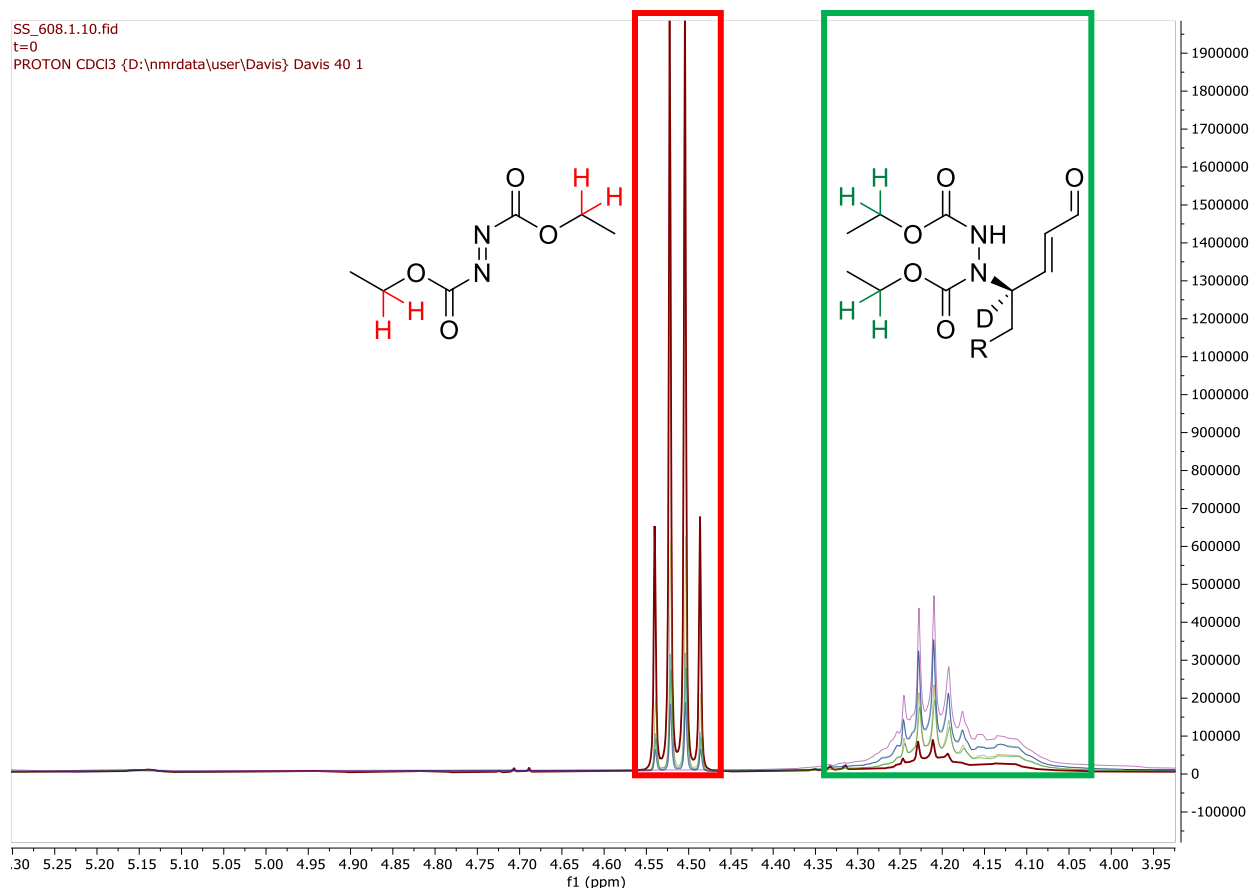


Figure 2.12: Stacked NMR segment of γ -amination reaction with deuterated enal. The signals on left (red) show the ethyl protons of DEAD, the signals on the right (green) show the ethyl protons of hydrazine moiety in the product.

2.3.4: Michael Addition pathway

Another plausible pathway for the γ -amination reaction is that after the formation of cycloadduct **DA-INT**, it could undergo a Michael addition. It is proposed that a water molecule could add at the β -carbon of **DA-INT** to result in the enamine intermediate **EN-1** which allows rotation around the α - β bond. The rotation which is followed by elimination of water could potentially result in iminium ion intermediate **INT 8**, the productive conformer leading to the observed product (Figure 2.8).

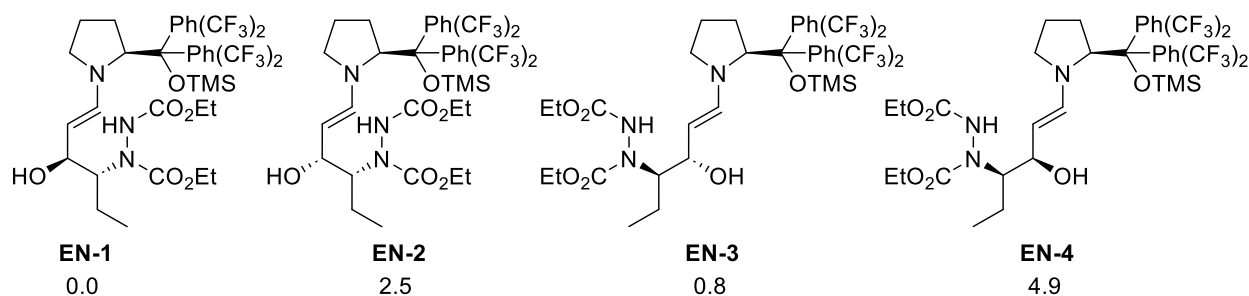


Figure 2.13: Michael addition intermediates.

We started with calculating the different configuration of the resulting enamine intermediates upon Michael Addition on **DA-INT** (Figure 2.13). The diastereomeric enamine intermediates **EN-1** and **EN-2**, which upon rotation would result in diastereomers **EN-3** and **EN-4** were calculated. It was determined that the enamine intermediate **EN-1** was thermodynamically favoured by 2.5 kcal/mol relative to the diastereomer **EN-2**. The rotation of **EN-1** results in **EN-3** which was determined to be slightly disfavoured by 0.8 kcal/mol while the diastereomer **EN-4** was found to disfavoured by 4.9 kcal/mol. The lack of thermodynamic preference for the enamine intermediate **EN-3** over **EN-1** upon rotation makes this pathway implausible.

2.4: Conclusions

Computational and experimental methods were utilized to study the aminocatalytic γ -amination reaction of enals with DEAD *via* dienamine activation. This reaction was investigated to rationalize the unexpected stereoselectivity of the product. Our calculations indicate that the reaction proceeds *via* a Diels-Alder type pathway, which is kinetically favoured compared to nucleophilic addition. The excellent regioselectivity is also a result of the nature of Diels-Alder reaction which takes place at the *ipso* and γ -carbon of the dienamine.

The γ -amination reaction results in product with *E*-configuration of the α,β -double bond and (*R*)-stereocenter. To understand the observed stereochemistry with *E*-configuration, two plausible

mechanisms were studied. Our calculations on the first mechanism consisting of downstream aminated dienamine suggested that the formation of aminated dienamine could be the driving force to result in intermediates with *E*-configuration. In order to obtain evidence of aminated dienamine, γ -amination reaction was performed with γ -deuterated-2,4-enal. The NMR monitoring of the reaction did not show any evidence of the downstream aminated dienamine. Furthermore, the productive intermediate with *E*-configuration containing (*R*)-stereocenter did not demonstrate thermodynamic preference. The intermediate resulting in product with (*S*)-stereocenter was thermodynamically preferred which is not observed experimentally.

The second mechanism consists of nucleophilic substitution of water molecule on the Diels-Alder cycloadduct **DA-INT**. This results in an enamine intermediate which, upon rotation, can lead to intermediate with (*E*)-configuration around the double bond. Our calculations indicate that there is no significant thermodynamic preference of intermediate resulting in product (*E*)-configuration around the α,β -double bond with (*R*)-stereocenter at the γ -position.

Overall, our mechanistic investigation suggests that the addition of DEAD to the dienamine proceeds *via* Diels-Alder pathway. However, the experimental and computational data did not support the proposed mechanism for the downstream reaction pathway. Therefore, new plausible mechanisms must be explored to rationalize the observed stereochemistry.

2.5: References

- (1) List, B.; Lerner, R. A.; Barbas, C. F. Proline-Catalyzed Direct Asymmetric Aldol Reactions. *J. Am. Chem. Soc.* **2000**, 122 (10), 2395–2396. <https://doi.org/10.1021/ja994280y>.

- (2) Ahrendt, K. A.; Borths, C. J.; MacMillan, D. W. C. New Strategies for Organic Catalysis: The First Highly Enantioselective Organocatalytic Diels - Alder Reaction. *J. Am. Chem. Soc.* **2000**, *122* (17), 4243–4244. <https://doi.org/10.1021/ja000092s>.
- (3) Bahmanyar, S.; Houk, K. N.; Martin, H. J.; List, B. Quantum Mechanical Predictions of the Stereoselectivities of Proline-Catalyzed Asymmetric Intermolecular Aldol Reactions. *J. Am. Chem. Soc.* **2003**, *125* (9), 2475–2479. <https://doi.org/10.1021/ja028812d>.
- (4) Burés, J.; Armstrong, A.; Blackmond, D. G. Explaining Anomalies in Enamine Catalysis: “Downstream Species” as a New Paradigm for Stereocontrol. *Acc. Chem. Res.* **2016**, *49* (2), 214–222. <https://doi.org/10.1021/acs.accounts.5b00394>.
- (5) Schmid, M. B.; Zeitler, K.; Gschwind, R. M. Distinct Conformational Preferences of Prolinol and Prolinol Ether Enamines in Solution Revealed by NMR. *Chem. Sci.* **2011**, *2* (9), 1793. <https://doi.org/10.1039/c1sc00274k>.
- (6) Schmid, M. B.; Zeitler, K.; Gschwind, R. M. Formation and Stability of Prolinol and Prolinol Ether Enamines by NMR: Delicate Selectivity and Reactivity Balances and Parasitic Equilibria. *J. Am. Chem. Soc.* **2011**, *133* (18), 7065–7074. <https://doi.org/10.1021/ja111544b>.
- (7) Bertelsen, S.; Marigo, M.; Brandes, S.; Dinér, P.; Jørgensen, K. A. Dienamine Catalysis: Organocatalytic Asymmetric γ -Amination of α,β -Unsaturated Aldehydes. *J. Am. Chem. Soc.* **2006**, *128* (39), 12973–12980. <https://doi.org/10.1021/ja064637f>.
- (8) Marcos, V.; Alemán, J. Old Tricks, New Dogs: Organocatalytic Dienamine Activation of α,β -Unsaturated Aldehydes. *Chem. Soc. Rev.* **2016**, *45* (24), 6812–6832. <https://doi.org/10.1039/c6cs00438e>.

- (9) Ramachary, D. B.; Reddy, Y. V. Dienamine Catalysis: An Emerging Technology in Organic Synthesis. *Eur. J. Org. Chem.* **2012**, 2012 (5), 865–887. <https://doi.org/10.1002/ejoc.201101157>.
- (10) Stiller, J.; Marqués-López, E.; Herrera, R. P.; Fröhlich, R.; Strohmann, C.; Christmann, M. Enantioselective α - and γ -Alkylation of α,β -Unsaturated Aldehydes Using Dienamine Activation. *Org. Lett.* **2011**, 13 (1), 70–73. <https://doi.org/10.1021/ol102559f>.
- (11) Kumar, I.; Ramaraju, P.; Mir, N. A. Asymmetric Trienamine Catalysis: New Opportunities in Amine Catalysis. *Org. Biomol. Chem.* **2013**, 11 (5), 709–716. <https://doi.org/10.1039/c2ob26681d>.
- (12) Zhou, Q.-Q.; Xiao, Y.-C.; Yuan, X.; Chen, Y.-C. Asymmetric Diels-Alder Reactions of 2,4,6-Trienals via Tetraenamine Catalysis. *Asian J. Org. Chem.* **2014**, 3 (4), 545–549. <https://doi.org/10.1002/ajoc.201400015>.
- (13) Stiller, J.; Poulsen, P. H.; Cruz, D. C.; Dourado, J.; Davis, R. L.; Jørgensen, K. A. Organocatalytic [4+2] Addition Reactions via Tetraenamine Intermediate. *Chem. Sci.* **2014**, 5 (5), 2052–2056. <https://doi.org/10.1039/c4sc00081a>.
- (14) Ouellet, S. G.; Tuttle, J. B.; MacMillan, D. W. C. Enantioselective Organocatalytic Hydride Reduction. *J. Am. Chem. Soc.* **2005**, 127 (1), 32–33. <https://doi.org/10.1021/ja043834g>.
- (15) Seegerer, A.; Hioe, J.; Hammer, M. M.; Morana, F.; Fuchs, P. J. W.; Gschwind, R. M. Remote-Stereocontrol in Dienamine Catalysis: Z-Dienamine Preferences and Electrophile–Catalyst Interaction Revealed by NMR and Computational Studies. *J. Am. Chem. Soc.* **2016**, 138 (31), 9864–9873. <https://doi.org/10.1021/jacs.6b04008>.
- (16) Becke, A. D. A New Mixing of Hartree–Fock and Local Density-functional Theories. *J. Chem. Phys.* **1993**, 98 (2), 1372–1377. <https://doi.org/10.1063/1.464304>.

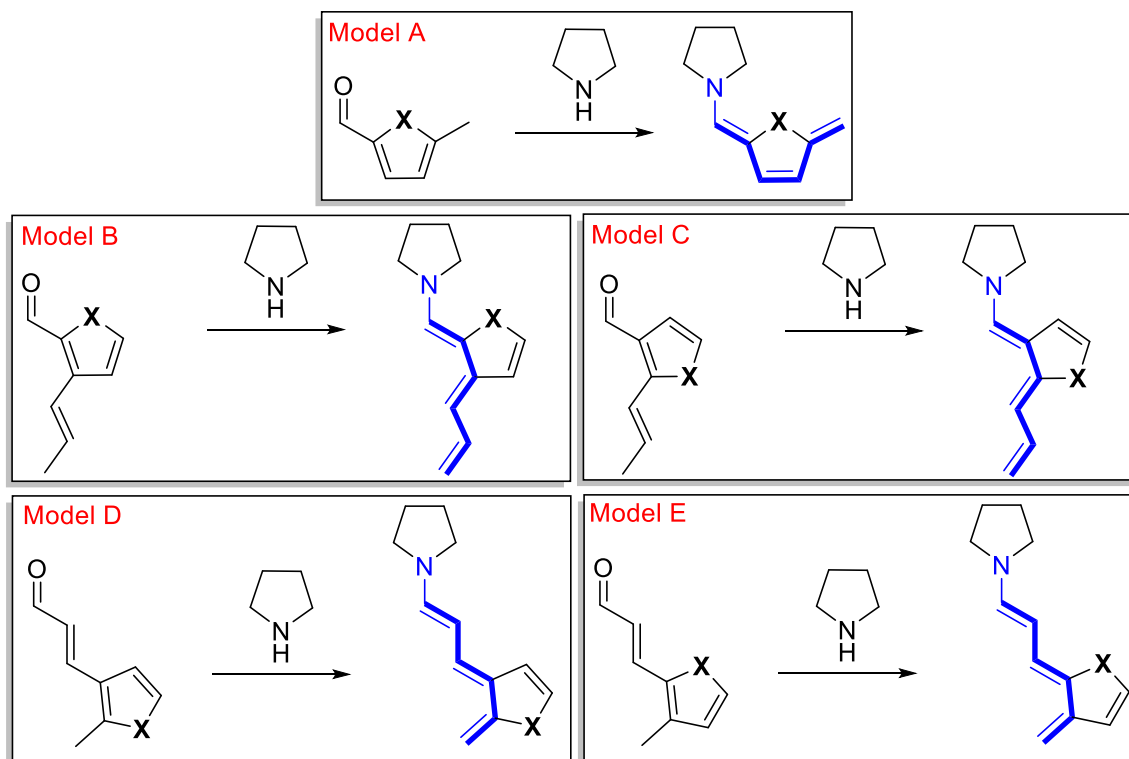
- (17) Becke, A. D. Density-functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, 98 (7), 5648–5652. <https://doi.org/10.1063/1.464913>.
- (18) Petersson, G. A.; Al-Laham, M. A. A Complete Basis Set Model Chemistry. II. Open-Shell Systems and the Total Energies of the First-Row Atoms. *J. Chem. Phys.* **1991**, 94, 6081–6090. <https://doi.org/10.1063/1.460447>.
- (19) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A Complete Basis Set Model Chemistry. I. The Total Energies of Closed-shell Atoms and Hydrides of the First-row Elements. *J. Chem. Phys.* **1998**, 89 (4), 2193. <https://doi.org/10.1063/1.455064>.
- (20) Tomasi, J.; Mennucci, B.; Cammi, R. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005**, 105 (8), 2999–3093. <https://doi.org/10.1021/cr9904009>.
- (21) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. a.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. a.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, a. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, a. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. a.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. a.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, a. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 09*, Gaussian, Inc., Wallin. 2009

- (22) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function. *Theor. Chem. Acc.* **2008**, *120* (1–3), 215–241. <https://doi.org/10.1007/s00214-007-0310-x>.
- (23) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7* (18), 3297–3305. <https://doi.org/10.1039/B508541A>.
- (24) Legault, C. Y. *CYLview20*;, Université de Sherbrooke, **2020** (<http://www.cylview.org>)

Chapter 3 : Exploring the Role of Aminocatalysis in the Dearomatization and Regioselectivity of Heteroaromatic Aldehydes.

3.1: Introduction

Heteroaromatic scaffolds (specifically furans, pyrrole and thiophenes) have recently gained attention as a substrate for asymmetric vinylogous aminocatalysis and have been used to form polyenamine intermediates for remote alkylation and numerous Diels-Alder reactions.¹⁻⁸ These heteroaromatic compounds appear to be a privileged scaffold for asymmetric aminocatalysis as they not only provide a rigid, conjugated backbone for improved stereocontrol but also have enhanced reactivity upon formation of the enamine due to conjugation of the polyenamine with the heteroatom of the aromatic ring. These features, paired with the driving force of regeneration of the aromatic ring upon reaction of the enamine, suggest there is a great deal of potential for further development in this area of remote functionalization of heteroaromatic aldehydes.



Scheme 3.1: Model systems studied in this work (X=O, NH, and S)

The relative stability of enamines can be readily assessed by examining the energies of the equilibrium between two carbonyls and their corresponding enamines (i.e.: carbonyl A + enamine B $\rightarrow$ enamine A + carbonyl B).⁹ However, one of the most interesting features of aminocatalytic reactions involving heteroaromatic aldehydes is the formation of dearomatized trienamine intermediates. Herein, we have examined a series of heteroaromatic aldehydes (Scheme 1) with particular emphasis on the effects that the formation of the iminium ion intermediates have in the dearomatization of these systems. The use of homodesmotic equations to study the aromaticity of 5-membered heteroaromatic rings has been explored in the literature.^{10–14} In this, we decided to employ a higher hierarchy of homodesmotic equations, hyperhomodesmotic equations, to more accurately assess the dearomatization penalty for the Model Systems depicted in Scheme 1.^{15,16} Hyperhomodesmotic equations allow for a systematic error cancelation and thus provide a good

estimation of the energy penalties for dearomatization of these systems.^{15,16} We have also studied the trienamine intermediates formed from these aldehydes and have employed computational methods for predicting the most reactive sites of the intermediates, including population analysis of the HOMOs and isosurfaces of Fukui functions.¹⁷

3.2: Computational methods

All structures were optimized in the gas phase using M06-2X¹⁸ with the double- ζ split valence 6-31+G(d,p) basis set^{19,20} and vibrational analysis verified that each structure was a minimum. All optimizations were performed in Gaussian 09.e01.²¹ Single point energies were calculated using M06-2X¹⁸ functional and the correlation-consistent basis set cc-pVTZ²² as well as the second order Møller-Plesset perturbation theory (MP2)^{23–26} with the cc-pVTZ²² basis set. Values discussed in test are free energies calculated at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p). MP2/cc-pVTZ//M06-2X/6-31+G(d,p) energies are included in tables and show the same trends as those calculated with M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p). Orbital coefficients were generated with QMForge v2.1.²⁷ Electrostatic potential-derived charges were calculated using CHelpG scheme.²⁸ The Fukui function describes the change of the electronic density $f(r)$ in a given point with respect to the change in the number of electrons, both calculated at the geometry of the neutral molecule. This approach has been used to predict reactivity in organic molecules.^{17,29–31} All 3D figures were generated using VESTA v3.5.5.³²

3.3: Results and Discussion

3.3.1: Model System A

To begin this study, we explored the simplest heteroaromatic system bearing an aldehyde and a methyl group at the 2- and 5-positions of the ring, respectively (Model System A, Scheme

1). This represents one of the first compounds that employed the dearomatization approach in the formation of polyenamines for the remote alkylation of furfural derivatives.^{33,34} We decided to focus on the influence that the *transient* iminium ion has on the formation of the dearomatized trienamine intermediate using the hyperhomodesmotic equations outlined in Table 3.1. The first equation examines the energetic cost of breaking the aromaticity of the furfural derivative by forming its enol tautomer while the second equation evaluates the same energetic penalty with the iminium ion derived from furfural.

Table 3.1: Hyperhomodesmotic equations used to assess the dearomatization of Model System A. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p). All reported values are in kcal/mol

(1)

A1; X = O
A2; X = NH
A3; X = S **A4** **A5; X = O**
A6; X = NH
A7; X = S **A8**

(2)

A9; X = O
A10; X = NH
A11; X = S **A12** **A13; X = O**
A14; X = NH
A15; X = S **A16**

	X = O	X = NH	X = S
Equation 1	11.1 (9.3)	16.8 (14.6)	11.5 (10.1)
Equation 2	5.4 (3.8)	15.0 (13.0)	5.1 (3.2)
$\Delta\Delta G_{(eq.2-eq.1)}$	-5.7 (-5.5)	-1.8 (-1.6)	-6.4 (-6.9)

In examining the energetics of equations 1 and 2, the dearomatization of the heteroaromatic ring in both the aldehydes **A1-3** (X = O, NH, S, respectively) and the

corresponding iminium ions **A9-11** is disfavored. However, the presence of the iminium ion decreases the energetic penalty for loss of aromaticity in all heterocycles **A9-11** when compared to the corresponding aldehydes **A1-3** (Table 3.1). Calculations on these equations with MP2/cc-pVTZ //M06-2X/6-31+G(d,p) show the same energetic trends with deviation of less than 0.4 kcal/mol for all systems. This decrease in the energy penalty suggests that the presence of the iminium ion facilitates dearomatization.

Perhaps the most interesting observation noted is in the comparison of the influence of the iminium ion across the three heterocyclic systems. The formation of the iminium ion in the furan and thiophene systems has a significant influence on the dearomatization, in each case lowering it by ~6 kcal/mol, relative to the corresponding aldehydes. On the other hand, the effect of the iminium ion in the pyrrole system is significantly less, lowering it by less than 2 kcal/mol relative to the aldehyde.

To understand how the choice of heteroatom in the heteroaromatic ring influences the energetic penalty for dearomatization in Model System A, we examined the geometries of all structures involved in equations 1 and 2. While no large geometric changes were noted in comparing the structures of aldehydes (**A1-3** and **A8**) and iminium ions (**A9-11** and **A16**), comparison of the enols and trienamines did reveal a significant change in geometry in **A14** relative to **A6** (X = NH). In trienamine **A14**, the pyrrolidine ring of the catalyst is bent so that the nitrogen lone pair is not fully aligned for donation into the π -system of the trienamine. This twisting appears to be due to steric clash of the alkyl ring of the catalyst with the N-H bond of the pyrrole and is not present in the furan- and thiophene-based systems (see supporting data). Comparison of the N_{cat}-C bond lengths of the enamines (1.36 Å for **A13**, 1.38 Å for **A12**, 1.36 Å for **A15**, and 1.39 Å for **A14**) suggests that trienamine **A14** is the least conjugated (see supporting

data). In the corresponding enolate **A6** the pyrrole NH does not encounter the same steric repulsion and is not bent out of conjugation, resulting in an increase in energy for the formation of trienamine in the pyrrole system.

Next, we wanted to assess the influence of the heteroaromatic ring on the regioselectivity of the addition reaction. To do this, we performed population analysis of the HOMO of the trienamine systems **A12-15** (Figure 3.1 and Table 3.2). In order to evaluate the possible synergistic effects between the conjugation provided by the aminocatalyst and the heteroatom, the all-carbon trienamine **A12** was also computed. Examination of the HOMO orbital coefficients of the trienamine derived from cyclopentadiene **A12** reveals that it follows the general vinylogy principle³⁵, with the α -carbon having the largest coefficient followed by γ -carbon and then the ε -carbon (Table 3.2). The presence of the heteroatom in the ring system of Model System A (trienamines **A13-15**) significantly increases the orbital coefficient at the ε -carbon whereas the orbital coefficients for β - and γ -carbons decrease relative to those in **A12**. An interesting feature of this model is the very low orbital coefficient observed at the γ -carbon in trienamines **A13-15**, when compared to **A12**. It would appear that the heteroatom in the ring is influencing the conjugated trienamine backbone in two ways; it donates into the terminal double bond, increasing the orbital coefficient at the ε -carbon and it also disrupts the donating abilities of the amine *via* cross-conjugation with the enamine, decreasing the orbital coefficients at the α - and γ -carbons. To further explore the electronic nature of these enamine intermediates isosurfaces of the Fukui function were also generated. Consistent with our orbital analysis of the Fukui isosurface shows the most nucleophilic site to be the ε -carbon of each heterocyclic enamine (see supporting data).

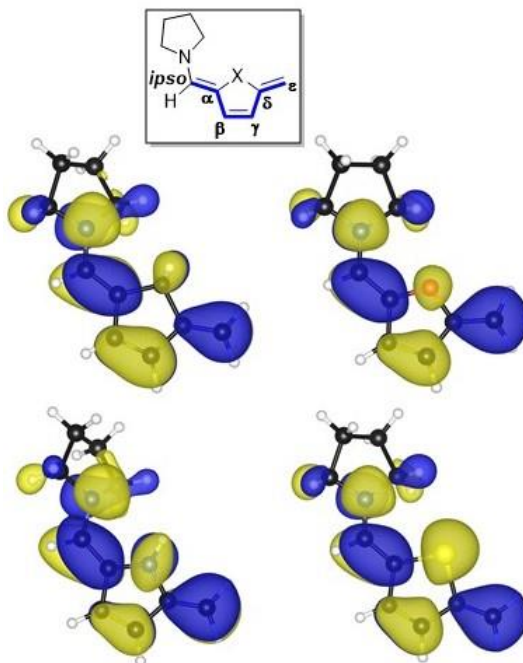


Figure 3.1: HOMO of trienamines A12-A15 for Model System A (isovalue 0.035)

Table 3.2: Orbital coefficients of the HOMO of trienamines A12-A15.

Carbon	A12 (X = CH ₂)	A13 (X = O)	A14 (X = NH)	A15 (X = S)
<i>ipso</i>	13.6	11.8	15.2	10.8
α	18.7	11.3	8.4	11.2
β	7.5	3.4	3.3	3.3
γ	16.0	8.0	5.6	7.6
δ	2.5	3.3	3.7	3.4
ϵ	12.3	19.7	20.6	16.7

Overall, the decreased energy penalty associated with the dearomatization of the trienamine system and the regiochemical preferences suggested by the orbital analysis of the various trienamines are in agreement with the experimental results reported by Albrecht and co-workers.^{33,34} Our results also suggest that other heteroaromatic rings follow a similar trend so, similar reactivity may be achieved employing those systems.

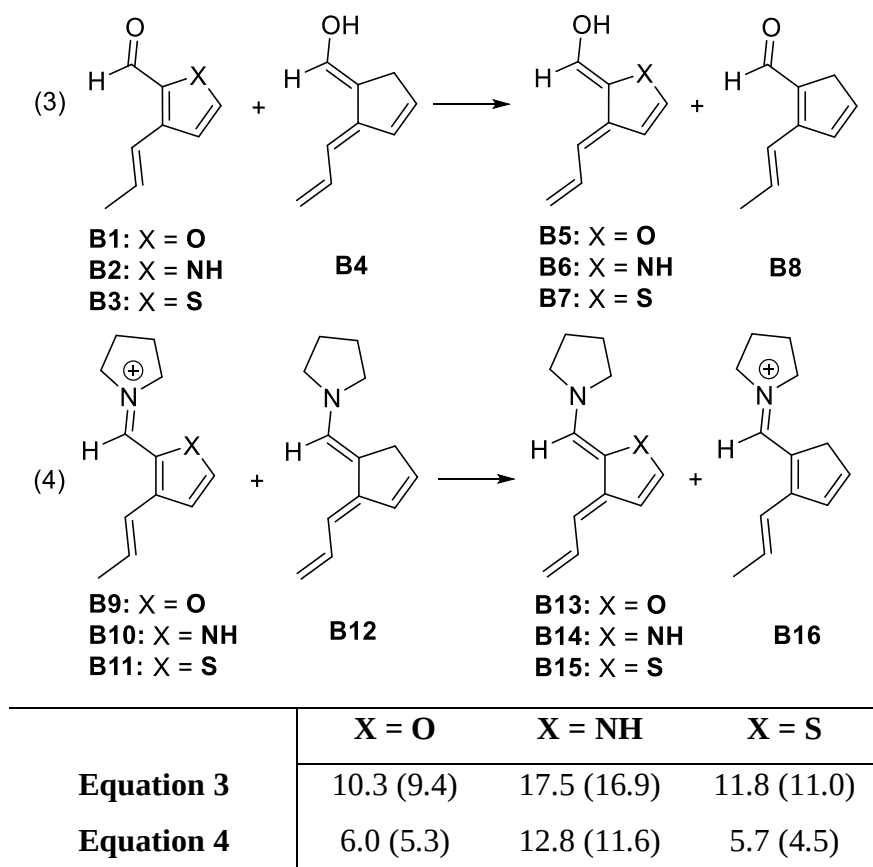
3.3.2: Model system B

Next, we explored a family of heterocyclic systems containing an allyl group on the 3-position of the ring (Model System B, Scheme 3.1). Upon deprotonation at the ϵ -carbon of the corresponding iminium ion, aromaticity in the ring is disrupted as the trienamine intermediate is formed. While these ortho-olefinated, heterocyclic aldehydes have been synthesized and have found use as intermediates in the design of photoswitches and optoelectronics,^{36–38} to the best of our knowledge, they have yet to be used as substrates in organocatalytic reactions. However, the rigidity provided by the heterocyclic scaffold suggests that they would serve as optimal substrates for organocatalytic remote functionalization and, therefore, we decided to perform a similar study to that made for Model System A to provide insights into what features this scaffold may present for future organocatalytic reaction development.

Assessment of the impact of the pyrrolidine catalyst on the energetic penalty for dearomatization of the substrate was achieved through hyperhomodesmotic equations 3 and 4 (Table 3.3). It was observed that dearomatization of aldehydes **B1-3** (eq. 3) and iminium ions **B9-11** (eq. 4) is, again, disfavored. Similar to Model System A, the addition of the aminocatalyst decreases the energetic penalty for the loss of aromaticity by 4-6 kcal/mol in all heterocycles **B9-11** when compared to the corresponding aldehydes **B1-3** (Table 3.3). Upon analyzing the geometries of structures involved in equations 3 and 4, no major changes were observed when

comparing the geometries of aldehyde (**B1-3** and **B8**) and corresponding enols (**B4-B7**). However, comparison of the iminium ions (**B9-B11** and **B16**) and trienamines (**B12-B15**) shows a significant geometric change in trienamine structures. While the dihedral angles between $C_{\text{cat}}-N_{\text{cat}}-C_{\text{ipso}}-C_{\alpha}$, in the parent iminium ions **B9-11** and **B16**, are fairly planar (between 0.6 and 2.7°), they are distorted in the enamines to 33.5° in **B12**, 4.2° in **B13**, 46.6° in **B14**, and 27.5° in **B15**. These changes are caused by increased steric repulsion between the CH_2 unit of the catalyst and hydrogens and/or lone pairs of X in the cyclic substrate (see supporting data). The loss of planarity in trienamines results in minimizing the steric clashes and consequently, favoring the dearomatization of iminium ions.

Table 3.3: Hyperhomodesmotic equations used to assess the dearomatization of Model System B. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.



$\Delta\Delta G_{(eq.4-eq.3)}$	-4.3 (-4.1)	-4.7 (-5.3)	-6.1 (-6.6)

To assess the influence of the heteroaromatic ring in Model System B on the potential regioselectivity of an addition reaction we performed a population analysis of the HOMO of the trienamine systems **B12-15** (Figure 3.3). It was observed that for all trienamines **B12-15**, the coefficient at γ -carbon is the higher than any of the other carbons in the trienamine backbone (Table 3.4). This appears to be the result of the cross conjugated nature of the π system.³⁹ This effect is enhanced in the heteroaromatic trienamines **B13-15** by the constructive donation from both the heteroatom in the ring and the N of the catalyst at the γ -carbon. The orbital coefficient on the α -carbon is lowered in these systems due to the cross-conjugation of the two heteroatoms. The increased nucleophilicity at the γ -carbon was also identified by the isosurfaces of the Fukui functions for **B13-15** (see supporting data).

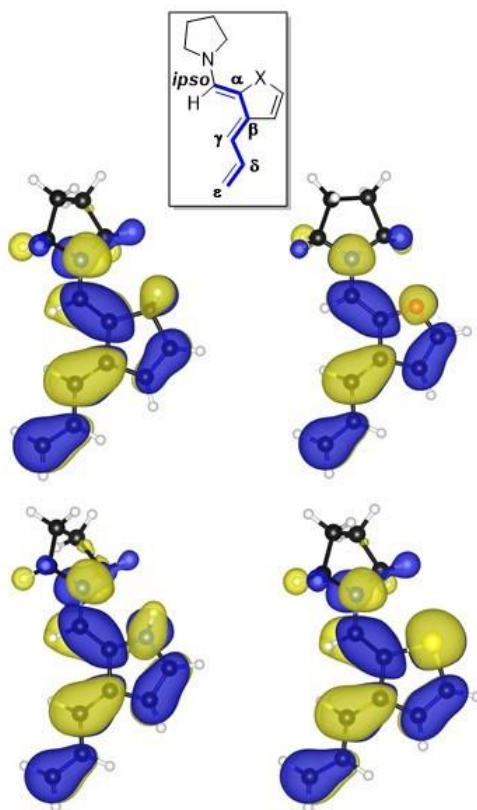


Figure 3.2: HOMO of trienamines **B12-B15** (isovalue 0.035).

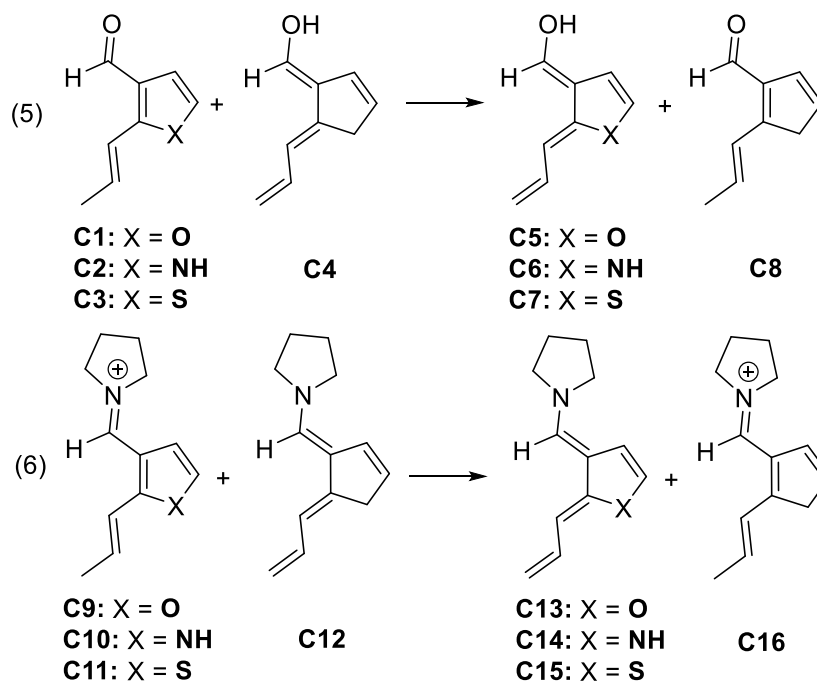
Table 3.4: Orbital coefficients of the HOMO of Model System B.

Carbon	B12 (X = CH ₂)	B13 (X = O)	B14 (X = NH)	B15 (X = S)
<i>ipso</i>	10.8	10.9	14.4	10.8
α	15.2	11.6	8.1	10.5
β	8.6	4.9	4.8	4.2
γ	21.0	21.4	19.4	17.8
δ	2.5	1.5	1.4	1.2
ϵ	12.4	11.2	10.1	9.0

3.3.3: Model System C

Swapping of the positions of the aldehyde and allyl groups in Model system B provided our next heteroaromatic aldehyde, Model System C (Scheme 1). This scaffold has been recently used by Chen and co-workers to perform stereoselective remote Michael additions.⁴⁰ In this case, the application of a bifunctional organocatalyst with the furfural derivatives allowed for the formation of the trienamine intermediate that then reacted with electron-deficient 3-olefinic oxindoles, giving the corresponding Michael adducts in good yields and enantioselectivities.

Table 3.5: Hyperhomodesmotic equations used to assess the dearomatization of Model System C. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p). All reported values are in kcal/mol



	X = O	X = NH	X = S
Equation 5	10.4 (10.3)	15.5 (15.6)	10.6 (10.3)
Equation 6	7.4 (7.8)	16.7 (17.6)	6.4 (6.3)
$\Delta\Delta G_{(eq.6-eq.5)}$	-3.0 (-2.4)	1.2 (2.1)	-3.7 (-4.0)

As with the previous model systems, the hyperhomodesmotic equations 5 and 6 (Table 3.5) suggest that the conversion of aldehydes **C1-3** and iminium ions **C9-11**, to the corresponding trienamines, is an unfavourable process. However, the penalty for loss of aromaticity in iminium ion **C9** ($X = O$) is over 2 kcal/mol lower than that of the parent aldehyde **C1**, suggesting the iminium ion is decreasing the penalty for dearomatization. This is also the case in the thiophene system (**C11** vs **C3**) where the presence of the iminium ion decreases the penalty for loss of aromaticity by nearly 4 kcal/mol. Conversely, the loss of aromaticity in iminium ion **C10** ($X = NH$) is 1-2 kcal/mol higher than that for the dearomatization of aldehyde **C2** (Table 3.5). This can be explained by the increased loss of delocalization of the pyrrole lone pair into the iminium ion upon formation of the trienamine. This delocalization can be seen in the increased length of the $C_\alpha-C_\beta$ double bond in **C10** (1.42 Å) relative to that in **C6** (1.40 Å). It is also indicated by a distortion in the planarity of the exocyclic double bond in **C10**, which is twisted out of the plane of the aromatic ring to avoid steric interactions between the N-H bond of the pyrrolidine and the C-H of the exocyclic double bond (see supporting data).

To assess the influence of the heteroaromatic ring in Model System C on the potential regioselectivity of an addition reaction, we performed a population analysis of the HOMO of the trienamines **C12-15** (Figure 3.5). Population analysis shows that for trienamine **C12** ($X = CH_2$) the vinylogy principle is obeyed, i.e. the highest orbital coefficient in the HOMO is at α -carbon followed by γ -carbon and finally ε -carbon. However, when $X =$ heteroatom, γ -carbon exhibits the highest orbital coefficient in the HOMO (Table 3.14). Similar to Model System B, there appears to be a synergistic effect between the N_{cat} and the heteroatom of the substrate ring which increase the electron density at carbon γ -carbon (Figure 3.5 and Table 3.6). It is also observed that α - and ε -carbons have similar values in their orbital coefficients which could indicate some cross

conjugation between the heteroatom and *ipso*-carbon. The increased nucleophilicity at the γ -carbon for our heterocyclic triamines was also identified by the Fukui isosurfaces for **C13-15** (see supporting data).

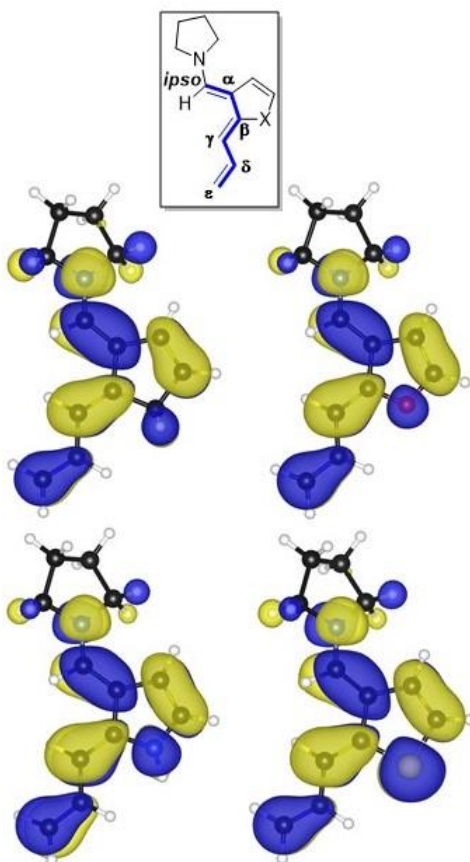


Figure 3.3: HOMO of the trienamines **C12-C15** for Model System C (isovalue (0.035)).

Table 3.6: Orbital coefficients for the HOMO of trienamines **C12-C15**.

Carbon	C12 (X = CH ₂)	C13 (X = O)	C14 (X = NH)	C15 (X = S)
<i>ipso</i>	13.2	11.2	10.7	10.3
α	19.0	12.6	10.2	11.4

β	4.7	3.7	3.0	3.4
γ	14.4	20.3	22.6	17.9
δ	1.3	1.6	1.2	1.1
ϵ	7.5	10.7	11.3	8.7

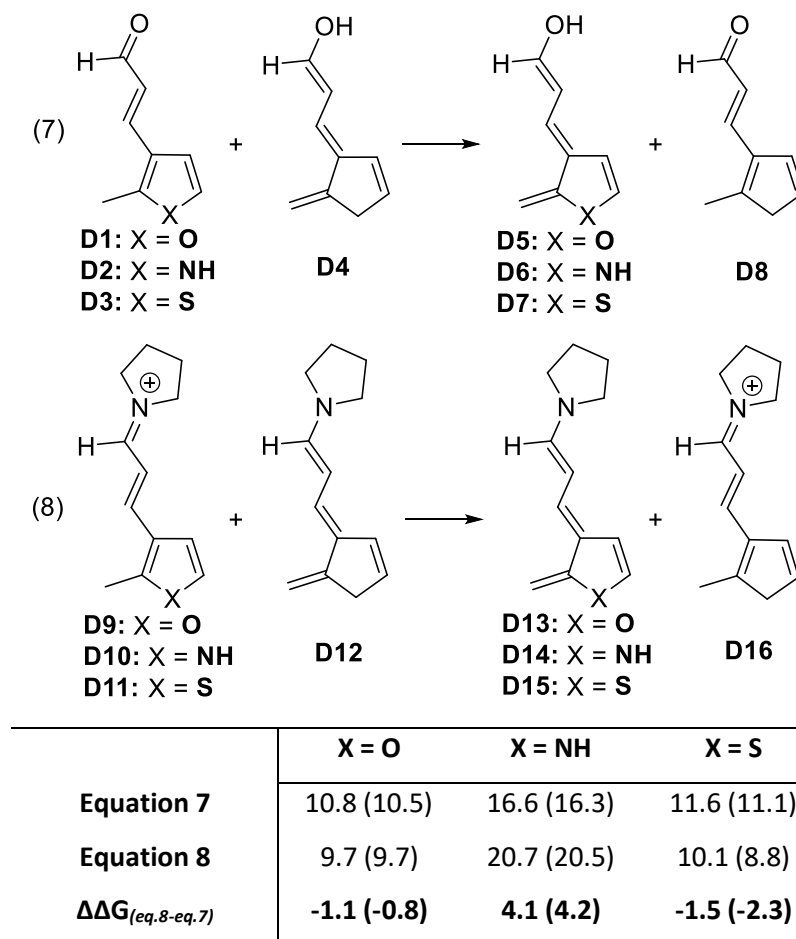
The orbital coefficients calculated for trienamine **C12** appear to be in contradiction to the work reported by Chen and co-workers,⁴⁰ where the authors observed functionalization at the ϵ -position. In spite of that, it is worth highlighting that the authors used a bifunctional H-bond/aminocatalyst and it is likely that the H-bond donor properties of the catalyst may have directed the electrophile to the more remote ϵ -carbon, overcoming the inherent nucleophilicity of the γ -carbon.

3.3.4: Model System D

Next, we explored Model System D where an α,β -unsaturated aldehyde is at the 3-position of the ring and a methyl substituent at the 2-position. The indole-based version of this system has been reported by Melchiorre and co-workers to undergo a Diels-Alder reaction *via* formation of an *ortho*-quinodimethane trienamine intermediate with indole rings.^{41,42} The authors also explored the reactivity of these systems towards Diels-Alder reaction using both a pyrrole and a furan system and achieved the same type of reactivity with 3-olefinic oxindoles as the dienophile.⁴³

Table 3.7: Hyperhomodesmotic equations used to assess the dearomatization of Model System D. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in

parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.



As with the previous model systems, hyperhomodesmotic equations 7 and 8 (Table 3.7) suggest that the conversion of aldehydes **D1-3** and iminium ions **D9-11** to the corresponding trienes is an unfavourable process. However, in this system, it appears that the formation of the iminium ions does not have a major influence in the energy penalty for loss of aromaticity when X = O or S. Iminium ions **D9** and **D11** (X = O and S, respectively) are favoured to undergo dearomatization by approximately 1 and 2 kcal/mol compared to their respective parent aldehydes **D1** and **D3**. On the other hand, when X = NH the loss of aromaticity in iminium ion **D10** (X = NH) is c.a. 4 kcal/mol higher than that for the dearomatization of aldehyde **D2** (Table 3.7). One possible

explanation to why the nitrogen system appears to be less favoured to undergo dearomatization relates to the stabilization of the iminium ion **D10**. Unlike the previous model systems, there does not appear to be any major steric constraints in this model system that force the π -system to distort thereby weakening donation from the heteroatoms. When comparing the bond distances between aldehyde **D2** (1.46 Å for $C_{\text{ipso}} - C_{\alpha}$, 1.35 Å for $C_{\alpha} - C_{\beta}$, 1.45 Å for $C_{\beta} - C_{\gamma}$, 1.39 Å for $C_{\gamma} - C_{\delta}$ and 1.36 Å for $C_{\delta} - N$) and iminium ion **D10** (1.38 Å for $C_{\text{ipso}} - C_{\alpha}$, 1.41 Å for $C_{\alpha} - C_{\beta}$, 1.41 Å for $C_{\beta} - C_{\gamma}$, 1.41 Å for $C_{\gamma} - C_{\delta}$ and 1.35 Å for $C_{\delta} - N$), it is clear that the nitrogen from the heteroaromatic ring is donating charge to the iminium ion (see supporting data). This effect stabilizes the iminium ion making less likely to undergo dearomatization.

Population analysis of the trienamines (Figure 3.7) shows that for this model, the ϵ -carbon carries the highest coefficient for the HOMO in the heteroaromatic trienamines **D13-15** (Table 3.8). This effect is similar to that found in Model System A and can be explained by the synergistic effect between the lone pair on the nitrogen of the aminocatalyst and the heteroatom in the aromatic ring, which combine to increase the electron density at the terminal position of the trienamine system (Figure 4). Fukui isosurfaces for **D13-15** also indicate that the ϵ -carbon of each of these heterocyclic triamines was the most nucleophilic (see supporting data). In the case of the cyclopentadiene derived trienamine **D12** ($X = \text{CH}_2$) the orbital coefficients at α - and γ -carbons are nearly equal in value. Similar trends were seen in Model System B however in this case it does not appear to be the result of the conjugated carbon π -system, as both models share the same carbon backbone, and instead is a combination of donation from N_{cat} and hyperconjugation with the C-H bonds of the sp^3 hybridized carbon in the ring.

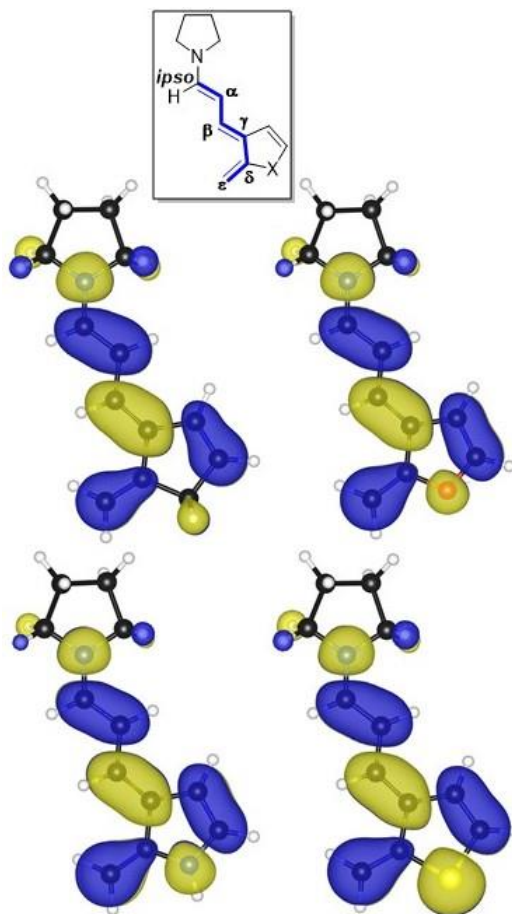


Figure 3.4 HOMO of the trienamines **D12-D15** for Model System D (isovalue 0.035).:

Table 3.8: Orbital coefficients for the HOMO of trienamines **D12-D15**.

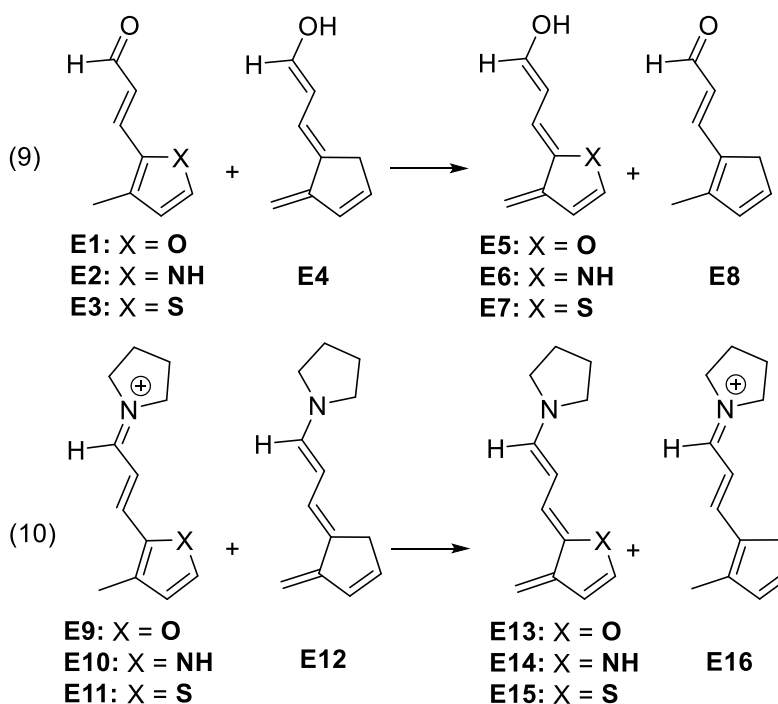
Carbon	D12 (X = CH ₂)	D13 (X = O)	D14 (X = NH)	D15 (X = S)
<i>Ipso</i>	10.7	8.6	9.1	8.0
α	16.7	10.2	12.9	10.8
β	11.0	12.0	11.2	10.3
γ	17.5	11.5	13.9	12.5
δ	1.4	1.1	1.2	1.3
ϵ	8.8	17.0	14.8	13.9

Our calculations show that aminocatalysis does not have a major influence on the dearomatization of this type of systems. Nonetheless, Melchiorre's work show that secondary amine catalysts can still be exploited with this scaffold for regio- and stereoselective Diels-Alder reactions.^{42,43}

3.3.5: Model system E.

Finally, we explored Model System E which contains an α,β -unsaturated aldehyde at the 2-position of the ring and a methyl substituent on 3-position. To the best of our knowledge, this system has not been explored in any asymmetric synthetic approach but, due to its similarities with the previous Model, we decided it would be interesting to explore it in this work.

Table 3.9: Hyperhomodesmotic equations used to assess the dearomatization of Model System E. Values in plain text are free energies at M06-2X/cc-pVTZ //M06-2X/6-31+G(d,p) and values in parentheses are free energies at MP2/cc-pVTZ//M06-2X/6-31+G(d,p)). All reported values are in kcal/mol.



X = O

X = NH

X = S

Equation 9	9.3 (8.8)	15.1 (14.2)	10.6 (9.7)
Equation 10	8.4 (7.7)	15.9 (14.9)	7.2 (6.0)
$\Delta\Delta G_{(eq.10-eq.9)}$	-0.9 (-1.1)	0.8 (0.7)	-3.4 (-3.5)

As with all previous model systems, hyperhomodesmotic equations 9 and 10 (Table 3.9) suggest that the conversion of aldehydes **E1-3** and iminium ions **E9-11** to the corresponding trienes is an unfavorable process. Similar to Model System D, it appears that the catalyst has little influence on the dearomatization step, with iminium ions **E9** and **E10** having an energy difference of approximately -1 kcal/mol and 1 kcal/mol, respectively, while iminium ion **E11** is slightly more favoured to undergo dearomatization when compared to their respective parent aldehydes (Table 3.9). Analysis of the geometries of the structures in each of the equations for this system show no major changes between the aldehydes (**E1-3**) and iminium ions (**E9-10**) nor between enols (**E5-7**) and trienamines (**E13-15**), with all systems remaining fairly planar (see supporting data).

Examination of the HOMO orbital coefficients of the trienamine derived from cyclopentadiene **E12** reveals that it follows the general vinylogy principle³⁵, with the α -carbon having the largest coefficient followed by γ -carbon and then the ε -carbon (Figure 3.9 and Table 3.10). The presence of the heteroatom in the ring system of Model System E (**E13-15**) significantly increases the orbital coefficients at the ε -carbons while also decreasing the orbital coefficients γ -carbons relative to those in **E12**. This trend is similar to that described in Model System A and is again the result of constructive donation into the ε -position by both heteroatoms. Isosurfaces generated using the Fukui function are consistent with our orbital analysis of the HOMO and show the ε -carbon of each heterocyclic enamine to be the most nucleophilic (see supporting data).

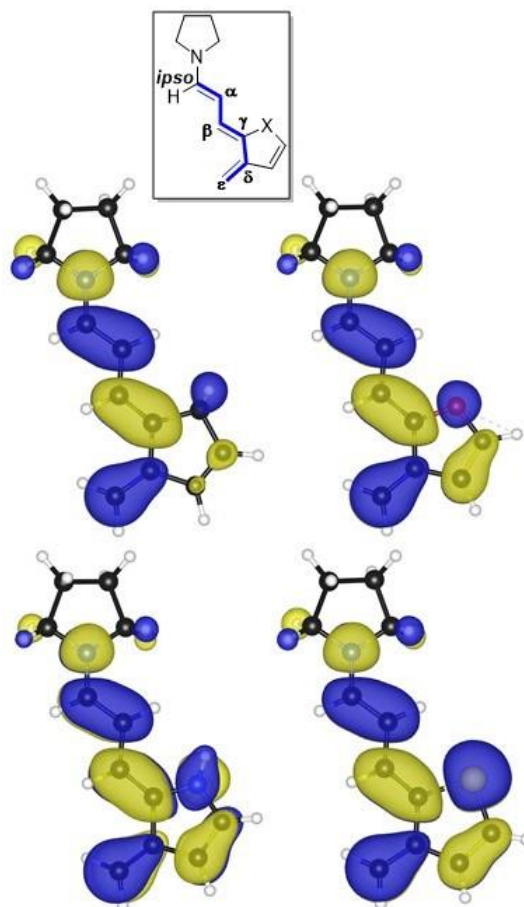


Figure 3.5: HOMO of the trienamines **E12-E15** for Model System E (isovalue 0.035).

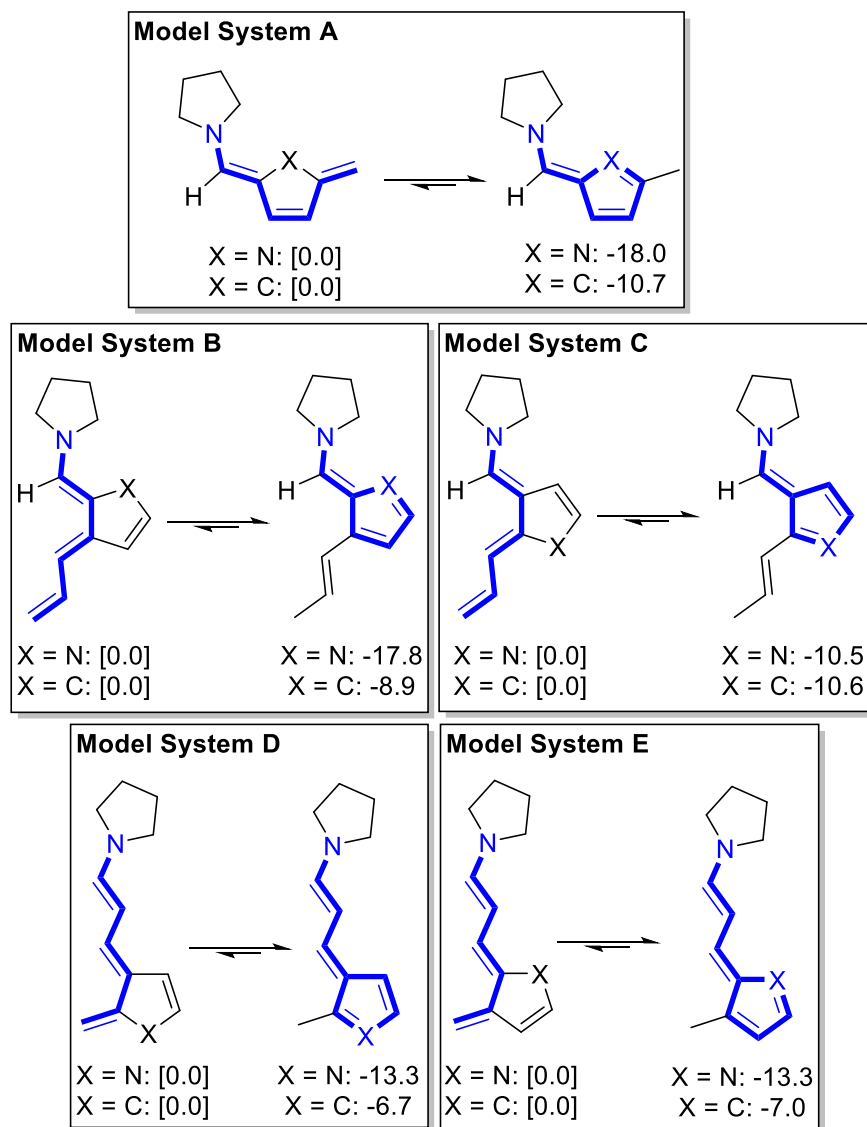
Table 3.10: Orbital coefficients for the HOMO of trienamines **E12-E15**.

Carbon	E12 (X = CH ₂)	E13 (X = NH)	E14 (X = O)	E15 (X = S)
<i>Ipso</i>	10.6	9.7	9.3	8.2
α	19.2	14.5	11.4	11.6
β	8.9	10.8	13.3	10.6
γ	18.5	13.0	11.1	11.9
δ	2.4	1.8	1.7	1.6
ϵ	12.7	15.5	15.3	13.5

3.3.6: Fulvene systems

During the study of the Model Systems illustrated in Scheme 3.1, it became evident that when $X = \text{CH}_2$ or NH another trienamine intermediate could be formed by deprotonation of X . This other possibility opens the doors to the formation of (hetero)fulvenes which can then be used as 6-electron systems for higher-order cycloadditions. In fact, some examples have been recently reported by Jørgensen and co-workers, such as [10+2]- and [10+4]-cycloadditions using isobenzofulevenes^{44–46} and hetero-[6+4]- and [6+2]-cycloadditions using 2-formyl substituted pyrroles, imidazoles and pyrazoles.⁴⁷

Consequently, we decided to explore the energy differences between the trienamines depicted in the previous models to the possible fulvenes (Scheme 3.2). It is clear from Scheme 3.2 that, in all Model Systems, the fulvenes are thermodynamically preferred over the trienamines previously explored. This feature expands the scope of these substrates as possible polyenes for high-order cycloadditions as well as non-classical modes of activation. In all cases when $X = \text{N}$, methylation of the nitrogen atom would prevent the formation of the fulvene and force formation of the trienamine while maintaining the observed trends in the orbital coefficients, for all models (see supporting information). Hyperhomodesmotic equations on the *N*-methylated systems indicate that the energetic penalties for dearomatization in these alkylated versions of Model Systems A and B are lower than those of the unprotected pyrrole systems presented in Tables 1 and 3. However, in the *N*-methylated versions of Model Systems C, D, and E, the energetic penalties for dearomatization increase relative to their respective unprotected pyrroles (see supporting information for details)



Scheme 3.2: Energy differences between linear trienamines and (hetero)fulvene systems for all Model Systems ($X = \text{CH}_2$ or NH ; relative free energies in kcal/mol calculated at the M06-2X/6-31+G(d,p) level of theory).

3.4: Conclusions

In conclusion, we investigated the influences of an aminocatalyst in the dearomatization of a series of heteroaromatic aldehydes in order to form a trienamine reactive intermediate. Our calculations suggest that all Models are good candidates for further synthetic studies with the furan and thiophen derived scaffolds being the most favourable as they possess a smaller energy penalty

for formation of the trienamine intermediate. Orbital analysis indicates that the closer the heteroatom in the aromatic ring is to the epsilon position of the trienamine the more likely it is for that carbon to possess a higher orbital coefficient in the HOMO. This would suggest an inherent regioselectivity for the more distal positions. Fukui functions were also calculated and follow a similar trend. Nonetheless, as experimental work cited in this paper has shown, this regioselectivity can be overridden by a careful choice of aminocatalyst and reaction conditions. Experimental work cited in this manuscript helps to support our findings for Model Systems A, C and D. Model Systems B and E, to the best of our knowledge, have yet to be used in asymmetric aminocatalysis but are promising scaffolds for further development in this area. Furthermore, it has been illustrated that when cyclopentadienes or pyrroles are used, it is thermodynamically possible to obtain electron-rich (hetero)fulvene systems that can be exploited in high-order cycloadditions.

3.5: References

- (1) Jensen, K. L.; Dickmeiss, G.; Jiang, H.; Albrecht, Ł.; Jørgensen, K. A. The Diarylprolinol Silyl Ether System: A General Organocatalyst. *Acc. Chem. Res.* **2012**, *45* (2), 248–264. <https://doi.org/10.1021/ar200149w>.
- (2) Kumar, I.; Ramaraju, P.; Mir, N. A. Asymmetric Trienamine Catalysis: New Opportunities in Amine Catalysis. *Org. Biomol. Chem.* **2013**, *11* (5), 709–716. <https://doi.org/10.1039/C2OB26681D>.
- (3) Jiang, H.; Albrecht, Ł.; Jørgensen, K. A. Aminocatalytic Remote Functionalization Strategies. *Chem. Sci.* **2013**, *4* (6), 2287–2300. <https://doi.org/10.1039/c3sc50405k>.
- (4) Jurberg, I. D.; Chatterjee, I.; Tannert, R.; Melchiorre, P. When Asymmetric Aminocatalysis Meets the Vinylogy Principle. *Chem. Commun.* **2013**, *49* (43), 4869–4883. <https://doi.org/10.1039/c3cc41270a>.
- (5) Klier, L.; Tur, F.; Poulsen, P. H.; Jørgensen, K. A. Asymmetric Cycloaddition Reactions Catalysed by Diarylprolinol Silyl Ethers. *Chem. Soc. Rev.* **2017**, *46* (4), 1080–1102. <https://doi.org/10.1039/C6CS00713A>.
- (6) Pawar, T. J.; Jiang, H.; Vázquez, M. A.; Villegas Gómez, C.; Cruz Cruz, D. Aminocatalytic Privileged Diversity-Oriented Synthesis (ApDOS): An Efficient Strategy to Populate Relevant Chemical Spaces. *Eur. J. Org. Chem.* **2018**, *2018* (16), 1835–1851. <https://doi.org/10.1002/ejoc.201800273>.
- (7) Reyes-Rodríguez, G. J.; Rezayee, N. M.; Vidal-Albalat, A.; Jørgensen, K. A. Prevalence of Diarylprolinol Silyl Ethers as Catalysts in Total Synthesis and Patents. *Chem. Rev.* **2019**, *119* (6), 4221–4260. <https://doi.org/10.1021/acs.chemrev.8b00583>.

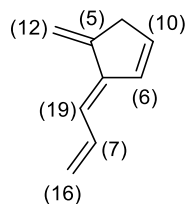
- (8) Przydacz, A.; Skrzyńska, A.; Albrecht, Ł. Breaking Aromaticity with Aminocatalysis: A Convenient Strategy for Asymmetric Synthesis. *Angew. Chem. Int. Ed.* **2019**, *58* (1), 63–73. <https://doi.org/10.1002/anie.201808197>.
- (9) Castro-Alvarez, A.; Carneros, H.; Costa, A. M.; Vilarrosa, J. Computer-Aided Insight into the Relative Stability of Enamines. *Synthesis* **2017**, *49* (24), 5285–5306. <https://doi.org/10.1055/s-0036-1590909>.
- (10) von Ragué Schleyer, P.; Jiao, H.; Goldfuss, B.; Freeman, P. K. Aromaticity and Antiaromaticity in Five-Membered C₄H₄X Ring Systems: “Classical” and “Magnetic” Concepts May Not Be “Orthogonal.” *Angew. Chem. Int. Ed. Engl.* **1995**, *34* (3), 337–340. <https://doi.org/10.1002/anie.199503371>.
- (11) Nyulászi, L.; Várnai, P.; Veszprémi, T. About the Aromaticity of Five-Membered Heterocycles. *J. Mol. Struct. THEOCHEM* **1995**, *358* (1), 55–61. [https://doi.org/10.1016/0166-1280\(95\)04338-1](https://doi.org/10.1016/0166-1280(95)04338-1).
- (12) Chesnut, D. B.; Davis, K. M. Resonance Revisited: A Consideration of the Calculation of Cyclic Conjugation Energies. *J. Comput. Chem.* **1997**, *18* (4), 584–593. [https://doi.org/10.1002/\(SICI\)1096-987X\(199703\)18:4<584::AID-JCC11>3.0.CO;2-G](https://doi.org/10.1002/(SICI)1096-987X(199703)18:4<584::AID-JCC11>3.0.CO;2-G).
- (13) Schleyer, P. R. von; Jiao, H. What Is Aromaticity? *Pure Appl. Chem.* **1996**, *68* (2), 209–218. <https://doi.org/10.1351/pac199668020209>.
- (14) Quiñonero, D.; Garau, C.; Frontera, A.; Ballester, P.; Costa, A.; Deyà, P. M. Quantification of Aromaticity in Oxocarbons: The Problem of the Fictitious “Nonaromatic” Reference System. *Chem. – Eur. J.* **2002**, *8* (2), 433–438. [https://doi.org/10.1002/1521-3765\(20020118\)8:2<433::AID-CHEM433>3.0.CO;2-T](https://doi.org/10.1002/1521-3765(20020118)8:2<433::AID-CHEM433>3.0.CO;2-T).

- (15) Wheeler, S. E.; Houk, K. N.; Schleyer, P. v. R.; Allen, W. D. A Hierarchy of Homodesmotic Reactions for Thermochemistry. *J. Am. Chem. Soc.* **2009**, *131* (7), 2547–2560. <https://doi.org/10.1021/ja805843n>.
- (16) Wheeler, S. E. Homodesmotic Reactions for Thermochemistry. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2* (2), 204–220. <https://doi.org/10.1002/wcms.72>.
- (17) Parr, R. G.; Yang, W. Density Functional Approach to the Frontier-Electron Theory of Chemical Reactivity. *J. Am. Chem. Soc.* **1984**, *106* (14), 4049–4050. <https://doi.org/10.1021/ja00326a036>.
- (18) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function. *Theor. Chem. Acc.* **2008**, *120* (1–3), 215–241.
- (19) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A Complete Basis Set Model Chemistry. I. The Total Energies of Closed-shell Atoms and Hydrides of the First-row Elements. *J. Chem. Phys.* **1998**, *89* (4), 2193. <https://doi.org/10.1063/1.455064>.
- (20) Petersson, G. A.; Al-Laham, M. A. A Complete Basis Set Model Chemistry. II. Open-Shell Systems and the Total Energies of the First-Row Atoms. *J. Chem. Phys.* **1991**, *94*, 6081–6090. <https://doi.org/10.1063/1.460447>.
- (21) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. a.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. a.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, a. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, a. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.;

- Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. a.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. a.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, a. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 09*, Gaussian, Inc., Wallin. 2009
- (22) Kendall, R. A.; Dunning, T. H.; Harrison, R. J. Electron Affinities of the First-row Atoms Revisited. Systematic Basis Sets and Wave Functions. *J. Chem. Phys.* **1992**, 96 (9), 6796–6806. <https://doi.org/10.1063/1.462569>.
- (23) Head-Gordon, M.; Pople, J. A.; Frisch, M. J. MP2 Energy Evaluation by Direct Methods. *Chem. Phys. Lett.* **1988**, 153 (6), 503–506. [https://doi.org/10.1016/0009-2614\(88\)85250-3](https://doi.org/10.1016/0009-2614(88)85250-3).
- (24) Sæbø, S.; Almlöf, J. Avoiding the Integral Storage Bottleneck in LCAO Calculations of Electron Correlation. *Chem. Phys. Lett.* **1989**, 154 (1), 83–89. [https://doi.org/10.1016/0009-2614\(89\)87442-1](https://doi.org/10.1016/0009-2614(89)87442-1).
- (25) Frisch, M. J.; Head-Gordon, M.; Pople, J. A. A Direct MP2 Gradient Method. *Chem. Phys. Lett.* **1990**, 166 (3), 275–280. [https://doi.org/10.1016/0009-2614\(90\)80029-D](https://doi.org/10.1016/0009-2614(90)80029-D).
- (26) Head-Gordon, M.; Head-Gordon, T. Analytic MP2 Frequencies without Fifth-Order Storage. Theory and Application to Bifurcated Hydrogen Bonds in the Water Hexamer. *Chem. Phys. Lett.* **1994**, 220 (1), 122–128. [https://doi.org/10.1016/0009-2614\(94\)00116-2](https://doi.org/10.1016/0009-2614(94)00116-2).

- (27) Tenderholt, A. L. QMForge, version 2.1 <https://sourceforge.net/projects/qmforge/files/qmforge/QMForge-2.1/%0A>. (accessed 2023-02-17).
- (28) Breneman, C. M.; Wiberg, K. B. Determining Atom-Centered Monopoles from Molecular Electrostatic Potentials. The Need for High Sampling Density in Formamide Conformational Analysis. *J. Comput. Chem.* **1990**, *11* (3), 361–373. <https://doi.org/10.1002/jcc.540110311>.
- (29) Geerlings, P.; De Proft, F.; Langenaeker, W. Conceptual Density Functional Theory. *Chem. Rev.* **2003**, *103* (5), 1793–1874. <https://doi.org/10.1021/cr990029p>.
- (30) Roy, R. K. Stockholders Charge Partitioning Technique. A Reliable Electron Population Analysis Scheme to Predict Intramolecular Reactivity Sequence. *J. Phys. Chem. A* **2003**, *107* (48), 10428–10434. <https://doi.org/10.1021/jp035848z>.
- (31) Liu, S.; Rong, C.; Lu, T. Information Conservation Principle Determines Electrophilicity, Nucleophilicity, and Regioselectivity. *J. Phys. Chem. A* **2014**, *118* (20), 3698–3704. <https://doi.org/10.1021/jp5032702>.
- (32) Momma, K.; Izumi, F. VESTA 3 for Three-Dimensional Visualization of Crystal, Volumetric and Morphology Data. *J. Appl. Crystallogr.* **2011**, *44* (6), 1272–1276. <https://doi.org/10.1107/S0021889811038970>.
- (33) Skrzynska, A.; Przydacz, A.; Albrecht, Ł. Organocatalytic Nonclassical Trienamine Activation in the Remote Alkylation of Furan Derivatives. *Org. Lett.* **2015**, *17* (22), 5682–5685.
- (34) Dyguda, M.; Przydacz, A.; Krzemińska, A.; Albrecht, Ł. On the Origins of Stereoselectivity in the Aminocatalytic Remote Alkylation of 5-Alkylfurfurals. *Org. Biomol. Chem.* **2019**, *17* (24), 6025–6031. <https://doi.org/10.1039/c9ob00914k>.

- (35) Fuson, R. C. The Principle of Vinylogy. *Chem. Rev.* **1935**, 16 (1), 1–27.
<https://doi.org/10.1021/cr60053a001>.
- (36) Nurkkala, L. J.; Steen, R. O.; Friberg, H. K. J.; Häggström, J. A.; Bernhardt, P. V.; Riley, M. J.; Dunne, S. J. The Effects of Pendant vs. Fused Thiophene Attachment upon the Luminescence Lifetimes and Electrochemistry of Tris(2,2'-Bipyridine)Ruthenium(II) Complexes. *Eur. J. Inorg. Chem.* **2008**, 2008 (26), 4101–4110.
<https://doi.org/10.1002/ejic.200800456>.
- (37) Škorić, I.; Kikaš, I.; Kovács, M.; Šindler-Kulyk, M.; Horváth, O. Synthesis, Spectroscopic Characterization and Photophysics of New Functionalized 2,3-Distyrylfurans: Substituent and Solvent Effects on Their Photobehavior. *J. Photochem. Photobiol. Chem.* **2010**, 211 (2), 152–161. <https://doi.org/10.1016/j.jphotochem.2010.02.013>.
- (38) Zhen, W.; Wang, F.; Zhao, M.; Du, Z.; Li, X. Rhodium(III)-Catalyzed Oxidative C–H Functionalization of Azomethine Ylides. *Angew. Chem. Int. Ed.* **2012**, 51 (47), 11819–11823.
<https://doi.org/10.1002/anie.201207204>.
- (39) Orbital coefficients on a model system containing only the carbon backbone of trienamine **B13** were examined and revealed the γ -C to have the highest orbital coefficient. This suggests the nature of the conjugation is the main factor leading to the high orbital coefficients in **B13-15**. Orbital coefficients for the carbon backbone are shown in parentheses in the image below.



- (40) Xu, C.-J.; Li, H.-W.; He, X.-L.; Du, W.; Chen, Y.-C. Asymmetric Direct Remote Michael Addition Reactions of Allyl Furfurals *via* Dearomative Trienamine and Tetraenamine Catalysis. *Asian J. Org. Chem.* **2019**, *8* (7), 1037–1040. <https://doi.org/10.1002/ajoc.201900197>.
- (41) Liu, Y.; Nappi, M.; Arceo, E.; Vera, S.; Melchiorre, P. Asymmetric Catalysis of Diels–Alder Reactions with in Situ Generated Heterocyclic *Ortho*-Quinodimethanes. *J. Am. Chem. Soc.* **2011**, *133* (38), 15212–15218. <https://doi.org/10.1021/ja206517s>.
- (42) Liu, Y.; Nappi, M.; Escudero-Adán, E. C.; Melchiorre, P. Multicatalytic Asymmetric Synthesis of Complex Tetrahydrocarbazoles *via* a Diels–Alder/Benzoin Reaction Sequence. *Org. Lett.* **2012**, *14* (5), 1310–1313. <https://doi.org/10.1021/ol300192p>.
- (43) Liu, Y.; Nappi, M.; Arceo, E.; Vera, S.; Melchiorre, P. Asymmetric Catalysis of Diels–Alder Reactions with in Situ Generated Heterocyclic *Ortho*-Quinodimethanes. *J. Am. Chem. Soc.* **2011**, *133* (38), 15212–15218. <https://doi.org/10.1021/ja206517s>.
- (44) Donslund, B. S.; Monleón, A.; Palazzo, T. A.; Christensen, M. L.; Dahlgaard, A.; Erickson, J. D.; Jørgensen, K. A. Organocatalytic Enantioselective Higher-Order Cycloadditions of In Situ Generated Amino Isobenzofulvenes. *Angew. Chem. Int. Ed.* **2018**, *57* (5), 1246–1250. <https://doi.org/10.1002/anie.201710694>.
- (45) Donslund, B. S.; Jessen, N. I.; Bertuzzi, G.; Giardinetti, M.; Palazzo, T. A.; Christensen, M. L.; Jørgensen, K. A. Catalytic Enantioselective [10+4] Cycloadditions. *Angew. Chem. - Int. Ed.* **2018**, *57* (40), 13182–13186. <https://doi.org/10.1002/anie.201807830>.
- (46) Chen, Y.-C.; Yang, Y.; Jiang, Y.; Du, W. Asymmetric Cross [10+2] Cycloadditions of 2-Alkylidene-1-indanones and Activated Alkenes under Phase-Transfer Catalysis. *Chem. - Eur. J.* <https://doi.org/10.1002/chem.201904930>.

- (47) Bertuzzi, G.; Thøgersen, M. K.; Giardinetti, M.; Vidal-Albalat, A.; Simon, A.; Houk, K. N.; Jørgensen, K. A. Catalytic Enantioselective Hetero-[6+4] and -[6+2] Cycloadditions for the Construction of Condensed Polycyclic Pyrroles, Imidazoles, and Pyrazoles. *J. Am. Chem. Soc.* **2019**, jacs.8b13659. <https://doi.org/10.1021/jacs.8b13659>.

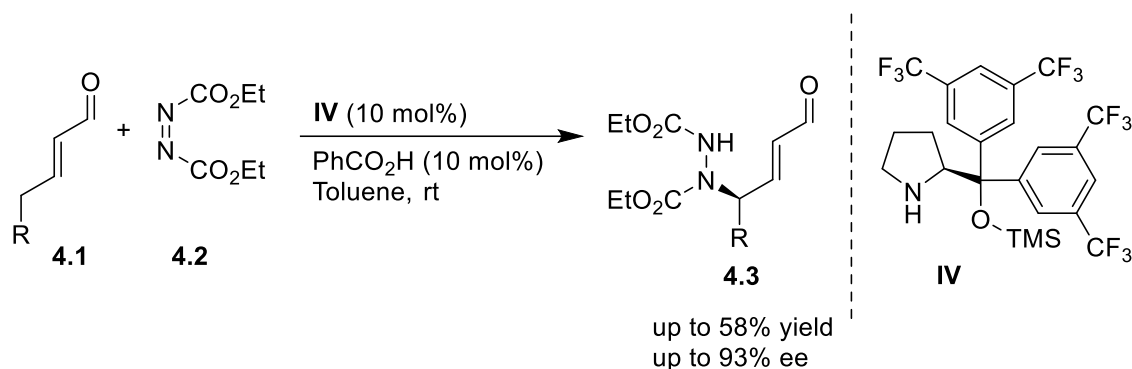
Chapter 4 : Exploring the Role of Substituents on Trienamine Backbone in Trienamine-Mediated Diels-Alder Reactions.

4.1: Introduction

The principle of vinylogy, reported by Fuson in 1935, states that the electronic effects of a functional group can be propagated through a conjugated π -system to a distal position.¹ Hence, by using poly-unsaturated carbonyl compounds, enamine activation has been extended to di-, tri-, and tetraenamine activation to give rise to vinylogous nucleophilicity at remote γ -, and ϵ - positions.²⁻⁹ This not only expanded the scope of aminocatalysis but has also demonstrated the ability of stereochemical induction at distal positions. However, there are various challenges in reaction development for remote functionalization *via* aminocatalysis such as the ability of catalyst to promote regioselectivity at remote positions. The order of nucleophilicity ($\alpha > \gamma > \epsilon$) for the vinylogous backbone makes the regioselectivity challenging, therefore, designing remote functionalization reactions must take electronics and sterics into account. In addition to this, the increased backbone conformational freedom with the increase in distance makes it challenging to perform stereoselective transformations.

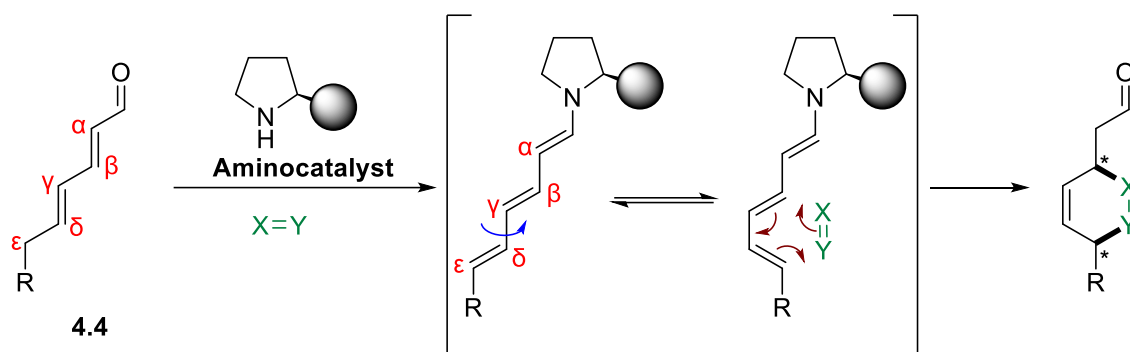
The first report using aminocatalysis which demonstrated stereochemical induction at a remote position was reported by Jørgensen.³ A dienamine mediated γ -functionalization of enals using diethyl azodicarboxylate (DEAD) catalyzed by diarylprolinol silylether was reported (Scheme 4.1). This was a significant report as 1) it showed the success of vinylogous nucleophilicity of dienamine intermediate, 2) it also provided perfect regioselectivity for the γ position, and 3) the ability of aminocatalyst to induce a new stereocenter at the distal γ -carbon. The authors suggested that the reaction proceeds *via* a Diels-Alder cycloaddition between the dienamine intermediate and DEAD to eventually result in mono-functionalized γ -aminated dienal.

This report revealed the potential of nucleophilic dienamine intermediate, however, the reaction follows a cycloaddition pathway rather than general nucleophilic addition which limits the number of examples with mono-functionalization at γ -position. Nonetheless, the vinylogous dienamine reactivity has been exploited to develop various stereoselective cycloaddition reactions.^{4,5}



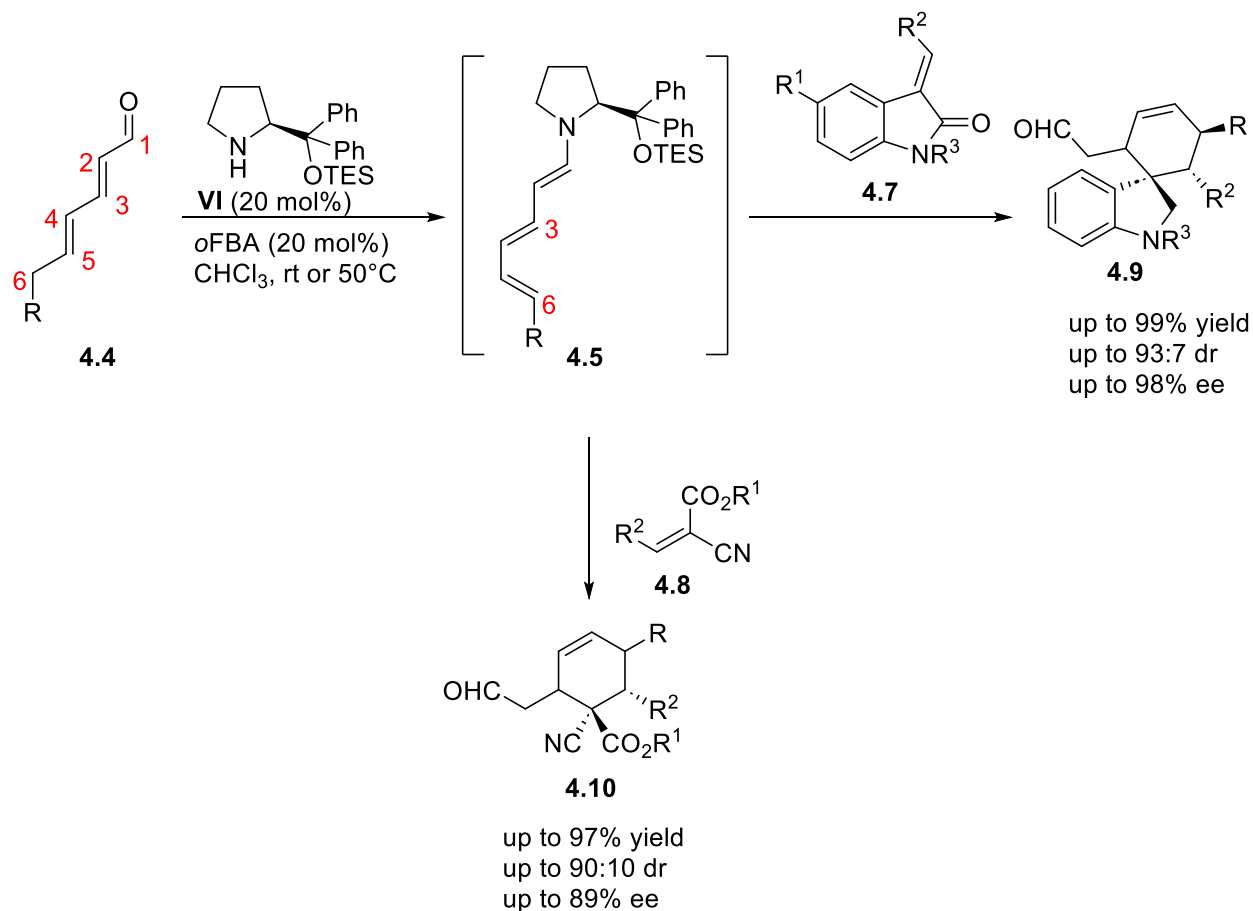
Scheme 4.1: Dienamine mediated γ -amination of α,β -unsaturated aldehydes.

Similarly, enamine activation has been further extended to trienamine which allows the vinylogous nucleophilicity to be further *transmitted* to more distal positions and further expand the scope of aminocatalytic reactions. Due to higher conformational freedom and vinylogous nucleophilicity of linear trienamine backbone, there have not been any reports of mono-functionalization at the remote ϵ -position. However, the single-bond rotation of the trienamine at γ - δ bond, results in the formation of a diene which has been shown to readily undergo cycloaddition reaction with various dienophiles (Scheme 4.2).



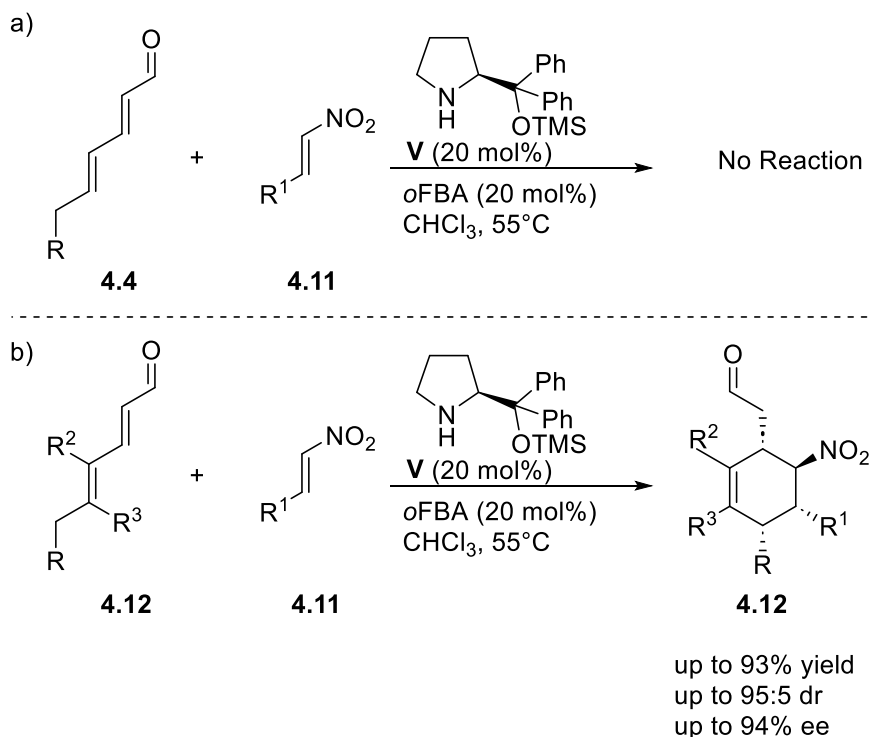
Scheme 4.2: General trienamine mediated Diels-Alder reaction.

Chen and Jørgensen utilized this strategy by reacting dienophiles with the terminal diene.¹⁰ This was the first example of stereoselective Diels-Alder reaction of 2,4-dienals with olefinic dienophiles such as 3-olefinic oxindoles and olefinic cyanoacetates (Scheme 4.3). This report not only demonstrated the ability of aminocatalyst to induce chirality at remote positions but also showed excellent regioselectivity by forming two new C-C bonds at β - and ϵ - positions exclusively. The authors did not observe reactivity with 1,4-*s-cis* diene because of the unfavorable steric interactions with the bulk of catalyst. Furthermore, the HOMO energy was significantly higher for 3,6-*s-cis* diene compared to 1,4-*s-cis* diene. Since the initial report by Jørgensen and Chen, there have been various examples of cycloaddition reactions using trienamine intermediate to form complex cyclic structures containing multiple stereocenters.^{6,11,12}



Scheme 4.3: Trienamine mediated enantioselective Diels-Alder reactions reported by Jørgensen and Chen.

In the same year, Chen published another report of Diels-Alder reaction with trienamine intermediates and nitroalkenes.¹³ The authors observed that trienamine intermediates resulting from unsubstituted 2,4-dienals, did not form any product (Scheme 4a). However, when the authors introduced alkyl substituents to the backbone of 2,4-dienals, successful reactions with nitroalkenes were performed (Scheme 4b). The authors proposed that the electron-donating ability of the alkyl substituents raises the HOMO energy of the trienamine intermediate. This approach of further raising the HOMO energy of the trienamine intermediate is significant since it not only expands the scope of trienamine mediated reactions but also allows to design novel reactions by tuning the HOMO-LUMO gap of substrates using appropriate substituents.



Scheme 4.4: HOMO-raising strategy through substitution on 2,4-dienals for Diels–Alder reactions with nitroalkenes reported by Chen. a) No reaction is observed with unsubstituted dienal and nitroalkenes via trienamine intermediate. b) Dienals with substituents at γ - and δ -carbons to enhance HOMO of trienamine for Diels–Alder reaction with nitroalkenes.

By understanding the impact of substituents at various positions of trienamine backbone, one can tune the electronics to result in desired reactivity and selectivity. This can aid in the design of trienamine mediated reactions utilizing a wide variety of substituted carbonyl compounds. Herein, an extensive computational analysis of trienamines formed from 2,4-hexadienal with various electron-donating (methyl, phenyl, and 4-methoxybenzene) and electron-withdrawing substituent such as (4-cyanobenzene) at the β -, γ -, δ - and ϵ -carbons is reported (Figure 1). The Diels–Alder reaction requires the *s-cis* diene conformation, therefore, the focus of this report is on three conformations of the substituted trienamine intermediates, 1) all-*trans* conformer, 2) conformer with 1,4-*s-cis* diene, and 3) conformer with 3,6-*s-cis* diene (Figure 4.1). This allows us to examine the conformations with *s-cis* diene moiety of substituted trienamine intermediate

substituted to study the thermodynamics and location of MO energy levels. An extensive orbital analysis is also performed to understand the orbital composition of trienamine intermediate.

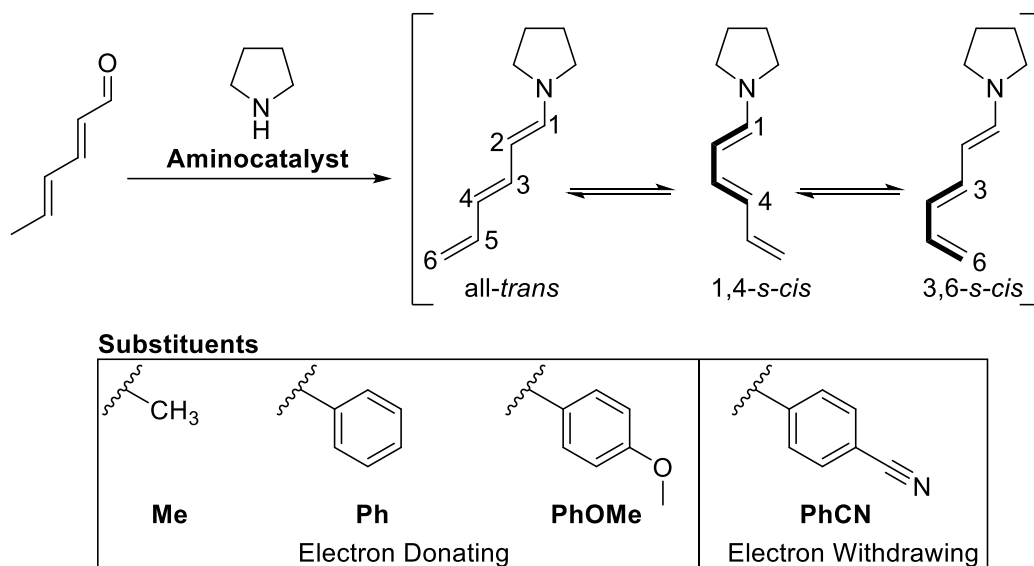


Figure 4.1: Conformations of trienamine intermediates and substituents studied in this report.

4.2: Computational methods

All structures were optimized in the gas phase using M06-2X¹⁴ with the double- ζ split valence 6-31+G(d,p) basis set^{15,16} and vibrational analysis verified that each structure was a minimum. All optimizations were performed on performed using Gaussian 09.e01.¹⁷ The orbital coefficients were calculated using Multiwfn v3.7.¹⁸ The 3D geometry figures were generated using CYLview20.¹⁹ The HOMO isosurfaces were generated using VESTA v3.5.5.²⁰

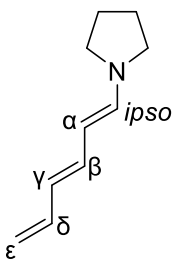
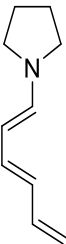
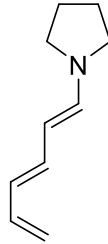
4.3: Results and Discussion

4.3.1: Unsubstituted Trienamines

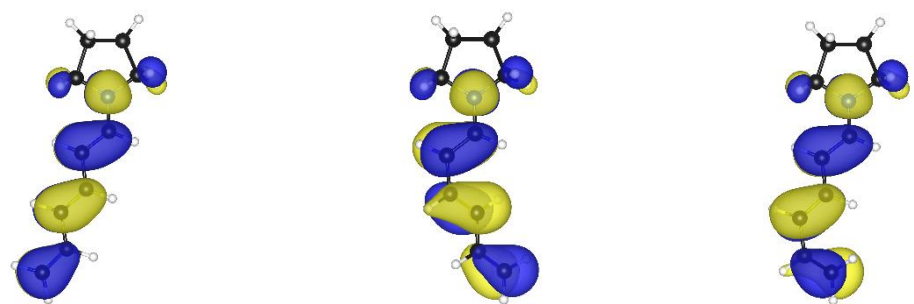
We began our investigation by computing the simplest unsubstituted trienamine intermediate, resulting from condensation of pyrrolidine with 2,4-hexadienal. The unsubstituted

trienamine system can be used as a reference for substituted trienamines. The lowest energy confirmation of the unsubstituted trienamine was the all-*trans* conformer **A1**. The 1,4-*s-cis* conformer **A2** and 3,6-*s-cis* conformer **A3** were 3.2 and 2.8 kcal/mol were higher in energy relative to **A1**, respectively (Table 4.1). The *s-cis* conformations in **A2** and **A3** lead to steric repulsions between the hydrogens at 1 and 4 positions for **A2**, and 3 and 6 positions for **A3**. The steric repulsions in **A2** and **A3** are evidenced by dihedral angles of the *pi*-backbone. The $\theta_{1-2-3-4}$, $\theta_{2-3-4-5}$, and $\theta_{3-4-5-6}$ for trienamine **A1** were determined to be 179.8°, 180.0° and 179.8°, respectively. The dihedral angle for 1,4-*s-cis* diene moiety for **A2** ($\theta_{1-2-3-4}$) and 3,6-*s-cis* diene moiety for **A3** ($\theta_{3-4-5-6}$) were determined to be 24.6° and 27.2°, respectively. See appendix for tabulated dihedral angle data. This causes distortion in the *pi*-backbone resulting in it being out of conjugation, leading to higher energy than **A1**. The increase in energy due to the steric repulsions also correlates with HOMO energies of the conformations of the trienamine intermediates. The HOMO of all *trans* trienamine **A1** was found to be -5.80 eV, whereas the HOMOs are lower in energy for **A2** (-5.91 eV), and **A3** (-5.84 eV). It is noteworthy that both **A2** and **A3** are thermodynamically similar in energy, however, **A3** which has a terminal diene, results in raised HOMO relative to **A2**. This suggests that the trienamine **A3** with 3,6-*s-cis* conformer may be more reactive than **A2**. This is also evident in the first report of trienamine mediated Diels-Alder reaction by Jørgensen; the authors only observed reactivity with the 3,6-*s-cis* diene.¹⁰

Table 4.1: Relative energies and HOMO locations of unsubstituted trienamine system. Relative free energies are in kcal/mol.

	 A1	 A2	 A3
Relative Energy (kcal/mol)	[0.0]	3.2	2.8
HOMO (eV)	-5.80	-5.91	-5.84

The population analysis of HOMO coefficients of the unsubstituted trienamine system was also performed (Table 4.2). The population analysis of unsubstituted trienamine reveals that the general vinylogy principle is followed where the α -carbon has the largest coefficient followed by γ -carbon and then ϵ -carbon, regardless of configuration. However, it is **important** to note that the distortion in the π -backbone of **A2** and **A3** impacts the HOMO coefficients. The distortion in 1,4-*s-cis* diene in **A2** causes the α,β -bond to twist to prevent steric clash between α and γ hydrogens. This results in the HOMO coefficient for γ -position to be 14.82 for **A2**, compared to 16.06 for **A1** and 16.97 for **A3**. Similarly, for 3,6-*s-cis* diene in **A3**, twisting occurs at γ,δ -bond resulting in the HOMO coefficient to be 9.83, compared to 12.01 for **A1** and 11.09 for **A3**.

Table 4.2: Orbital coefficients of HOMOs of trienamine **A1-A3**.


	A1	A2	A3
<i>ipso</i>	10.67	10.62	10.88
α	17.27	18.84	17.91
β	8.75	8.52	8.52
γ	16.06	14.82	16.97
δ	4.51	4.21	4.11
ϵ	12.01	11.09	9.83

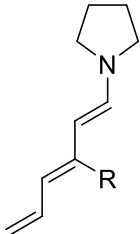
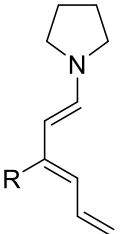
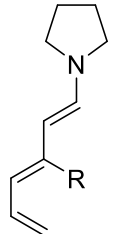
4.3.2: β -Substituted Trienamines

Next, we explored the trienamine intermediates with substituents at the β -carbon for which there have not been any trienamine mediated reactions reported. This was done using a range of electron donating and withdrawing substituents at the β -carbon. Beginning with electron donating substituents, all *trans* trienamine intermediates were determined to be energetically favourable for methyl (**B1**), phenyl (**C1**), and 4-methoxybenzene (**D1**) substituents (Table 4.3). In contrast to the configurations of the unsubstituted trienamine, the β -substituted trienamines with 1,4-*s-cis* configuration were thermodynamically more favourable than the 3,6-*s-cis* configuration for methyl, phenyl, and 4-methoxybenzene substituents. The methyl substituted trienamine **B2** with 1,4-*s-cis* configuration was determined to be 1.4 kcal/mol higher in energy than **B1**, whereas the trienamine **B3** was higher in energy by 3.1 kcal/mol (Table 4.3). This is due to the increased

repulsions between the methyl group in **B3** and the hydrogen at 6-position. The dihedral angle $\theta_{1-2-3-4}$ for 1,4-*s-cis* diene moiety in **B2** was found to be 31.6° , whereas the 3,6-*s-cis* diene moiety was determined to be further twisted with $\theta_{3-4-5-6}$ to be 36.73° . The geometric configuration of **B2** forces the methyl group to face away from the π -backbone resulting in thermodynamic preference over **B3**. This observation is also reflected in both phenyl and 4-methoxybenzene substituents.

For trienamines with aryl substituents, the rotation of aryl ring relative to the π -backbone depended on the trienamine conformation as shown in Figure 4.2. The phenyl substituent of the intermediates **C1** and **C3** rotates to minimize steric repulsions with hydrogens at *ipso* and ε -positions for **C1**, and *ipso* and ε -positions for **C3**. The rotation configures the phenyl ring to be almost perpendicular to the π -backbone. The $C_\alpha-C_\beta-C_{Ph}=C_{Ph}$ was determined to be 69.1° and 73.5° for **C1** and **C3**, respectively, whereas it was determined to be 132.8° for **C2**. This rotation of phenyl ring also has an impact of its conjugation with the π -backbone which is discussed further below.

Table 4.3: Relative energies and HOMO locations of trienamines **B1-B3**, **C1-C3**, **D1-D3**, and **E1-E3**. All free energies are reported in kcal/mol.

		 B1: R = CH ₃ C1: R = Ph D1: R = PhOMe E1: R = PhCN	 B2: R = CH ₃ C2: R = Ph D2: R = PhOMe E2: R = PhCN	 B3: R = CH ₃ C3: R = Ph D3: R = PhOMe E3: R = PhCN
Relative Energy (kcal/mol)	R=CH ₃	[0.0]	1.4	3.1
	R=Ph	[0.0]	2.6	4.6
	R=PhOMe	[0.0]	2.5	4.1

	R=PhCN	[0.0]	2.8	4.0
<i>HOMO</i> (eV)	R=CH ₃	-5.78	-5.90	-5.84
	R=Ph	-5.80	-5.98	-5.82
	R=PhOMe	-5.76	-5.90	-5.76
	R=PhCN	-6.10	-6.27	-6.13

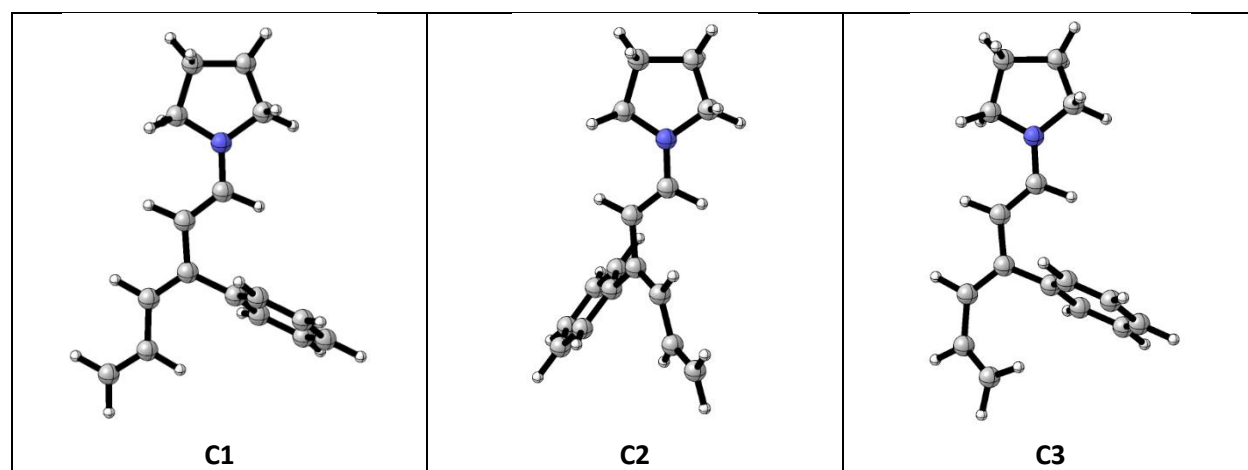


Figure 4.2: Three dimensional structures of trienamines **C1-C3**.

The HOMO analysis revealed that the β -substituted trienamine with 1,4-*s-cis* configuration had lower HOMOs level relative to the 3,6-*s-cis* configuration for all electron donating substituents. The HOMO of trienamine **B2** was found to be located at -5.90 eV however **B3** was -5.84 eV. The energy of the HOMO of β -substituted trienamines with 3,6-*s-cis* diene rises with substituents containing higher electron donating ability (Table 4.3). This suggests that the 1,4-*s-cis* diene configuration with electron donating substituents at the beta position of trienamines are thermodynamically favoured, however, the β -substituted trienamines containing the 3,6-*s-cis* diene are more likely to undergo Diels-Alder reaction. This is because the trienamines containing 1,4-*s-cis* diene are less planar relative to trienamines with 3,6-*s-cis* diene with aryl substituents.

Geometric analysis shows that the dihedral angle of diene moiety in trienamine **D2** is 33.04°, whereas the dihedral of terminal diene in trienamine **D3** is 19.73° (See Appendix).

Trienamine with 4-cyanobenzene, an electron withdrawing group, substituted at the beta position was also examined. Similar to trienamines with electron donating substituents, trienamine **E2** with 1,4-*s-cis* diene configuration was more thermodynamic favourable relative to trienamine **E3** containing 3,6-*s-cis* diene. Similarly, the HOMO for **E3**, -6.13 eV, is located higher than for **E2**, -6.27 eV (Table 4.3).

The MO analysis of β -substituted trienamine suggests that the vinylogy principle is followed regardless of electronics of substituents (Table 4.4-4.7). Upon geometric analysis of trienamine intermediates with aryl substituents, it was determined that the rotation of aryl substituent with respect to the *pi*-backbone. The phenyl substituent for **C1** and **C3** is out of conjugation due to its almost perpendicular alignment to the *pi*-backbone, whereas the phenyl substituent is for **C2** is more in alignment with the backbone. The figures shown in Table 4.5 of C1-C3 show that phenyl substituent in **C1** and **C3** have no contribution to the HOMO, whereas the substituent shows conjugation with the backbone in **C2**, consistent with twisting of the phenyl ring. This phenomenon is present for all aryl substituents (Table 4.5-4.7)

Overall, the substituents at the β -position demonstrate thermodynamic preference for trienamine with 1,4-*s-cis* diene moiety, however, HOMO energy is also lowered for 1,4-*s-cis* diene configuration. The 3,6-*s-cis* diene configuration is thermodynamically disfavoured, regardless of substituent at the β -position. Furthermore, the HOMO of the trienamine with 3,6-*s-cis* configuration is raised as the electron donating ability of a substituent increases. However, there have not been any reported examples of β -substituted trienamine mediated Diels-Alder reactions which could be explained by the thermodynamically disfavoured 3,6-*s-cis* diene configuration.

Table 4.4: Orbital coefficients of HOMOs of trienamine **B1-B3**

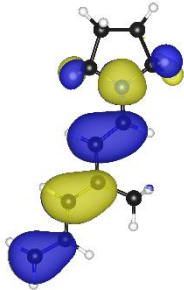
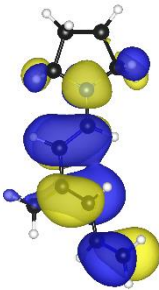
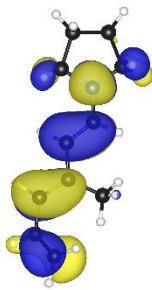
			
	B1	B2	B3
<i>ipso</i>	10.77	10.19	11.15
α	18.21	18.17	18.21
β	8.45	8.54	7.99
γ	15.66	15.02	16.46
δ	4.24	4.18	3.53
ε	11.35	10.93	7.89

Table 4.5: Orbital coefficients of HOMOs of trienamine **C1-C3**

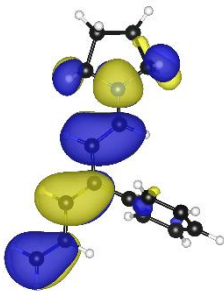
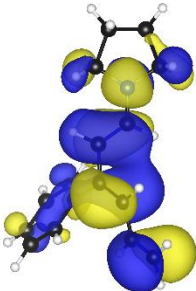
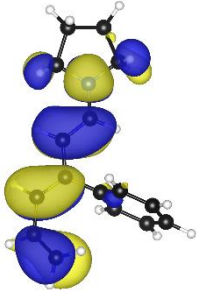
			
	C1	C2	C3
<i>ipso</i>	10.35	9.66	10.47
α	17.10	17.03	17.37
β	8.25	8.00	8.07
γ	15.77	14.80	16.30
δ	4.37	4.21	4.29
ε	11.66	10.94	10.47

Table 4.6: Orbital coefficients of HOMOs of trienamine **D1-D3**

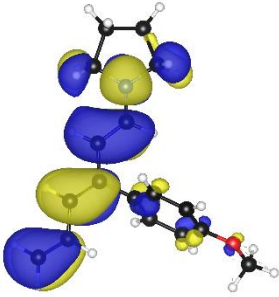
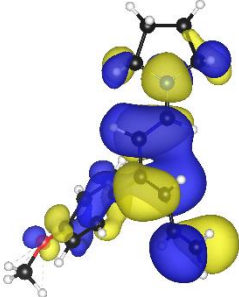
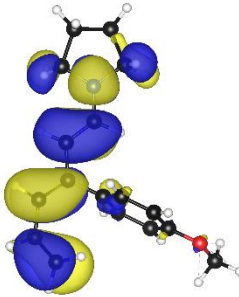
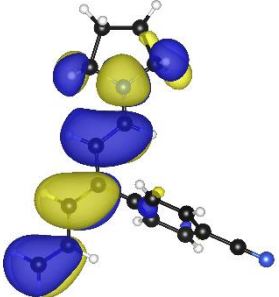
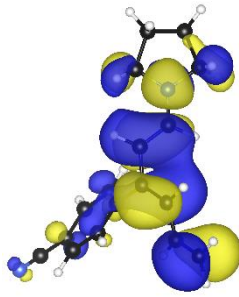
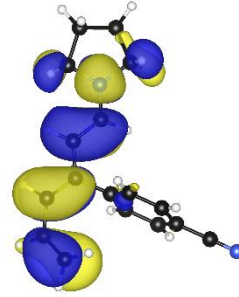
			
	D1	D2	D3
<i>ipso</i>	10.17	9.17	10.39
α	16.59	15.79	17.08
β	8.29	8.08	8.10
γ	15.99	15.50	16.44
δ	4.40	4.32	4.32
ϵ	11.82	11.40	10.62

Table 4.7: Orbital coefficients of HOMOs of trienamine **E1-E3**

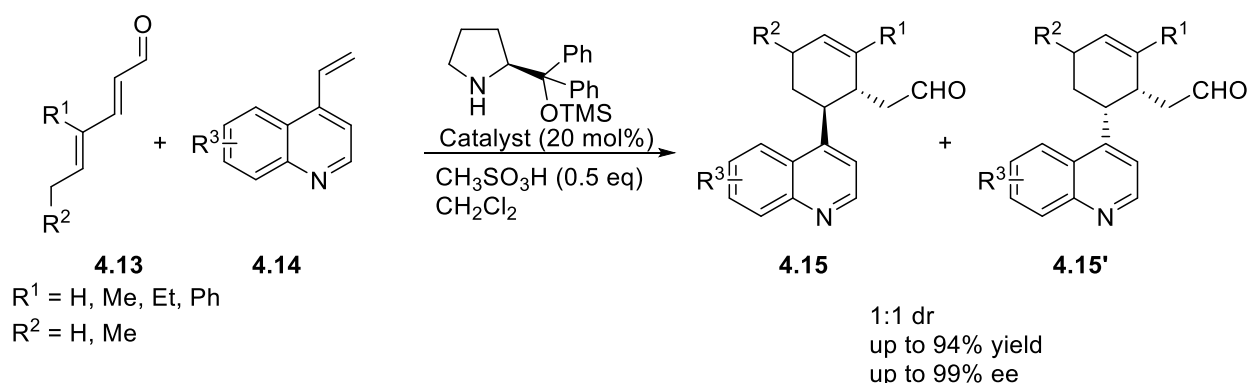
			
	E1	E2	E3
<i>ipso</i>	10.22	9.65	10.33
α	17.58	18.10	18.04
β	8.03	7.71	7.80
γ	15.31	14.24	15.95
δ	4.33	4.08	4.12
ϵ	11.41	10.50	9.89

4.3.3: γ -Substituted Trienamines

The γ -substituted 2,4-dienals have been heavily utilized in trienamine mediated Diels-Alder reactions. One of the first trienamine mediated Diels-Alder reaction reported by Chen¹³ utilized alkyl and aryl substituents at the γ -position of 2,4-dienals to react with nitroalkenes. The

authors observed no reaction when unsubstituted trienamine intermediate was employed. It was proposed that electron donating substituents were employed to further raise the HOMO energy level for successful Diels-Alder reaction with nitroalkenes.¹³

Recently, Wang and coworkers reported a trienamine mediated cycloaddition reaction between γ -substituted 2,4-dienals and vinylquinolines to result in novel chiral quinoline compounds of biological interest (Scheme 5).²¹ The authors employed alkyl and aryl substituents to react with various substituted vinylquinolines. Since Chen's initial report, electron-donating aryl and alkyl substituents at γ -position have been most commonly used.^{11,22-29} Hence, we explored the γ -substituted trienamines.



Scheme 4.5: Trienamine mediated [4+2] cycloaddition reaction between γ -substituted 2,4-dienals and vinylquinolines reported by Wang et al.

Similar to the unsubstituted trienamine, the γ -substituted trienamines with 1,4-*s-cis* diene configuration were slightly higher in energy than 3,6-*s-cis* diene configuration. The methyl substituted trienamine with 1,4-*s-cis* diene configuration, **F2**, was determined to be 4.2 kcal/mol higher than trienamine with all *trans* configuration **F1**, whereas, the trienamine with 3,6-*s-cis* diene configuration, **F3**, was 3.3 kcal/mol higher than **F1** (Table 4.8). The 1,4-*s-cis* configuration for **F2** results in repulsions between the methyl group and hydrogen at *ipso* position. In **F3**, the methyl substituent points away from the pi-backbone resulting in repulsions only by protons at 3- and 6-

position. This trend is also observed with other substituents, regardless of its electron donating or electron withdrawing capabilities. However, the difference in energy between the trienamine with 1,4-*s-cis* diene configuration and 3,6-diene configuration decreases when the substituent is an aryl group. The phenyl substituted trienamine **G2** and trienamine **G3** are 2.9 and 2.5 kcal/mol higher in energy, respectively, than the all-*trans* trienamine **G1** (Table 4.8). In trienamine **G2**, the lack of proton-proton repulsions, present in **F2**, and the ring being able to configure such that the repulsions between the *ipso* group and the phenyl group decrease significantly resulting in lowered energy for **G2**.

Table 4.8: Relative energies and HOMO locations of trienamines **F1-F3**, **G1-G3**. All free energies are reported in kcal/mol.

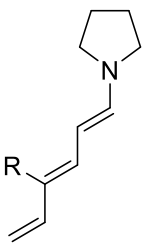
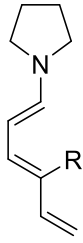
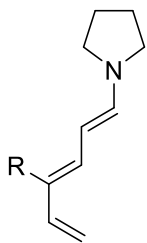
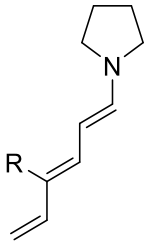
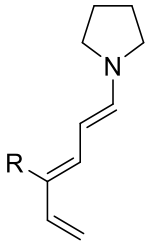
		 F1: R = CH ₃ G1: R = Ph	 F2: R = CH ₃ G2: R = Ph	 F3: R = CH ₃ G3: R = Ph
Relative Energy (kcal/mol)	R=CH ₃	[0.0]	4.2	3.3
	R=Ph	[0.0]	2.9	2.5
HOMO (eV)	R=CH ₃	-5.75	-5.91	-5.75
	R=Ph	-5.78	-5.80	-5.79

Table 4.9: Relative energies and HOMO locations of trienamines **H1**, **H2**, **I1**, and **I2**. All free energies are reported in kcal/mol.

		 H1: R = PhOMe I1: R = PhCN	 H2: R = PhOMe I2: R = PhCN
Relative Energy (kcal/mol)	R=PhOMe	[0.0]	2.7
	R=PhCN	[0.0]	2.7
HOMO (eV)	R=PhOMe	-5.71	-5.69
	R=PhCN	-6.09	-6.12

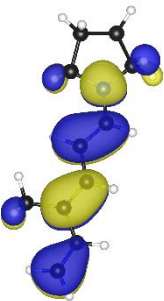
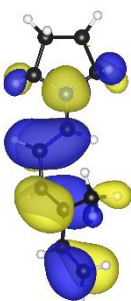
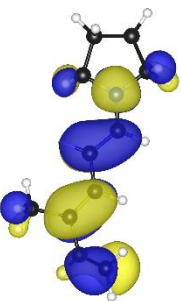
The HOMOs of 3,6-*s-cis* diene configuration for gamma substituted trienamines are higher in energy than 1,4-*s-cis* diene configuration. The HOMO of methyl substituted trienamine, **F1**, with all *trans* configuration, is located at -5.75 eV which gets lowered to -5.91 eV when 1,4-*s-cis* diene configuration for **F2** is studied. However, the HOMO of trienamine **F3** with 3,6-*s-cis* diene configuration remains unchanged from trienamine **F1** at -5.75 eV. This suggests that trienamine **F3** containing the terminal 3,6-*s-cis* diene is geometrically and electronically configured to undergo Diels-Alder reaction.

When comparing the HOMO of methyl substituted trienamine **F1** with unsubstituted trienamine **A1**, it was determined that the methyl group raises the HOMO of trienamine intermediate, from -5.80 eV (**A1**) to -5.75 eV (**F1**) due to its electron donating ability into the *pi*-backbone. This phenomenon is also present when the substituent is an electron donating aryl group,

however, when replaced with an electron withdrawing aryl group such as 4-cyanobenzene, the reactivity of trienamine decreases. The HOMO of 4-cyanobenzene substituted trienamine, **I1**, with all *trans* configuration is located at -6.09 eV which slightly lowers to -6.12 eV for **I2** when the trienamine contains a 3,6-*s-cis* diene configuration (Table 4.9). In contrast, the HOMO of 4-methoxybenzene substituted trienamine **H1** with all-*trans* configuration is located at -5.71 eV which raises by a small increment to -5.69 eV for trienamine **H2** consisting of 3,6-*s-cis* diene configuration (Table 4.9). Similar to aryl substituents at the β -positions, the aryl substituents are twisted out of plane with respect to the *pi*-backbone, therefore the *pi*-system of the aryl ring is not in conjugation with the trienamine backbone. This suggests that the *pi*-system of the aryl ring may have minimal contribution to the HOMO.

The molecular orbital analysis suggests that the vinylogy principle is followed for γ -substituted trienamine regardless of nature of substituents (Table 4.10-4.12). The analysis of γ -substituted trienamines indicates that the HOMO level of gamma substituted trienamine increases as the electron donating abilities of the substituent increase. The thermodynamic preference of 3,6-*s-cis* diene as well as the increase in reactivity has made γ -substituted trienamines an attractive option for reaction development.

Table 4.10: Orbital coefficients of HOMOs of trienamine **F1-F3**

			
	F1	F2	F3
<i>ipso</i>	10.54	10.37	10.84
α	16.78	18.50	17.48
β	9.43	8.91	9.56

γ	15.80	13.87	16.64
δ	3.99	3.09	3.54
ε	11.13	7.42	8.30

Table 4.11: Orbital coefficients of HOMOs of trienamine **G1-G3**

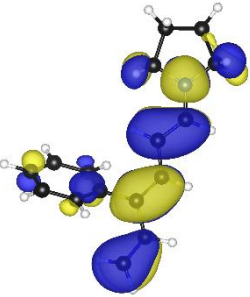
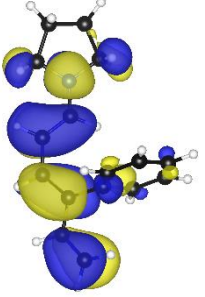
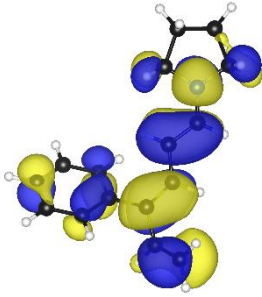
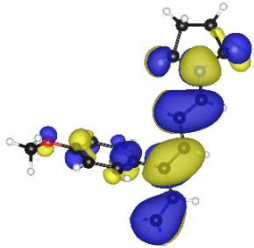
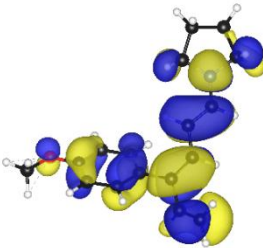
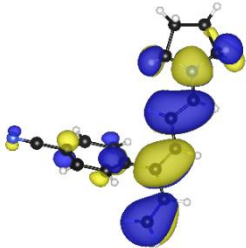
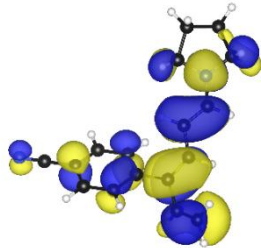
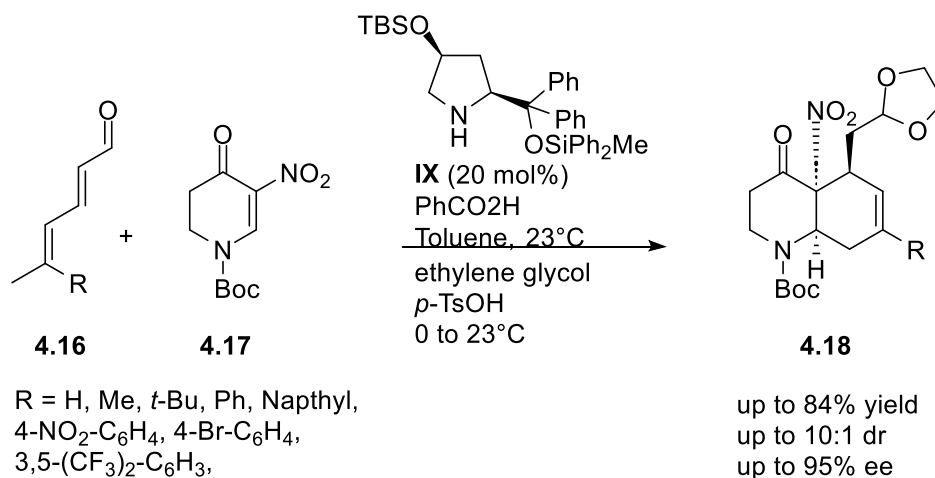
			
	G1	G2	G3
<i>ipso</i>	10.29	9.92	10.27
α	16.56	19.17	16.49
β	8.77	8.16	8.75
γ	15.12	13.96	15.43
δ	4.14	2.84	3.21
ε	11.08	6.89	7.57

Table 4.12: Orbital coefficients of HOMOs of trienamine **H1, H2, I1, and I2**.

				
	H1	H2	I1	I2
<i>ipso</i>	10.16	10.02	9.90	9.81
α	16.11	15.55	16.92	16.78
β	8.91	8.98	8.29	8.19
γ	14.93	14.79	15.26	15.62
δ	4.04	3.03	4.20	3.27
ε	10.86	7.22	11.20	7.63

4.3.4: δ -Substituted Trienamines

Next, we explored the δ -substituted trienamines which have been employed in various trienamine mediated Diels-Alder reactions.^{12,22,24,30–35} However, substituents at δ -position are not as widely reported as the γ -position, and the most common substituents utilized at the δ -position are electron-donating alkyl and aryl groups. Recently, Ishikawa *et al.* reported trienamine mediated Diels-Alder reaction between δ -substituted 2,4-dienals and 5-nitro-2,3-dihydro-4-pyridones to obtain octahydroquinolines enantioselectivity (Scheme 4.6).¹² This report utilized various electron-donating and electron-withdrawing aryl substituents at the δ -position. The scope of dienals used showed the presence of substituents at the δ -position on the trienamine did not exhibit a significant impact on yield of reaction. This is due to the dienophile **4.17** containing electron withdrawing nitro substituent which significantly lower the LUMO level.

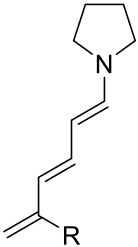
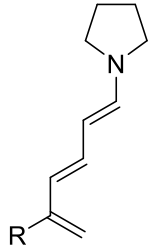


Scheme 4.6: Trienamine mediated Diels-Alder reaction between δ -substituted 2,4-dienals and 5-nitro-2,3-dihydro-4-pyridones, reported by Ishikawa *et al.*

The δ -substituted trienamines revealed a smaller energy difference between the all-*trans* and 3,6-*s-cis* diene configurations, relative to each other. However, the all-*trans* configuration was determined to be thermodynamically favoured. The methyl substituted trienamine **J2** with 3,6-*s-cis* diene configuration was determined to be 1.9 kcal/mol higher than all-*trans* trienamine **J1**. Interestingly, this energy difference decreases significantly for aryl substituents due to the ability

to rotate to minimize steric repulsions. (Table 4.13). The phenyl substituted trienamine **K2** with 3,6-*s-cis* diene was determined to be 1.2 kcal/mol higher relative to **K1** (Table 4.13). The preference for all-*trans* over 3,6-*s-cis* diene configuration is negligible for 4-methoxybenzene suggesting that thermodynamics of the trienamine intermediate may not be a major factor.

Table 4.13: Relative energies and HOMO locations of trienamines **J1**, **J2**, **K1**, **K2**, **L1**, **L2**, **M1**, and **M2**. All free enrgies are reported in kcal/mol.

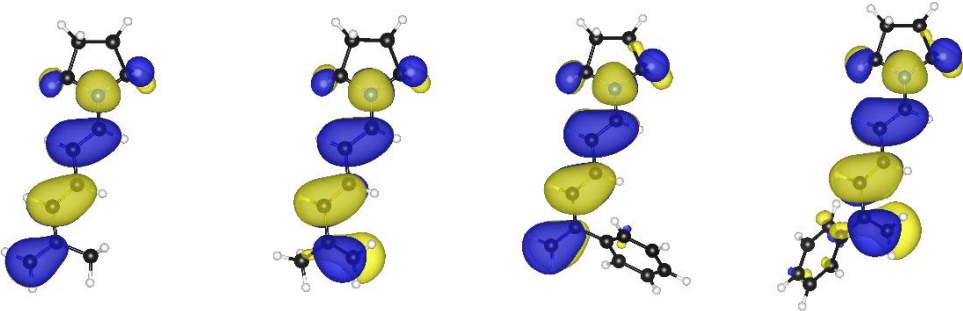
		 J1 : R = CH ₃ K1 : R = Ph L1 : R = PhOMe M1 : R = PhCN	 J2 : R = CH ₃ K2 : R = Ph L2 : R = PhOMe M2 : R = PhCN
Relative Energy (kcal/mol)	R=CH ₃	[0.0]	1.9
	R=Ph	[0.0]	1.2
	R=PhOMe	[0.0]	0.3
	R=PhCN	[0.0]	-0.2
HOMO (eV)	R=CH ₃	-5.79	-5.83
	R=Ph	-5.83	-5.93
	R=PhOMe	-5.78	-5.88
	R=PhCN	-6.09	-6.19

The HOMOs of δ - substituted trienamine reveals preference for all-*trans* configuration over 3,6-*s-cis* diene configuration for electron donating and electron withdrawing substituents. The

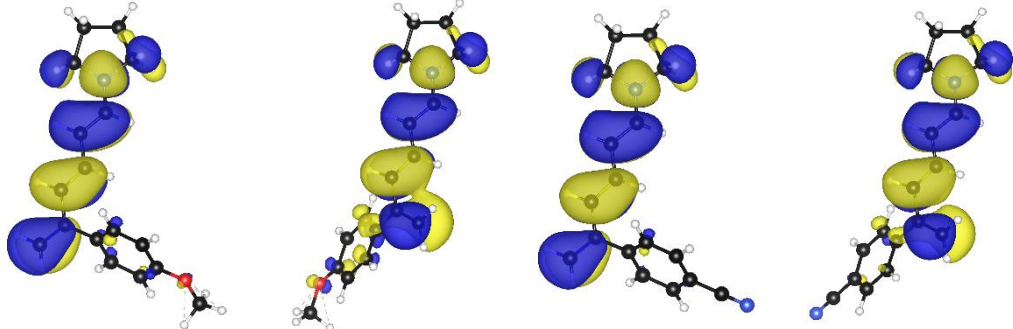
HOMO of phenyl substituted trienamine **K1** with all *trans* configuration is -5.83 eV which lowers to -5.93 eV when rotation around the γ - δ bond results in trienamine **K2** with 3,6-*s-cis* diene (Table 4.13). Similarly, when the substituent is an electron withdrawing group such as 4-cyanobenzene, the HOMO of **M1** lowers from -6.09 eV to -6.19 eV for trienamine **M2** (Table 4.13). This is due to the twisting of *pi*-backbone in 3,6-*s-cis*-diene configuration resulting in the backbone to be out of conjugation. The $\theta_{C3-C4-C5-C6}$ for **K1** and **K2** were determined to be 170.0° and 34.0° , respectively. The molecular orbital analysis suggests that the vinylogy principle is followed for δ -substituted trienamine regardless of nature of substituents (Table 4.14, 4.15).

Overall, the analysis of δ -substituted trienamines indicates that the energy difference between all-*trans* configuration and 3,6-*s-cis* diene configuration is relatively small. The aryl substituted trienamines do not demonstrate any significant thermodynamic preference for all-*trans* or 3,6-*s-cis* diene configuration. The HOMO level of δ -substituted trienamine was found to be higher for all-*trans* configuration relative to 3,6-*s-cis* diene configuration.

Table 4.14: Orbital coefficients of HOMOs of trienamine **J1**, **J2**, **K1**, and **K2**



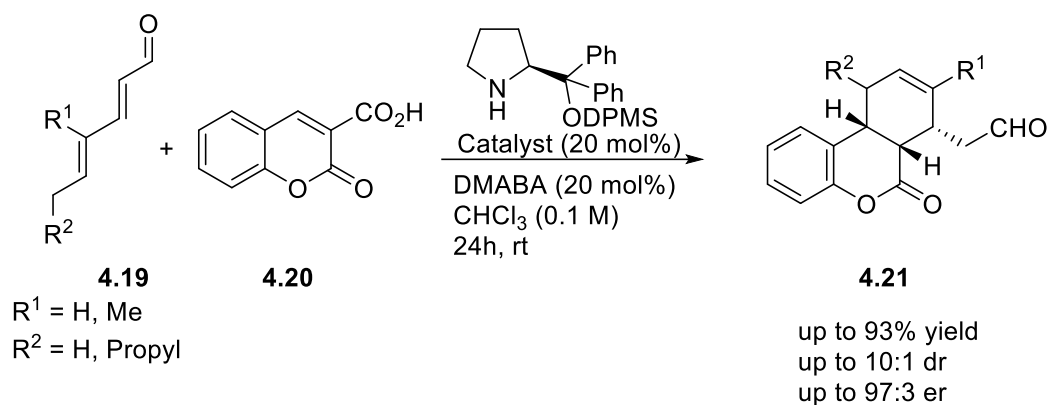
	J1	J2	K1	K2
<i>ipso</i>	10.83	10.83	10.55	10.64
α	17.56	17.93	17.37	18.10
β	8.70	8.41	8.37	8.04
γ	15.62	16.79	15.85	16.23
δ	4.26	4.00	4.20	3.69
ϵ	11.35	9.70	11.76	9.54

Table 4.15: Orbital coefficients of HOMOs of trienamine **L1**, **L2**, **M1**, and **M2**


	L1	L2	M1	M2
<i>ipso</i>	10.47	10.46	10.39	10.57
α	17.08	17.66	18.14	19.08
β	8.39	7.96	7.89	7.57
γ	15.65	15.83	16.04	16.54
δ	4.28	3.79	3.93	3.39
ϵ	12.10	10.03	11.08	8.57

4.3.5: ϵ -Substituted Trienamines

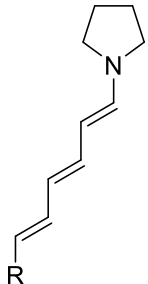
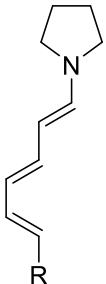
Finally, we explored ϵ -substituted trienamines which have not been widely utilized, relative to γ -substitution, in trienamine mediated Diels-Alder reactions. However, substituents with electron-donating abilities such as alkyl groups have been commonly utilized at the ϵ -position.^{10,24,36–41} Albrecht and co-workers reported a trienamine mediated cycloaddition using dienophiles activated by carboxylic acids. Upon reaction with a trienamine intermediate, the dienophile undergoes decarboxylation to synthesize biologically relevant 3,4-hydrocoumarins (Scheme 4.7).²⁴



Scheme 4.7: Trienamine mediated Diels-Alder reaction between ϵ -substituted 2,4-Dienals and Coumarin-3-carboxylic acids, reported by Albrecht et al.

Similar to γ -substituted trienamines, the ϵ -substituted trienamines showed similar thermodynamic preference for all *trans* conformer. The Van Der Waals repulsions are increased for 3,6-*s-cis* diene conformer resulting in 2-4 kcal/mol higher in energy than all-*trans* conformers, regardless of substituents (Table 4.16). The orbital analysis of epsilon substituted trienamines revealed that the HOMO gets raised as the electron donating ability of the substituent increases. The HOMO of phenyl substituted trienamine **O1** with all *trans* configuration is located at -5.66 eV which gets lowered to -5.74 eV for trienamine **O2** with the 3,6-*s-cis* diene configuration (Table 4.16). When the substituent is more electron donating such as 4-methoxy benzene, the HOMO of trienamine **P1** was determined to be located at -5.53 eV which gets lowered to -5.63 eV for trienamine **P2**. However, the electron withdrawing substituent 4-cyanobenzene lowers the HOMO to -5.98 eV and -6.03 eV for trienamines **Q1** and **Q2**, respectively (Table 4.16).

Table 4.16: Relative energies and HOMO locations of trienamines **N1**, **N2**, **O1**, **O2**, **P1**, **P2**, **Q1**, and **Q2**. All free energies are reported in kcal/mol.

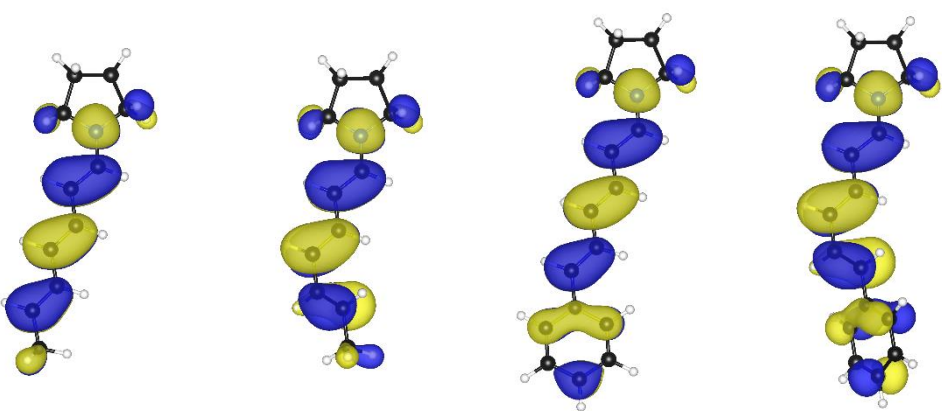
		 N1: R = CH₃ O1: R = Ph P1: R = PhOMe Q1: R = PhCN	 N2: R = CH₃ O2: R = Ph P2: R = PhOMe Q2: R = PhCN
Relative Energy (kcal/mol)	R=CH ₃	[0.0]	2.5
	R=Ph	[0.0]	3.4
	R=PhOMe	[0.0]	3.8
	R=PhCN	[0.0]	3.1
HOMO (eV)	R=CH ₃	-5.66	-5.74
	R=Ph	-5.66	-5.74
	R=PhOMe	-5.53	-5.63
	R=PhCN	-5.98	-6.03

While performing orbital analysis on epsilon substituted trienamines, it was revealed that the HOMO of trienamines gets raised when an aryl substituent is at ϵ -position compared to other positions of the trienamine regardless of the all-*trans* or 3,6-*s-cis* diene configuration. This is because the aryl substituents at the ϵ -position are fully in conjugation with the pi-backbone, however, this conjugation is disrupted for substituents at β -, γ -, or δ - position.

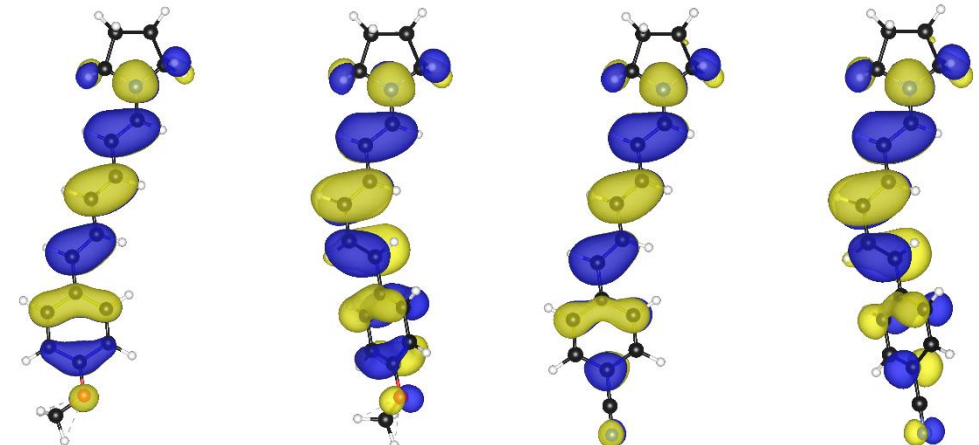
This is evident when comparing the location of HOMO for substituents at the nucleophilic (γ - and ε -) and electrophilic (β - and δ -) positions of the trienamine. The HOMO of trienamine **A1** is located at -5.80 eV which raises to -5.71 eV for γ -substituted trienamine **H1**. Substitution at ε -position results in raising the HOMO level further to -5.53 eV for trienamine **P1**. Similarly, the HOMO of trienamine is slightly raised to -5.76 eV for β -substituted trienamine **D1** and -5.78 eV for δ -substituted **L1** compared to unsubstituted trienamine **A1**. This also suggests that g - and e -substituted trienamines may be the most appealing candidates for trienamine mediated reaction development.

The orbital analysis for ε -substituted trienamines revealed that the vinylogy principle is not followed for aryl substituents (Table 4.18, 4.19). The calculations showed the orbital composition at the α and γ carbons to be equivalent for aryl substituents ($\alpha \approx \gamma > \varepsilon$) regardless of conformation. The calculated orbital composition for phenyl substituted trienamine **O2** for α -carbon is 14.74 which is slightly less than γ -carbon composition, 14.80.

Table 4.17: Orbital coefficients of HOMOs of trienamine **N1**, **N2**, **O1**, and **O2**



	N1	N2	O1	O2
<i>ipso</i>	10.63	10.91	9.29	9.61
α	16.33	17.20	13.70	14.74
β	9.27	8.93	8.81	8.53
γ	15.48	16.41	13.58	14.80
δ	5.20	4.67	5.72	5.30
ε	11.34	9.09	11.40	9.96

Table 4.18: Orbital coefficients of HOMOs of trienamine **P1**, **P2**, **Q1**, and **Q2**


	P1	P2	Q1	Q2
<i>ipso</i>	8.84	9.15	9.11	9.42
α	12.40	13.49	14.44	15.37
β	8.88	8.53	8.13	7.96
γ	12.54	13.72	14.13	15.33
δ	6.34	5.92	4.93	4.60
ϵ	10.92	9.70	11.49	10.09

4.4: Conclusions

In conclusion, the impact of electron donating and electron withdrawing substituents at different positions of the trienamine intermediate was investigated. Our calculations suggest that electron donating substituents raise the HOMO of the trienamine intermediate to undergo Diels-Alder reactions. This effect is prominent especially for nucleophilic positions (γ , ϵ) of the trienamine intermediate. It was also determined that the 1,4-*s-cis* diene moiety is less likely to undergo Diels-Alder reaction due to lower HOMO energy when compared to 3,6-*s-cis* diene configuration. Furthermore, the 3,6-*s-cis* diene configuration is also thermodynamically preferred for γ , and ϵ -substituted trienamine intermediates, making them *viable* candidates for Diels-Alder reaction development. The 1,4-*s-cis* diene configuration is thermodynamically favoured for the β - and δ -substituted trienamines, however, the HOMO level is lower compared to the 3,6-*s-cis* diene

configuration. Orbital analysis indicates that vinylogy principle is followed in all trienamine intermediates regardless of the nature of the substituent and its position on the trienamine backbone.

Our calculations also indicate that the aryl substituents are out of conjugation, with respect to the *pi*-backbone, for all trienamine intermediates except for the ϵ -substituted trienamine. The aryl substituents at the ϵ -position increase are fully in conjugation with the backbone resulting in highest HOMO location. This feature of ϵ -substituted trienamine intermediates can be exploited to expand the scope of trienamine mediated Diels-Alder cycloaddition.

4.5: References

- (1) Fuson, R. C. The Principle of Vinylogy. *Chem. Rev.* **1935**, 16 (1), 1–27.
<https://doi.org/10.1021/cr60053a001>.
- (2) List, B. The Ying and Yang of Asymmetric Aminocatalysis. *Chem. Commun.* **2006**, No. 8, 819–824. <https://doi.org/10.1039/b514296m>.
- (3) Bertelsen, S.; Marigo, M.; Brandes, S.; Dinér, P.; Jørgensen, K. A. Dienamine Catalysis: Organocatalytic Asymmetric γ -Amination of α,β -Unsaturated Aldehydes. *J. Am. Chem. Soc.* **2006**, 128 (39), 12973–12980. <https://doi.org/10.1021/ja064637f>.
- (4) Marcos, V.; Alemán, J. Old Tricks, New Dogs: Organocatalytic Dienamine Activation of α,β -Unsaturated Aldehydes. *Chem. Soc. Rev.* **2016**, 45 (24), 6812–6832.
<https://doi.org/10.1039/c6cs00438e>.
- (5) Ramachary, D. B.; Reddy, Y. V. Dienamine Catalysis: An Emerging Technology in Organic Synthesis. *Eur. J. Org. Chem.* **2012**, 2012 (5), 865–887.
<https://doi.org/10.1002/ejoc.201101157>.
- (6) Kumar, I.; Ramaraju, P.; Mir, N. A. Asymmetric Trienamine Catalysis: New Opportunities in Amine Catalysis. *Org. Biomol. Chem.* **2013**, 11 (5), 709–716.
<https://doi.org/10.1039/c2ob26681d>.
- (7) Halskov, K. S.; Johansen, T. K.; Davis, R. L.; Steurer, M.; Jensen, F.; Jørgensen, K. A. Cross-Trienamines in Asymmetric Organocatalysis. *J. Am. Chem. Soc.* **2012**, 134 (31), 12943–12946. <https://doi.org/10.1021/ja3068269>.
- (8) Stiller, J.; Poulsen, P. H.; Cruz, D. C.; Dourado, J.; Davis, R. L.; Jørgensen, K. A. Organocatalytic [4+2] Addition Reactions via Tetraenamine Intermediate. *Chem. Sci.* **2014**, 5 (5), 2052–2056. <https://doi.org/10.1039/c4sc00081a>.

- (9) Przydacz, A.; Skrzynska, A.; Albrecht, L. Breaking Aromaticity with Aminocatalysis: A Convenient Strategy for Asymmetric Synthesis. *Angew. Chem. Int. Ed Engl.* **2019**, *58* (1), 63–73. <https://doi.org/10.1002/anie.201808197>.
- (10) Jia, Z. J.; Jiang, H.; Li, J. L.; Gschwend, B.; Li, Q. Z.; Yin, X.; Grouleff, J.; Chen, Y. C.; Jørgensen, K. A. Trienamines in Asymmetric Organocatalysis: Diels-Alder and Tandem Reactions. *J. Am. Chem. Soc.* **2011**, *133* (13), 5053–5061. <https://doi.org/10.1021/ja1112194>.
- (11) Donslund, B. S.; Nielsen, R. P.; Mønsted, S. M. N.; Jørgensen, K. A. Benzofulvenes in Trienamine Catalysis: Stereoselective Spiroindene Synthesis. *Angew. Chem. Int. Ed.* **2016**, *55* (37), 11124–11128. <https://doi.org/10.1002/anie.201605079>.
- (12) Inoshita, T.; Goshi, K.; Morinaga, Y.; Umeda, Y.; Ishikawa, H. Enantioselective Construction of Octahydroquinolines via Trienamine-Mediated Diels–Alder Reactions. *Org. Lett.* **2019**, *21* (8), 2903–2907. <https://doi.org/10.1021/acs.orglett.9b00932>.
- (13) Jia, Z.-J.; Zhou, Q.; Zhou, Q.-Q.; Chen, P.-Q.; Chen, Y.-C. Exo-Selective Asymmetric Diels–Alder Reaction of 2,4-Dienals and Nitroalkenes by Trienamine Catalysis. *Angew. Chem. Int. Ed.* **2011**, *50* (37), 8638–8641. <https://doi.org/10.1002/anie.201102013>.
- (14) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function. *Theor. Chem. Acc.* **2008**, *120* (1–3), 215–241. <https://doi.org/10.1007/s00214-007-0310-x>.
- (15) Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. A Complete Basis Set Model Chemistry. I. The Total Energies of Closed-shell Atoms and

- Hydrides of the First-row Elements. *J. Chem. Phys.* **1998**, *89* (4), 2193.
<https://doi.org/10.1063/1.455064>.
- (16) Petersson, G. A.; Al-Laham, M. A. A Complete Basis Set Model Chemistry. II. Open-Shell Systems and the Total Energies of the First-Row Atoms. *J. Chem. Phys.* **1991**, *94*, 6081–6090. <https://doi.org/10.1063/1.460447>.
- (17) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; X. Li, M. C.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ort, J. V.; Fox, D. J. Gaussian 09, Revision. <http://gaussian.com/g09citation/> (accessed 2018-11-30).
- (18) Lu, T.; Chen, F. Multiwfn: A Multifunctional Wavefunction Analyzer. *J. Comput. Chem.* **2012**, *33* (5), 580–592. <https://doi.org/10.1002/jcc.22885>.
- (19) CYLview Visualization Software. <https://www.cylview.org/> (accessed 2023-05-09).
- (20) Momma, K.; Izumi, F. VESTA 3 for Three-Dimensional Visualization of Crystal, Volumetric and Morphology Data. *J. Appl. Crystallogr.* **2011**, *44* (6), 1272–1276. <https://doi.org/10.1107/S0021889811038970>.
- (21) Chen, J.; Fu, Y.; Yu, Y.; Wang, J. R.; Guo, Y. W.; Li, H.; Wang, W. Enantioselective [4 + 2] Cycloaddition Reaction of Vinylquinolines with Dienals Enabled by Synergistic Organocatalysis. *Org. Lett.* **2020**, *22* (15), 6061–6066. <https://doi.org/10.1021/acs.orglett.0c02137>.
- (22) Lu, J.-B.; Shi, C.-H.; Hu, D.; Gao, X.-Y.; Chen, Z.-C.; Du, W.; Chen, Y.-C. Regioselectivity Umpolung in Asymmetric Diels–Alder Reaction of Ortho-Formyl-Substituted Cinnamates and Dienals via Double Aminocatalysis. *Org. Lett.* **2021**, *23* (1), 145–149. <https://doi.org/10.1021/acs.orglett.0c03862>.

- (23) Barløse, C. L.; Østergaard, N. L.; Bitsch, R. S.; Iversen, M. V.; Jørgensen, K. A. A Direct Organocatalytic Enantioselective Route to Functionalized *Trans*-Diels–Alder Products Having the Norcarane Scaffold. *Angew. Chem. Int. Ed.* **2021**, *60* (33), 18318–18327. <https://doi.org/10.1002/anie.202106598>.
- (24) Albrecht, A.; Bojanowski, J.; Kot, A.; Sieroń, L. Decarboxylative, Trienamine Mediated Cycloaddition for the Synthesis of 3,4-Dihydrocoumarin Derivatives. *Org. Biomol. Chem.* **2019**, *17* (17), 4238–4242. <https://doi.org/10.1039/C9OB00386J>.
- (25) Yuan, X.; Zhang, S.-J.; Du, W.; Chen, Y.-C. Asymmetric Diels–Alder Cycloadditions of Trifluoromethylated Dienophiles Under Trienamine Catalysis. *Chem. – Eur. J.* **2016**, *22* (31), 11048–11052. <https://doi.org/10.1002/chem.201600989>.
- (26) Zhu, K.; Huang, H.; Wu, W.; Wei, Y.; Ye, J. Aminocatalyzed Asymmetric Diels–Alder Reaction of 2,4-Dienals and Rhodanine/Hydantoin Derivatives. *Chem. Commun.* **2013**, *49* (21), 2157–2159. <https://doi.org/10.1039/C3CC00023K>.
- (27) Zhou, Q.-Q.; Yuan, X.; Xiao, Y.-C.; Dong, L.; Chen, Y.-C. Aminocatalytic Asymmetric Diels–Alder Reaction of Phosphorus Dienophiles and 2,4-Dienals. *Tetrahedron* **2013**, *69* (48), 10369–10374. <https://doi.org/10.1016/j.tet.2013.10.001>.
- (28) Liu, J.-X.; Zhou, Q.-Q.; Deng, J.-G.; Chen, Y.-C. An Asymmetric Normal-Electron-Demand Aza-Diels–Alder Reaction via Trienamine Catalysis. *Org. Biomol. Chem.* **2013**, *11* (47), 8175–8178. <https://doi.org/10.1039/C3OB41698D>.
- (29) Albrecht, L.; Cruz Acosta, F.; Fraile, A.; Albrecht, A.; Christensen, J.; Jørgensen, K. A. Enantioselective H-Bond-Directing Approach for Trienamine-Mediated Reactions in Asymmetric Synthesis. *Angew. Chem. Int. Ed.* **2012**, *51* (36), 9088–9092. <https://doi.org/10.1002/anie.201204790>.

- (30) Albrecht, A.; Skrzyńska, A.; Pietrzak, A.; Bojanowski, J.; Albrecht, Ł. Asymmetric Aminocatalysis in the Synthesis of δ -Lactone Derivatives. *Asian J. Org. Chem.* **2016**, 5 (9), 1115–1119. <https://doi.org/10.1002/ajoc.201600272>.
- (31) Hejmanowska, J.; Jasiński, M.; Mlostoń, G.; Albrecht, Ł. Taming of Thioketones: The First Asymmetric Thia-Diels–Alder Reaction with Thioketones as Heterodienophiles. *Eur. J. Org. Chem.* **2017**, 2017 (5), 950–954. <https://doi.org/10.1002/ejoc.201601307>.
- (32) Li, Y.; Barløse, C.; Jørgensen, J.; Carlsen, B. D.; Jørgensen, K. A. Asymmetric Catalytic Aza-Diels–Alder/Ring-Closing Cascade Reaction Forming Bicyclic Azaheterocycles by Trienamine Catalysis. *Chem. – Eur. J.* **2017**, 23 (1), 38–41. <https://doi.org/10.1002/chem.201604310>.
- (33) Skrzyńska, A.; Drelich, P.; Frankowski, S.; Albrecht, Ł. Synthesis of γ,γ -Disubstituted Butenolides through a Doubly Vinylogous Organocatalytic Cycloaddition. *Chem. – Eur. J.* **2018**, 24 (62), 16543–16547. <https://doi.org/10.1002/chem.201804650>.
- (34) Ming, Y.-C.; Lv, X.-J.; Liu, M.; Liu, Y.-K. Synthesis of Chiral Polycyclic Tetrahydrocarbazoles by Enantioselective Aminocatalytic Double Activation of 2-Hydroxycinnamaldehydes with Dienals. *Org. Lett.* **2021**, 23 (16), 6515–6519. <https://doi.org/10.1021/acs.orglett.1c02309>.
- (35) Mitkari, S. B.; Medina-Ortíz, A.; Olivares-Romero, J. L.; Vázquez, M. A.; Peña-Cabrera, E.; Villegas Gómez, C.; Cruz Cruz, D. Organocatalytic Cascade Reactions for the Diversification of Thiopyrano-Piperidone Fused Rings Utilizing Trienamine Activation. *Chem. – Eur. J.* **2021**, 27 (2), 618–621. <https://doi.org/10.1002/chem.202004553>.

- (36) Li, X.; Lin, M.-H.; Han, Y.; Wang, F.; Cheng, J.-P. Asymmetric Diels–Alder Reaction of 3-Olefinic Benzofuran-2-Ones and Polyenals: Construction of Chiral Spirocyclic Benzofuran-2-Ones. *Org. Lett.* **2014**, *16* (1), 114–117. <https://doi.org/10.1021/ol403094a>.
- (37) Poulsen, P. H.; Feu, K. S.; Paz, B. M.; Jensen, F.; Jørgensen, K. A. Organocatalytic Asymmetric 1,6-Addition/1,4-Addition Sequence to 2,4-Dienals for the Synthesis of Chiral Chromans. *Angew. Chem.* **2015**, *127* (28), 8321–8325. <https://doi.org/10.1002/ange.201503370>.
- (38) Gu, J.; Xiao, B.-X.; Chen, Y.-R.; Du, W.; Chen, Y.-C. Asymmetric Diels–Alder and Cascade Reaction of Quinone Imine Ketals and 2,4-Dienals: Construction of Chiral Benzo[de]Quinolone Derivatives. *Adv. Synth. Catal.* **2016**, *358* (2), 296–302. <https://doi.org/10.1002/adsc.201500860>.
- (39) Maurya, V.; Appayee, C. Catalytic Asymmetric Synthesis of 3,4-Disubstituted Cyclohexadiene Carbaldehydes: Formal Total Synthesis of Cyclobakuchiols A and C. *Org. Lett.* **2018**, *20* (13), 4111–4115. <https://doi.org/10.1021/acs.orglett.8b01667>.
- (40) Jiang, H.; Zhou, L.; Mao, B.; Yuan, C.; Wang, W.; Wu, Y.; Zhang, C.; Guo, H. Organocatalytic Enantioselective [3+2] Cycloaddition of Azomethine Ylides with 2,4-Dienals: Construction of Remote Stereogenic Centers via 1,6-Addition Reaction. *Adv. Synth. Catal.* **2020**, *362* (24), 5716–5720. <https://doi.org/10.1002/adsc.202000813>.
- (41) Roy, S.; Pradhan, S.; Kumar, K.; Chatterjee, I. Asymmetric Organocatalytic Double 1,6-Addition: Rapid Access to Chiral Chromans with Molecular Complexity. *Org. Chem. Front.* **2020**, *7* (11), 1388–1394. <https://doi.org/10.1039/D0QO00354A>.

Chapter 5 : Electron-deficient 1,2-cyclohexadienes: Mechanistic investigation of unprecedented dimerization.

5.1: Introduction

Highly reactive intermediates such as strained cyclic intermediates: arynes, cyclic alkynes, and cyclic allenes have played an important role in organic chemistry in a wide variety of chemical transformations. From being a curiosity to experimental validation, small strained cyclic intermediates have recently been utilized in a wide variety of applications. These intermediates are usually short-lived species generated in-situ and consumed during the desired reaction. The most popular of these intermediates are strained cyclic compounds such as benzyne¹ (**5.1**), cyclohexyne² (**5.2**), and 1,2-cyclohexadiene³ (**5.3**) (Figure 5.1). These intermediates have been widely utilized in various applications such as natural product synthesis, ligand design, and material science.^{4–12}

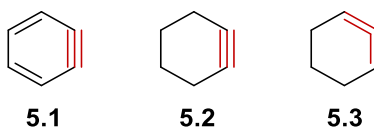


Figure 5.1: Cyclic strained reactive intermediates

The main focus of this chapter is on cyclic allenes, specifically 1,2-cyclohexadienes which were first experimentally validated by Wittig in 1966³. Over the decades, the interest in studying cyclic allenes has mostly been theoretical to understand its structure and reactivity. The earlier studies have determined that the reactivity of cyclic allenes is correlated with ring strain energy^{13–16}. The bending and twisting of an acyclic allene's linear and orthogonal geometry to set into a ring gives rise to its ring strain¹⁷.

In 2006, Johnson *et al.* published a comprehensive report estimating the strain of cyclic allenes using computational methods. This report revealed that the ring strain energy increases as

the ring size decreases¹³. The authors studied cyclic allenes ranging from 1,2-cyclononadiene **5.8** (strain energy (SE) = 2 kcal/mol) to 1,2-cyclobutadiene **5.4** (SE = 65 kcal/mol) (Figure 5.2). Further analysis of this study demonstrates that the correlation of ring strain with the ring size is a result of the bending angle of the 3-carbon allene moiety and it was determined the twisting of allenes decreases with the higher ring size. The calculations determine the bending angle of 1,2-cyclohexadiene **5.3** to be 133.3° and the ring strain to be 32 kcal/mol.

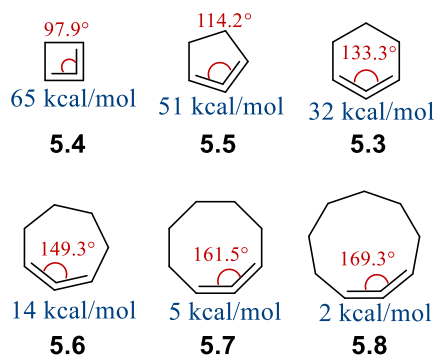
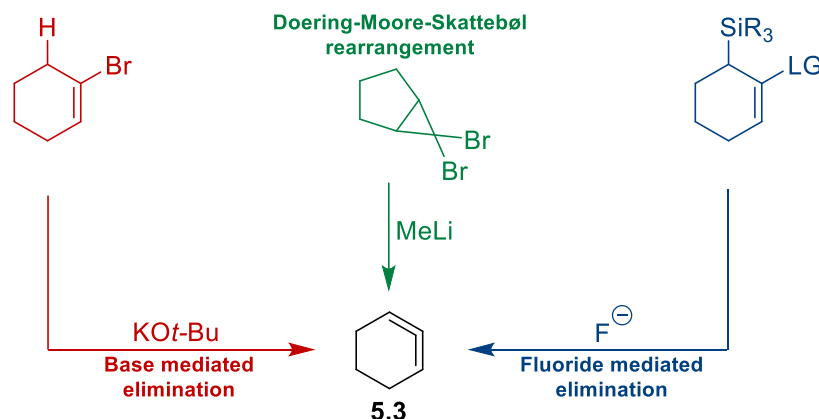


Figure 5.2: Bending angle and strain energies for cyclic allenes.

5.2: Generation of cyclic allenes

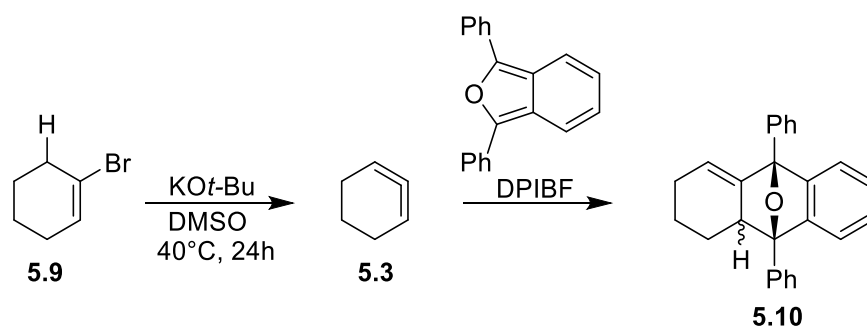
In order to take advantage of the reactive intermediate 1,2-cyclohexadiene **5.3** in chemical transformations, various methods to generate them have been reported. The most common methods are generation of the cyclic allene through base elimination¹⁸, fluoride promoted elimination¹⁹, and Doering-Moore-Skattebøl rearrangement²⁰ (Scheme 5.1). These methods to generate 1,2-cyclohexadienes will be discussed in subsections below.



Scheme 5.1: Common methods to generate 1,2-cyclohexadiene

5.2.1: Base mediated elimination

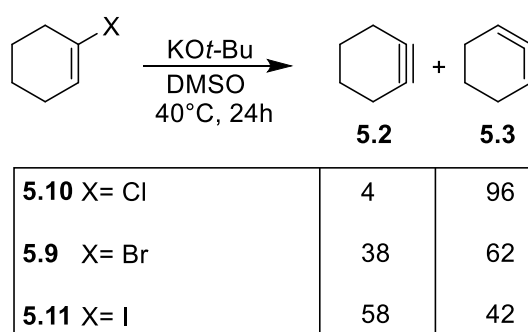
One of the most common methods to generate 1,2-cyclohexadiene **5.3** is *via* base mediated elimination. The experimental validation of 1,2-cyclohexadiene **5.3**, performed by Wittig and Fritze³, developed and utilized base promoted elimination. In the presence of strong base, KO*t*-Bu, 1-bromocyclohexene resulted in 1,2-cyclohexadiene intermediate at 40°C. This intermediate was trapped with diphenylisobenzofuran (DPIBF) *via* Diels-Alder reaction which resulted in a mixture of endo and exo cycloadducts (Scheme 5.2).



Scheme 5.2: Generation of 1,2-cyclohexadiene via base elimination and trapping with DPIBF.

One of the major advantages of this method is being able to generate 1,2-cyclohexadienes at mild temperatures, however, the strong base could be incompatible with a more functionalized

substrate which may result in side reactions. The studies performed on base promoted elimination for different halo-cyclohexene substrates, there is the possibility of a competing reaction of further elimination to result in cyclohexyne². In the presence of KO*t*-Bu in DMSO, 1-chlorocyclohexene resulted in 1,2-cyclohexadiene as the major product (96:4 cyclohexadiene:cyclohexyne), however, a greater mixture of 1,2-cyclohexadiene and cyclohexyne was observed when 1-bromocyclohexene (62:38) and 1-iodocyclohexene (42:58) were utilized. (Scheme 5.3).

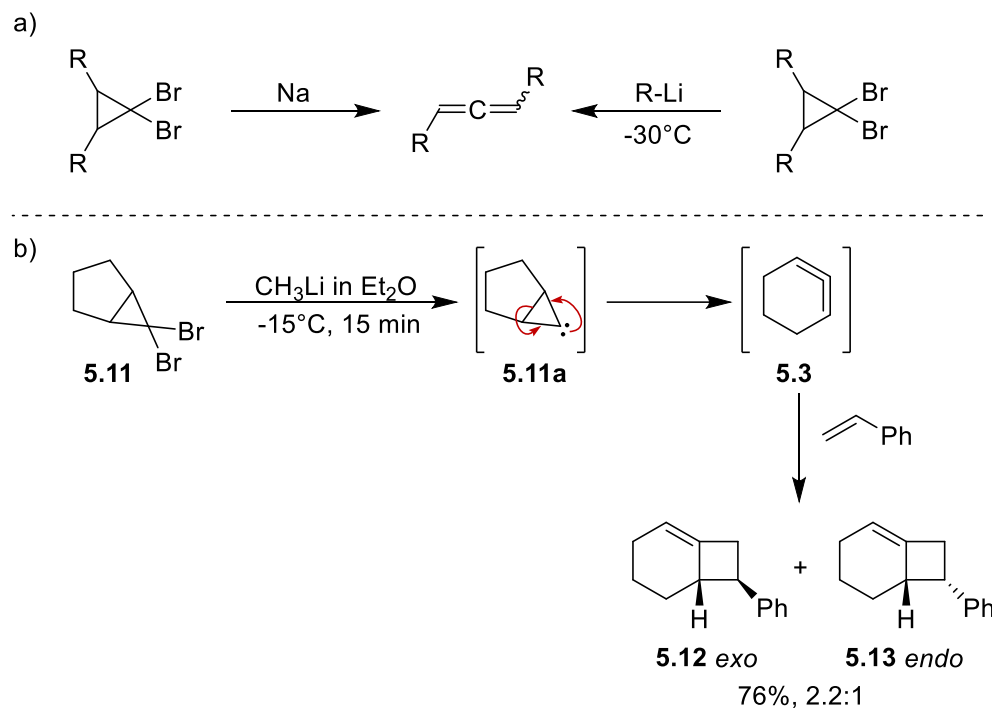


Scheme 5.3: Comparison of generation of cyclohexyne and 1,2-cyclohexadiene with different 1-chlorocyclohexenes

5.2.2: Doering-Moore-Skattebøl rearrangement

One of the earliest methods to generate allenes was pioneered by Doering who treated 1,1-dibromocyclopropanes with sodium metal at elevated temperatures²¹. Moore and Skattebøl later demonstrated the synthesis of allenes, with higher yields, by treating the 1,1-dibromocyclopropane with organolithium reagents at low temperatures (Scheme 5.4a)^{22,23}. This methodology is known as Doering-Moore-Skattebøl (DMS) rearrangement which has been utilized to synthesize cyclic allenes such as 1,2-cyclohexadiene. Moore and Moser reported that slow addition of methyllithium to 6,6-dibromobicyclo[3.1.0]hexane dissolved in styrene resulted in 1,2-cyclohexadiene which was trapped by styrene with a good yield (Scheme 5.4b)²⁰. The cycloadducts were isolated as a mixture of diastereomers (*exo:endo* 2.2:1). This methodology is a well-optimized way to generate

cyclic allenes, however, the use of organolithium reagents may not be compatible with various functional groups. One of the main disadvantages of this method is also the synthesis of starting material containing the 1,1-dibromocyclopropane moiety.

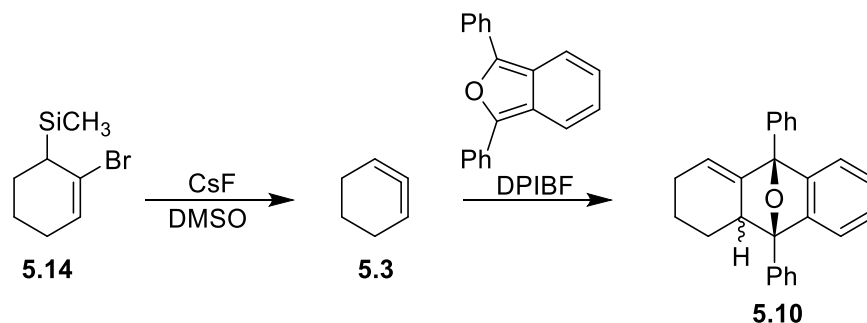


Scheme 5.4: a) Allene synthesis via Doering-Moore-Skattebøl reaction. b) Generation of 1,2-cyclohexadiene via Doering-Moore-Skattebøl reaction.

5.2.3: Fluoride mediated elimination

One of the most common methods for desilylation is by using a fluoride anion. This method to break carbon-silicon bonds was utilized to synthesize cyclic allenes by Shakespeare and Johnson. The authors reported the generation of 1,2-cyclohexadiene using 1-bromo-6-(trimethylsilyl)-cyclohexene in the presence of cesium fluoride (Scheme 5.5)¹⁹. The allene intermediate was trapped with DPIBF to result in a cycloadduct. This method has now been established to generate cyclic allenes with relatively mild reaction conditions compared to the

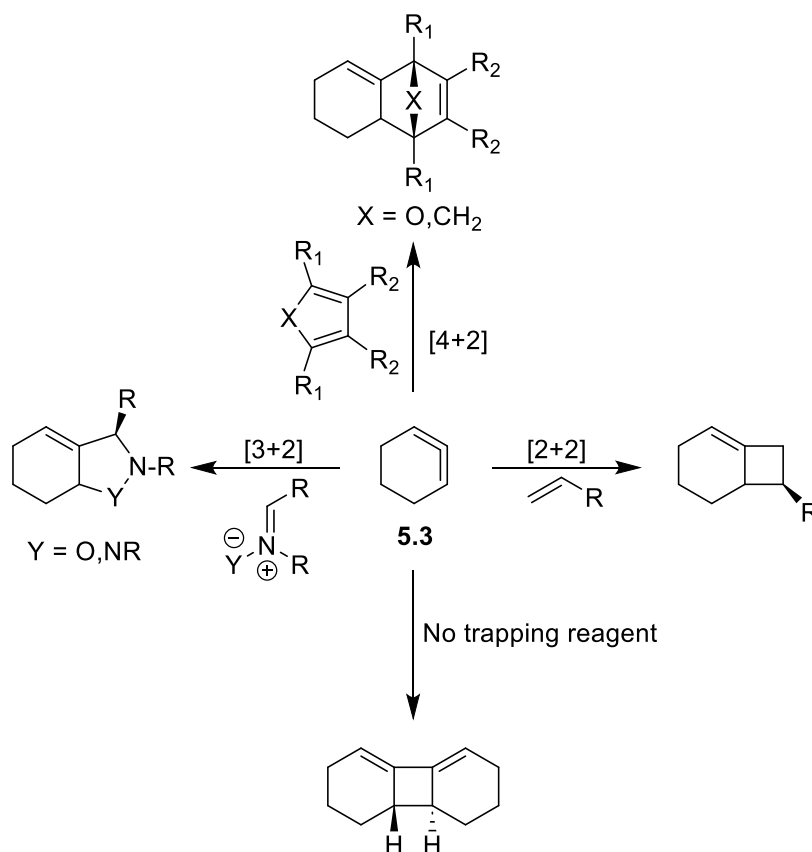
previous methods. This method has also allowed access to a larger scope of functionalized 1,2-cyclohexadienes^{24–26} (ref of garg, west, and mori, and garg).



Scheme 5.5: Generation of 1,2-cyclohexadiene via fluoride mediated elimination

5.3: Reactivity of 1,2-cyclohexadiene: Trapping and Dimerization

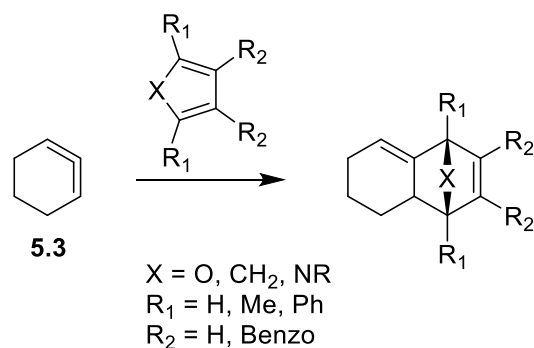
After generation of the cyclic allene 1,2-cyclohexadiene, there are various possibilities to utilize this reactive intermediate. The two well established reactions are dimerization and trapping of the 1,2-cyclohexadienes. In presence of a trapping reagent, the intermediate can undergo cycloaddition reactions which depend heavily on the nature of trapping reagent (Scheme 5.6). In the absence of a trapping reagent, the 1,2-cyclohexadiene can react with itself *via* dimerization (Scheme 5.6) which can react further and a mixture of oligomerization products would be obtained.



Scheme 5.6: Common reactions of 1,2-cyclohexadiene intermediate.

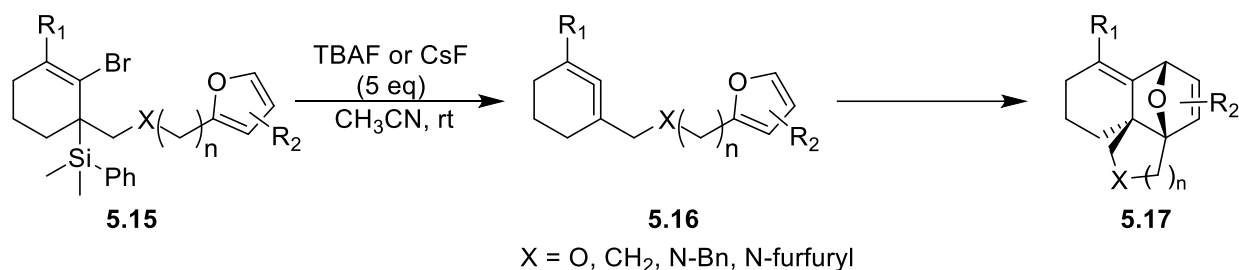
5.3.1: Trapping of 1,2-cyclohexadienes via cycloaddition reactions

One of the earliest and most common methods of trapping the 1,2-cyclohexadiene intermediate is *via* Diels-Alder reaction. This method was also utilized in early cyclic allene studies to experimentally validate the 1,2-cyclohexadiene intermediate (Scheme 5.2)³. The large scope of cyclic 1,3-dienes, such as furans, pyrroles, cyclopentadienes and cyclohexadienes, can be used to react with **5.3** *via* Diels-Alder reaction to obtain cycloadducts (Scheme 5.7)^{24,27–31}. Various functionalized 1,2-cyclohexadienes, hetroocyclic allenes, and other cyclic allenes have been utilized for trapping *via* [4+2] cycloaddition.



Scheme 5.7: Trapping of 1,2-cyclohexadiene via [4+2] cycloaddition reaction.

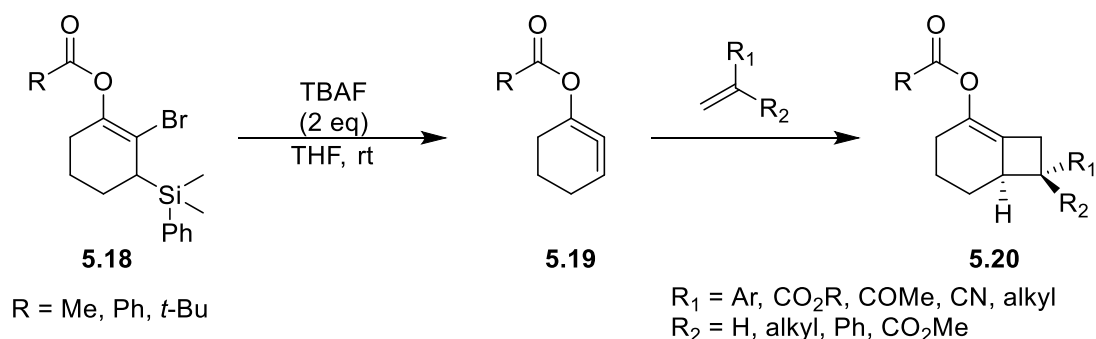
Recently, West and co-workers reported intramolecular [4+2] cycloaddition reaction between furan trap which is tethered to the allene precursor³². The authors utilized a complex allene precursor **5.15** to which fluoride promoted elimination method was applied to synthesize the cyclic allene intermediate **5.16**. This allene would then undergo Diels-Alder reaction with the tethered furan to obtain complex polycyclic cycloadducts **5.17** (Scheme 5.8). This strategy not only allows the synthesis of complex molecules but also lowers the equivalence of the trapping reagent required.



Scheme 5.8: Trapping of in-situ generated 1,2-cyclohexadiene via intramolecular [4+2] cycloaddition reaction.

Similar to [4+2] cycloaddition reaction with cyclic allenes, there have also been reports of [2+2] cycloaddition reactions. One of the earliest trapping reactions on 1,2-cyclohexadiene was performed with styrenes by Moore and Moser (Scheme 5.4b)²⁰. This methodology allowed to form diastereomeric mixture of bicyclic cycloadducts containing cyclobutanes.

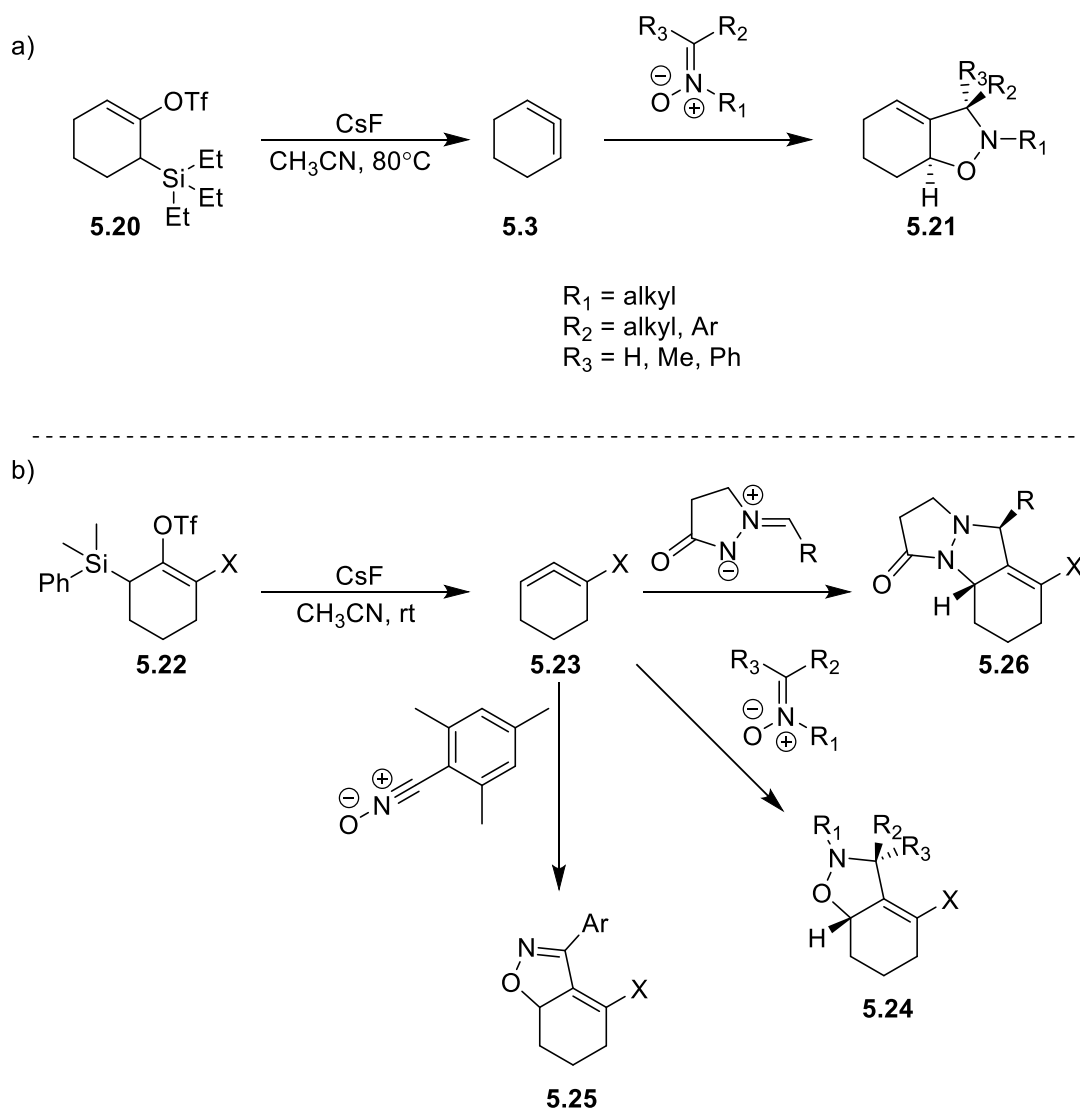
Recently, West and coworkers reported a [2+2] cycloaddition reaction with various styrenes to trap acyloxy-1,2-cyclohexadienes³³. A large scope of styrenes were reacted with various acyloxy 1,2-cyclohexadienes **5.19** generated *via* fluoride promote elimination from precursors **5.18**. The resulting cycloadducts were isolated with moderate diastereoselectivity to afford bicyclo[4.2.0]octenes **5.20** with a preference of *exo* isomer.



Scheme 5.9: Generation and trapping of acyloxy 1,2-cyclohexadienes with styrenes.

Recently, independent works by West and Garg have also demonstrated trapping of 1,2-cyclohexadiene and its derivatives using 1,3-dipoles to result in complex polycyclic compounds. Garg and coworkers utilized nitron to access isoxazolidine cycloadducts **5.21** by using allylic silane triflate allene precursors **5.20** (Scheme 5.10a)²⁴.

West and coworkers also generated 1,2-cyclohexadienes using allylic silane triflates **5.22**³⁴. This report utilized 1,3-dipoles such as nitrile oxides, and azomethine imines in addition to nitrones to undergo cycloaddition reactions with cyclic allenes (Scheme 5.10b). Recent studies have also reported that trapping with 1,3-dipoles can be performed with heterocyclic allenes to give access to complex heterocyclic compounds³⁵.

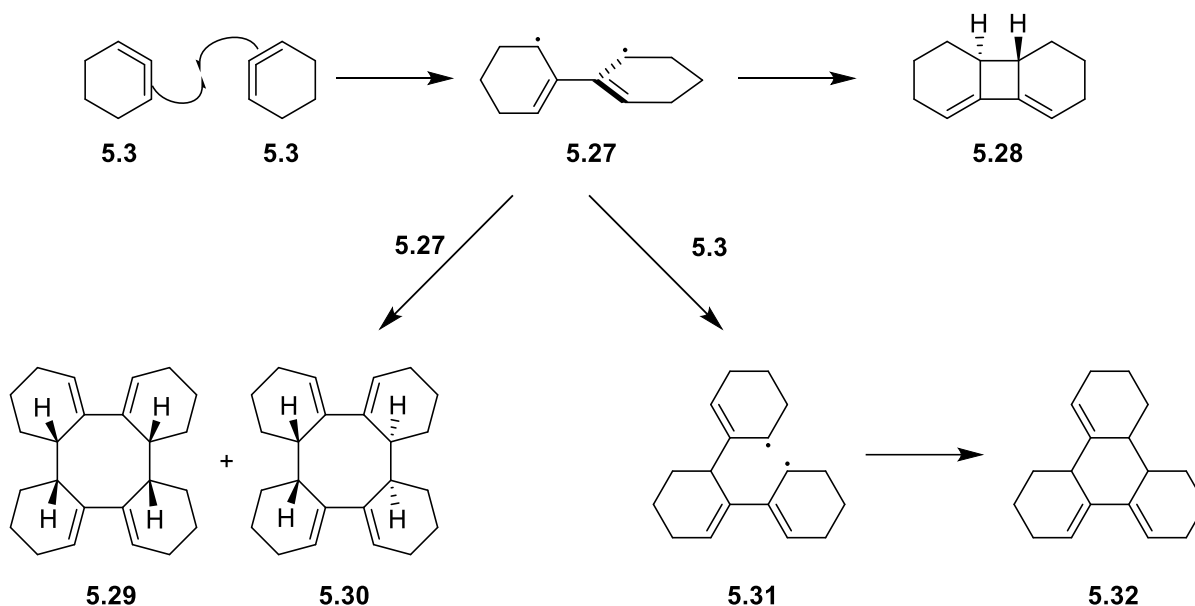


Scheme 5.10: a) [3+2] cycloaddition of 1,2-cyclohexadiene and nitrones by Garg. b) [3+2] cycloaddition of 1,2-cyclohexadiene and 1,3-dipoles by West.

5.3.2: Dimerization

One of the major challenges with cyclic allene intermediates is its tendency to dimerize and sometime oligomerize. In early cyclic allene research³⁶, Wittig reported the isolated dimer **5.28** of 1,2-cyclohexadiene **5.3**³. However, Moser and Moore investigated the formation of dimers and oligomers after the generation of 1,2-cyclohexadiene (Scheme 5.11)³⁷. The authors proposed that the 1,2-cyclohexadiene intermediate reacts with itself to form the diradical **5.27**. After the

formation of **5.27**, the temperature plays a major role³⁸. They observed that if the reaction was at room temperature, the diradical **5.27** quickly forms the dimer **5.28**. However, when the reaction is performed at -78°C the diradical **5.27** reacts further with either **5.27** to result in tetramers **5.29** and **5.30** or with another 1,2-cyclohexadiene **5.3** molecule to form the trimer **5.32**.



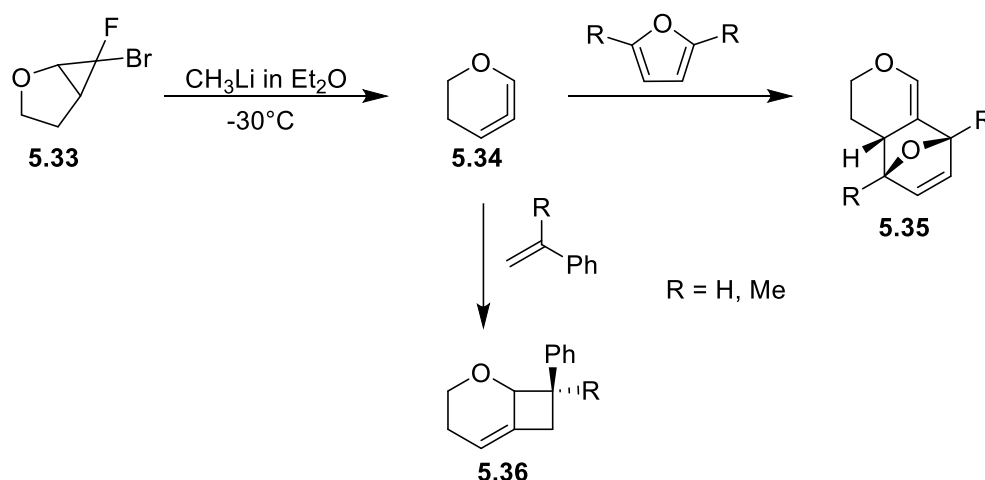
Scheme 5.11: Dimer, trimer, and tetramer products of 1,2-cyclohexadiene.

5.4: Polar Cyclic Allenes

After methods for generation and trapping of cyclic allenes were established, there have recently been attempts to study the reactivity of 1,2-cyclohexadiene in the presence of electron-donating or electron withdrawing groups.

Christl reported the generation of oxygen containing cyclic allenes which were then trapped using furans and styrenes³⁹. The authors used Doering-Moore-Skattlebøl rearrangement to generate 1-oxa-2,3-cyclohexadiene **5.34** from the allene precursor **5.33**. The resulting allenes were trapped furans and styrenes to result in cycloadducts with an oxane moiety (Scheme 5.12).

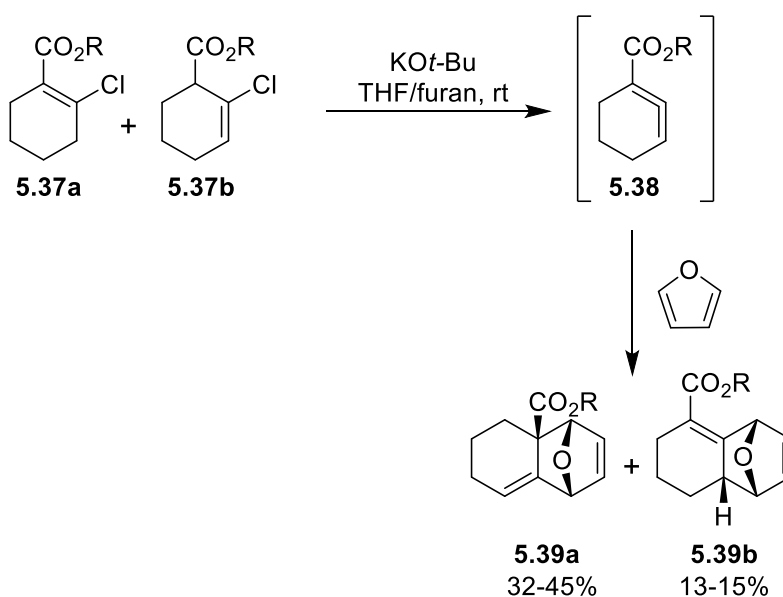
Interestingly, the authors observed different chemoselectivity with different trapping reagents. The reaction with styrenes takes place at the enol ether double bond whereas the reaction with furans takes place at the most remote double bond from the oxygen. The authors proposed that, according to frontier molecular orbital theory, the electron-rich enol ether double bond would be less active towards an electron-rich diene such as furan, which is chemoselective towards the remote double bond. Hence, the trapping reaction with furan was proposed as a one-step Diels-Alder reaction. For the reaction with styrene, a stepwise radical pathway is proposed. Since the alkoxy substituent would be better at stabilizing the radical intermediate, the reaction takes place at the 2-position of the allene.



Scheme 5.12: Generation and trapping of 1-oxa-2,3-cyclohexadiene with furans and styrenes.

By utilizing fluoride promoted elimination of allene precursor **5.22**, West and coworkers reported generation of 1-acetoxy-1,2-cyclohexadiene **5.23**³³. This allene with electron donating acetoxy group was trapped with furans and 1,3-dipoles to result in a huge variety of cycloadducts (Scheme 5.10b). The allene **5.23** demonstrated similar chemoselectivity as oxaallenes where the most remote double bond reacted with the diene.

Similarly, there have been various reports of investigating the reactivity of allenes with an electron withdrawing group. Nendel and coworkers reported the generation of alkyl 1,2-cyclohexadiene carboxylates **5.38** *via* base promoted elimination⁴⁰. The authors use a mixture of allene precursor regioisomers **5.37a** and **5.37b** which resulted in the same allene **5.38**. It was determined that the trapping reaction with furans formed a mixture of regioisomeric **5.39a** and **5.39b** (Scheme 5.13).



Scheme 5.13: Generation and trapping of ester-substituted 1,2-cyclohexadienes.

5.5: Mechanistic investigation of dimerization and trapping of electron deficient 1,2-cyclohexadienes.

There have been studies of cyclic allenes with electron withdrawing groups such as esters⁴⁰, however, reports with other substituents such as keto- or cyano-substituted cyclic allenes have been very limited. The West group, our experimental collaborators, planned to explore the reactivity of keto- and cyano-substituted 1,2-cyclohexadienes. There were four suitable substrates identified for this study with different electron withdrawing groups where three substrates

contained 2-aryl groups and one substrate employed a 2-cyano group (Figure 5.3). The synthesis of **5.40a** – **5.40c**, was performed in two steps from morpholinocyclohexene **5.41** with moderate yields (Scheme 5.14a).⁴¹ The synthesis of **5.40d** was also performed in two steps by performing Thorpe-Ziegler reaction on 1,5-dicyanopentane **5.43** followed by sulfonylation reaction (Scheme 5.14b).^{42,43}

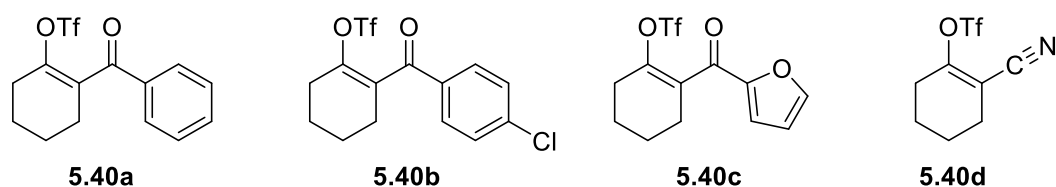
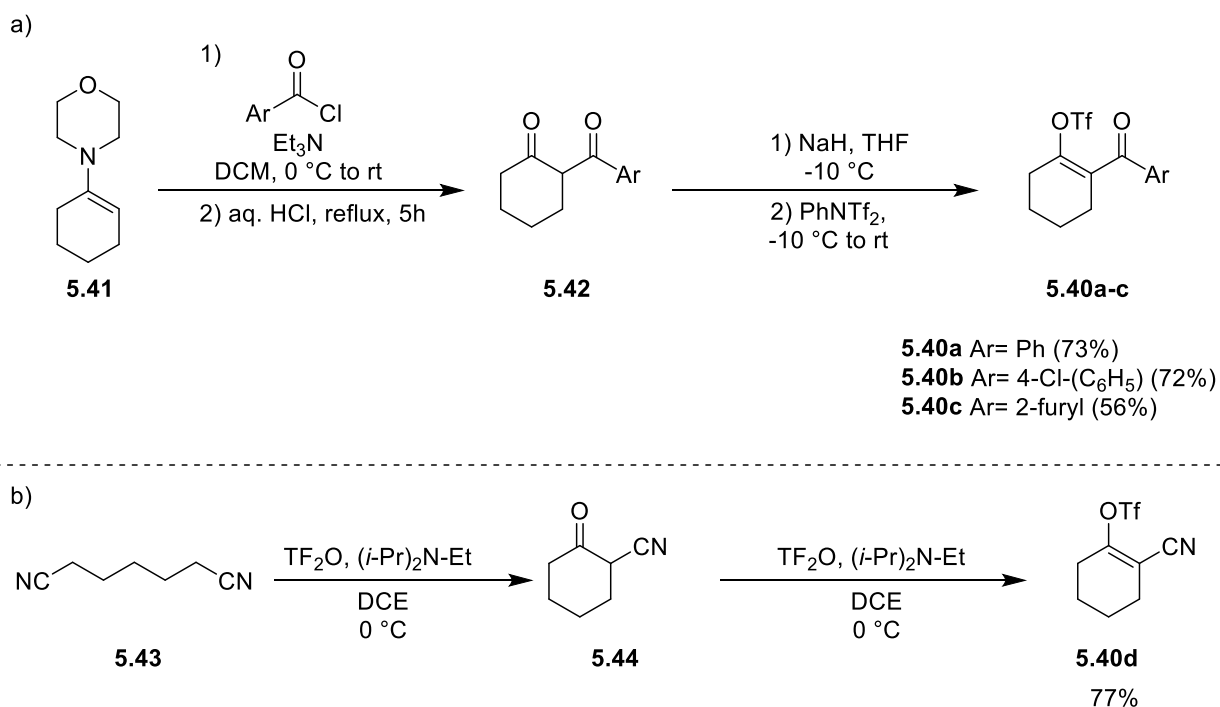


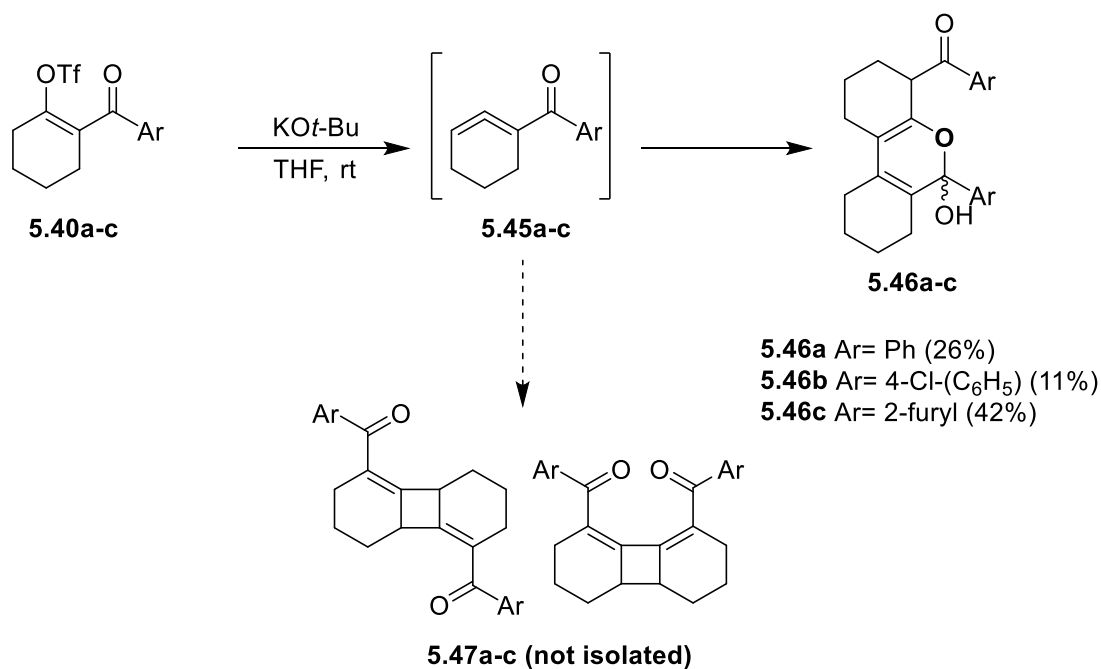
Figure 5.3: Precursors for electron deficient 1,2-cyclohexadienes



Scheme 5.14: a) Synthesis of 2-aryl enol triflate allene precursors. b) Synthesis of 2-cyano enol triflate allene precursor.

During the optimization of conditions for generation of electron deficient keto-1,2-cyclohexadienes **5.40a-c**, an unprecedented dimerization of the cyclic allene **5.45a-c** was

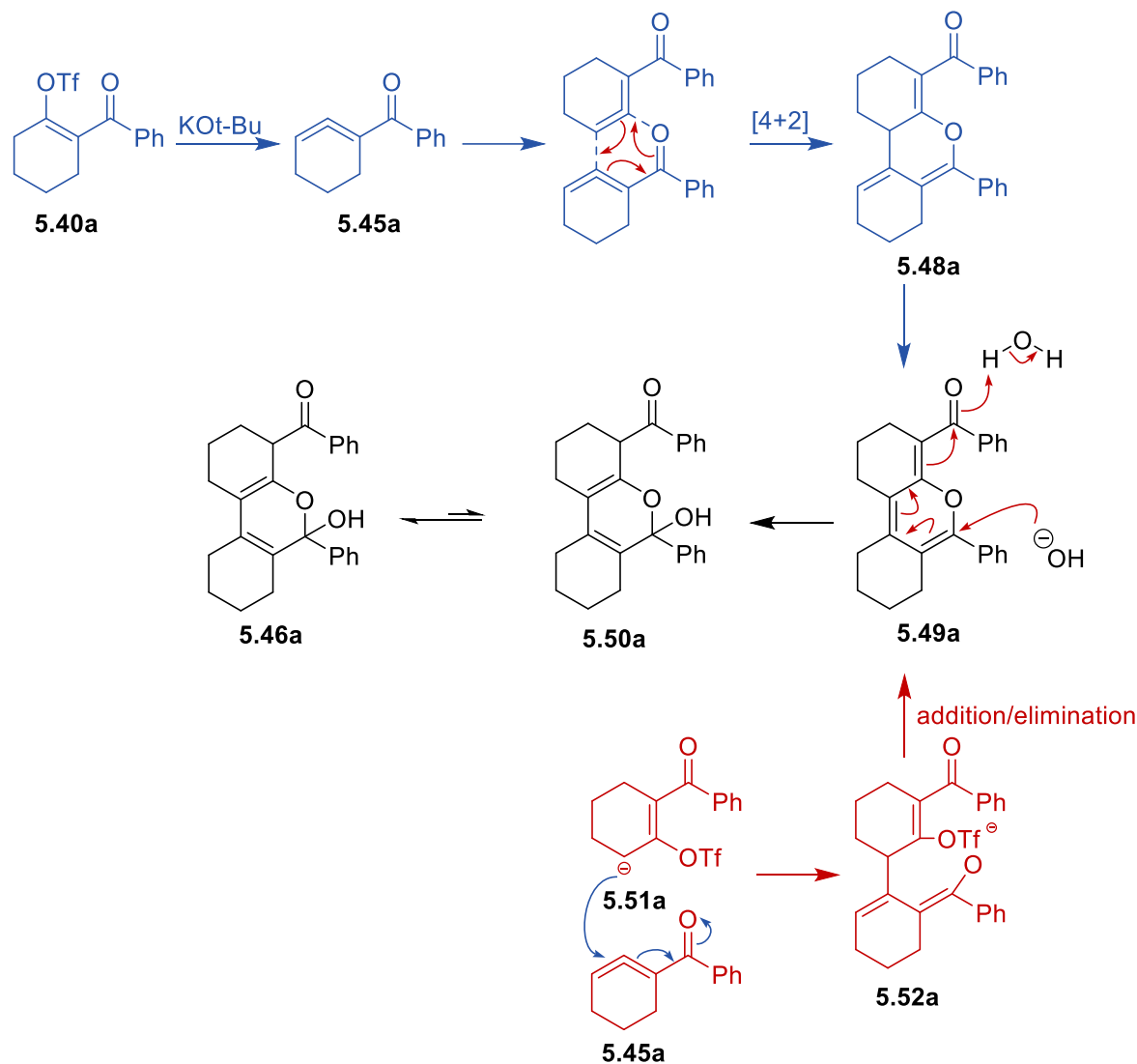
observed. In the absence of any trapping reagent, following the treatment of allene precursor **5.40a-c** with KO^tBu in THF at room temperature, unexpected type of dimerization products **5.46a-c** were isolated. The expected products **5.47a-c** resulting from [2+2] dimerization were not isolated (Scheme 5.15).



Scheme 5.15: Unexpected dimerization of 2-aryl 1,2-cyclohexadienes.

There were two pathways hypothesized where the formation of dimer could proceed 1) *via* hetero-Diels-Alder, or 2) stepwise nucleophilic substitution (Scheme 5.16). Once the cyclic allene **5.45a** is generated, two **5.45a** molecules can react with each other in a hetero-Diels-Alder fashion to generate **5.48a**. This, upon isomerization and followed by an aqueous workup, would result in **5.50a** and lead to the isolated product **5.46a** as a result of tautomerization. In contrast, the conjugate base **5.51a** of allene precursor **5.40a** would act as a nucleophile and attack the cyclic allene **5.45a** at the central carbon to result in enolate **5.52a**. A subsequent Michael addition of enolate oxygen

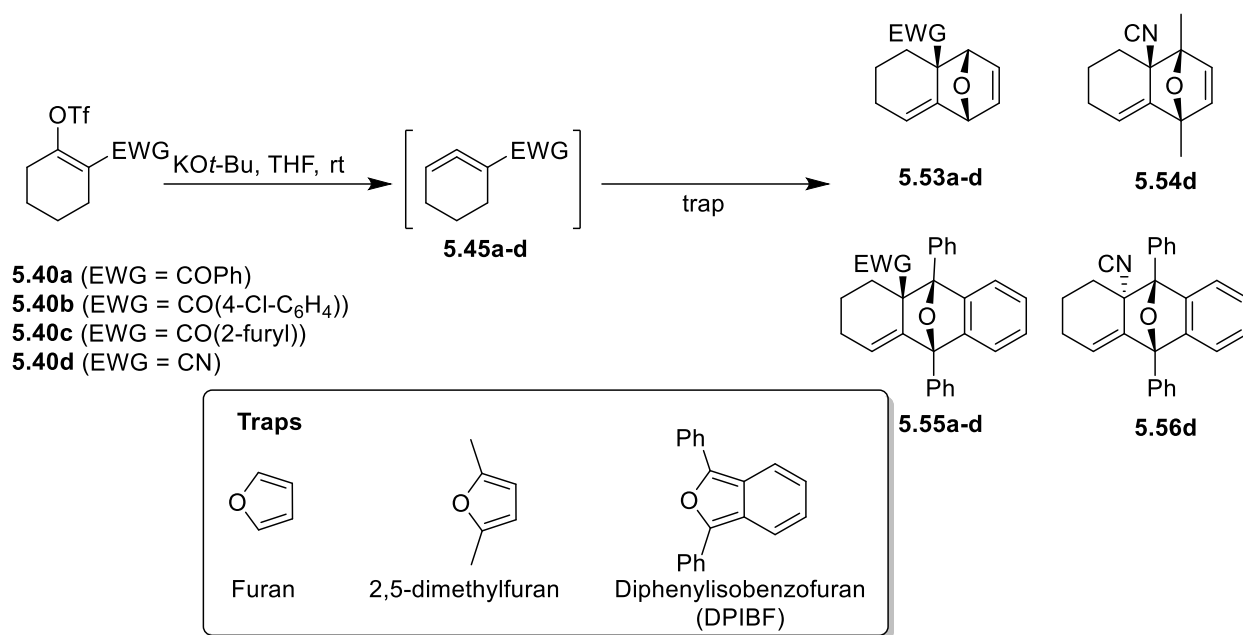
and elimination of triflate anion would result in intermediate **5.49a** that will tautomerize to form the isolated product **5.46a**.



Scheme 5.16: Possible mechanisms for the formation of 5.46a

The cyclic allenes were generated using base (KOtBu) promoted elimination to result in keto- and cyano-substituted cyclic allenes. Furthermore, trapping reactions using furan, 1,3-dimethylfuran, and 1,3-diphenylisobenzofuran (DPIBF) were performed (Scheme 5.17). Interestingly, complete regioselectivity was observed with the trapping reagent reacting with the

more electron-deficient double bond of the allene, which was expected. This is a normal demand Diels-Alder reaction where the electron-rich diene such as furan reacts with the electron-deficient double bond of the allene acting as the electron-poor dienophile. This finding contrasts with reports of trapping reaction with ester substituted cyclic allenes where a mixture of regioisomers are obtained.⁴⁰ This variability in the regioselectivity could be the result of stronger electron withdrawing effect of keto- and cyano- substituents relative to esters. Additionally, complete diastereoselectivity favouring the *endo* cycloadducts was also observed. However, the cyano-substituted allene **45d** resulted in both *endo* and *exo* cycloadducts in a 3:1 ratio (Table 5.1).



Scheme 5.17: Generation of electron deficient 1,2-cyclohexadienes and trapping reactions with furans.

Entry	Substrate	Trap	Product (s) (Yield %)
1	5.40a	Furan	5.53a (50)
2	5.40b	Furan	5.53b (82)
3	5.40c	Furan	5.53c (60)

4	5.40d	Furan	5.53d (45)
5	5.40d	2,5-Dimethylfuran	5.54d (20)
6	5.40a	DPIBF	5.55a (20)
7	5.40b	DPIBF	5.55b (23)
8	5.40c	DPIBF	5.55c (36)
9	5.40d	DPIBF	5.55d (36) + 5.56d (12)

Table 5.1: Diels-Alder trapping of electron deficient 1,2-cyclohexadienes with furans

5.6: Computational study of observed experimental results: dimerization and selectivity of trapping reactions.

Using DFT methods, we set out to examine the unprecedented dimerization of electron deficient 1,2-cyclohexadiene **5.45a-c**. The mechanistic pathway to understand the observed regio- and diastereoselectivities of the trapping reaction was also explored by DFT methods. This mechanistic investigation will provide insights into reactivity of cyclic allenes with electron withdrawing substituents which may aid in further reaction developments with such intermediates.

5.6.1: Computational methods

All structures were optimized using M06-2X⁴⁴ with the double- ζ split valence 6-31+G(d,p) basis set. Solvation with tetrahydrofuran was performed using the Integration Equation Formalism Polarizable Continuum Model (IEFPCM)⁴⁵ model and vibrational analysis verified that each structure was either a minimum or transition state. All optimizations were performed in Gaussian 09.e01.⁴⁶ Non-covalent interaction (NCI)^{47,48} plots were used to further elucidate the secondary orbital interactions in cycloaddition transition state structures. NCI figures were generated on VMD⁴⁹ with isovalue of 0.3 and the remaining figures were created using Vesta⁵⁰.

5.6.2: Investigation of dimerization

The mechanism of dimerization was examined *via* DFT calculations employing the M062x/6-31+G(d,p) functional with SMD solvent model (THF). Our model indicates that the [4+2] cycloaddition occurs in a concerted asynchronous manner with the carbon-carbon bond forming earlier than the carbon-oxygen bond (2.20 Å vs 2.90 Å, respectively, in the transition state structure). Despite the asynchronicity of the transition state structure, intrinsic reaction coordinate (IRC) calculations indicate that this transition state leads directly to reactants and products. This reaction occurs with a barrier of 17.7 kcal/mol and the resulting [4+2] adduct is favoured by 90.5 kcal/mol, relative to the starting allenes (Figure 5.5a).

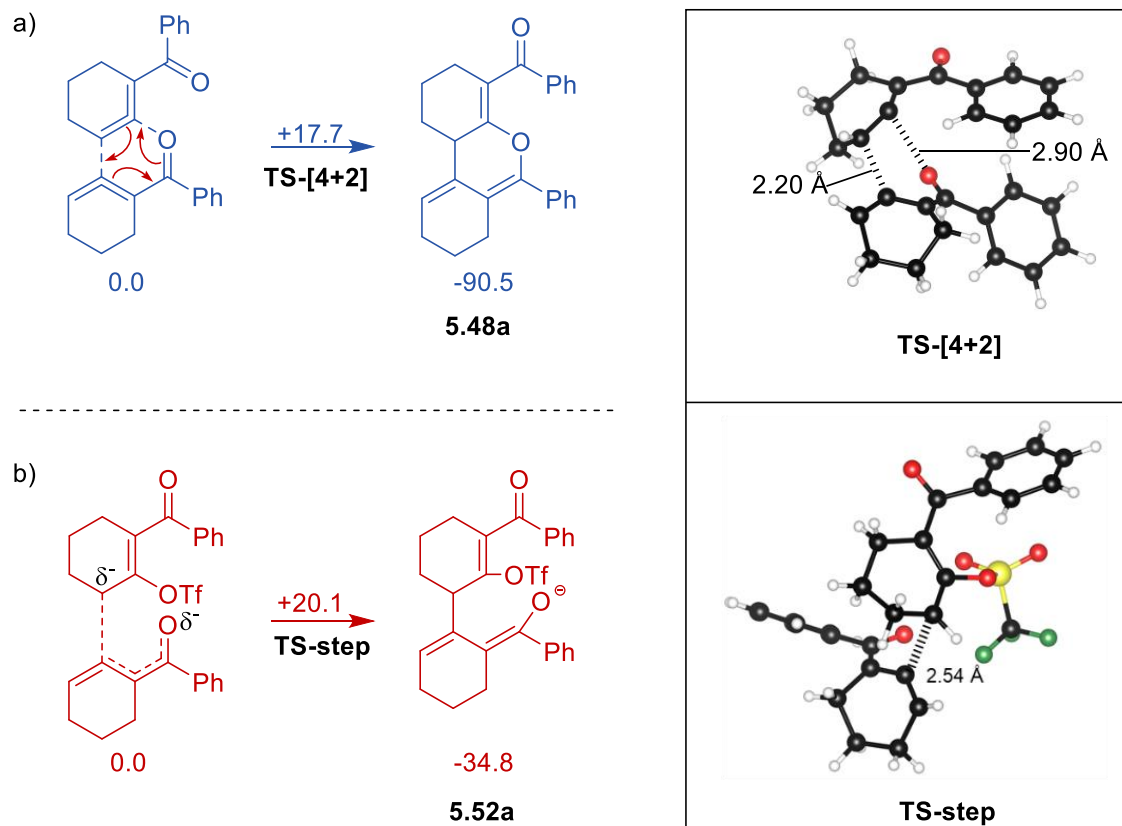


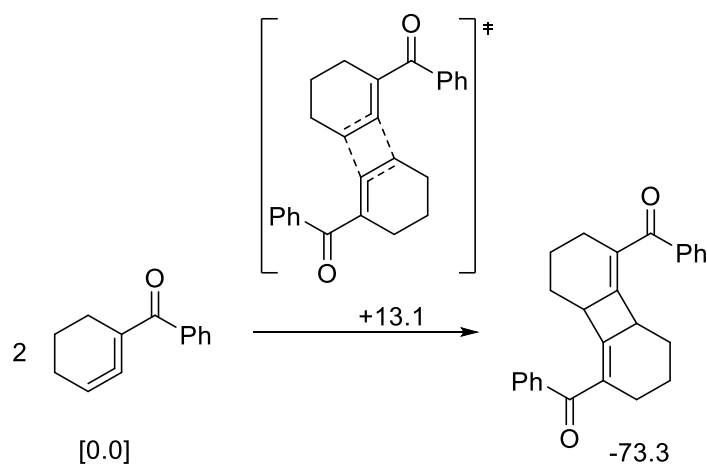
Figure 5.4: DFT investigation of a) concerted allene dimerization and b) stepwise anionic addition pathways leading to formation of **5.46a**. Reported values are Gibbs Free energies and are reported in kcal/mol.

Studies on the nucleophilic attack of **5.45a** by the conjugate base **5.51a** show that it proceeds with a barrier of 19.1 kcal/mol and results in the formation of an intermediate that is favoured by 42.3 kcal/mol, relative to the combined energies of **5.45a** and conjugate base **5.51a** (Figure 5.5b). These results suggest that either addition pathway is plausible under the given reaction conditions and would likely be dependent on the lifetime of the anionic intermediate and rate of formation of the allene.

5.6.3: Discussion of [2+2] dimerization of **5.45a**

The dimerization of **5.45a** via a [2+2] cycloaddition was also considered and found to be 4.6 kcal/mol lower in energy than the [4+2] pathway (Scheme 5.18). Similar to [4+2], the transition

state was also determined to be concerted asynchronous in nature. This is consistent with previous studies on allene dimerization however it is not consistent with the observed product distribution and suggests that this system may be more complex than initially expected.



Scheme 5.18: [2+2] dimerization of 5.45a. Reported values are Gibbs Free energies and are reported in kcal/mol.

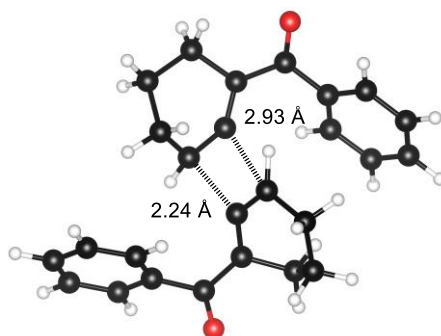
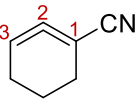


Figure 5.5: Transition state structure of [2+2] dimerization of 5.45a.

5.6.4: Computational investigation of trapping reactions of 5.45a-d with furans.

To examine the nature of the mechanism and to understand the observed regio- and diastereo-selectivities of the trapping reactions, DFT calculations were performed on the Diels–Alder reactions of allenes (5.45a-d) with furan, 2,5-dimethyl furan, and DPIBF. Herein, we present

the results of the computations performed on allene **5.45d** with furan. The calculations on all other allenes (**5.45a,b,c**) and dienes followed similar energetic trends and are presented following the discussion of **5.45d**.

Examination of the cycloaddition occurring across the 1,2 bond of allene **5.45d** reveals that both the *endo* and *exo* additions (**TS1** and **TS2** respectively) proceed in a concerted, asynchronous fashion, with the transition state structure for the *endo* addition being  favoured by 2.1 kcal/mol (Figure 5.6). The formation of the *endo* adduct is exergonic by 38.9 kcal/mol, and its formation is favoured by 0.8 kcal/mol over that of the *exo* product. The energetic favourability of the *endo* pathway can be justified by secondary orbital interactions between the lone pair on the furan oxygen and the electron withdrawing group at C1 of the allene.

Noncovalent interaction (NCI) analysis on **TS1** and **TS2** confirmed larger, favourable electrostatic interactions in **TS1** (where the O of the furan is interacting with the cyano group) as compared to **TS2** (where the C3/C4 2-carbon unit of the furan is interacting with the cyano group). In contrast to the cycloaddition occurring across the 1,2 bond of **5.45d**, the addition across the 2,3 bond of **5.45d** occurs *via* a stepwise mechanism with the bond between C2 of the allene and the furan forming first. The transition states for the first addition step for both the *endo* (**TS3**) and *exo* (**TS4**) approaches of the allene are nearly equal in energy, with the *exo* addition being lower in energy by 0.4 kcal/mol (Fig. 5.6b). The stepwise nature of the addition across the 2,3-bond is likely the result of poor orbital overlap between the furan and the orbital at C3 of the allene. In the LUMO of **5.45d**, the orbital coefficient on C3 is smaller than that of C1 or C2 (Fig. 5.6c). Comparison of all four transition state structures (**TS1**, **TS2**, **TS3**, **TS4**) shows the *endo* addition of furan across the C1-C2 bond of the allene to be favoured by ~3 kcal/mol over all other approaches. This is

consistent with the experimental observations and with previous reports on electron deficient allenes undergoing preferential cycloaddition proximal to the EWG.^{24,28,29,32,34,35,40,51}

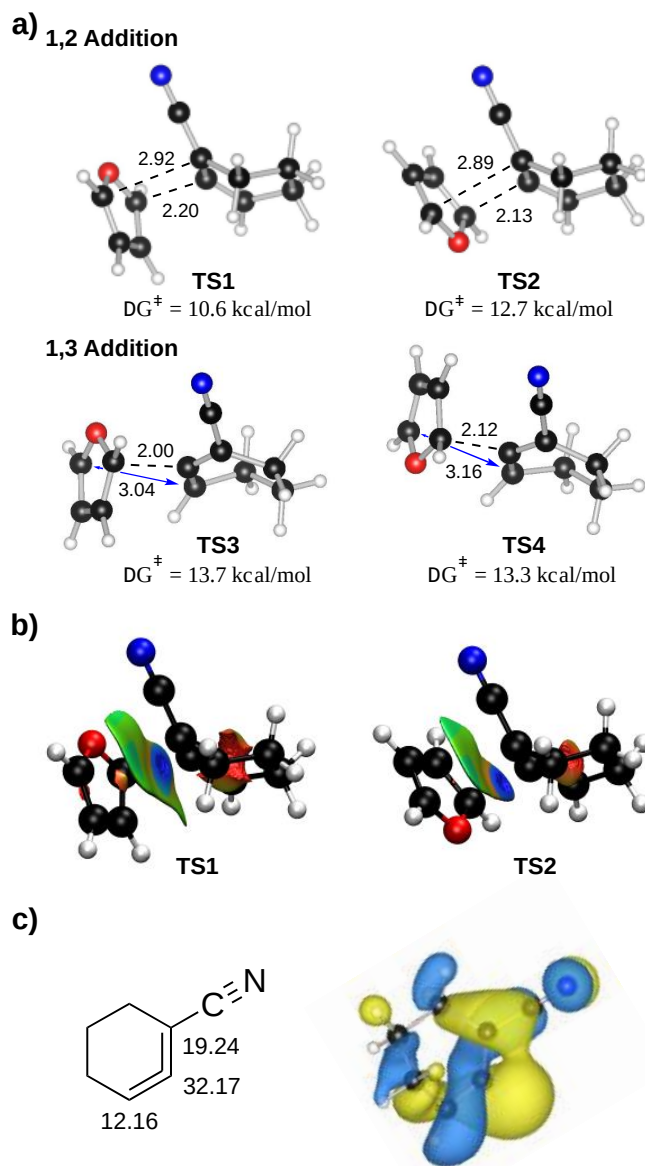
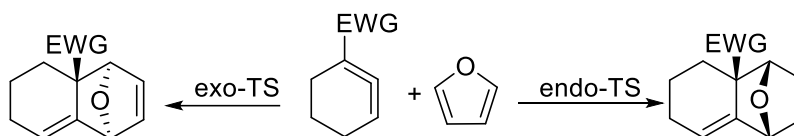


Figure 5.6: a) Optimized transition state structures leading to the possible diastereomers and regioisomers for the addition of furan with allene **5.45d**. The bond lengths are reported in Ångstroms. Reported values are Gibbs Free energies and are reported in kcal/mol. B) NCI figures (isovalue of 0.4) of **TS1** and **TS2**. Blue = strong attractive interactions, green = weak attractive

interactions, red = strong repulsive interactions. C) LUMO coefficients (left) and its depiction (right) of allene **5.45d**.

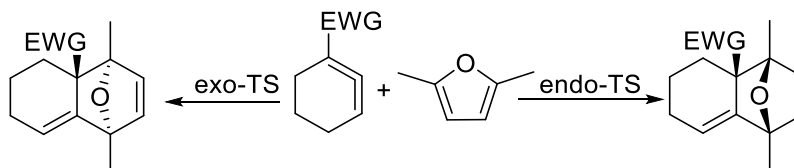
The results of computations performed on the Diels-Alder reactions of allenes **5.45a-5.45d** with furan, 2,5-dimethylfuran, and DPIBF are presented in Table 5.2, 5.3, and 5.4. It was determined that the formation of endo product was thermodynamically favoured for all trapping reactions except for the case of **5.45d** and **DPIBF**. The difference in barrier between endo pathway and exo pathway was determined to be 0.1 kcal/mol.

Table 5.2: Energies of trapping reactions with furan. All free energies reported in kcal/mol



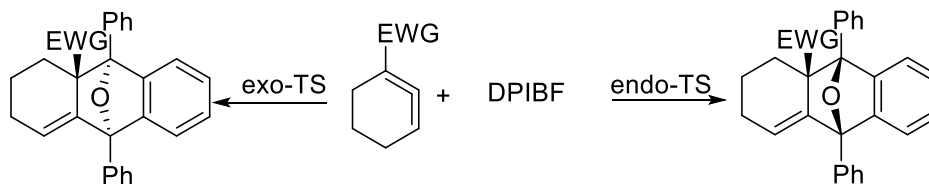
Allene	Exo	Exo-TS	SM	Endo-TS	Endo
5.45a	-24.1	+14.8	[0.0]	+14.4	-23.7
5.45b	-27.5	+10.5	[0.0]	+9.4	-27.9
5.45c	-29.3	+11.6	[0.0]	+10.4	-29.1
5.45d	-29.4	+12.7	[0.0]	+10.6	-30.4

Table 5.3: Energies of trapping reactions with 2,5-dimethylfuran. All free energies reported in kcal/mol.



Allene	Exo	Exo-TS	SM	Endo-TS	Endo
5.45a	-21.4	+15.4	[0.0]	+13.5	-20.5
5.45b	-25.3	+11.3	[0.0]	+9.1	-24.8
5.45c	-27.0	+11.1	[0.0]	+9.6	-27.4
5.45d	-30.4	+12.3	[0.0]	+9.0	-31.5

Table 5.4: Energies of trapping reactions with DPIBF. All free energies reported in kcal/mol.



Allene	Exo	Exo-TS	SM	Endo-TS	Endo

5.45a	-35.0	+9.7	[0.0]	+8.6	-35.7
5.45b	-39.4	+5.5	[0.0]	+4.1	-40.2
5.45c	-40.9	+4.7	[0.0]	+4.3	-41.5
5.45d	-46.6	+6.0	[0.0]	+5.9	-45.1

In order to understand the observation of both endo and exo product for allene **5.45d** with DPIBF, the transition state structures were examined. In figure 5.7, the cyano group is directly on top the pi-system of isobenzofuran moiety of DPIBF, for exo TS, which might result in favourable secondary orbital interactions to lower the barrier. This interaction is absent in the endo TS. The HOMOs of furans and the LUMO of allene **5.45d** is shown in figure 5.8. This interaction is absent in the endo TS.

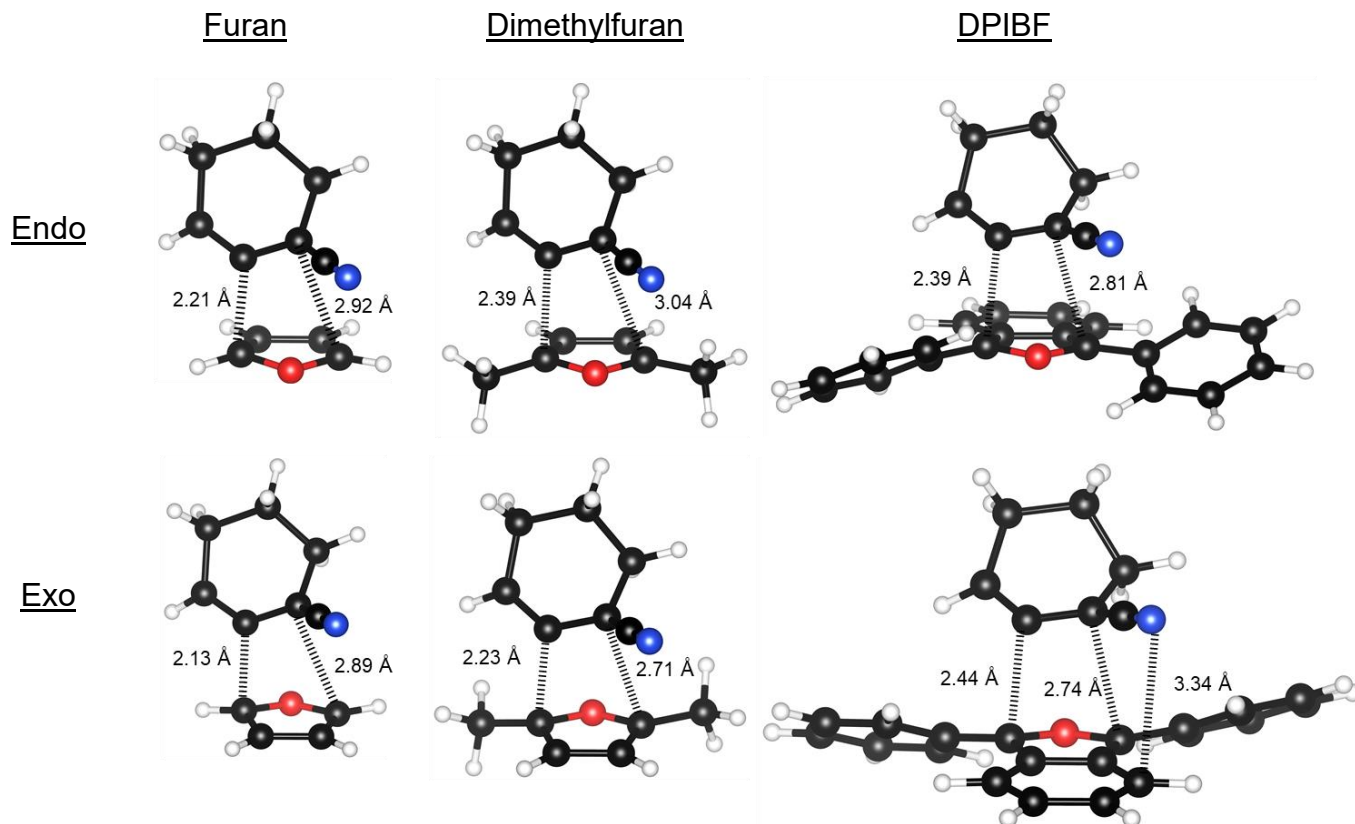


Figure 5.7: Transition state structures for trapping of allene 5.45d with furan (left), 2,5-Dimethylfuran (center), and DPIBF (right) for endo approach (top) and exo approach (bottom).

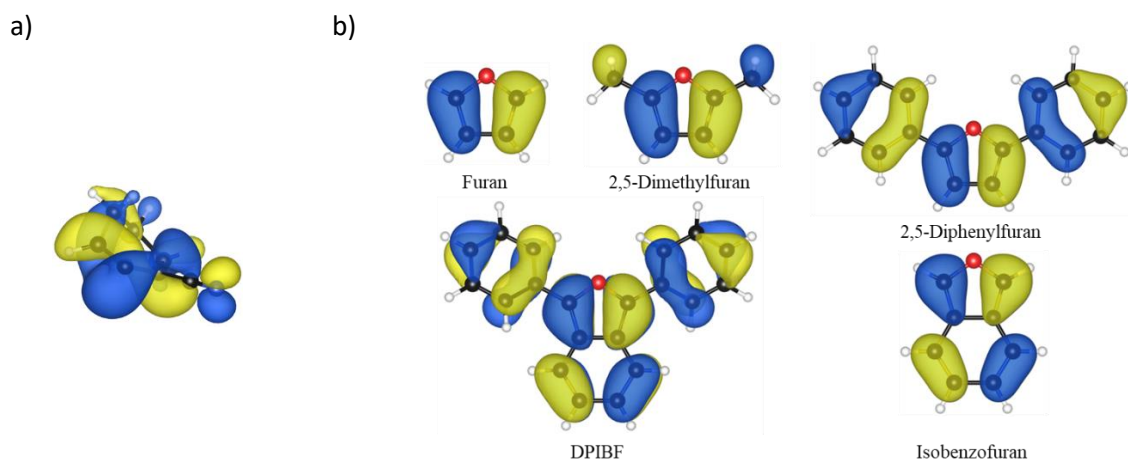


Figure 5.8: a) LUMO of allene 5.45d. b) HOMOs of various furans

In order to gain more insight about this favourable orbital interaction, barriers for formation of endo and exo cycloadducts with 2,5-diphenylfuran and isobenzofuran were also calculated. The barriers for endo and exo products with various furans are shown in Table 5.5. The difference in

barriers between formation endo and exo cycloadduct is 1.5 kcal/mol for diphenylfuran and 1.0 kcal/mol for isobenzofuran, favouring the endo. Similar to DPIBF exo-TS, favourable interactions in the exo approach for isobenzofuran can be observed (Figure 5.9). This favourable interaction helps explain the presence of exo adduct from **5.45d** and DPIBF.

*Table 5.5: Transition state energies of trapping allene **5.45d** with various dienes. All free energies are reported in kcal/mol. The energy values are relative to allene **5.45d** and diene.*

	Furan	Dimethylfuran	DPIBF	Isobenzofuran	Diphenylfuran
Endo-TS	10.6	9.0	5.9	6.7	11.0
Exo-TS	12.7	12.3	6.0	7.7	12.5

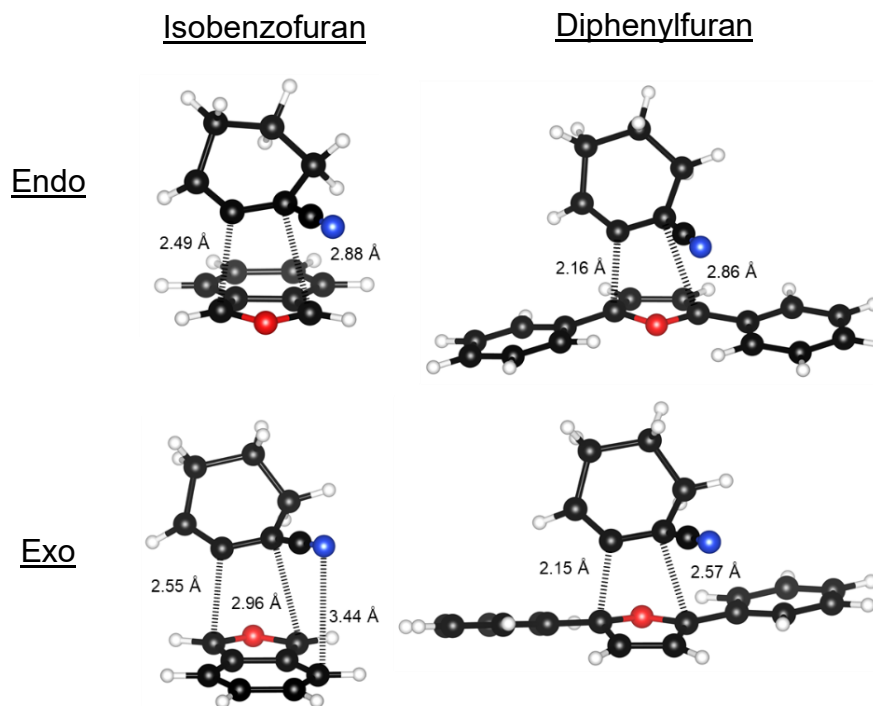
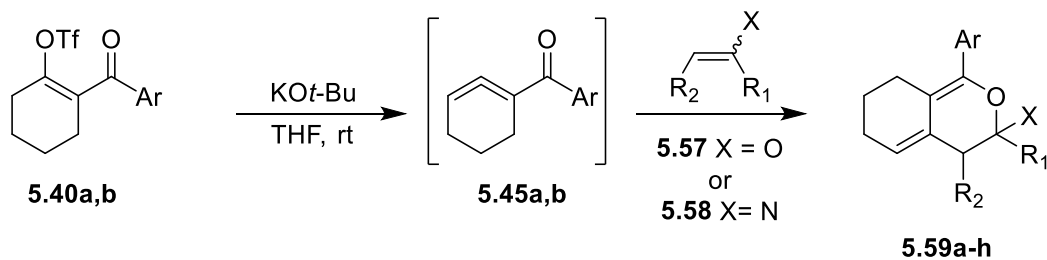
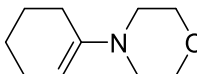
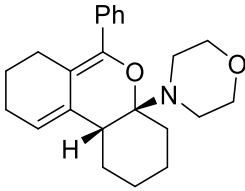
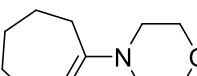
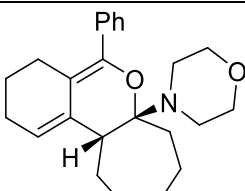
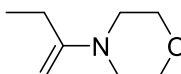
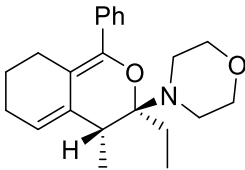
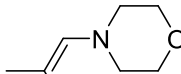
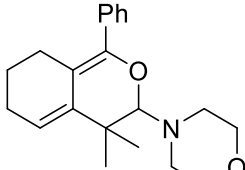


Figure 5.9: Transition state structures of trapping of allene **5.45d** with isobenzofuran (left) and 2,5-Diphenylfuran (right) for endo approach (top) and exo approach (bottom).

5.6.5: Investigation of trapping reactions of cyclic allenes with enamines

Due to confirmation of hetero-Diels-Alder dimerization mechanism for the formation of **5.46a-c**, curiosity surfaced of cyclic allenes **5.45a-c** could react as heterodienes with an olefinic trap in [4+2] cycloaddition pathway. It was proposed that this process could occur *via* inverse electron-demand, in which the LUMO of the heterodyne (cyclic allene) and the HOMO of an electron rich dienophile would be the principle frontier molecular orbital interactions. Therefore, the 2-keto aroyl cyclic allenes were generated and trapped with various electron-rich heterodienophiles (Table 5.6). The resulting cycloadducts **5.59a-g** were isolated as single diastereomer which suggests a concerted cycloaddition pathway rather than a stepwise mechanism.



Entry	Substrate	Trap	Product (isolated yield)
1	5.40a	 5.57a	--
2	5.40a	 5.57b	--
3	5.40a	 5.58a	 5.59a
4	5.40a	 5.58b	 5.59b
5	5.40a	 5.58c	 5.59c
6	5.40a	 5.58d	 5.59d

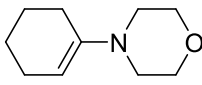
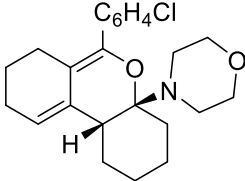
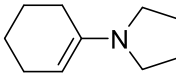
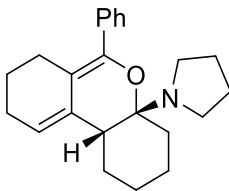
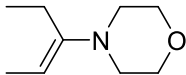
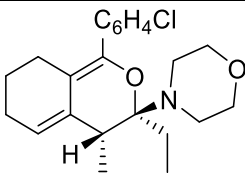
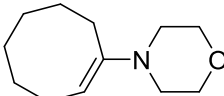
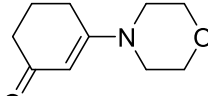
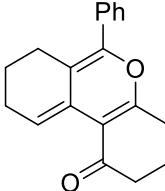
7	5.40b	 5.58a	 5.59e
8	5.40a	 5.58e	 5.59f
9	5.40b	 5.58c	 5.59g
10	5.40a	 5.58f	--
11	5.40a	 5.58g	 5.59h

Table 5.6: Hetero-Diels-Alder trapping of 2-keto aroyl cyclohexadienes derived from **5.40a**, **5.40b** with electron-rich heterodienophiles

As in the dimerization process shown in Scheme 5.15, the formation of cycloadducts **5.59** could conceivably arise by either a pericyclic Diels–Alder process, or *via* stepwise ionic addition of the nucleophilic enamines to the electron-deficient allenes. Retention of stereochemical information in the two cases involving acyclic enamine **5.58c** offers evidence for a concerted mechanism. DFT calculations on the cycloaddition of allene **5.45a** with enamine **5.58a** indicate that the [4 + 2] cycloaddition occurs in a concerted asynchronous manner, with the carbon–carbon

bond forming earlier than the carbon–oxygen bond (2.57 and 3.12 Å, respectively) (Figure. 5.10a). The cycloaddition occurs with a barrier of 12.4 kcal/mol and is exergonic by 52.4 kcal/mol. As shown in Figure. 5.10, the cycloaddition occurs through a transition state structure (**TS5**) that places the N of the enamine directly over the C of the carbonyl on the allene. This allows for favourable secondary orbital interactions, as indicated by the NCI plot of **TS5** (Fig. 5.10b).¹⁹ The concerted nature of this reaction is consistent with the mechanism calculated for the dimerization of **5a** and with the observed stereochemistry of **16c** and **16g**.

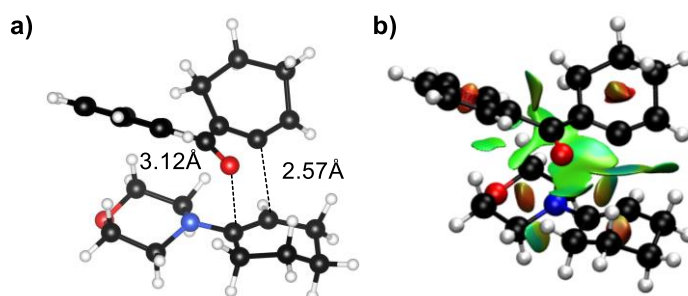


Figure 5.10: Optimized transition state structure **TS5** for the favoured diastereomer of the cycloaddition of **5.45a** with **5.58a**. b) NCI plot of **TS5**.

We further examined the reactivity of enamine **5.58a** with **5.45a** to determine if a [2+2] product (**5.60a**) was plausible (Figure 5.11). The DFT calculations suggest that the observed product **5.59a** is thermodynamically favoured by 21.5 kcal/mol compared to **5.60a**. The calculations also suggest that the formation of **5.60a** proceeds *via* stepwise ionic addition of nucleophilic **5.58a** to electron deficient **5.45a**. The first step to form **5.60-INT** has a barrier of 16.2 kcal/mol (3.8 kcal/mol higher than [4+2] barrier) and is exergonic by 20.3 kcal/mol. Additionally, relative to **5.60-INT**, the second step proceeds with a barrier of 11.6 kcal/mol, resulting in **17a**. Hence, the formation of **16a** is both kinetically and thermodynamically favoured than **5.60a**.

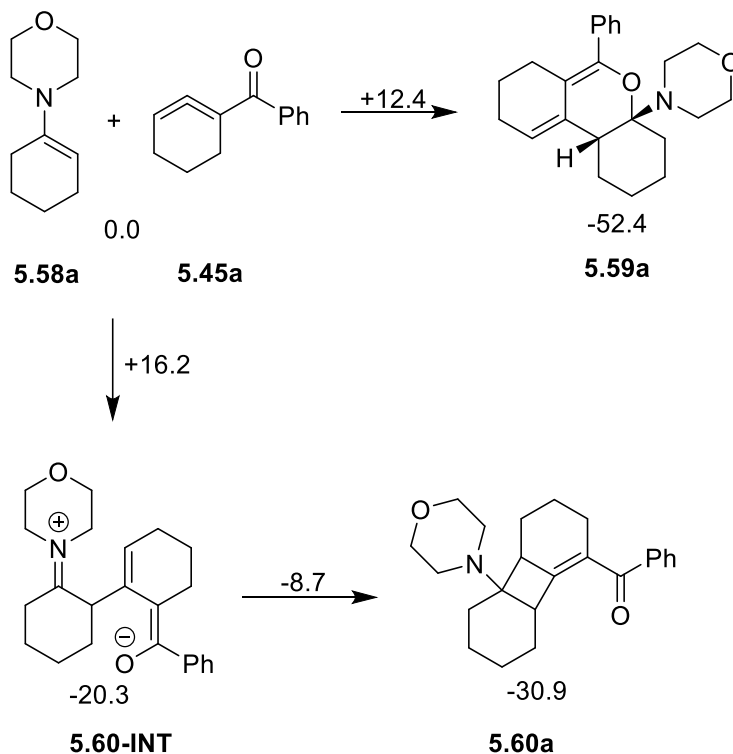


Figure 5.11: Examination of reactivity of enamine **5.58a** with allene **5.45a**. Comparison of [4+2] pathway leading to **5.59a** and stepwise pathway leading **5.60a**. Energies are reported in kcal/mol.

5.7: Conclusions

In this chapter, DFT methods were utilized to investigate the reactivity of cyclic allenes with electron-withdrawing substituents. The experimental results of tapping allenes with different 1,3-dienes, as well as, dimerization reaction of allenes were rationalized using computational methods. The electron deficient allenes were determined to undergo dimerization *via* an asynchronous hetero-Diels-Alder pathway which was kinetically favoured compared to the stepwise pathway. The resulting cycloadduct was found to be thermodynamically highly favourable relative to the stepwise-pathway intermediate.

The trapping reactions of cyclic allenes with 1,3-dienes resulted in cycloadducts with excellent regio- and diastereo-selectivity. The DFT calculations suggest a hetero-Diels-Alder process in a concerted asynchronous manner. The calculations suggest that the Diels-Alder reaction of 1,3-dienes with allenes across the 1,2-bond is kinetically favoured due to favourable orbital overlap compared to 2,3-bond, resulting in high regioselectivity. Furthermore, the trapping reactions were observed with high *endo* diastereoselectivity as a result of thermodynamic favourability due to favourable secondary orbital interactions, compared to *exo* selectivity.

Additionally, the electron-deficient cyclic allenes with electron withdrawing substituents allowed to expand the scope by trapping them with enamines as electron-rich hetero-dienophiles to result in complex polycyclic compounds. The trapping of allenes with enamines also followed a hetero-Diels-Alder pathway in a concerted, asynchronous manner. The results presented in chapter will aid in development of a diverse set of electron deficient cyclic allenes and electron-rich trapping reagents to expand the scope of reactive intermediates in organic chemistry.

5.8: References

- (1) Roberts, J. D.; Simmons, H. E. Jr.; Carlsmith, L. A.; Vaughan, C. W. REARRANGEMENT IN THE REACTION OF CHLOROBENZENE-1-C14 WITH POTASSIUM AMIDE1. *J. Am. Chem. Soc.* **1953**, 75 (13), 3290–3291. <https://doi.org/10.1021/ja01109a523>.
- (2) Bottini, A. T.; Corson, F. P.; Fitzgerald, R.; Frost, K. A. Reactions of 1-Halocyclohexenes and Methyl Substituted 1-Halocyclohexenes with Potassium t-Butoxide. *Tetrahedron* **1972**, 28 (19), 4883–4904. [https://doi.org/10.1016/0040-4020\(72\)88141-9](https://doi.org/10.1016/0040-4020(72)88141-9).
- (3) Wittig, G.; Fritze, P. On the Intermediate Occurrence of 1,2-Cyclohexadiene. *Angew. Chem. Int. Ed. Engl.* **1966**, 5 (9), 846–846. <https://doi.org/10.1002/anie.196608461>.
- (4) Pellissier, H.; Santelli, M. The Use of Arynes in Organic Synthesis. *Tetrahedron* **2003**, 59 (6), 701–730. [https://doi.org/10.1016/S0040-4020\(02\)01563-6](https://doi.org/10.1016/S0040-4020(02)01563-6).
- (5) Wenk, H. H.; Winkler, M.; Sander, W. One Century of Aryne Chemistry. *Angew. Chem. Int. Ed.* **2003**, 42 (5), 502–528. <https://doi.org/10.1002/anie.200390151>.
- (6) Gampe, C. M.; Carreira, E. M. Arynes and Cyclohexyne in Natural Product Synthesis. *Angew. Chem. Int. Ed.* **2012**, 51 (16), 3766–3778. <https://doi.org/10.1002/anie.201107485>.
- (7) Tadross, P. M.; Stoltz, B. M. A Comprehensive History of Arynes in Natural Product Total Synthesis. *Chem. Rev.* **2012**, 112 (6), 3550–3577. <https://doi.org/10.1021/cr200478h>.
- (8) Dubrovskiy, A. V.; Markina, N. A.; Larock, R. C. Use of Benzyne for the Synthesis of Heterocycles. *Org. Biomol. Chem.* **2012**, 11 (2), 191–218. <https://doi.org/10.1039/C2OB26673C>.
- (9) Su, Q.; Ding, J.; Du, Z.; Lai, Y.; Li, H.; Ouyang, M.-A.; Song, L.; Lin, R. Recent Advances in the Reactions of Cyclic Carbynes. *Molecules* **2020**, 25 (21), 5050. <https://doi.org/10.3390/molecules25215050>.
- (10) Goetz, A. E.; Shah, T. K.; Garg, N. K. Pyridynes and Indolynes as Building Blocks for Functionalized Heterocycles and Natural Products. *Chem. Commun.* **2015**, 51 (1), 34–45. <https://doi.org/10.1039/c4cc06445c>.
- (11) Agard, N. J.; Prescher, J. A.; Bertozzi, C. R. A Strain-Promoted [3 + 2] Azide–Alkyne Cycloaddition for Covalent Modification of Biomolecules in Living Systems. *J. Am. Chem. Soc.* **2004**, 126 (46), 15046–15047. <https://doi.org/10.1021/ja044996f>.
- (12) Ippoliti, F. M.; Adamson, N. J.; Wonilowicz, L. G.; Nasrallah, D. J.; Darzi, E. R.; Donaldson, J. S.; Garg, N. K. Total Synthesis of Lissodendoric Acid A via Stereospecific Trapping of a Strained Cyclic Allene. *Science* **2023**, 379 (6629), 261–265. <https://doi.org/10.1126/science.ade0032>.

- (13) Daoust, K. J.; Hernandez, S. M.; Konrad, K. M.; Mackie, I. D.; Winstanley, J.; Johnson, R. P. Strain Estimates for Small-Ring Cyclic Allenes and Butatrienes. *J. Org. Chem.* **2006**, *71* (15), 5708–5714. <https://doi.org/10.1021/jo060698k>.
- (14) Dillon, P. W.; Underwood, G. R. Cyclic Allenes. I. Electronic Structure and Probable Deformation of the Allene Linkage When Included in a Ring. INDO-MO [Intermediate Neglect of Differential Overlap-Molecular Orbital] Study. *J. Am. Chem. Soc.* **1974**, *96* (3), 779–787. <https://doi.org/10.1021/ja00810a023>.
- (15) Schmidt, M. W.; Angus, R. O.; Johnson, R. P. Small Ring Cyclic Allenes: An Ab Initio Study of the Structure of 1,2-Cyclohexadiene. *J. Am. Chem. Soc.* **1982**, *104* (24), 6838–6839. <https://doi.org/10.1021/ja00388a087>.
- (16) Angus, R. O.; Schmidt, M. W.; Johnson, R. P. Small-Ring Cyclic Cumulenes: Theoretical Studies of the Structure and Barrier to Inversion in Cyclic Allenes. *J. Am. Chem. Soc.* **1985**, *107* (3), 532–537. <https://doi.org/10.1021/ja00289a002>.
- (17) Johnson, R. P. Strained Cyclic Cumulenes. *Chem. Rev.* **1989**, *89* (5), 1111–1124. <https://doi.org/10.1021/cr00095a009>.
- (18) Wittig, G.; Fritze, P. On the Intermediate Occurrence of 1,2-Cyclohexadiene. *Angew. Chem. Int. Ed. Engl.* **1966**, *5* (9), 846–846. <https://doi.org/10.1002/anie.196608461>.
- (19) Shakespeare, W. C.; Johnson, R. P. 1,2,3-Cyclohexatriene and Cyclohexen-3-Yne: Two New Highly Strained C₆H₆ Isomers. *J. Am. Chem. Soc.* **1990**, *112* (23), 8578–8579. <https://doi.org/10.1021/ja00179a050>.
- (20) Moore, W. R.; Moser, W. R. Reaction of 6,6-Dibromobicyclo[3.1.0]Hexane with Methyllithium. Efficient Trapping of 1,2-Cyclohexadiene by Styrene. *J. Org. Chem.* **1970**, *35* (4), 908–912. <https://doi.org/10.1021/jo00829a008>.
- (21) von E. Doering, W.; LaFlamme, P. M. A Two-Step of Synthesis of Allenes from Olefins. *Tetrahedron* **1958**, *2* (1), 75–79. [https://doi.org/10.1016/0040-4020\(58\)88025-4](https://doi.org/10.1016/0040-4020(58)88025-4).
- (22) Skattebøl, L. Chemistry of Gem-Dihalocyclopropanes. V.1 Formation of Tricyclo[4.1.0.0^{4,6}]Heptane and Derivatives. *J. Org. Chem.* **1966**, *31* (9), 2789–2794. <https://doi.org/10.1021/jo01347a014>.
- (23) Moore, W. R.; Ward, H. R. The Formation of Allenes from Gem-Dihalocyclopropanes by Reaction with Alkylolithium Reagents^{1,2}. *J. Org. Chem.* **1962**, *27* (12), 4179–4181. <https://doi.org/10.1021/jo01059a013>.
- (24) Barber, J. S.; Styduhar, E. D.; Pham, H. V.; McMahon, T. C.; Houk, K. N.; Garg, N. K. Nitron Cycloadditions of 1,2-Cyclohexadiene. *J. Am. Chem. Soc.* **2016**, *138* (8), 2512–2515. <https://doi.org/10.1021/jacs.5b13304>.
- (25) Lofstrand, V. A.; West, F. G. Efficient Trapping of 1,2-Cyclohexadienes with 1,3-Dipoles. *Chem. - Eur. J.* **2016**, *22* (31), 10763–10767. <https://doi.org/10.1002/chem.201602201>.

- (26) Inoue, K.; Nakura, R.; Okano, K.; Mori, A. One-Pot Synthesis of Silylated Enol Triflates from Silyl Enol Ethers for Cyclohexynes and 1,2-Cyclohexadienes. *Eur. J. Org. Chem.* **2018**, 2018 (25), 3343–3347. <https://doi.org/10.1002/ejoc.201800353>.
- (27) Bottini, A. T.; Hilton, L. L.; Plott, J. Relative Reactivities of 1,2-Cyclohexadiene with Conjugated Dienes and Styrene. *Tetrahedron* **1975**, 31 (17), 1997–2001. [https://doi.org/10.1016/0040-4020\(75\)80186-4](https://doi.org/10.1016/0040-4020(75)80186-4).
- (28) Barber, J. S.; Yamano, M. M.; Ramirez, M.; Darzi, E. R.; Knapp, R. R.; Liu, F.; Houk, K. N.; Garg, N. K. Diels-Alder Cycloadditions of Strained Azacyclic Allenes. *Nat. Chem.* **2018**, 10 (9), 953–960. <https://doi.org/10.1038/s41557-018-0080-1>.
- (29) McVeigh, M. S.; Kelleghan, A. V.; Yamano, M. M.; Knapp, R. R.; Garg, N. K. Silyl Tosylate Precursors to Cyclohexyne, 1,2-Cyclohexadiene, and 1,2-Cycloheptadiene. *Org. Lett.* **2020**, 22 (11), 4500–4504. <https://doi.org/10.1021/acs.orglett.0c01510>.
- (30) Lofstrand, V. A.; McIntosh, K. C.; Almeahadi, Y. A.; West, F. G. Strain-Activated Diels–Alder Trapping of 1,2-Cyclohexadienes: Intramolecular Capture by Pendent Furans. *Org Lett* **2019**, 21, 6231–6234. <https://doi.org/10.1021/acs.orglett.9b02085>.
- (31) Wang, B.; Constantin, M. G.; Singh, S.; Zhou, Y.; Davis, R. L.; West, F. G. Generation and Trapping of Electron-Deficient 1,2-Cyclohexadienes. Unexpected Hetero-Diels-Alder Reactivity. *Org. Biomol. Chem.* **2021**, 19 (2), 399–405. <https://doi.org/10.1039/d0ob02285c>.
- (32) Lofstrand, V. A.; McIntosh, K. C.; Almeahadi, Y. A.; West, F. G. Strain-Activated Diels–Alder Trapping of 1,2-Cyclohexadienes: Intramolecular Capture by Pendent Furans. *Org. Lett.* **2019**, 21 (16), 6231–6234. <https://doi.org/10.1021/acs.orglett.9b02085>.
- (33) Jankovic, Christian. L.; West, F. G. 2 + 2 Trapping of Acyloxy-1,2-Cyclohexadienes with Styrenes and Electron-Deficient Olefins. *Org. Lett.* **2022**, 24 (51), 9497–9501. <https://doi.org/10.1021/acs.orglett.2c03978>.
- (34) Lofstrand, V. A.; West, F. G. Efficient Trapping of 1,2-Cyclohexadienes with 1,3-Dipoles. *Chem. - Eur. J.* **2016**, 22 (31), 10763–10767. <https://doi.org/10.1002/chem.201602201>.
- (35) Almeahadi, Y. A.; West, F. G. A Mild Method for the Generation and Interception of 1,2-Cycloheptadienes with 1,3-Dipoles. *Org. Lett.* **2020**, 22 (15), 6091–6095. <https://doi.org/10.1021/acs.orglett.0c02172>.
- (36) Ball, W. J.; Landor, S. R. 442. Allenes. Part III. The Synthesis of Cyclic Allenes. *J. Chem. Soc. Resumed* **1962**, No. 0, 2298–2304. <https://doi.org/10.1039/JR9620002298>.
- (37) Moore, W. R.; Moser, W. R. Reaction of 6,6-Dibromobicyclo[3.1.0]Hexane with Methylolithium. Evidence for the Generation of 1,2-Cyclohexadiene and 2,2'-Dicyclohexenylene. *J. Am. Chem. Soc.* **1970**, 92 (18), 5469–5474. <https://doi.org/10.1021/ja00721a028>.

- (38) Bottini, A. T.; Corson, F. P.; Fitzgerald, R.; Frost, K. A. Reactions of 1-Halocyclohexenes and Methyl Substituted 1-Halocyclohexenes with Potassium t-Butoxide. *Tetrahedron* **1972**, 28 (19), 4883–4904. [https://doi.org/10.1016/0040-4020\(72\)88141-9](https://doi.org/10.1016/0040-4020(72)88141-9).
- (39) Christl, M.; Braun, M. Generation and Interception of 1-OXA-2, 3-Cyclohexadiene and 1, 2, 4-Cyclohexatriene. *Strain Its Implic. Org. Chem. Org. Stress React.* **1989**, 121–131.
- (40) Nendel, M.; Tolbert, L. M.; Herring, L. E.; Islam, Md. N.; Houk, K. N. Strained Allenes as Dienophiles in the Diels–Alder Reaction: An Experimental and Computational Study. *J. Org. Chem.* **1999**, 64 (3), 976–983. <https://doi.org/10.1021/jo982091c>.
- (41) Fos, E.; Borràs, L.; Gasull, M.; Mauleón, D.; Carganico, G. Synthesis of Isomeric Series of Aryltetrahydrobenz-Isioxazoles and Arylcyclopentisoxazoles. *J. Heterocycl. Chem.* **1992**, 29 (1), 203–208. <https://doi.org/10.1002/jhet.5570290137>.
- (42) Lin, H. S.; Rampersaud, A. A.; Zimmerman, K.; Steinberg, M. I.; Boyd, D. B. Nonpeptide Angiotensin II Receptor Antagonists: Synthetic and Computational Chemistry of N-[[4-[2-(2H-Tetrazol-5-Yl)-1-Cycloalken-1-Yl]Phenyl]Methyl]Imidazole Derivatives and Their in Vitro Activity. *J. Med. Chem.* **1992**, 35 (14), 2658–2667. <https://doi.org/10.1021/jm00092a017>.
- (43) Jia, Z.; Gálvez, E.; Sebastián, R. M.; Pleixats, R.; Álvarez-Larena, Á.; Martin, E.; Vallribera, A.; Shafir, A. An Alternative to the Classical α -Arylation: The Transfer of an Intact 2-Iodoaryl from ArI(O₂CCF₃)₂. *Angew. Chem. Int. Ed.* **2014**, 53 (42), 11298–11301. <https://doi.org/10.1002/anie.201405982>.
- (44) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function. *Theor. Chem. Acc.* **2008**, 120 (1–3), 215–241.
- (45) Tomasi, J.; Mennucci, B.; Cammi, R. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005**, 105 (8), 2999–3093. <https://doi.org/10.1021/cr9904009>.
- (46) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; X. Li, M. C.; Marenich, A.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ort, J. V.; Fox, D. J. Gaussian 09, Revision. <http://gaussian.com/g09citation/> (accessed 2018-11-30).
- (47) Johnson, E. R.; Keinan, S.; Mori-Sánchez, P.; Contreras-García, J.; Cohen, A. J.; Yang, W. Revealing Noncovalent Interactions. *J. Am. Chem. Soc.* **2010**, 132 (18), 6498–6506. <https://doi.org/10.1021/ja100936w>.
- (48) Contreras-García, J.; Johnson, E. R.; Keinan, S.; Chaudret, R.; Piquemal, J.-P.; Beratan, D. N.; Yang, W. NCIPLOT: A Program for Plotting Non-Covalent Interaction Regions. *J. Chem. Theory Comput.* **2011**, 7 (3), 625–632. <https://doi.org/10.1021/ct100641a>.

- (49) Humphrey, W.; Dalke, A.; Schulten, K. VMD: Visual Molecular Dynamics. *J. Mol. Graph.* **1996**, *14* (1), 33–38. [https://doi.org/10.1016/0263-7855\(96\)00018-5](https://doi.org/10.1016/0263-7855(96)00018-5).
- (50) Momma, K.; Izumi, F. VESTA 3 for Three-Dimensional Visualization of Crystal, Volumetric and Morphology Data. *J. Appl. Crystallogr.* **2011**, *44* (6), 1272–1276. <https://doi.org/10.1107/S0021889811038970>.
- (51) Yamano, M. M.; Knapp, R. R.; Ngamnithiporn, A.; Ramirez, M.; Houk, K. N.; Stoltz, B. M.; Garg, N. K. Cycloadditions of Oxacyclic Allenes and a Catalytic Asymmetric Entryway to Enantioenriched Cyclic Allenes. *Angew. Chem. Int. Ed.* **2019**, *58* (17), 5653–5657. <https://doi.org/10.1002/anie.201900503>.

Chapter 6 : Conclusions and Future Work

The development of computational methods such as Density Functional Theory (DFT) has become an important tool in a chemist's toolkit to understand and rationalize the observed experimental results. The significant development in computational abilities has allowed to develop models to predict stereoselectivity in enantioselective aminocatalytic reactions. In this dissertation, an overview of computational and experimental methods utilized to investigate aminocatalytic remote functionalization reactions were presented. The employment of computational chemistry as a tool to aid in reaction development was also presented.

In Chapter 2, calculations were performed to investigate the first report of remote functionalization by aminocatalysis. The observed stereochemistry of the product contains (*E*)-configuration around the α,β -double bond of enal with (*R*)-stereocenter at the γ -position. We investigated the mechanism of dienamine mediated γ -amination reaction of enals with DEAD, reported by Jorgenson. Consistent with previous studies, calculations suggest that *ipso* and γ -positions of dienamine intermediate and DEAD undergo a Diels-Alder cycloaddition reaction which was the kinetically favoured over mono-addition of DEAD. The excellent regioselectivity is due to ring-opening of the cycloadduct which also rationalizes the (*R*)-stereocenter observed in the product. The ring-opening of the cycloadduct directly results in (*Z*)-configuration, hence, two plausible downstream reaction pathways were examined to rationalize the experimentally observed stereochemistry. The first mechanism consisted of formation of downstream aminated dienamine intermediate which, upon rotation, results in (*E*)-configuration. By performing and closely monitoring the γ -amination reaction with γ -deuterated enal, in combination with DFT calculations suggest that the formation of downstream second dienamine intermediate is unlikely. The (*E*)-configuration with (*S*)-stereocenter was determined to be more thermodynamically

favoured than (*R*)-stereocenter. The second mechanism employed nucleophilic substitution of water molecule on the Diels-Alder cycloadduct to result in enamine intermediates which allows rotation to result in (*E*)-configuration. However, the calculations performed suggest that there was no significant thermodynamic preference for the enamine intermediate which would eventually result in the observed product. Further conformational analysis and rotational barriers between the enamine intermediate need to be calculated to reject the Michael addition pathway. Hence, further calculations and other downstream mechanisms must be explored to rationalize the observed stereochemistry.

In Chapter 3, a DFT study was performed to investigate the role of aminocatalysts to activate various model heteroaromatic aldehyde scaffolds by promoting the loss of aromaticity to form the reactive trienamine intermediate. Several hyperhomodesmotic equations were used to examine the energy penalty for dearomatization of heteroaromatic aldehydes. It was determined that the condensation of aminocatalyst results in iminium ions which decrease the cost for dearomatization, when compared to the parent aldehyde. This makes the heteroaromatic aldehydes excellent candidates to expand the scope of aminocatalytic reactions. Populations analysis of the trienamine intermediates was also performed which suggested that the largest HOMO coefficient is a result of the synergy between catalyst and the heteroatom of the aromatic ring. Additionally, this feature can be exploited by utilizing scaffolds to increase the electron density at remote positions to develop novel asymmetric remote functionalization methods.

Furthermore, we demonstrated that the nitrogen containing heteroaromatic aldehydes and all-carbon systems could give rise to fulvene which were determined to be thermodynamically more favoured than trienamine intermediates. Exploration of these fulvene systems may aid in novel approaches in stereoselective cycloaddition reactions.

In Chapter 4, computational methods were utilized to assess the influence of substituents at different positions of the trienamine intermediate. It was determined that the 3,6-*s-cis* diene configuration is thermodynamically preferred for γ , δ , and ϵ -substituted trienamines regardless of the nature of the substituent. The location of HOMO energy level and orbital coefficients were also calculated. Generally, the HOMO energy was raised as the electron donating nature of the substituent is increased. It was determined that electron donating substituents at the nucleophilic (γ and ϵ) positions raise the HOMO energy level of trienamine intermediate with 3,6-*s-cis* diene configuration significantly. For β -substituted trienamines, 1,4-*s-cis* diene configuration was thermodynamically more favoured, however, HOMO energy is raised for 3,6-*s-cis* diene configuration. Furthermore, the analysis of aryl substituent demonstrated the twisting of aryl ring to minimize steric repulsions which consequently results in aryl ring being out of conjugation, minimizing its impact on MO coefficients. In all cases, the MO analysis suggested that the vinylogy principle was followed regardless of the nature and position of substituent. By tuning the substituents on the trienamine backbone and utilizing dienophile with lowered LUMO, this study can aid in trienamine mediated Diels-Alder reaction development. This project will be applied on reported trienamine mediated Diels-Alder reactions to study the role of steric bulk of the aminocatalyst on HOMOs. The impact of LUMO-lowering in dienophiles will also be studied which can then help in expanding the scope of substituted 2,4-dienals and dienophiles.

In Chapter 5, computational investigation on the reactivity of electron deficient cyclic allenes was presented. The project was done in collaboration with West research group in University of Alberta who performed the experimental work referenced in this chapter. Our collaborators observed an unprecedented dimerization of electron-deficient cyclic allenes. Our calculations indicate that the dimerization proceeds *via* concerted asynchronous Diels-Alder

pathway. Furthermore, the trapping of cyclic allenes with electron rich dienes such as furans was investigated to gain insights on the observed regio- and stereoselectivity. It was determined that the trapping reactions also proceed *via* hetero-Diels-Alder pathway and the observed stereoselectivity is a result of secondary orbital interactions. The observed regioselectivity was determined to be a result of kinetic preference. The reaction of dienes with 1,2-bond of allene was kinetically favoured than the reaction with 2,3-bond of cyclic allene. The computational investigation led to the development of novel trapping method of cyclic allenes with enamines to result in complex polycyclic compounds. This novel trapping method was also determined to proceed *via* hetero-Diels-Alder pathway.

Appendix

Supporting data

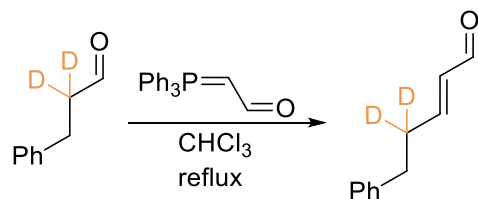
A1: Experimental Data and Procedures

General

The proton nuclear magnetic resonance spectra ^1H -NMR were recorded at 400 MHz and coupling constants (J) are reported in Hertz (Hz). Standard notation is used to describe the multiplicity of signals observed in ^1H -NMR spectra: broad (br), multiplet (m), singlet (s), doublet (d), triplet (t), quartet (q), etc. Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 100 MHz. The chemical shifts are reported on the δ scale (ppm) relative to residual solvent peaks: CDCl_3 (7.26 ppm, ^1H ; 77.16, ^{13}C). Purification of reaction products was carried out by flash chromatography using 40-63 μm (230-400 mesh) silica gel (Silicycle). Thin layer chromatography (TLC) were carried out on silica gel plates, using UV light, KMnO_4 dip, or dinitrophenylhydrazine (DNP) dip for detection. High-resolution mass spectrometry (HRMS) data were collected using ESI technique.

Commercially available starting materials were purchased from Sigma and Fisher, and used without further purification. 2- d_2 -3-phenyl-propanal was synthesized using the literature procedure (*J. Label. Compd. Radiopharm.* **2010**, 53 (8), 556–558)

Preparation of γ -deuterated-aldehyde

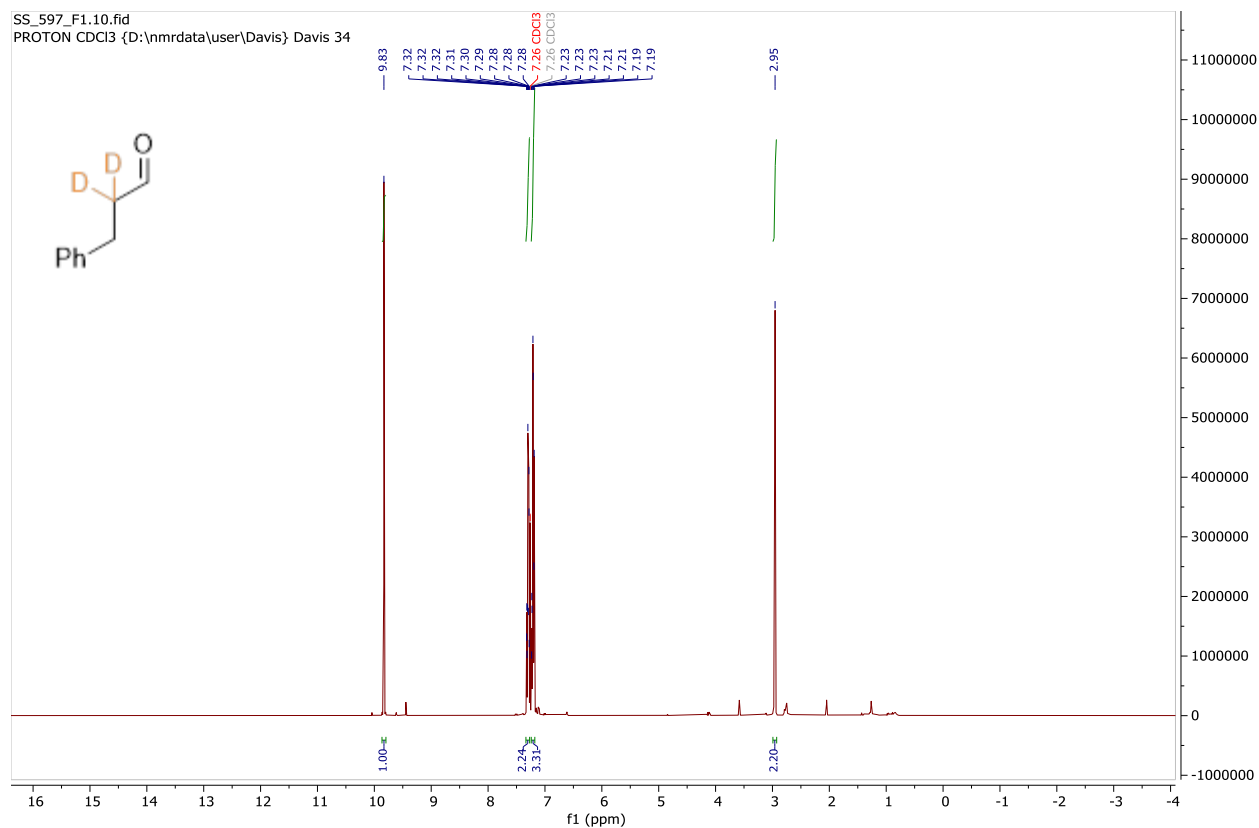


To a solution of triphenylphosphoranylidene)-acetaldehyde (2343 mg, 7.7 mmol, 1.1eq) in CHCl_3 (23 mL) was added 2-*d*₂-3-phenyl-propanal (953 mg, [0.3M] in CHCl_3 , 1.0 eq) and the mixture was refluxed overnight. The solvent was evaporated in vacuo and the residue was taken up in hexanes. The triphenylphosphine oxide solid was filtered and the resulting filtrate was evaporated under vacuum. The resulting oil was purified by flash column chromatography (9:1 Petroleum Ether: Diethyl Ether) to afford 4-*d*₂-5-phenyl-2-pentenal as clear oil (29%).

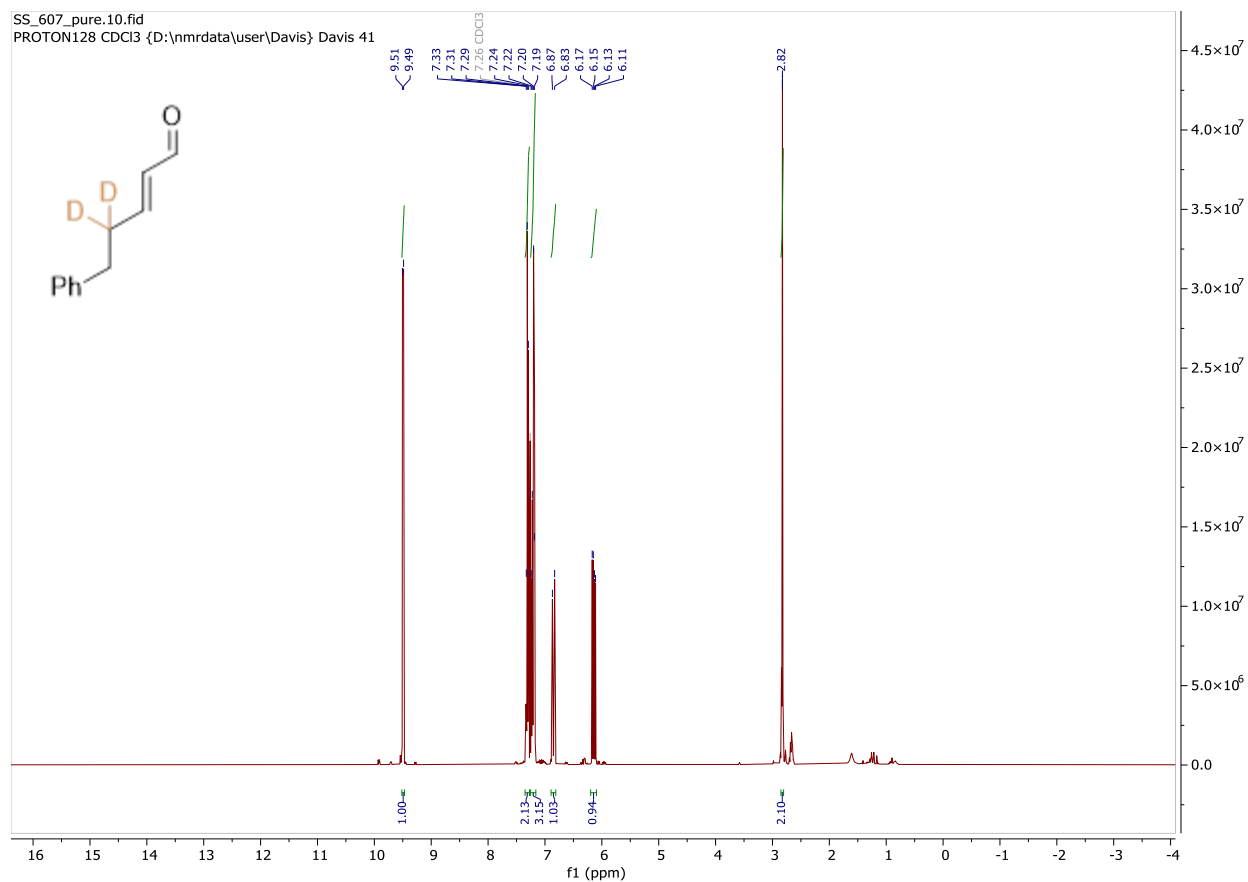
¹H NMR (400 MHz, CDCl_3): δ = 9.50 (d, J =7.9 Hz, 1H), 7.34-7.27 (m, 2H), 7.24-7.17 (m, 3H), 6.85 (d, J = 15.6 Hz, 1H), 6.14 (dd, 15.6, 7.9 Hz, 1H), 2.82 (s, 2H).

¹³C NMR (100 MHz, CDCl_3): δ = 194.1, 157.3, 140.4, 133.6, 128.7, 128.5, 126.5, 34.2, 34.1.

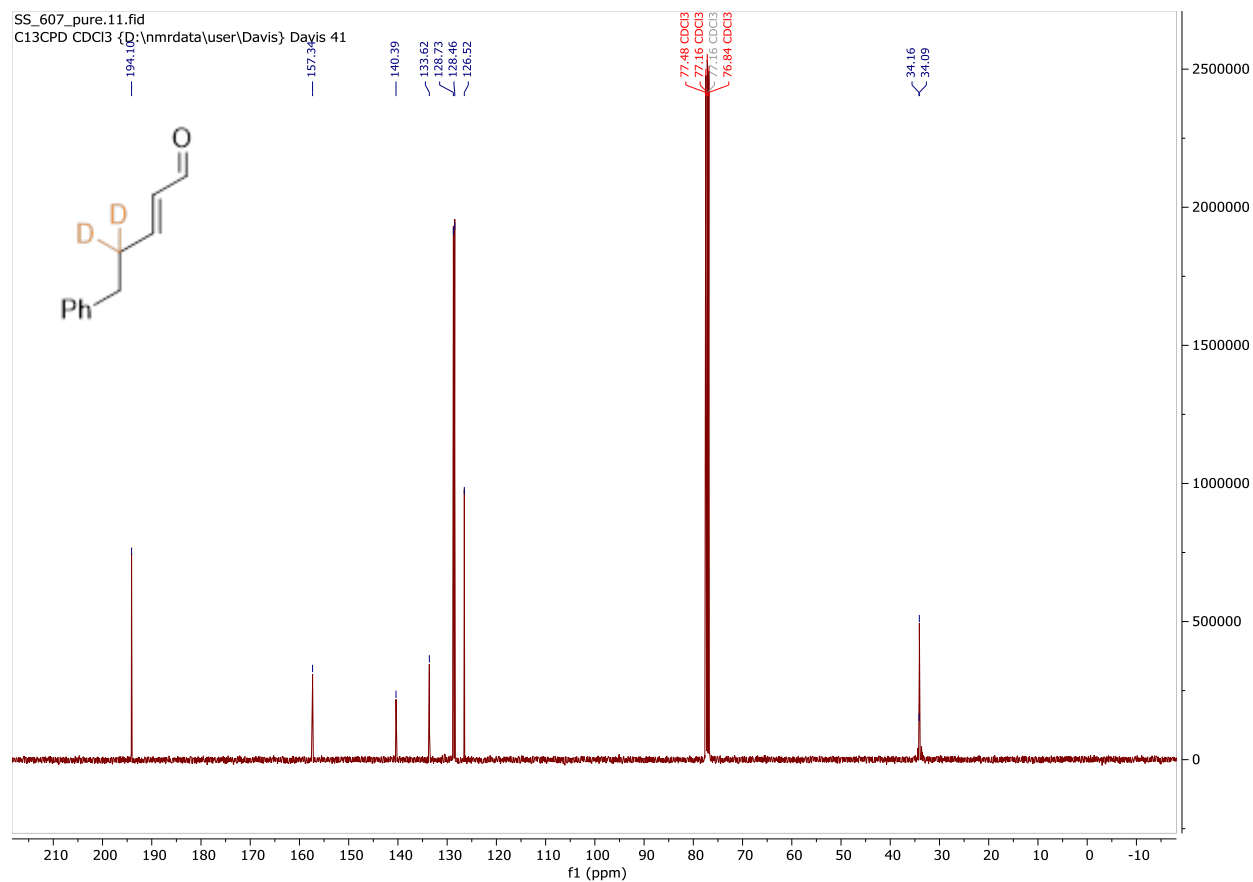
HRMS ESI Calcd for $\text{C}_{11}\text{H}_9\text{D}_2\text{O}$ $[\text{M}-\text{H}]^-$: 161.0940; found: 161.094



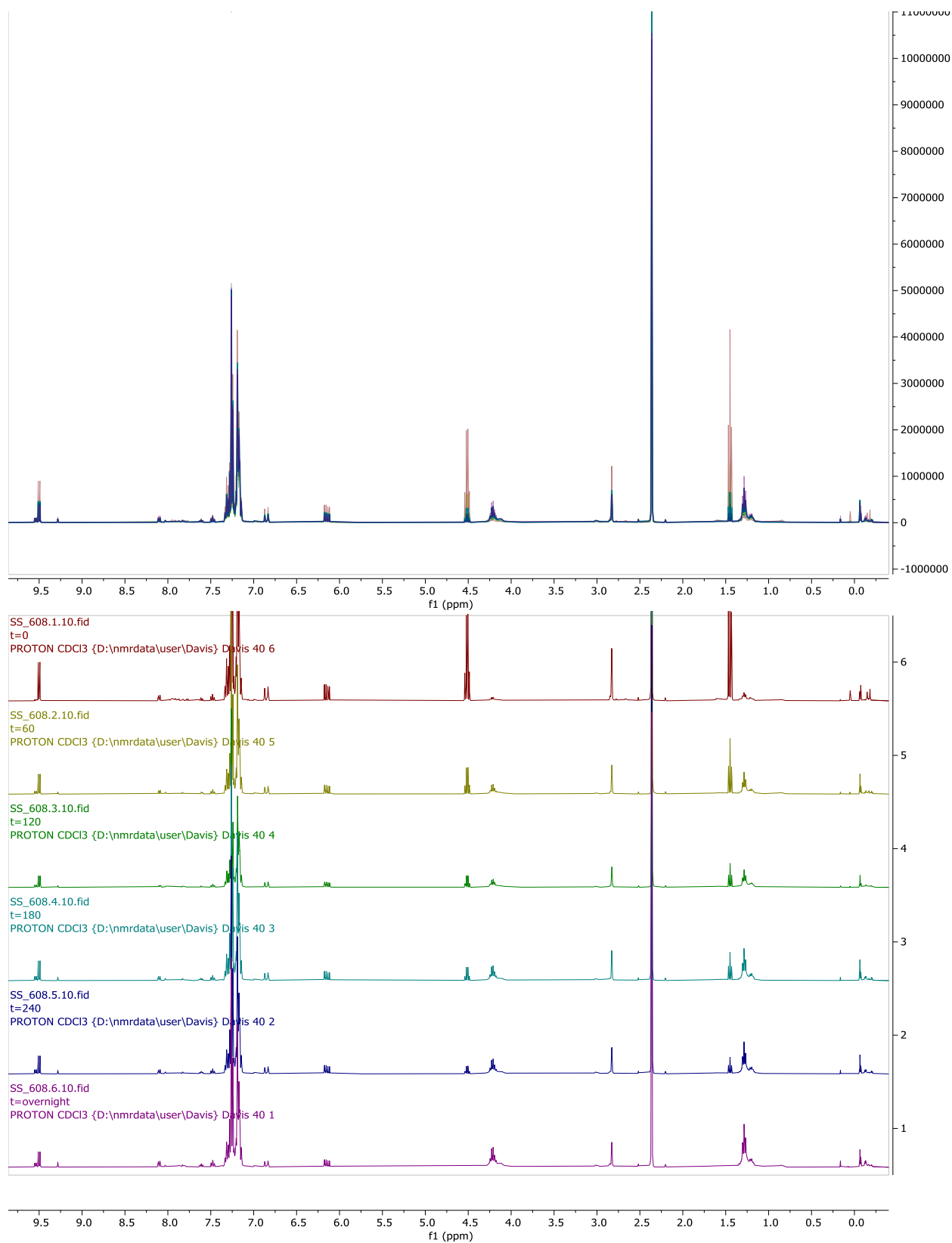
¹H NMR spectrum of 2-d₂-3-phenyl-propanal (400 MHz in CDCl₃)



¹H NMR spectrum of 4-*d*₂-5-phenyl-2-pentenal (400 MHz in CDCl₃)



¹³C NMR spectrum of 4-d₂-5-phenyl-2-pentalenal (100 MHz in CDCl₃)



^1H NMR monitoring study of γ -amination reaction between 4- d_2 -5-phenyl-2-pental and DEAD shown in Scheme 2.3. (400 MHz in CDCl_3)

A2: Supporting Data for Chapter 3

A.2.1: Geometry Analysis of all Model systems.

Model System A

Table A1: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the aldehydes and enols of model system A.

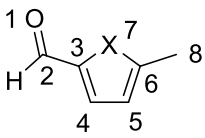
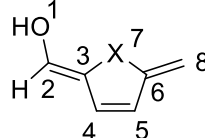
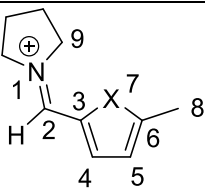
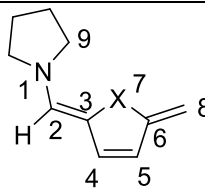
						
Atom numbers	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.21	1.22	1.21	1.36	1.37	1.36
2,3	1.46	1.45	1.46	1.34	1.34	1.34
3,4	1.37	1.39	1.37	1.45	1.46	1.46
4,5	1.42	1.41	1.42	1.35	1.35	1.34
5,6	1.37	1.39	1.37	1.46	1.47	1.46
6,7	1.35	1.36	1.73	1.34	1.35	1.34
7,3	1.36	1.37	1.73	1.38	1.39	1.78
1,2,3,4	180.00	180.00	180.00	1.37	1.39	1.77
3,4,5,6	0.00	0.00	0.00	179.97	179.99	179.98
2,3,7,6	180.00	180.00	179.99	0.01	0.00	0.00
NH,7,3,4	N.A.	180.00	N.A.	179.96	180.00	179.99
NH,7,6,5	N.A.	180.00	N.A.	N.A.	180.00	N.A.

Table A2: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the iminium ions and enamines of model system A.

						
Atom numbers	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.30	1.31	1.30	1.36	1.39	1.36
2,3	1.41	1.40	1.42	1.35	1.35	1.36
3,4	1.38	1.41	1.39	1.43	1.46	1.45
4,5	1.41	1.39	1.40	1.35	1.35	1.35
5,6	1.38	1.40	1.38	1.45	1.47	1.46
6,8	1.35	1.35	1.72	1.34	1.35	1.34
6,7	1.37	1.39	1.75	1.38	1.40	1.78
7,3	179.90	179.03	179.97	1.39	1.40	1.78
1,2,3,4	0.08	0.15	0.08	179.73	175.57	179.23
3,4,5,6	179.56	179.38	179.17	0.00	0.60	0.11

2,3,7,6	N.A.	178.38	N.A.	179.52	175.85	177.78
NH,7,3,4	N.A.	178.53	N.A.	N.A.	155.38	N.A.
NH,7,6,5	178.93	178.69	178.86	N.A.	155.61	N.A.
9,1,2,3	1.30	1.31	1.30	7.63	48.20	19.30

Model System B

Table A3: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the aldehydes and enols of model system B.

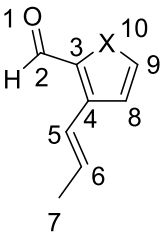
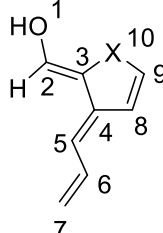
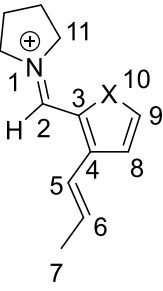
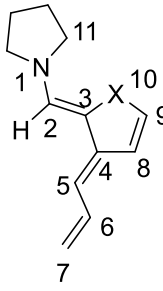
						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.21	1.22	1.21	1.36	1.37	1.36
2,3	1.46	1.45	1.46	1.34	1.34	1.34
3,4	1.38	1.40	1.39	1.47	1.48	1.48
4,5	1.46	1.46	1.47	1.35	1.36	1.36
5,6	1.34	1.34	1.34	1.45	1.47	1.45
6,7	1.50	1.50	1.50	1.34	1.34	1.34
4,8	1.43	1.42	1.43	1.46	1.46	1.46
8,9	1.36	1.38	1.37	1.34	1.35	1.34
9,10	1.34	1.36	1.71	1.36	1.38	1.75
3,10	1.46	1.37	1.73	1.39	1.40	1.79
1,2,3,4	179.97	179.99	179.55	179.98	179.92	179.00
2,3,4,5	0.00	0.01	1.38	0.01	0.06	9.93
3,4,5,6	179.97	179.95	165.74	180.00	179.99	178.60
4,5,6,7	179.99	179.99	179.66	180.00	179.99	179.61
1,2,3,10	0.03	0.00	0.86	0.02	0.06	3.69
3,4,8,9	0.01	0.01	0.26	0.01	0.01	4.10
NH,10,3,4	N.A.	179.98	N.A.	N.A.	179.83	N.A.
NH,10,8,9	N.A.	179.97	N.A.	N.A.	179.82	N.A.

Table A4: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the iminium ions and enamines of model system B.

						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.30	1.31	1.30	1.36	1.38	1.36
2,3	1.41	1.40	1.41	1.35	1.35	1.36
3,4	1.40	1.42	1.41	1.46	1.47	1.47
4,5	1.45	1.46	1.46	1.36	1.36	1.36
5,6	1.34	1.34	1.34	1.45	1.45	1.45
6,7	1.49	1.49	1.49	1.34	1.34	1.34
4,8	1.43	1.41	1.42	1.46	1.46	1.46
8,9	1.36	1.39	1.37	1.34	1.35	1.34
9,10	1.34	1.35	1.70	1.36	1.39	1.75
3,10	1.41	1.39	1.73	1.40	1.42	1.79
1,2,3,4	179.60	177.64	178.70	179.31	176.04	177.23
2,3,4,5	1.49	2.71	6.13	3.10	12.75	20.13
3,4,5,6	177.45	166.90	157.80	178.63	178.21	174.55
4,5,6,7	179.85	179.33	178.96	179.79	179.74	179.20
1,2,3,10	1.73	4.66	6.79	1.38	7.46	13.06
3,4,8,9	0.04	0.28	0.25	0.78	3.28	6.65
NH,10,3,4	N.A.	177.35	N.A.	N.A.	148.74	N.A.
NH,10,8,9	N.A.	177.65	N.A.	N.A.	146.10	N.A.
11,1,2,3	0.64	2.69	2.08	4.15	46.61	27.45

Model System C

Table A5: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the aldehydes and enols of model system C.

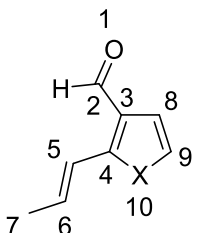
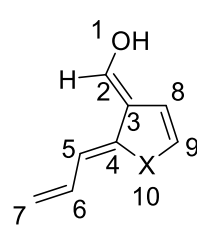
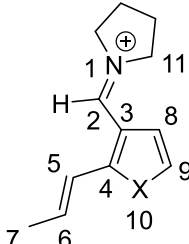
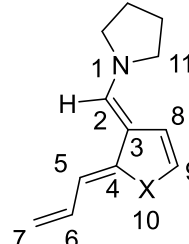
						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.21	1.21	1.21	1.35	1.35	1.35
2,3	1.46	1.46	1.47	1.35	1.35	1.35
3,4	1.38	1.40	1.38	1.47	1.48	1.48
4,5	1.45	1.46	1.46	1.34	1.36	1.35
5,6	1.34	1.34	1.34	1.45	1.45	1.45
6,7	1.50	1.50	1.50	1.34	1.34	1.34
3,8	1.44	1.43	1.43	1.47	1.47	1.46
8,9	1.35	1.37	1.36	1.34	1.35	1.34
9,10	1.37	1.38	1.73	1.37	1.39	1.75
4,10	1.35	1.36	1.73	1.39	1.40	1.79
1,2,3,4	179.90	179.98	180.00	179.99	179.83	180.00
2,3,4,5	0.03	0.00	0.08	0.06	6.23	0.01
3,4,5,6	179.84	178.60	178.71	180.00	177.92	180.00
4,5,6,7	179.99	179.91	179.91	180.00	177.52	179.97
1,2,3,8	0.09	0.10	0.10	0.04	2.15	0.00
10,4,5,6	0.14	1.33	1.32	0.01	2.67	0.00
10,4,3,8	0.01	0.00	0.05	0.02	3.84	0.01
NH,10,4,3	N.A.	179.60	N.A.	N.A.	165.45	N.A.
NH,10,9,8	N.A.	179.61	N.A.	N.A.	164.52	N.A.

Table A6: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the iminium ions and enamines of model system C.

						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.30	1.30	1.30	1.36	1.36	1.36
2,3	1.41	1.41	1.42	1.36	1.36	1.37
3,4	1.40	1.38	1.41	1.47	1.47	1.47
4,5	1.44	1.46	1.46	1.35	1.37	1.36
5,6	1.34	1.34	1.34	1.45	1.44	1.45
6,7	1.49	1.49	1.49	1.34	1.35	1.34
3,8	1.45	1.44	1.44	1.47	1.47	1.46
8,9	1.35	1.36	1.36	1.34	1.35	1.34
9,10	1.37	1.38	1.73	1.37	1.39	1.76
4,10	1.33	1.35	1.71	1.38	1.40	1.78
1,2,3,4	177.29	176.99	175.13	176.95	176.46	173.00
2,3,4,5	1.33	2.96	4.10	7.02	13.30	15.02
3,4,5,6	179.38	153.17	153.05	178.87	175.01	177.75
4,5,6,7	179.89	178.25	178.43	179.63	176.16	179.34
1,2,3,8	4.12	6.95	9.50	7.84	11.06	14.42
10,4,5,6	1.07	27.06	28.60	2.37	6.55	5.04
10,4,3,8	0.16	0.37	1.28	2.22	6.09	6.24
NH,10,4,3	N.A.	175.29	N.A.	N.A.	160.87	N.A.
NH,10,9,8	N.A.	175.33	N.A.	N.A.	158.80	N.A.
11,1,2,3	1.23	2.02	2.60	14.74	16.78	22.09

Model System D

Table A7: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the aldehydes and enols of model system D.

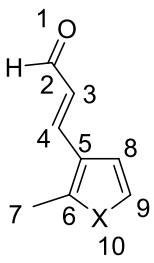
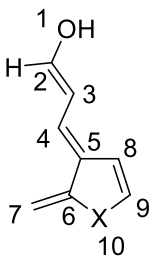
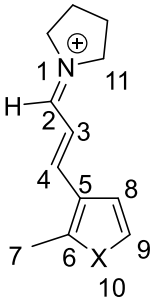
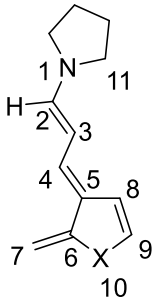
						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.21	1.21	1.21	1.36	1.36	1.36
2,3	1.47	1.46	1.47	1.34	1.34	1.34
3,4	1.35	1.35	1.35	1.44	1.44	1.44
4,5	1.45	1.45	1.46	1.35	1.35	1.36
5,6	1.37	1.39	1.38	1.48	1.49	1.49
6,7	1.49	1.49	1.50	1.34	1.34	1.34
5,8	1.44	1.44	1.44	1.46	1.46	1.46
8,9	1.35	1.37	1.36	1.34	1.35	1.34
9,10	1.36	1.38	1.72	1.37	1.38	1.76
6,10	1.35	1.36	1.73	1.39	1.40	1.78
1,2,3,4	179.99	179.99	180.00	179.95	179.92	179.94
2,3,4,5	180.00	180.00	180.00	179.95	179.93	179.90
3,4,5,6	179.97	179.97	179.98	180.00	179.99	179.99
4,5,6,7	0.01	0.01	0.00	0.03	0.04	0.05
3,4,5,8	0.04	0.03	0.02	0.01	0.01	0.03
10,6,5,4	180.00	180.00	180.00	179.98	179.97	179.96
10,6,5,8	0.01	0.00	0.00	0.01	0.02	0.03
NH,10,6,5	N.A.	180.00	N.A.	N.A.	180.00	N.A.
NH,10,9,8	N.A.	180.00	N.A.	N.A.	180.00	N.A.

Table A8: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the iminium ions and enamines of model system D.

						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.30	1.31	1.30	1.36	1.36	1.35
2,3	1.37	1.38	1.37	1.36	1.36	1.36
3,4	1.42	1.41	1.43	1.44	1.44	1.44
4,5	1.39	1.41	1.40	1.36	1.36	1.36
5,6	1.48	1.41	1.50	1.48	1.49	1.48
6,7	1.48	1.49	1.50	1.34	1.35	1.34
5,8	1.45	1.44	1.44	1.46	1.46	1.46
8,9	1.35	1.36	1.35	1.34	1.35	1.34
9,10	1.37	1.39	1.73	1.37	1.39	1.76
6,10	1.33	1.35	1.71	1.39	1.40	1.79
1,2,3,4	179.82	179.86	179.79	179.97	179.77	179.62
2,3,4,5	179.77	179.65	179.76	179.97	179.60	179.47
3,4,5,6	179.95	178.68	179.76	179.97	179.84	179.95
4,5,6,7	0.13	1.73	0.28	0.03	6.72	1.44
3,4,5,8	0.11	1.07	0.22	0.06	1.80	0.52
10,6,5,4	179.96	179.76	179.94	179.99	173.98	178.75
10,6,5,8	0.01	0.04	0.05	0.04	4.69	0.85
NH,10,6,5	N.A.	180.00	N.A.	N.A.	162.70	N.A.
NH,10,9,8	N.A.	179.99	N.A.	N.A.	161.33	N.A.
11,1,2,3	0.47	0.51	0.49	0.14	0.79	0.03

Model System E

Table A9: Bond lengths ($\text{\AA}$) and dihedral angles ($^\circ$) for the aldehydes and enols of model system E.

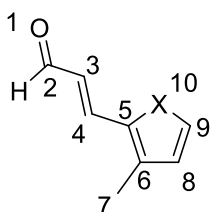
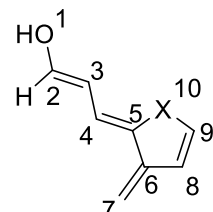
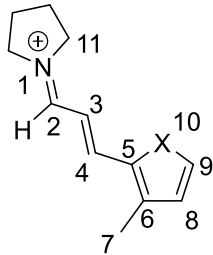
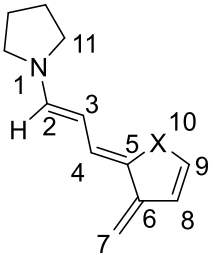
						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.21	1.21	1.21	1.35	1.36	1.35
2,3	1.47	1.46	1.47	1.34	1.34	1.35
3,4	1.35	1.35	1.35	1.45	1.45	1.45
4,5	1.44	1.44	1.45	1.34	1.35	1.35
5,6	1.37	1.39	1.38	1.48	1.49	1.48
6,7	1.49	1.50	1.50	1.34	1.34	1.35
6,8	1.43	1.42	1.43	1.47	1.47	1.47
8,9	1.36	1.38	1.37	1.34	1.35	1.34
9,10	1.35	1.36	1.72	1.37	1.39	1.76
5,10	1.36	1.38	1.74	1.39	1.41	1.78
1,2,3,4	179.98	179.99	179.96	180.00	178.36	180.00
2,3,4,5	179.99	180.00	179.97	179.97	173.67	179.97
3,4,5,6	179.99	179.99	179.57	180.00	176.72	179.99
4,5,6,7	0.03	0.02	0.09	0.01	7.41	0.11
3,4,5,10	0.01	0.01	0.28	0.00	3.20	0.02
10,5,6,8	0.01	0.01	0.04	0.00	5.65	0.06
7,6,5,10	179.98	179.98	179.78	180.00	172.53	179.92
NH,10,5,4	N.A.	0.01	N.A.	N.A.	28.96	N.A.
NH,10,9,8	N.A.	179.99	N.A.	N.A.	150.06	N.A.

Table A10: Bond lengths (Å) and dihedral angles (°) for the iminium ions and enamines of model system D.

						
Bond	X=O	X=NH	X=S	X=O	X=NH	X=S
1,2	1.30	1.31	1.30	1.36	1.36	1.35
2,3	1.41	1.41	1.41	1.36	1.36	1.36
3,4	1.37	1.38	1.37	1.44	1.44	1.44
4,5	1.47	1.40	1.41	1.35	1.35	1.35
5,6	1.38	1.42	1.40	1.47	1.48	1.48
6,7	1.49	1.50	1.50	1.35	1.35	1.35
6,8	1.42	1.40	1.41	1.47	1.47	1.47
8,9	1.37	1.39	1.37	1.34	1.35	1.34
9,10	1.34	1.35	1.71	1.36	1.39	1.75
5,10	1.37	1.39	1.74	1.40	1.41	1.78
1,2,3,4	179.87	179.89	179.72	179.63	179.56	179.49
2,3,4,5	179.73	179.73	179.65	179.71	175.65	179.62
3,4,5,6	179.95	179.41	179.74	179.94	177.28	179.80
4,5,6,7	0.04	0.36	0.24	0.02	7.91	1.04
3,4,5,10	0.43	0.42	0.51	0.08	3.01	0.18
10,5,6,8	0.02	0.00	0.01	0.02	5.84	0.57
7,6,5,10	179.95	179.56	179.76	179.96	172.34	179.31
NH,10,5,4	N.A.	0.47	N.A.	N.A.	29.25	N.A.
NH,10,9,8	N.A.	179.64	N.A.	N.A.	149.33	N.A.
11,1,2,3	0.43	0.42	0.51	0.22	3.42	0.32

A.2.2: Charge Analysis and Fukui function Isosurfaces for all Model systems

Table A 11: ESP charges of trienamines A12-15.

Carbon	A12 (X = CH ₂)	A13 (X = O)	A14 (X = NH)	A15 (X = S)
<i>ipso</i>	-0.085	-0.363	-0.153	-0.154
<i>α</i>	-0.150	0.266	0.151	0.044
<i>β</i>	-0.143	-0.228	-0.145	-0.136
<i>γ</i>	-0.211	-0.221	-0.220	0.249
<i>δ</i>	0.138	0.425	0.459	0.356
<i>ε</i>	-0.562	-0.691	-0.751	-0.621

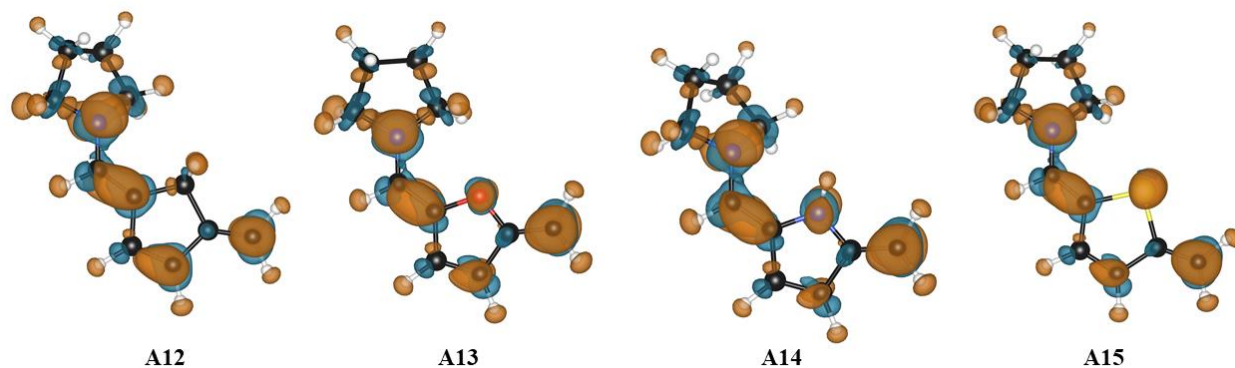


Figure A 1: Electrophilic Fukui function $f^-(r)$ for trienamines **A12-15** (isovalue 0.003).

Table A 12: ESP charges of trienamines **B12-B15**.

Carbon	B12 (X = CH ₂)	B13 (X = O)	B14 (X = NH)	B15 (X = S)
<i>ipso</i>	-0.033	-0.297	-0.109	-0.091
<i>α</i>	-0.272	0.130	0.039	-0.076
<i>β</i>	0.148	0.097	0.204	0.221
<i>γ</i>	-0.312	-0.323	-0.363	-0.333
<i>δ</i>	0.091	0.088	0.121	0.078
<i>ε</i>	-0.460	-0.488	-0.491	-0.460

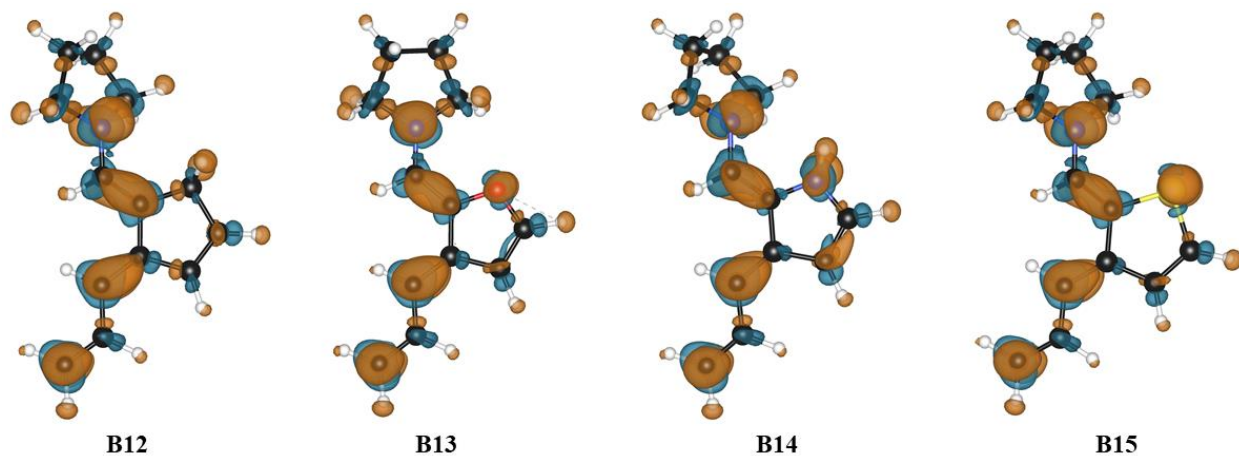


Figure A 2: Electrophilic Fukui function $f^-(r)$ for trienamines **B12-15** (isovalue 0.003).

Table A 13: ESP charges of trienamines **C12-C15**.

Carbon	C12 (X = CH ₂)	C13 (X = O)	C14 (X = NH)	C15 (X = S)
<i>ipso</i>	-0.152	-0.278	-0.249	-0.240
<i>α</i>	0.019	0.107	0.137	0.167
<i>β</i>	-0.143	0.189	0.137	-0.024

γ	-0.238	-0.385	-0.397	-0.218
δ	0.051	0.186	0.152	-0.096
ε	-0.443	-0.519	-0.526	-0.486

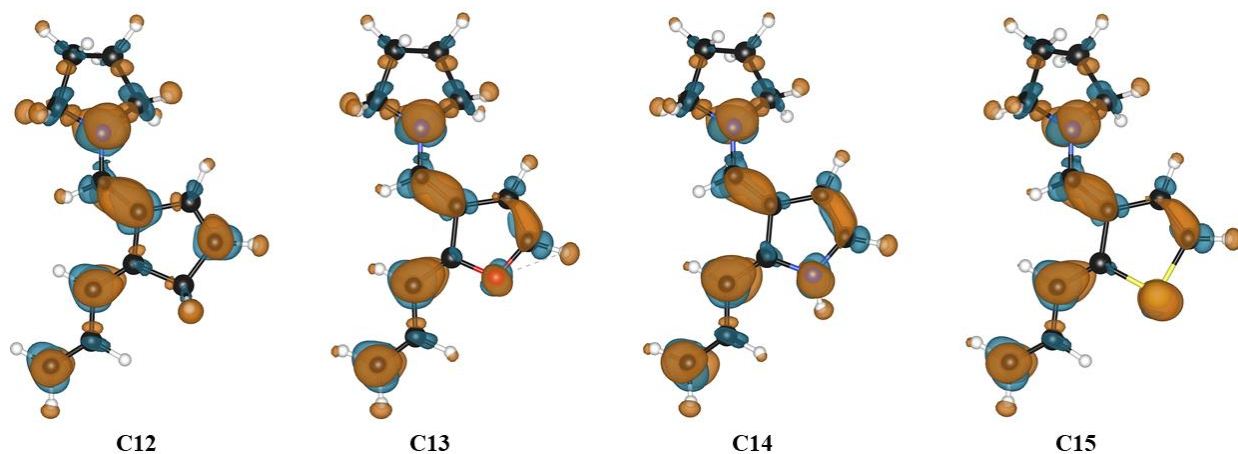


Figure A 3: Electrophilic Fukui function $f^-(r)$ for trienamines **C12-15** (isovalue 0.003).

Table A 14: ESP charges of trienamines **D12-D15**.

Carbon	D12 (X = CH ₂)	D13 (X = O)	D14 (X = NH)	D15 (X = S)
<i>ipso</i>	-0.159	-0.173	-0.131	-0.107
α	-0.150	-0.120	-0.156	-0.164
β	-0.197	-0.260	-0.254	-0.272
γ	0.065	0.126	0.141	0.189
δ	-0.009	0.301	0.258	0.130
ε	-0.473	-0.590	-0.635	-0.515

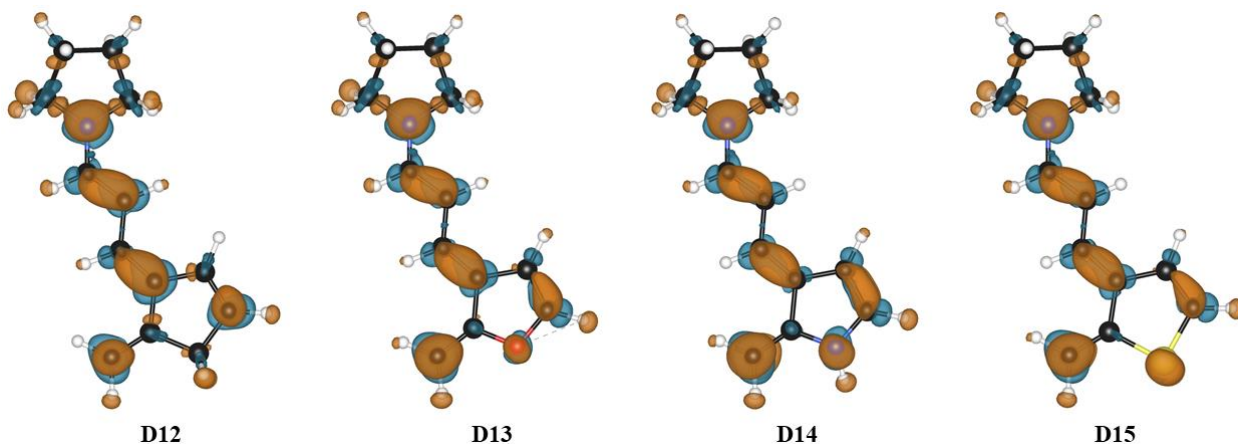
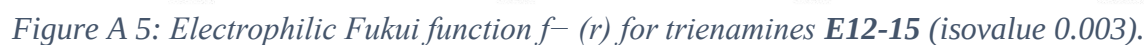


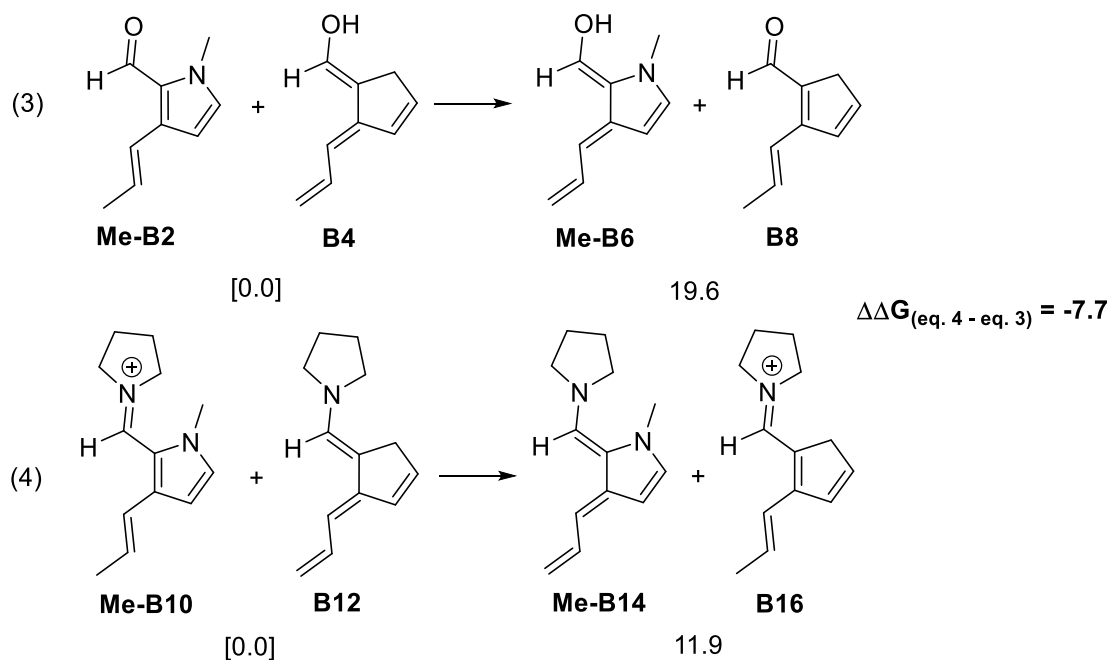
Figure A 4: Electrophilic Fukui function $f^-(r)$ for trienamines **D12-15** (isovalue 0.003).

Table A 15: ESP charges of trienamines **E12-E15**.

Carbon	E12 (X = CH ₂)	E13 (X = O)	E14 (X = NH)	E15 (X = S)
<i>ipso</i>	-0.150	-0.189	-0.177	-0.181
<i>α</i>	-0.179	-0.059	-0.102	-0.162
<i>β</i>	-0.130	-0.269	-0.227	-0.089
<i>γ</i>	-0.220	0.128	0.044	-0.101
<i>δ</i>	0.283	0.318	0.381	0.429
<i>ε</i>	-0.590	-0.660	-0.658	-0.676

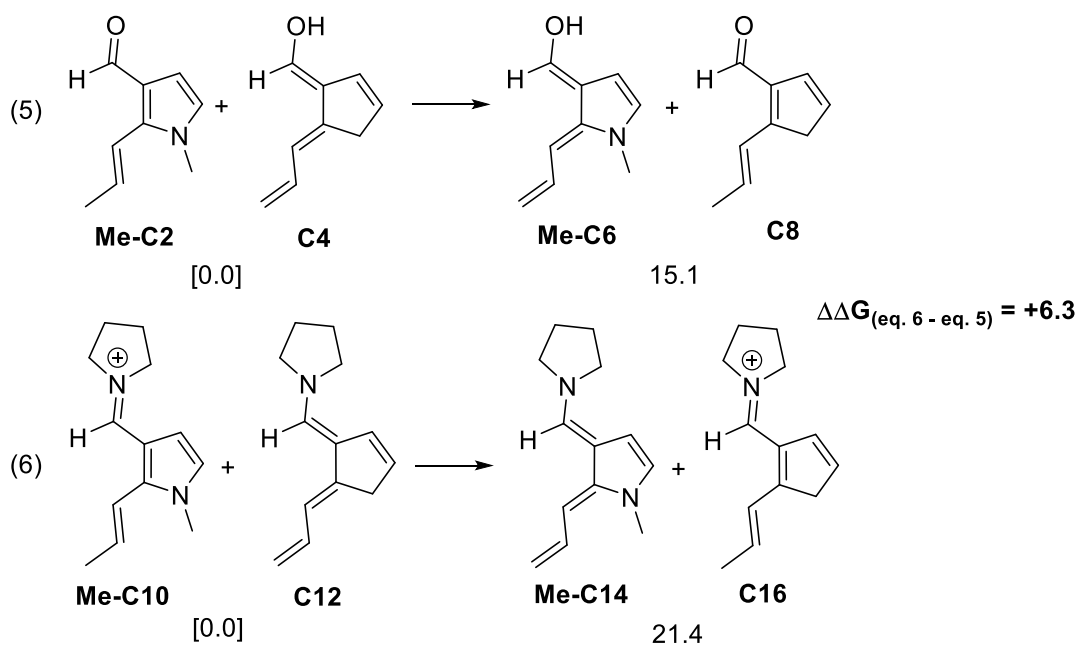


Model System B



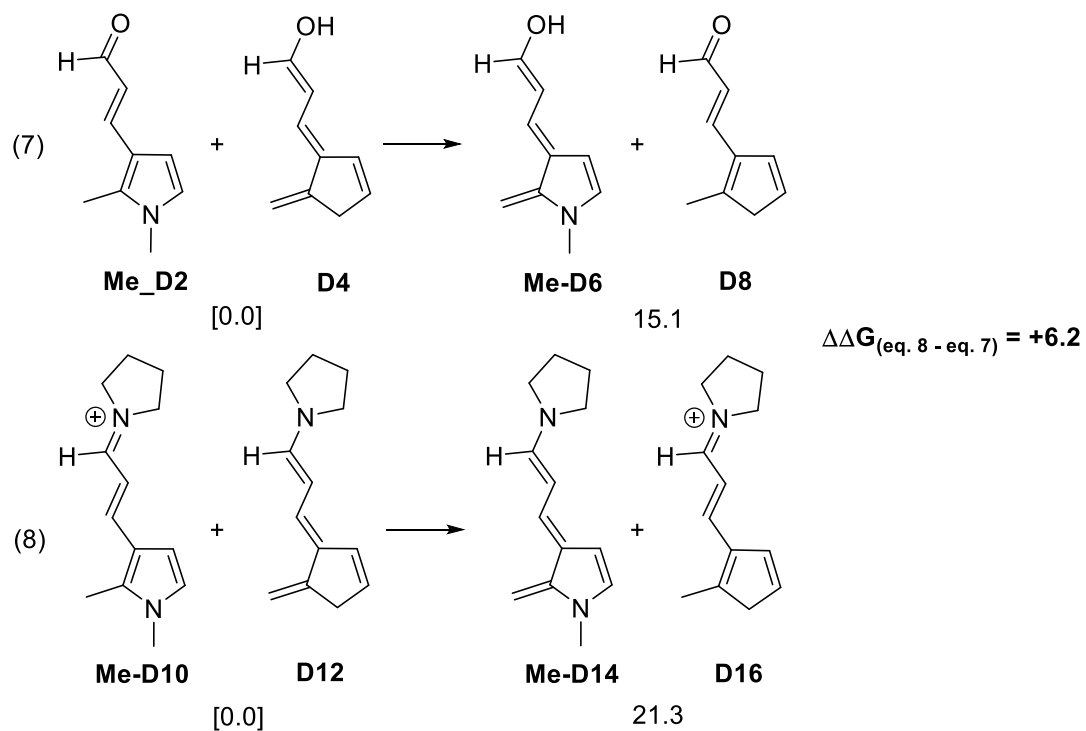
Scheme A2: Hyperhomodesmotic equations for the *N*-methyl derivative of model system B (relative energies in kcal/mol)

Model System C



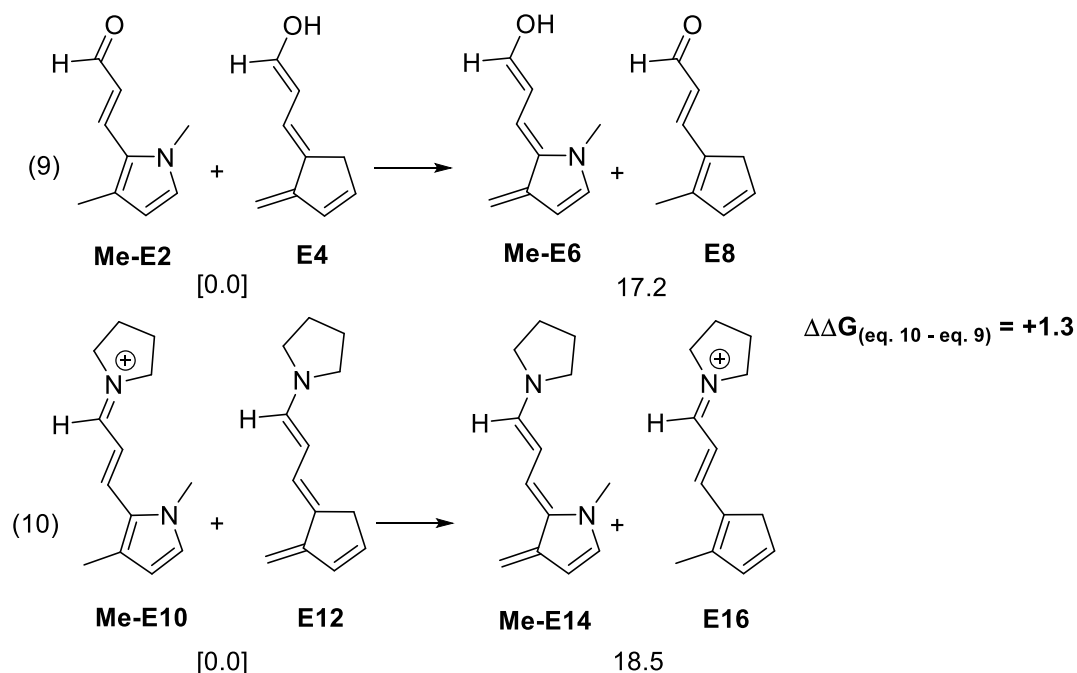
Scheme A3: Hyperhomodesmotic equations for the *N*-methyl derivative of model system C (relative energies in kcal/mol).

Model System D



Scheme A4: Hyperhomodesmotic equations for the N-methyl derivative of model system D (relative energies in kcal/mol).

Model System E



Scheme A5: Hyperhomodesmotic equations for the N-methyl derivative of model system B (relative energies in kcal/mol).

Table A 16: Orbital coefficients of the HOMO of N-Me trienamines

Carbon	Model System A	Model System B	Model System C	Model System D	Model System E
<i>ipso</i>	18.7	14.0	10.5	8.2	9.1
α	10.3	8.3	9.4	9.2	10.2
β	2.8	5.2	2.8	11.9	13.3
γ	6.2	19.3	22.8	10.5	9.8
δ	2.0	1.5	1.2	1.0	1.5
ϵ	20.4	10.1	11.6	17.8	15.3

Table A 17: Comparison of Orbital coefficients of the HOMOs of N-H-trienamines and N-Me trienamines.

Carbon	A14	Me-A14	B14	Me-B14	C14	Me-C14	D14	Me-D14	E14	Me-E14
<i>ipso</i>	15.2	18.7	14.4	14.0	10.7	10.5	9.1	8.2	9.3	9.1
α	8.4	10.3	8.1	8.3	10.2	9.4	12.9	9.2	11.4	10.2
β	3.3	2.8	4.8	5.2	3.0	2.8	11.2	11.9	13.3	13.3
γ	5.6	6.2	19.4	19.3	22.6	22.8	13.9	10.5	11.1	9.8
δ	3.7	2.0	1.4	1.5	1.2	1.2	1.2	1.0	1.7	1.5
ϵ	20.6	20.4	10.1	10.1	11.3	11.6	14.8	17.8	15.3	15.3

A3: Dihedral angles of trienamine backbone for Chapter 4

Table A 18: Dihedral angles of trienamine backbone for A1-A3

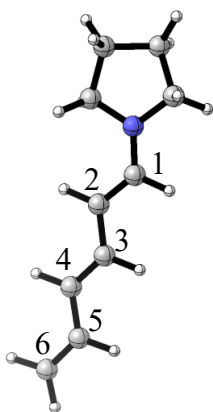
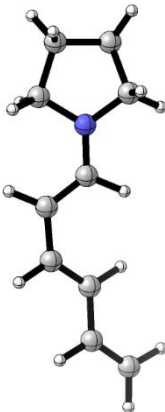
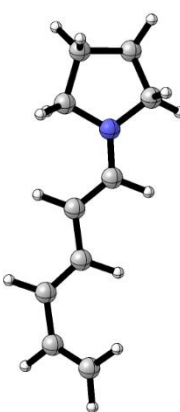
			
	A1	A2	A3
1,2,3,4	-179.75°	-24.61°	-178.37°
2,3,4,5	179.96°	176.78°	-178.50°
3,4,5,6	-179.84°	-179.73°	27.22°

Table A19: Dihedral angles of trienamine backbone for B1-B3

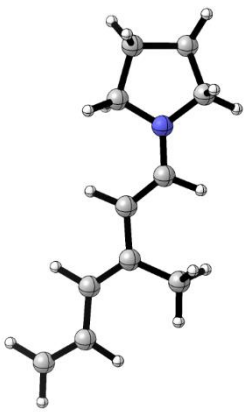
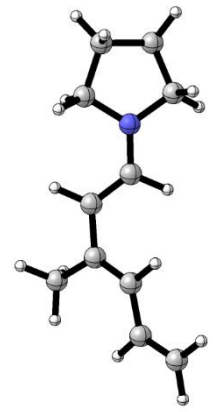
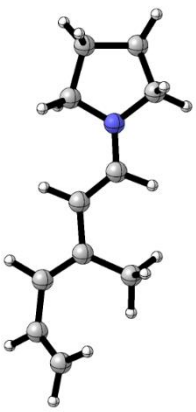
			
	B1	B2	B3
1,2,3,4	-179.87°	31.62°	176.17°
2,3,4,5	179.96°	-174.13°	-178.02°
3,4,5,6	-179.92°	-178.92°	36.73°

Table A20: Dihedral angles of trienamine backbone for **C1-C3**

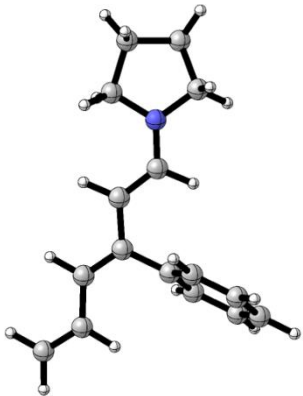
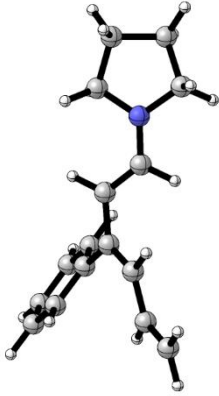
			
	C1	C2	C3
1,2,3,4	-173.62°	33.96°	-175.27°
2,3,4,5	-177.55°	-169.26°	-178.54°
3,4,5,6	-177.72°	-176.33°	20.68°

Table A21: Dihedral angles of trienamine backbone for **D1-D3**

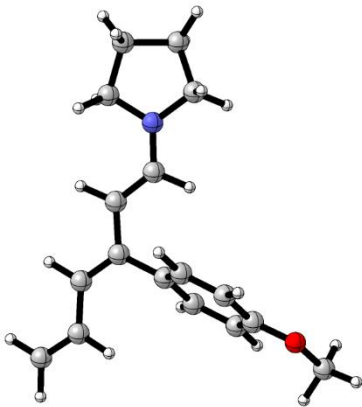
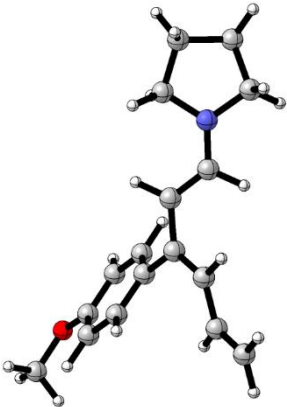
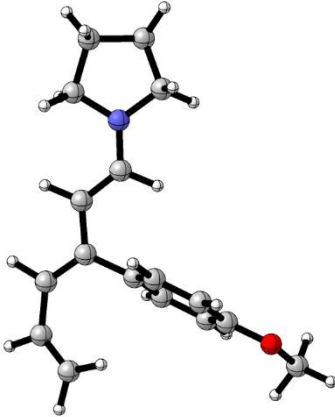
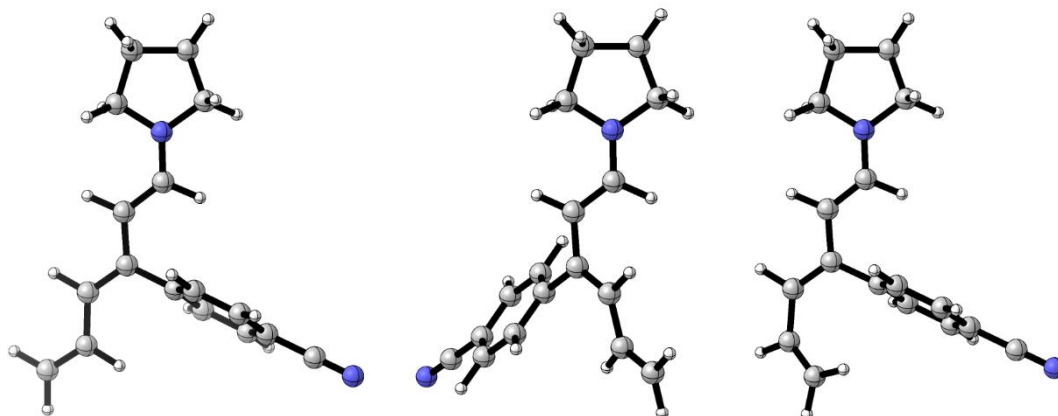
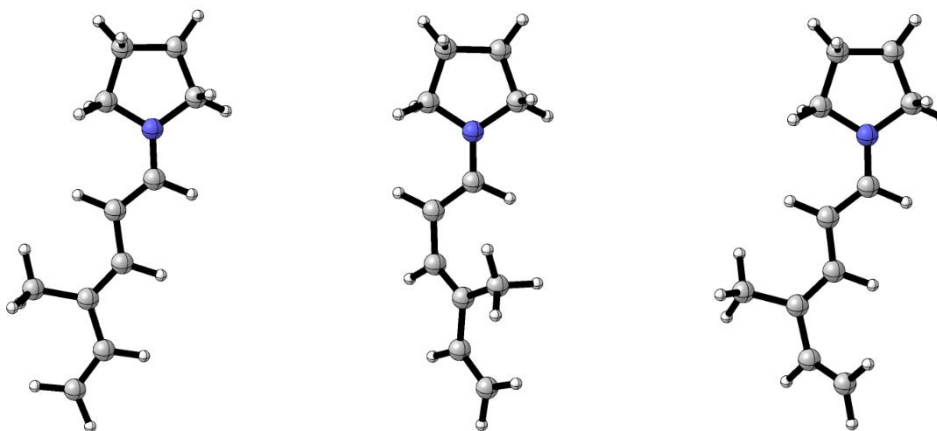
			
	D1	D2	D3
1,2,3,4	-172.08°	33.04°	-174.79°
2,3,4,5	-176.03°	-169.18°	-177.63°
3,4,5,6	-178.16°	-175.38°	19.73°

Table A22: Dihedral angles of trienamine backbone for **E1-E3**



	E1	E2	E3
1,2,3,4	-173.86°	32.32°	-173.98°
2,3,4,5	-177.13°	-169.30°	-178.43°
3,4,5,6	-178.53°	-176.11°	23.90°

Table A 23: Dihedral angles of trienamine backbone for **F1-F3**



	F1	F2	F3
1,2,3,4	-179.87°	34.13°	-176.46°
2,3,4,5	-179.94°	-175.80°	-176.79°
3,4,5,6	179.97°	175.30°	33.17°

Table A24: Dihedral angles of trienamine backbone for **G1-G3**

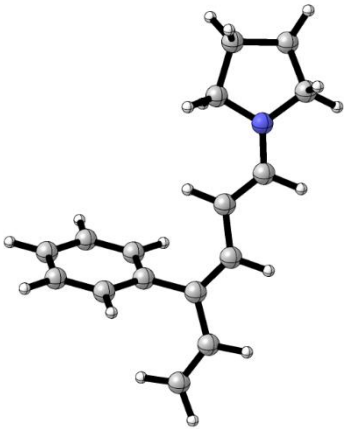
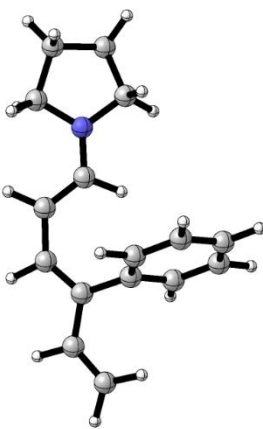
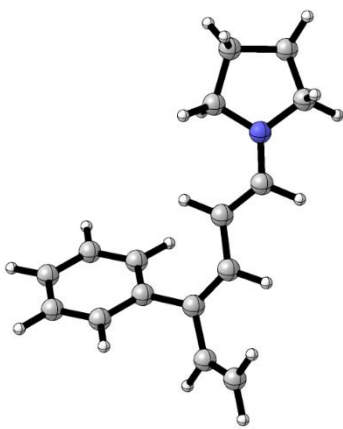
			
	G1	G2	G3
1,2,3,4	-178.50°	18.05°	-176.56°
2,3,4,5	-178.27°	-178.27°	-172.83°
3,4,5,6	-174.78°	-177.85°	33.73°

Table A 25: Dihedral angles of trienamine backbone for **H1, H2**

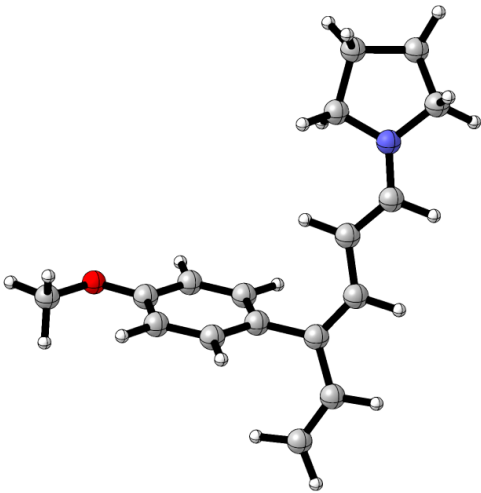
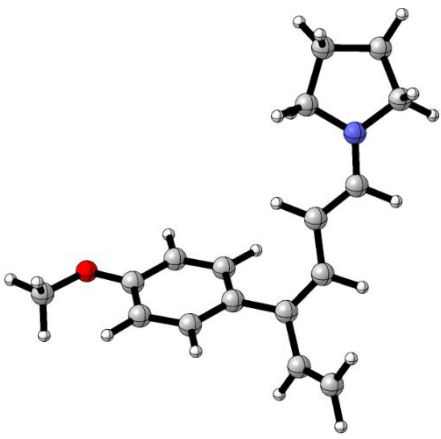
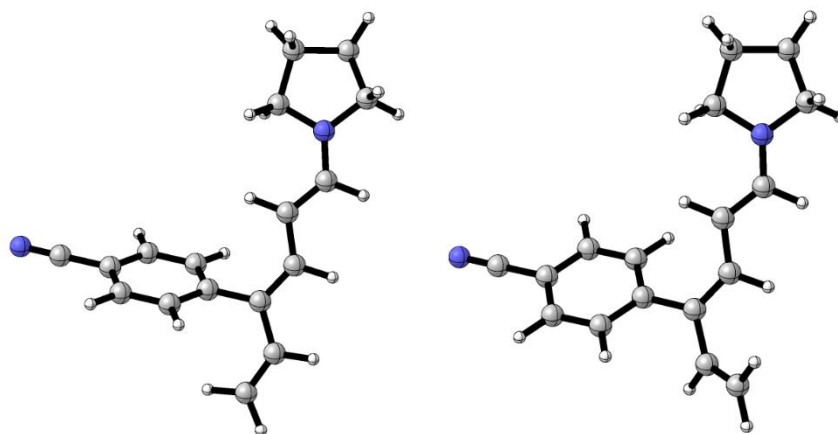
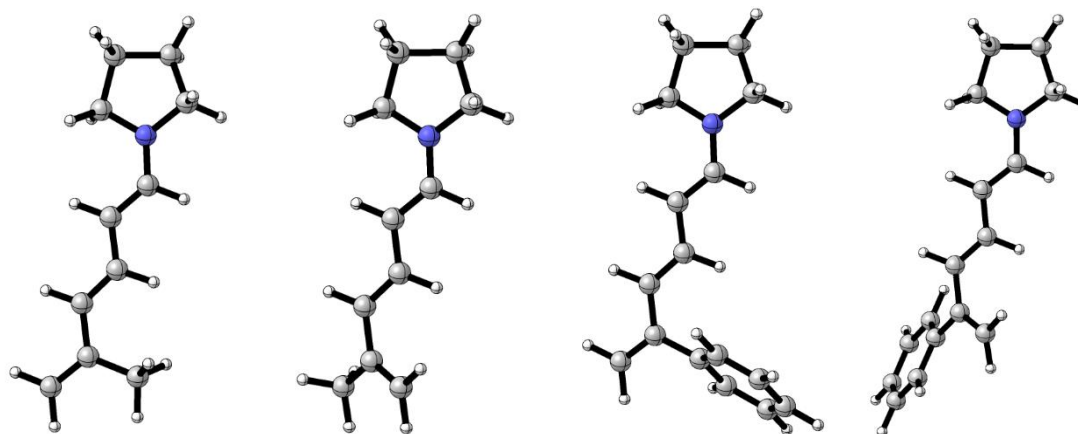
		
	H1	H2
1,2,3,4	-179.76°	-176.44°
2,3,4,5	-178.04°	-172.93°
3,4,5,6	-175.67°	34.03°

Table A26: Dihedral angles of trienamine backbone for **I1**, **I2**



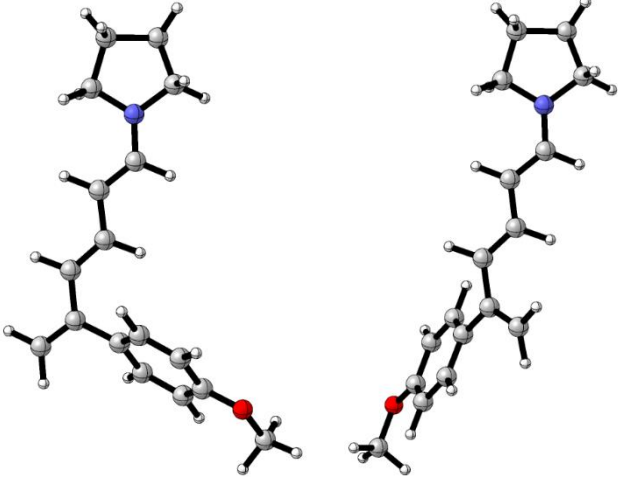
	I1	I2
1,2,3,4	-179.73°	-175.80°
2,3,4,5	-177.71°	-171.94°
3,4,5,6	-174.72°	33.65°

Table A27: Dihedral angles of trienamine backbone for **J1**, **J2**, **K1**, and **K2**



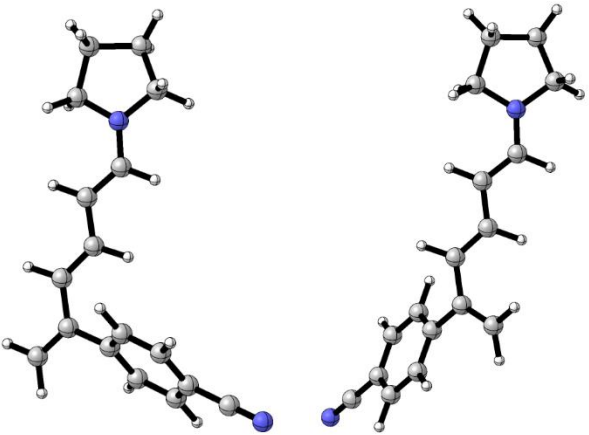
	J1	J2	K1	K2
1,2,3,4	-179.57°	-178.56°	-179.35°	-178.28°
2,3,4,5	179.94°	-179.19°	177.97°	-177.58°
3,4,5,6	-179.93°	30.16°	-179.35°	-178.28°

Table A28: Dihedral angles of trienamine backbone for **L1**, **L2**



	L1	L2
1,2,3,4	-179.70°	177.66°
2,3,4,5	178.65°	-178.25°
3,4,5,6	-168.92°	35.79°

Table A29: Dihedral angles of trienamine backbone for **M1**, **M2**



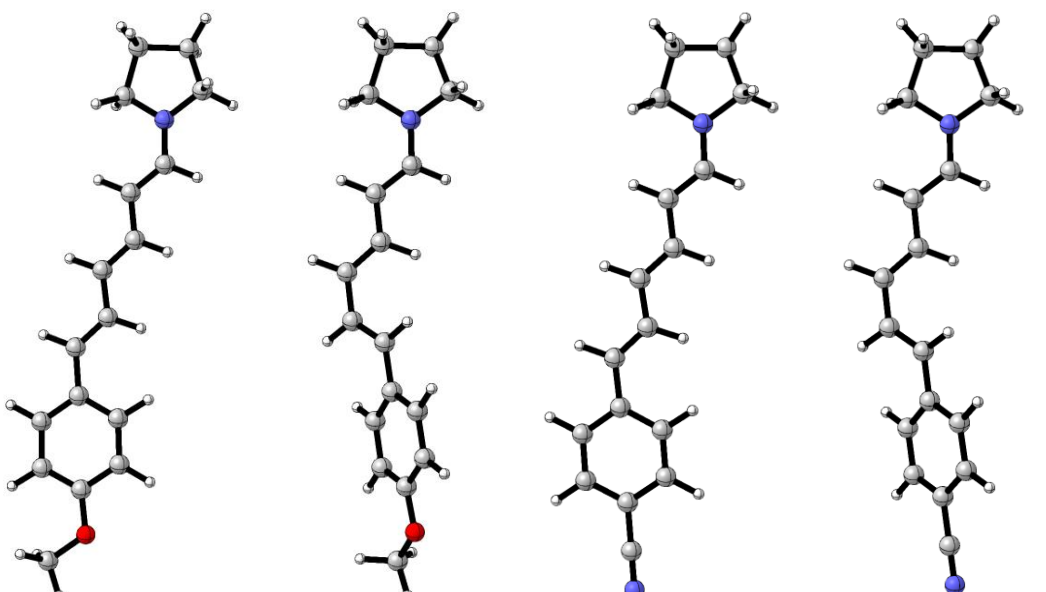
	M1	M2
1,2,3,4	-179.29°	-177.66°
2,3,4,5	179.15°	-177.89°
3,4,5,6	-168.18°	34.59°

Table A30: Dihedral angles of trienamine backbone for **N1**, **N2**, **O1**, and **O2**



	N1	N2	O1	O2
1,2,3,4	-179.82°	-178.27°	-179.78°	-177.91°
2,3,4,5	179.96°	-177.98°	179.83°	-178.03°
3,4,5,6	-179.93°	30.52°	-179.54°	27.14°

Table A31: Dihedral angles of trienamine backbone for **P1**, **P2**, **P3**, and **P4**

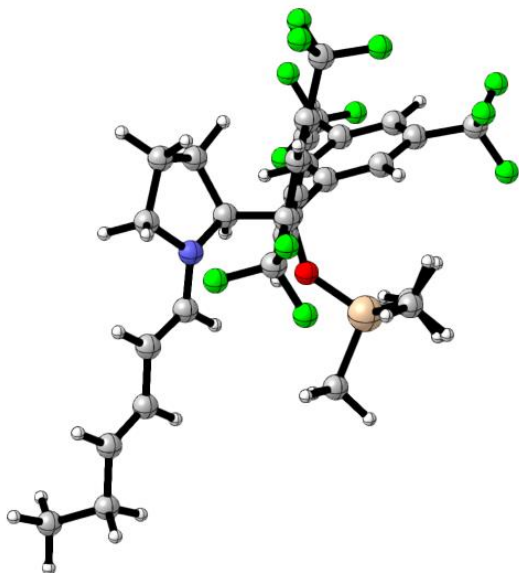


	P1	P2	Q1	Q2
1,2,3,4	-179.80°	-177.89°	-179.70°	-177.60°
2,3,4,5	179.92°	-177.79°	-179.77°	-178.16°
3,4,5,6	179.99°	27.88°	-179.57°	24.98°

A4: Energies and Reaction Coordinates

A.4.1: Energies and Reaction Coordinates for Chapter 2

Dienamine A



HF (B3LYP/6-31G(d)) = -2779.5033766 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.569260 (Hartree/Particle)

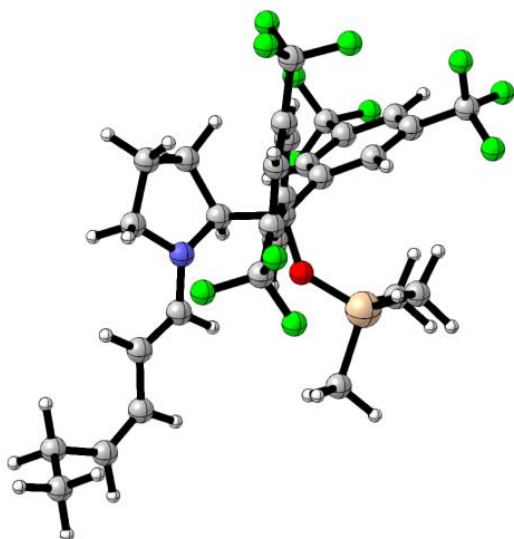
Thermal correction = 0.482236 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.661205	-2.159084	-0.200289
2	6	0	-5.315956	-2.209322	-0.159899
3	6	0	-4.412505	-1.350977	-0.901322
4	6	0	-3.063164	-1.465843	-0.808685
5	7	0	-2.129555	-0.705441	-1.478803
6	6	0	-0.709474	-1.046650	-1.480788
7	6	0	-0.218197	-0.551204	-2.859865
8	6	0	-1.213634	0.549229	-3.276770
9	6	0	-2.531433	0.134921	-2.608564
10	1	0	-4.857710	-0.591529	-1.540623
11	1	0	-2.629969	-2.206583	-0.143933
12	1	0	-0.613539	-2.133865	-1.389248
13	1	0	0.816083	-0.196569	-2.847549
14	1	0	-0.264047	-1.386682	-3.567101
15	1	0	-0.887029	1.526128	-2.911244
16	1	0	-1.314048	0.622497	-4.363264
17	1	0	-3.116319	0.997418	-2.264431
18	1	0	-3.172511	-0.446408	-3.289413

19	6	0	0.061944	-0.466261	-0.221120
20	8	0	-0.614398	-1.056238	0.883687
21	14	0	-0.471963	-1.199066	2.565941
22	6	0	-0.313218	0.470686	3.434292
23	1	0	-0.280086	0.301790	4.518579
24	1	0	0.600655	1.011972	3.165417
25	1	0	-1.164279	1.128900	3.228090
26	6	0	-2.097229	-2.019705	3.040408
27	1	0	-2.177844	-3.020970	2.601104
28	1	0	-2.174275	-2.127607	4.129282
29	1	0	-2.958009	-1.434641	2.698221
30	6	0	0.962855	-2.320236	3.065895
31	1	0	0.802353	-2.663633	4.096229
32	1	0	1.014403	-3.210282	2.428004
33	1	0	1.938393	-1.825664	3.035342
34	6	0	1.540209	-0.911283	-0.193678
35	6	0	2.436275	-0.283449	0.682925
36	6	0	2.016176	-1.997865	-0.937171
37	6	0	3.752228	-0.725268	0.814341
38	1	0	2.110067	0.564209	1.275056
39	6	0	3.339727	-2.430474	-0.816455
40	1	0	1.368443	-2.531809	-1.620130
41	6	0	4.218465	-1.801783	0.061430
42	1	0	5.241449	-2.143915	0.160797
43	6	0	-0.098506	1.059864	-0.195844
44	6	0	0.839218	1.932591	-0.761354
45	6	0	-1.284543	1.601869	0.310913
46	6	0	0.602411	3.309453	-0.801181
47	1	0	1.761445	1.549767	-1.183230
48	6	0	-1.517695	2.977030	0.268800
49	1	0	-2.030337	0.942926	0.735642
50	6	0	-0.577848	3.843574	-0.285421
51	1	0	-0.761144	4.910593	-0.316419
52	6	0	-7.584409	-3.065399	0.565663
53	1	0	-8.221279	-2.468252	1.237361
54	1	0	-6.995706	-3.730682	1.211237
55	6	0	-8.497952	-3.906686	-0.344272
56	1	0	-9.179281	-4.530669	0.246473
57	1	0	-9.108586	-3.264969	-0.991116
58	1	0	-7.906714	-4.563954	-0.992014
59	1	0	-4.846445	-2.956646	0.484903
60	6	0	4.640586	-0.086246	1.848416
61	6	0	3.823981	-3.558140	-1.690985
62	6	0	-2.829051	3.493273	0.796485
63	6	0	1.661484	4.223979	-1.357672
64	9	0	-3.854397	3.169008	-0.026711
65	9	0	-2.836220	4.835091	0.934995
66	9	0	-3.118207	2.957500	2.005929
67	9	0	1.140838	5.388223	-1.800545
68	9	0	2.592221	4.535476	-0.425645
69	9	0	2.320979	3.653552	-2.391527
70	9	0	4.405240	1.238184	1.965303
71	9	0	4.429292	-0.630825	3.073086
72	9	0	5.948944	-0.247579	1.565173
73	9	0	2.867313	-4.496385	-1.869047
74	9	0	4.170667	-3.115513	-2.922252
75	9	0	4.906591	-4.172458	-1.170837
76	1	0	-7.141171	-1.417986	-0.843751

Dienamine B



HF (B3LYP/6-31G(d)) = -2779.5010527 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.569160 (Hartree/Particle)

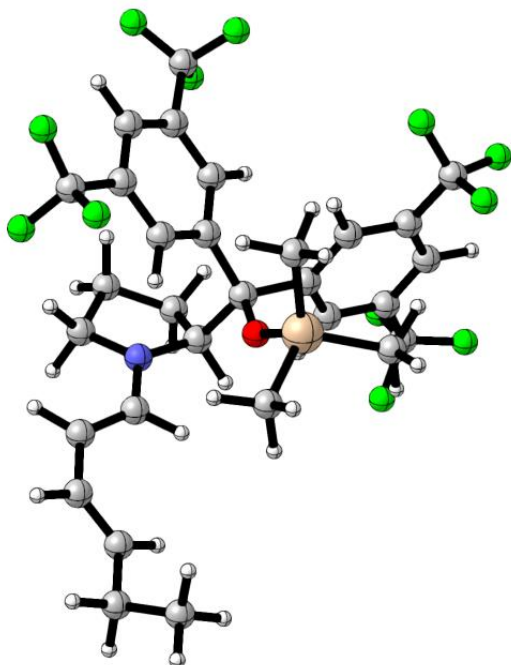
Thermal correction = 0.480521 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.149362	-3.468706	0.030323
2	6	0	-4.823114	-3.219370	0.009972
3	6	0	-4.104496	-2.253890	-0.800198
4	6	0	-2.757024	-2.112698	-0.707910
5	7	0	-1.975230	-1.232397	-1.423154
6	6	0	-0.515322	-1.319395	-1.429835
7	6	0	-0.122705	-0.787351	-2.827357
8	6	0	-1.305935	0.089525	-3.280036
9	6	0	-2.521933	-0.545682	-2.595039
10	1	0	-4.669342	-1.625576	-1.482802
11	1	0	-2.199399	-2.720231	-0.002440
12	1	0	-0.228123	-2.369587	-1.311285
13	1	0	0.826371	-0.244629	-2.829120
14	1	0	-0.006504	-1.640061	-3.505212
15	1	0	-1.173796	1.122615	-2.948428
16	1	0	-1.413932	0.105388	-4.368167
17	1	0	-3.271512	0.197930	-2.296764
18	1	0	-3.026272	-1.275229	-3.248120
19	6	0	0.147357	-0.580601	-0.192348
20	8	0	-0.379467	-1.273443	0.934836
21	14	0	0.005803	-1.535109	2.564274
22	6	0	0.297322	0.067609	3.519938
23	1	0	0.293823	-0.157762	4.594423

24	1	0	1.261271	0.535870	3.294754
25	1	0	-0.494340	0.802986	3.337606
26	6	0	-1.536732	-2.397268	3.210328
27	1	0	-1.718336	-3.337022	2.676030
28	1	0	-1.429858	-2.636199	4.275569
29	1	0	-2.428959	-1.771664	3.095270
30	6	0	1.493002	-2.682001	2.743142
31	1	0	1.590773	-2.995014	3.790590
32	1	0	1.369439	-3.588215	2.138821
33	1	0	2.435701	-2.207610	2.452457
34	6	0	1.685217	-0.716401	-0.192663
35	6	0	2.461253	0.151389	0.586753
36	6	0	2.345625	-1.762767	-0.850152
37	6	0	3.840385	-0.020405	0.711653
38	1	0	1.986706	0.968470	1.117107
39	6	0	3.728388	-1.924640	-0.738143
40	1	0	1.796146	-2.477515	-1.449297
41	6	0	4.488396	-1.058035	0.045346
42	1	0	5.558037	-1.195938	0.143807
43	6	0	-0.317165	0.883413	-0.166516
44	6	0	0.374809	1.905279	-0.827876
45	6	0	-1.528991	1.200420	0.456597
46	6	0	-0.123557	3.210611	-0.848742
47	1	0	1.309194	1.696027	-1.336263
48	6	0	-2.024991	2.505149	0.432027
49	1	0	-2.083583	0.420457	0.961961
50	6	0	-1.327167	3.521565	-0.217752
51	1	0	-1.711392	4.534193	-0.231096
52	6	0	-7.223555	-2.787730	-0.774788
53	1	0	-7.757896	-3.538635	-1.377488
54	1	0	-6.786559	-2.080931	-1.489228
55	6	0	-8.249286	-2.052413	0.106997
56	1	0	-9.047486	-1.608153	-0.499692
57	1	0	-8.716118	-2.739023	0.823743
58	1	0	-7.768721	-1.251505	0.679941
59	1	0	-4.197374	-3.811811	0.680596
60	6	0	0.684970	4.296070	-1.508613
61	6	0	-3.355600	2.785607	1.078728
62	6	0	4.616063	0.953401	1.560065
63	6	0	4.403813	-3.026819	-1.513378
64	9	0	5.849210	0.497987	1.858456
65	9	0	3.978874	1.202363	2.729334
66	9	0	4.765586	2.144472	0.938082
67	9	0	5.592056	-3.368403	-0.973518
68	9	0	4.640138	-2.657214	-2.793773
69	9	0	3.641402	-4.141730	-1.563450
70	9	0	-0.083507	5.338017	-1.890935
71	9	0	1.633143	4.786870	-0.676722
72	9	0	1.329081	3.840280	-2.607300
73	9	0	-3.545820	4.103246	1.303005
74	9	0	-4.382228	2.361001	0.305554
75	9	0	-3.472292	2.149538	2.266292
76	1	0	-6.505633	-4.236829	0.717932

Dienamine C



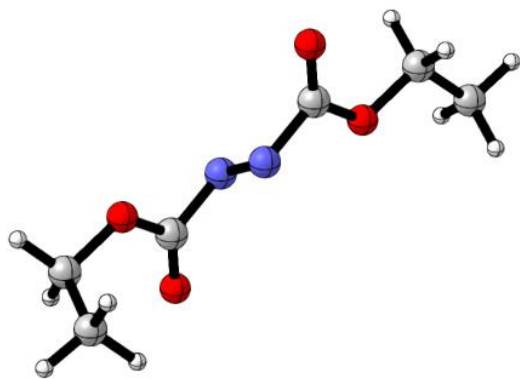
HF (B3LYP/6-31G(d)) = -2779.4979275 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.568863 (Hartree/Particle)
 Thermal correction = 0.481663 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.332323	-3.333678	0.589362
2	6	0	5.461928	-2.010029	0.799162
3	6	0	4.462007	-1.087585	1.333478
4	6	0	3.122402	-1.281629	1.240832
5	7	0	2.145340	-0.473681	1.777534
6	6	0	0.729225	-0.816205	1.711918
7	6	0	0.146225	-0.184157	2.996692
8	6	0	1.107654	0.965121	3.358815
9	6	0	2.468946	0.507979	2.814296
10	1	0	4.840061	-0.180253	1.799279
11	1	0	2.734741	-2.129464	0.685613
12	1	0	0.636743	-1.907738	1.722807
13	1	0	-0.885721	0.157203	2.878621
14	1	0	0.148650	-0.940482	3.789301
15	1	0	0.795761	1.896145	2.878904
16	1	0	1.141421	1.147656	4.436490
17	1	0	3.049945	1.341823	2.399776
18	1	0	3.089578	0.029756	3.587498
19	6	0	0.049395	-0.367922	0.348591
20	8	0	0.810725	-1.047232	-0.643399
21	14	0	0.828295	-1.305945	-2.317314
22	6	0	0.688465	0.294818	-3.310798
23	1	0	0.752970	0.051020	-4.379404

24	1	0	-0.259607	0.823259	-3.160235
25	1	0	1.500168	0.994066	-3.082294
26	6	0	2.517342	-2.084866	-2.594349
27	1	0	2.604070	-3.043747	-2.070585
28	1	0	2.687500	-2.270956	-3.661952
29	1	0	3.323412	-1.438403	-2.230506
30	6	0	-0.515944	-2.517772	-2.855892
31	1	0	-0.260375	-2.914784	-3.847009
32	1	0	-0.580743	-3.369524	-2.168758
33	1	0	-1.510227	-2.067264	-2.931496
34	6	0	-1.419050	-0.834804	0.252824
35	6	0	-2.232707	-0.335597	-0.773282
36	6	0	-1.962112	-1.817620	1.089095
37	6	0	-3.533090	-0.802575	-0.961847
38	1	0	-1.851428	0.430170	-1.439540
39	6	0	-3.271424	-2.273114	0.910576
40	1	0	-1.379137	-2.251862	1.890714
41	6	0	-4.067262	-1.774149	-0.117433
42	1	0	-5.078447	-2.135231	-0.260163
43	6	0	0.198540	1.152128	0.194394
44	6	0	-0.799725	2.059240	0.567182
45	6	0	1.429957	1.662746	-0.232776
46	6	0	-0.577128	3.437973	0.497094
47	1	0	-1.760642	1.703663	0.921394
48	6	0	1.650972	3.038617	-0.292300
49	1	0	2.221126	0.978310	-0.510586
50	6	0	0.650075	3.939644	0.067495
51	1	0	0.823148	5.007381	0.016739
52	6	0	6.381509	-4.212160	-0.035183
53	1	0	6.656173	-5.018273	0.663135
54	1	0	7.294336	-3.627478	-0.209378
55	6	0	5.922369	-4.853821	-1.357242
56	1	0	6.699606	-5.507299	-1.771131
57	1	0	5.020747	-5.460714	-1.208250
58	1	0	5.686554	-4.086098	-2.102818
59	1	0	6.425966	-1.556600	0.556787
60	6	0	-4.322350	-0.301044	-2.141831
61	6	0	-3.838084	-3.276049	1.882160
62	6	0	3.013290	3.521199	-0.710304
63	6	0	-1.701472	4.374816	0.851640
64	9	0	3.940744	3.259294	0.242941
65	9	0	3.042378	4.849406	-0.941738
66	9	0	3.432424	2.901453	-1.838543
67	9	0	-1.262521	5.626418	1.100143
68	9	0	-2.610948	4.461747	-0.146945
69	9	0	-2.370695	3.952623	1.949225
70	9	0	-4.132264	1.020342	-2.345739
71	9	0	-3.944218	-0.929355	-3.283766
72	9	0	-5.646389	-0.507547	-1.995677
73	9	0	-2.902141	-4.163389	2.287001
74	9	0	-4.310898	-2.671132	2.997007
75	9	0	-4.860234	-3.975775	1.347531
76	1	0	4.403560	-3.831202	0.876718

DEAD



HF (B3LYP/6-31G(d)) = -645.0194751 Hartrees

Imaginary Frequencies: none found

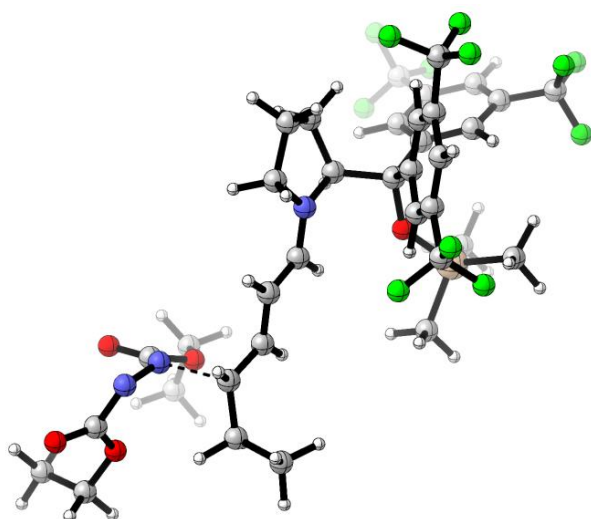
Zero-point correction = 0.171505 (Hartree/Particle)

Thermal correction = 0.128213 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	-0.279067	-0.213454	-0.644452
2	7	0	0.214071	0.457518	0.282776
3	6	0	-1.655410	-0.596117	-0.393261
4	6	0	1.590738	0.839524	0.031384
5	8	0	1.884446	1.994100	-0.161768
6	8	0	-1.948049	-1.757093	-0.238532
7	8	0	2.401400	-0.203135	0.149513
8	8	0	-2.461245	0.455361	-0.467821
9	6	0	-3.892408	0.190425	-0.337930
10	1	0	-4.358128	1.009844	-0.887835
11	1	0	-4.111984	-0.756848	-0.835351
12	6	0	3.829081	0.081927	0.035645
13	1	0	4.017848	0.462410	-0.972062
14	1	0	4.077245	0.869068	0.753017
15	6	0	4.569640	-1.210011	0.312342
16	1	0	4.289241	-1.984450	-0.408035
17	1	0	5.647503	-1.035070	0.229721
18	1	0	4.355377	-1.576294	1.320971
19	6	0	-4.309113	0.174493	1.122241
20	1	0	-5.395611	0.049680	1.188599
21	1	0	-3.835488	-0.655569	1.654248
22	1	0	-4.038614	1.113468	1.614798

TS 1



HF (B3LYP/6-31G(d)) = -3424.4936703 Hartrees

Imaginary Frequencies: 1 (-328.74 cm⁻¹)

Zero-point correction = 0.742978 (Hartree/Particle)

Thermal correction = 0.635589 Hartrees

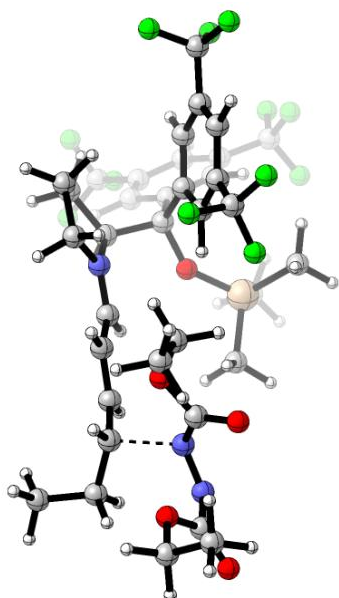
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.990129	1.091319	0.529535
2	6	0	-3.717885	0.471769	0.559257
3	6	0	-2.706326	0.750049	-0.363491
4	6	0	-1.518664	0.030956	-0.371854
5	7	0	-0.510872	0.188780	-1.242174
6	6	0	0.683329	-0.670680	-1.253414
7	6	0	1.165048	-0.580213	-2.717427
8	6	0	0.636411	0.764581	-3.259175
9	6	0	-0.625203	1.053644	-2.431356
10	1	0	-2.873851	1.535606	-1.094821
11	1	0	-1.354011	-0.732277	0.380831
12	1	0	0.359115	-1.683987	-1.003344
13	1	0	2.249328	-0.672007	-2.813447
14	1	0	0.723357	-1.410483	-3.277881
15	1	0	1.373878	1.559373	-3.129448
16	1	0	0.406424	0.705911	-4.325840
17	1	0	-0.702808	2.104039	-2.131306
18	1	0	-1.543911	0.789367	-2.968714
19	6	0	1.723151	-0.285283	-0.123785
20	8	0	1.000143	-0.494011	1.083235
21	14	0	1.345566	-0.821552	2.719342
22	6	0	2.572572	0.396849	3.476364
23	1	0	2.542416	0.283237	4.568007
24	1	0	3.607225	0.215771	3.166410
25	1	0	2.321585	1.439514	3.251594
26	6	0	-0.343732	-0.621920	3.523269
27	1	0	-1.075466	-1.316099	3.093456

28	1	0	-0.282737	-0.831929	4.598022
29	1	0	-0.735372	0.394893	3.405698
30	6	0	1.951868	-2.591660	2.944973
31	1	0	1.986596	-2.829339	4.015935
32	1	0	1.273090	-3.310249	2.471091
33	1	0	2.955571	-2.755647	2.540140
34	6	0	2.953666	-1.218088	-0.152821
35	6	0	4.144165	-0.815816	0.463385
36	6	0	2.894372	-2.520563	-0.667584
37	6	0	5.231181	-1.684408	0.576681
38	1	0	4.230897	0.184031	0.872562
39	6	0	3.990086	-3.380085	-0.574574
40	1	0	1.994610	-2.894198	-1.139764
41	6	0	5.166833	-2.972805	0.053921
42	1	0	6.010098	-3.646967	0.139587
43	6	0	2.112961	1.197995	-0.248341
44	6	0	3.114210	1.631565	-1.127361
45	6	0	1.418284	2.161538	0.486049
46	6	0	3.407317	2.989122	-1.263296
47	1	0	3.683208	0.914622	-1.708811
48	6	0	1.734645	3.517335	0.369999
49	1	0	0.627907	1.851149	1.157590
50	6	0	2.726969	3.944608	-0.507908
51	1	0	2.969563	4.996116	-0.599679
52	6	0	-5.867091	1.055437	1.762627
53	1	0	-5.856279	0.047118	2.193178
54	1	0	-6.899227	1.262907	1.464057
55	6	0	-5.431829	2.086316	2.818493
56	1	0	-6.112798	2.071208	3.677581
57	1	0	-4.419048	1.883392	3.186032
58	1	0	-5.439222	3.101916	2.405148
59	1	0	-3.548916	-0.324930	1.280974
60	7	0	-5.980054	0.285797	-0.908504
61	7	0	-6.998677	1.066055	-1.228854
62	6	0	-8.293342	0.685314	-0.887004
63	8	0	-8.396304	-0.251952	0.105050
64	8	0	-9.268905	1.199744	-1.413123
65	6	0	-6.102355	-1.111154	-0.905409
66	8	0	-6.698681	-1.729248	-1.771683
67	8	0	-5.333636	-1.697101	0.046987
68	6	0	-9.732785	-0.685044	0.431907
69	1	0	-9.647384	-1.087831	1.445075
70	1	0	-10.391622	0.187321	0.446804
71	6	0	-5.205726	-3.135502	-0.044713
72	1	0	-5.177529	-3.423704	-1.097747
73	1	0	-4.237087	-3.350772	0.415671
74	1	0	-5.016640	2.042553	0.000700
75	6	0	1.003209	4.493665	1.253452
76	6	0	4.417022	3.416698	-2.295776
77	6	0	3.910522	-4.747395	-1.205558
78	6	0	6.455845	-1.198641	1.307990
79	6	0	-10.244954	-1.736735	-0.541931
80	1	0	-11.235782	-2.084546	-0.225852
81	1	0	-10.329130	-1.315429	-1.546880
82	1	0	-9.569452	-2.597125	-0.580023
83	6	0	-6.334596	-3.840921	0.690480
84	1	0	-7.294146	-3.626533	0.212611
85	1	0	-6.171964	-4.924842	0.670478

86	1	0	-6.380697	-3.517918	1.735793
87	9	0	1.285013	5.775171	0.948855
88	9	0	-0.335620	4.333913	1.160927
89	9	0	1.327719	4.304949	2.555594
90	9	0	3.850533	3.482102	-3.525614
91	9	0	4.934488	4.632360	-2.030337
92	9	0	5.443044	2.542597	-2.385253
93	9	0	6.162663	-0.907338	2.599204
94	9	0	6.943634	-0.065586	0.757312
95	9	0	7.445462	-2.111209	1.313919
96	9	0	4.242121	-4.703985	-2.516278
97	9	0	4.745711	-5.623877	-0.612089
98	9	0	2.661264	-5.257594	-1.133229

TS 2



HF (B3LYP/6-31G(d)) = -3424.4942779 Hartrees

Imaginary Frequencies: 1 (-347.34 cm^{-1})

Zero-point correction = 0.743461 (Hartree/Particle)

Thermal correction = 0.639686 Hartrees

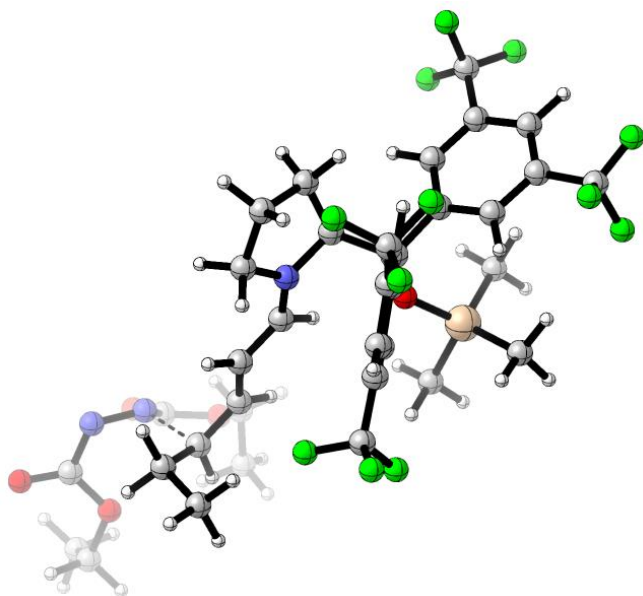
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.838853	-1.870726	1.185021
2	6	0	3.425042	-1.963720	1.217852
3	6	0	2.519488	-1.027932	1.711792
4	6	0	1.154846	-1.253453	1.556827
5	7	0	0.163583	-0.491481	2.028298
6	6	0	-1.255498	-0.830247	1.833327
7	6	0	-1.938571	-0.154701	3.039967
8	6	0	-1.030855	1.034138	3.422638

9	6	0	0.380850	0.618818	2.975165
10	1	0	2.885148	-0.129023	2.195882
11	1	0	0.829153	-2.125902	1.000980
12	1	0	-1.333693	-1.919221	1.876772
13	1	0	-2.963022	0.159227	2.826583
14	1	0	-1.984309	-0.875199	3.863314
15	1	0	-1.343343	1.943908	2.906099
16	1	0	-1.064498	1.239244	4.495390
17	1	0	0.926176	1.436157	2.491192
18	1	0	0.991680	0.250082	3.807595
19	6	0	-1.784064	-0.429650	0.392884
20	8	0	-0.884998	-1.085963	-0.485213
21	14	0	-0.702675	-1.443498	-2.143545
22	6	0	-0.764196	0.110348	-3.210777
23	1	0	-0.621948	-0.178355	-4.260104
24	1	0	-1.717735	0.647027	-3.150543
25	1	0	0.034540	0.815009	-2.954623
26	6	0	1.006259	-2.219449	-2.205686
27	1	0	1.037612	-3.158857	-1.640544
28	1	0	1.277249	-2.455595	-3.241897
29	1	0	1.785156	-1.560659	-1.806537
30	6	0	-1.980242	-2.700624	-2.732172
31	1	0	-1.611750	-3.165448	-3.655859
32	1	0	-2.121795	-3.502096	-1.997732
33	1	0	-2.959285	-2.266376	-2.953683
34	6	0	-3.218349	-0.958663	0.162119
35	6	0	-3.931265	-0.516856	-0.960514
36	6	0	-3.819311	-1.929459	0.972256
37	6	0	-5.190671	-1.030436	-1.267768
38	1	0	-3.504560	0.239725	-1.609594
39	6	0	-5.088010	-2.432568	0.672066
40	1	0	-3.319001	-2.318388	1.849246
41	6	0	-5.782683	-1.992308	-0.451782
42	1	0	-6.761817	-2.390720	-0.688789
43	6	0	-1.696219	1.098227	0.223943
44	6	0	-2.772559	1.948633	0.502286
45	6	0	-0.469592	1.673569	-0.127738
46	6	0	-2.627329	3.336404	0.421628
47	1	0	-3.738778	1.540081	0.774604
48	6	0	-0.324581	3.059200	-0.189908
49	1	0	0.374854	1.034813	-0.352958
50	6	0	-1.401990	3.903034	0.078931
51	1	0	-1.290270	4.978584	0.012993
52	1	0	3.000691	-2.854023	0.749471
53	7	0	5.097753	-1.170148	-0.603525
54	7	0	5.883254	-1.932804	-1.361477
55	6	0	7.252820	-1.704935	-1.311933
56	8	0	7.693743	-0.993779	-0.220541
57	8	0	8.017248	-2.151516	-2.155191
58	6	0	5.279013	0.213633	-0.572234
59	8	0	5.728796	0.859109	-1.504967
60	8	0	4.731370	0.787746	0.535134
61	6	0	9.104490	-0.703298	-0.183604
62	1	0	9.323499	-0.536388	0.875256
63	1	0	9.655752	-1.581692	-0.529637
64	6	0	4.692696	2.232810	0.533816
65	1	0	4.467144	2.581220	-0.475748
66	1	0	3.855341	2.482878	1.188681

67	6	0	1.036151	3.644110	-0.459108
68	6	0	-3.798883	4.217152	0.773118
69	6	0	-5.733213	-3.420736	1.610404
70	6	0	-5.866538	-0.585929	-2.538912
71	6	0	9.454220	0.519583	-1.019775
72	1	0	10.525019	0.738984	-0.929933
73	1	0	9.223824	0.338275	-2.072735
74	1	0	8.890774	1.396655	-0.685973
75	6	0	5.994505	2.826628	1.049086
76	1	0	6.820704	2.576098	0.378437
77	1	0	5.911235	3.918486	1.102758
78	1	0	6.226435	2.449551	2.051099
79	9	0	-3.923183	4.355047	2.114810
80	9	0	-4.962667	3.698525	0.324744
81	9	0	-3.674210	5.455420	0.255555
82	9	0	0.966210	4.876064	-0.997935
83	9	0	1.740863	3.758583	0.699870
84	9	0	1.767001	2.868894	-1.286416
85	9	0	-4.816009	-4.204996	2.218745
86	9	0	-6.601585	-4.228197	0.968691
87	9	0	-6.423453	-2.791567	2.589639
88	9	0	-5.701175	0.736836	-2.752980
89	9	0	-5.344704	-1.224447	-3.615336
90	9	0	-7.189600	-0.839549	-2.527890
91	6	0	5.615581	-3.168008	1.179655
92	1	0	6.647424	-2.961332	0.886380
93	1	0	5.199307	-3.839715	0.420645
94	6	0	5.608799	-3.854967	2.556270
95	1	0	6.217772	-4.765953	2.532722
96	1	0	6.021615	-3.197675	3.331110
97	1	0	4.594819	-4.135504	2.864809
98	1	0	5.277599	-1.073915	1.779357

TS 3



HF (B3LYP/6-31G(d)) = -3424.4963429 Hartrees

Imaginary Frequencies: 1 (-316.31 cm⁻¹)

Zero-point correction = 0.743856 (Hartree/Particle)

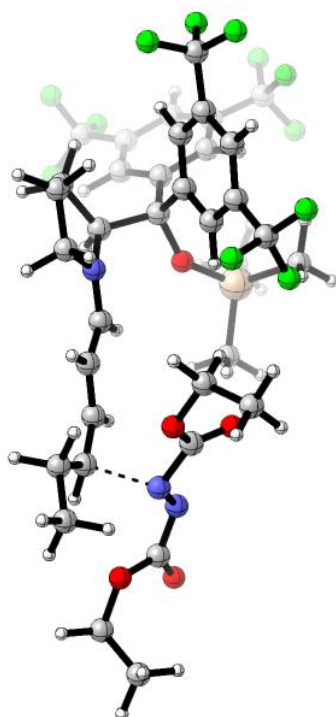
Thermal correction = 0.639483 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.935123	0.447468	0.115507
2	6	0	-3.614260	-0.067003	0.044569
3	6	0	-2.592098	0.404957	-0.777620
4	6	0	-1.360212	-0.241107	-0.803281
5	7	0	-0.313186	0.104792	-1.558049
6	6	0	0.968766	-0.620811	-1.553105
7	6	0	1.593034	-0.235654	-2.911978
8	6	0	0.962726	1.114224	-3.314557
9	6	0	-0.393547	1.153549	-2.593154
10	1	0	-2.757347	1.276192	-1.401669
11	1	0	-1.194325	-1.095803	-0.156909
12	1	0	0.742302	-1.689094	-1.508897
13	1	0	2.683620	-0.190873	-2.875384
14	1	0	1.329431	-1.007028	-3.642531
15	1	0	1.589461	1.952508	-3.003740
16	1	0	0.836633	1.188861	-4.397357
17	1	0	-0.597186	2.124971	-2.130064
18	1	0	-1.228853	0.918089	-3.262488
19	6	0	1.822071	-0.327459	-0.249002
20	8	0	1.027577	-0.861868	0.803351
21	14	0	1.280286	-1.552915	2.341514
22	6	0	2.308775	-0.451477	3.476776
23	1	0	2.182747	-0.800710	4.509910
24	1	0	3.380753	-0.484241	3.256787
25	1	0	1.980560	0.593695	3.445176
26	6	0	-0.478065	-1.694121	2.995220
27	1	0	-1.098143	-2.323721	2.346142
28	1	0	-0.479984	-2.148272	3.993501
29	1	0	-0.962896	-0.714538	3.076911
30	6	0	2.054846	-3.263977	2.201011
31	1	0	2.043532	-3.750306	3.184907
32	1	0	1.492030	-3.904207	1.511802
33	1	0	3.095262	-3.233906	1.862251
34	6	0	3.181214	-1.056288	-0.290138
35	6	0	4.235498	-0.608513	0.512925
36	6	0	3.367848	-2.243914	-1.012151
37	6	0	5.427351	-1.329713	0.610065
38	1	0	4.133615	0.308620	1.081102
39	6	0	4.567530	-2.951090	-0.931737
40	1	0	2.581330	-2.646206	-1.637640
41	6	0	5.605986	-2.505314	-0.112713
42	1	0	6.530332	-3.065223	-0.037094
43	6	0	1.968582	1.193185	-0.063031
44	6	0	2.949749	1.931391	-0.735588
45	6	0	1.047496	1.885275	0.728880
46	6	0	2.998743	3.322326	-0.624389
47	1	0	3.689895	1.430420	-1.350048
48	6	0	1.104155	3.275575	0.844263

49	1	0	0.281288	1.333310	1.257676
50	6	0	2.077257	4.007218	0.166633
51	1	0	2.122539	5.085504	0.257931
52	6	0	-5.223490	1.863126	-0.328529
53	1	0	-6.306386	1.978555	-0.421426
54	1	0	-4.816380	2.044942	-1.329259
55	6	0	-4.688037	2.909367	0.664609
56	1	0	-4.986245	3.917067	0.353133
57	1	0	-5.090853	2.740295	1.670468
58	1	0	-3.594865	2.891595	0.736790
59	1	0	-3.405580	-0.956497	0.633552
60	7	0	-5.912905	-0.652211	-1.125429
61	7	0	-6.794290	0.037948	-1.844991
62	6	0	-8.062911	0.227310	-1.310680
63	8	0	-8.138465	0.100687	0.056208
64	8	0	-9.020958	0.554002	-1.994939
65	6	0	-6.304982	-1.849422	-0.520245
66	8	0	-7.194192	-2.570690	-0.941684
67	8	0	-5.459385	-2.216951	0.483586
68	6	0	-9.450854	0.250380	0.632244
69	1	0	-9.264018	0.528563	1.673666
70	1	0	-9.966455	1.072147	0.128100
71	6	0	-5.654283	-3.546827	1.014459
72	1	0	-5.938599	-4.215740	0.199585
73	1	0	-4.669088	-3.835570	1.392114
74	1	0	-5.475361	0.149113	1.010398
75	6	0	0.053903	3.972177	1.670398
76	6	0	4.013743	4.077012	-1.441772
77	6	0	4.763822	-4.188225	-1.771782
78	6	0	6.486138	-0.831693	1.559515
79	6	0	-10.259537	-1.035925	0.539189
80	1	0	-11.226028	-0.906695	1.041093
81	1	0	-10.442515	-1.294803	-0.506829
82	1	0	-9.728211	-1.866295	1.015056
83	6	0	-6.694092	-3.558623	2.124438
84	1	0	-7.674676	-3.276601	1.731574
85	1	0	-6.769903	-4.564553	2.553581
86	1	0	-6.419805	-2.862652	2.924448
87	9	0	6.093711	-0.991093	2.848046
88	9	0	6.722334	0.486824	1.387284
89	9	0	7.654969	-1.482799	1.411372
90	9	0	5.342555	-3.891005	-2.957511
91	9	0	3.590821	-4.798919	-2.046189
92	9	0	5.560083	-5.086513	-1.156361
93	9	0	5.205115	3.441104	-1.469837
94	9	0	4.223047	5.322756	-0.974655
95	9	0	3.603518	4.193815	-2.729509
96	9	0	0.399180	5.238947	1.972113
97	9	0	-1.129658	4.024982	1.011461
98	9	0	-0.175233	3.319729	2.831352

TS 4



HF (B3LYP/6-31G(d)) = -3424.5064821 Hartrees

Imaginary Frequencies: 1 (-322.46 cm⁻¹)

Zero-point correction = 0.744314 (Hartree/Particle)

Thermal correction = 0.641766 Hartrees

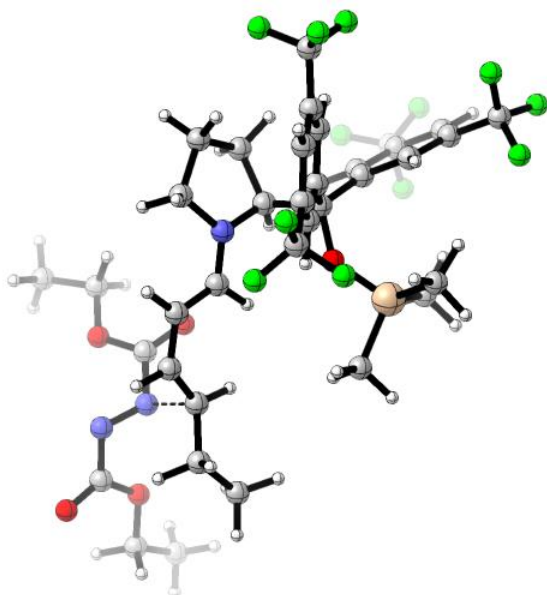
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.282633	-0.839524	1.551665
2	6	0	3.901148	-1.094228	1.387218
3	6	0	2.824755	-0.332545	1.873055
4	6	0	1.524109	-0.698984	1.566216
5	7	0	0.401148	-0.120115	2.030559
6	6	0	-0.930950	-0.721867	1.845306
7	6	0	-1.713457	-0.221505	3.079180
8	6	0	-1.031015	1.095546	3.498274
9	6	0	0.433410	0.914999	3.077498
10	1	0	3.013809	0.518940	2.518320
11	1	0	1.355511	-1.539099	0.901446
12	1	0	-0.801188	-1.806612	1.867771
13	1	0	-2.780907	-0.095840	2.884735
14	1	0	-1.617278	-0.965009	3.877698
15	1	0	-1.477366	1.948708	2.982433
16	1	0	-1.120336	1.278053	4.572207
17	1	0	0.882285	1.836738	2.691706
18	1	0	1.057923	0.559655	3.907878
19	6	0	-1.562986	-0.418100	0.426700
20	8	0	-0.600081	-0.922170	-0.484676
21	14	0	-0.475290	-1.410716	-2.116186

22	6	0	-0.812431	0.022290	-3.297604
23	1	0	-0.653173	-0.324714	-4.326810
24	1	0	-1.840666	0.397946	-3.240490
25	1	0	-0.134567	0.866049	-3.129270
26	6	0	1.308085	-1.977301	-2.244140
27	1	0	1.505226	-2.821191	-1.571666
28	1	0	1.514351	-2.324696	-3.264219
29	1	0	2.033415	-1.188096	-2.018925
30	6	0	-1.618035	-2.858657	-2.522047
31	1	0	-1.224951	-3.366225	-3.412540
32	1	0	-1.645307	-3.597450	-1.712732
33	1	0	-2.646099	-2.559240	-2.745274
34	6	0	-2.900577	-1.174012	0.247630
35	6	0	-3.749315	-0.817406	-0.808676
36	6	0	-3.269635	-2.272498	1.033837
37	6	0	-4.916056	-1.533791	-1.074744
38	1	0	-3.500223	0.027027	-1.441831
39	6	0	-4.448651	-2.977276	0.778849
40	1	0	-2.650979	-2.608788	1.855654
41	6	0	-5.279711	-2.618467	-0.279762
42	1	0	-6.187047	-3.173927	-0.483816
43	6	0	-1.743381	1.099915	0.239413
44	6	0	-2.898438	1.767745	0.665444
45	6	0	-0.710636	1.856059	-0.323951
46	6	0	-3.017461	3.152139	0.526952
47	1	0	-3.725827	1.214346	1.094560
48	6	0	-0.843011	3.237328	-0.482648
49	1	0	0.186986	1.354978	-0.661362
50	6	0	-1.994193	3.897264	-0.055669
51	1	0	-2.099808	4.967103	-0.189758
52	6	0	5.801908	0.223705	2.493657
53	1	0	5.670941	-0.170854	3.514308
54	1	0	5.185732	1.123871	2.426286
55	6	0	7.273622	0.592579	2.282598
56	1	0	7.596240	1.317949	3.038150
57	1	0	7.919798	-0.288211	2.357435
58	1	0	7.421650	1.029258	1.292188
59	1	0	3.654277	-1.955787	0.767454
60	7	0	5.657714	-0.425311	-0.298584
61	7	0	5.704783	-1.467726	-1.108964
62	6	0	6.829985	-2.262979	-0.983813
63	8	0	7.684116	-1.942571	0.041414
64	8	0	7.034489	-3.209964	-1.732044
65	6	0	4.687833	0.533370	-0.744360
66	8	0	4.031196	0.479290	-1.762430
67	8	0	4.721583	1.602631	0.080570
68	6	0	8.867223	-2.760026	0.156838
69	1	0	9.165064	-2.664656	1.205068
70	1	0	8.604065	-3.800156	-0.050982
71	6	0	3.855660	2.704977	-0.275424
72	1	0	2.944280	2.307194	-0.721272
73	1	0	3.615204	3.184588	0.676393
74	1	0	5.932636	-1.704896	1.487604
75	6	0	0.283881	4.027650	-1.094719
76	6	0	-4.240934	3.844072	1.068710
77	6	0	-4.848406	-4.102965	1.698459
78	6	0	-5.728043	-1.173621	-2.291117
79	6	0	9.970746	-2.279216	-0.774334

80	1	0	10.878749	-2.873461	-0.617472
81	1	0	9.662148	-2.388871	-1.817517
82	1	0	10.208892	-1.227445	-0.584038
83	6	0	4.544063	3.672238	-1.224893
84	1	0	4.773617	3.181406	-2.174906
85	1	0	3.876594	4.517685	-1.425112
86	1	0	5.472744	4.056697	-0.790749
87	9	0	-4.111346	4.094249	2.394102
88	9	0	-5.351567	3.089696	0.920614
89	9	0	-4.464652	5.027340	0.462260
90	9	0	-0.154763	5.150466	-1.697023
91	9	0	1.189414	4.411230	-0.157867
92	9	0	0.960956	3.305128	-2.015346
93	9	0	-5.556003	-3.645691	2.757795
94	9	0	-3.770394	-4.748052	2.196685
95	9	0	-5.618351	-5.015363	1.071499
96	9	0	-5.821464	0.164054	-2.451293
97	9	0	-5.153211	-1.663292	-3.417472
98	9	0	-6.979591	-1.669771	-2.234320

TS 5



HF (B3LYP/6-31G(d)) = -3424.5016314 Hartrees

Imaginary Frequencies: 1 (-254.50 cm⁻¹)

Zero-point correction = 0.742750 (Hartree/Particle)

Thermal correction = 0.636566 Hartrees

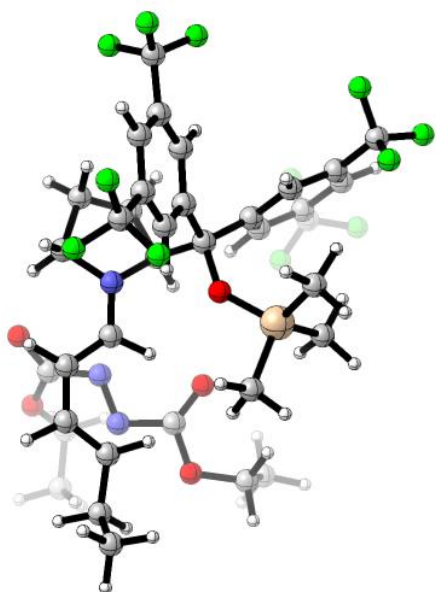
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.337783	-0.860708	-0.919909
2	6	0	-3.826094	-1.857044	-0.066065

3	6	0	-2.644281	-1.863150	0.692036
4	6	0	-1.671148	-0.872905	0.623442
5	7	0	-0.575123	-0.811459	1.393673
6	6	0	0.380182	0.304915	1.324190
7	6	0	0.987663	0.335807	2.743577
8	6	0	0.833290	-1.092188	3.306342
9	6	0	-0.384240	-1.675557	2.571778
10	1	0	-2.497610	-2.697799	1.371062
11	1	0	-1.754330	-0.079030	-0.103940
12	1	0	-0.194509	1.211059	1.118417
13	1	0	2.024094	0.680831	2.754978
14	1	0	0.409347	1.042215	3.347852
15	1	0	1.725376	-1.691916	3.113259
16	1	0	0.677595	-1.083518	4.388183
17	1	0	-0.230277	-2.715508	2.264020
18	1	0	-1.295135	-1.638037	3.181963
19	6	0	1.383438	0.169587	0.107440
20	8	0	0.539411	0.233273	-1.035144
21	14	0	0.675448	0.656905	-2.679360
22	6	0	2.069969	-0.260676	-3.562888
23	1	0	1.940717	-0.124431	-4.644728
24	1	0	3.066543	0.117390	-3.311714
25	1	0	2.051067	-1.338779	-3.367359
26	6	0	-0.987194	0.109974	-3.367152
27	1	0	-1.813970	0.631049	-2.870814
28	1	0	-1.050576	0.334170	-4.438968
29	1	0	-1.145506	-0.967418	-3.243276
30	6	0	0.874450	2.518671	-2.892299
31	1	0	0.779922	2.774453	-3.955453
32	1	0	0.094263	3.066713	-2.351597
33	1	0	1.846626	2.887865	-2.550727
34	6	0	2.382863	1.346156	0.070339
35	6	0	3.588699	1.216087	-0.628245
36	6	0	2.074691	2.602586	0.610322
37	6	0	4.453382	2.300023	-0.789982
38	1	0	3.859602	0.262156	-1.064865
39	6	0	2.947537	3.681504	0.461587
40	1	0	1.153459	2.765068	1.155581
41	6	0	4.143227	3.541943	-0.242531
42	1	0	4.816286	4.382096	-0.361233
43	6	0	2.087884	-1.197610	0.156191
44	6	0	3.218254	-1.424187	0.951812
45	6	0	1.559912	-2.274825	-0.559796
46	6	0	3.797764	-2.691821	1.027411
47	1	0	3.664131	-0.612445	1.515989
48	6	0	2.161997	-3.534100	-0.507851
49	1	0	0.675963	-2.126972	-1.167020
50	6	0	3.281394	-3.756817	0.289467
51	1	0	3.744304	-4.734759	0.332874
52	6	0	-5.281435	-1.259722	-2.029636
53	1	0	-6.219014	-1.623000	-1.583571
54	1	0	-4.859325	-2.127378	-2.556316
55	6	0	-5.550601	-0.135698	-3.032675
56	1	0	-6.263741	-0.459176	-3.799022
57	1	0	-5.963520	0.739601	-2.525217
58	1	0	-4.626018	0.161899	-3.542798
59	1	0	-4.463342	-2.733217	0.056893
60	7	0	-5.610181	0.086855	0.359162

61	7	0	-6.685832	-0.573304	0.714219
62	6	0	-7.802275	-0.358272	-0.093101
63	8	0	-7.797807	0.814524	-0.793726
64	8	0	-8.762710	-1.114853	-0.090727
65	6	0	-4.755544	0.508041	1.391655
66	8	0	-3.647914	0.991357	1.186152
67	8	0	-5.331691	0.469483	2.609059
68	6	0	-8.993708	1.081929	-1.550118
69	1	0	-9.111971	0.313543	-2.322675
70	1	0	-9.860081	1.011942	-0.884674
71	6	0	-4.573998	1.070756	3.679310
72	1	0	-4.349898	2.110108	3.417107
73	1	0	-3.620755	0.540998	3.782739
74	1	0	-3.728538	0.017480	-1.105475
75	6	0	-5.414311	0.971646	4.938877
76	1	0	-5.638812	-0.072859	5.176903
77	1	0	-4.871482	1.411473	5.782840
78	1	0	-6.360708	1.507856	4.818716
79	6	0	-8.857987	2.468897	-2.152610
80	1	0	-9.757766	2.714125	-2.727898
81	1	0	-8.733368	3.223275	-1.368903
82	1	0	-7.994906	2.525178	-2.824192
83	6	0	1.591175	-4.629048	-1.369939
84	6	0	4.945896	-2.908845	1.976926
85	6	0	5.734752	2.085970	-1.553414
86	6	0	2.552605	5.028194	1.013338
87	9	0	0.263955	-4.780768	-1.162889
88	9	0	2.178464	-5.820657	-1.144633
89	9	0	1.747877	-4.341384	-2.684664
90	9	0	4.500004	-3.033926	3.251997
91	9	0	5.644499	-4.024404	1.688237
92	9	0	5.807996	-1.868878	1.967557
93	9	0	1.875082	4.908996	2.176616
94	9	0	3.626819	5.811027	1.243832
95	9	0	1.747841	5.695884	0.156324
96	9	0	5.499655	1.463947	-2.734026
97	9	0	6.595037	1.301402	-0.866883
98	9	0	6.368401	3.243766	-1.822263

DA-TS



HF (B3LYP/6-31G(d)) = -3424.5049204 Hartrees

Imaginary Frequencies: 1 (-213.51 cm⁻¹)

Zero-point correction = 0.744156 (Hartree/Particle)

Thermal correction = 0.639740 Hartrees

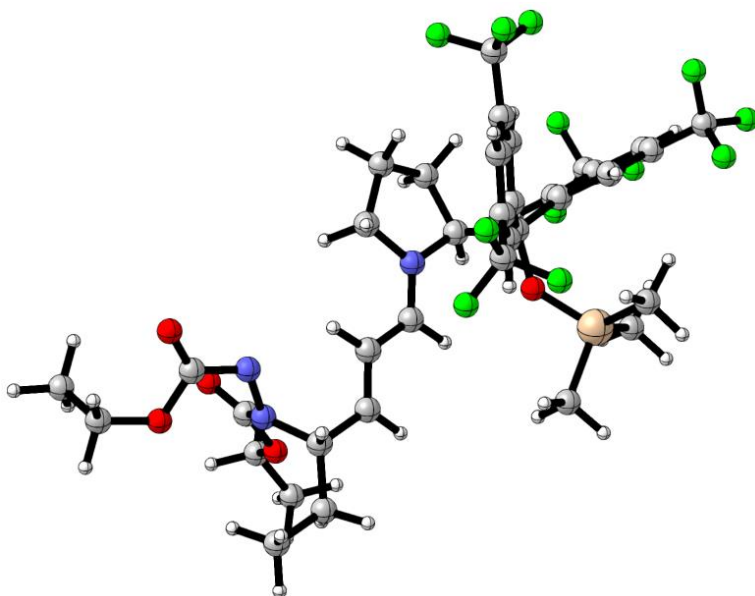
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.010491	-1.551207	-0.389877
2	6	0	2.850798	-2.695497	-0.323782
3	6	0	4.037994	-2.723033	0.384104
4	6	0	4.567175	-1.643754	1.116827
5	7	0	4.576242	-0.116067	-0.380907
6	6	0	4.105497	0.968443	0.407256
7	8	0	3.035153	1.548010	0.312739
8	7	0	3.704762	-0.398097	-1.343112
9	6	0	4.251103	-1.041853	-2.465777
10	8	0	5.516163	-0.735777	-2.865763
11	6	0	6.163586	0.541393	-2.668288
12	6	0	7.462144	0.361937	-1.902154
13	8	0	3.621655	-1.827010	-3.155671
14	8	0	5.070739	1.315601	1.285471
15	6	0	4.789839	2.438711	2.155048
16	6	0	5.078606	3.763472	1.465788
17	1	0	2.104665	-0.769987	0.348307
18	1	0	2.613392	-3.542466	-0.958369
19	1	0	4.695563	-3.572072	0.199571
20	1	0	3.750407	2.381961	2.487401
21	1	0	5.450383	2.282971	3.011166
22	1	0	6.359500	0.921457	-3.677975
23	1	0	4.406152	3.911806	0.616524
24	1	0	4.928793	4.587613	2.172493
25	1	0	6.113729	3.798787	1.110933

26	1	0	7.257066	0.021406	-0.884576
27	1	0	8.104929	-0.370640	-2.401790
28	1	0	8.002020	1.315245	-1.856118
29	1	0	5.492580	1.238013	-2.165038
30	6	0	5.955769	-1.723723	1.696041
31	1	0	6.608658	-2.267146	1.002178
32	1	0	6.358465	-0.711457	1.791110
33	1	0	3.865393	-1.047650	1.695363
34	7	0	0.872174	-1.486859	-1.099699
35	6	0	0.152897	-0.203597	-1.200525
36	6	0	0.593201	-2.397157	-2.234025
37	6	0	-0.377016	-0.205929	-2.650327
38	1	0	0.894472	0.582490	-1.043680
39	6	0	-0.916949	-0.015763	-0.052834
40	6	0	-0.500588	-1.690194	-3.047992
41	1	0	0.273614	-3.377378	-1.864089
42	1	0	1.515431	-2.509993	-2.809674
43	1	0	-1.316672	0.340748	-2.763665
44	1	0	0.365011	0.288493	-3.285492
45	8	0	-0.165455	-0.100785	1.152544
46	6	0	-1.598056	1.367596	-0.148910
47	6	0	-1.936583	-1.168935	-0.084030
48	1	0	-1.490210	-2.081856	-2.801769
49	1	0	-0.349163	-1.834814	-4.121027
50	14	0	-0.164545	0.600908	2.696556
51	6	0	-2.813888	1.589342	0.508216
52	6	0	-0.987692	2.461666	-0.779634
53	6	0	-3.067044	-1.145935	-0.910532
54	6	0	-1.700579	-2.316445	0.678546
55	6	0	-1.766768	0.265595	3.640345
56	6	0	1.252133	-0.303064	3.545577
57	6	0	0.214515	2.444480	2.628156
58	6	0	-3.396180	2.858029	0.548625
59	1	0	-3.312795	0.769313	1.011203
60	6	0	-1.580078	3.724577	-0.754228
61	1	0	-0.035706	2.356199	-1.282899
62	6	0	-3.931187	-2.240737	-0.972582
63	1	0	-3.290048	-0.270830	-1.510764
64	6	0	-2.571870	-3.406727	0.620711
65	1	0	-0.832162	-2.351848	1.323800
66	1	0	-1.604972	0.482214	4.704349
67	1	0	-2.606785	0.884727	3.309935
68	1	0	-2.066051	-0.786441	3.563721
69	1	0	2.209565	-0.068823	3.066894
70	1	0	1.326168	-0.004113	4.598302
71	1	0	1.116100	-1.390144	3.516712
72	1	0	0.447993	2.808968	3.637078
73	1	0	1.087354	2.627783	1.991110
74	1	0	-0.619821	3.042341	2.247794
75	6	0	-2.786523	3.936237	-0.086079
76	6	0	-4.709203	3.028559	1.267052
77	6	0	-0.938148	4.873165	-1.490373
78	6	0	-3.692170	-3.381223	-0.206424
79	6	0	-5.083388	-2.202621	-1.940743
80	6	0	-2.250947	-4.623340	1.448047
81	1	0	-3.233712	4.922502	-0.051671
82	9	0	-4.702502	2.390107	2.462520
83	9	0	-5.735385	2.508920	0.556866

84	9	0	-4.997343	4.324176	1.501290
85	9	0	-1.103938	6.040245	-0.830092
86	9	0	0.385916	4.686975	-1.666598
87	9	0	-1.483733	5.036992	-2.718245
88	1	0	-4.368734	-4.225743	-0.248474
89	9	0	-4.669245	-2.482161	-3.200762
90	9	0	-6.042252	-3.098603	-1.629846
91	9	0	-5.661801	-0.981992	-1.983743
92	9	0	-1.154707	-5.263085	0.977012
93	9	0	-3.261008	-5.516794	1.462495
94	9	0	-1.982835	-4.290557	2.731907
95	6	0	5.973335	-2.411998	3.074234
96	1	0	6.990918	-2.435557	3.480979
97	1	0	5.337636	-1.878742	3.791258
98	1	0	5.610360	-3.444025	3.010599

INT 1



HF (B3LYP/6-31G(d)) = -3424.5157551 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.745967 (Hartree/Particle)

Thermal correction = 0.640939 Hartrees

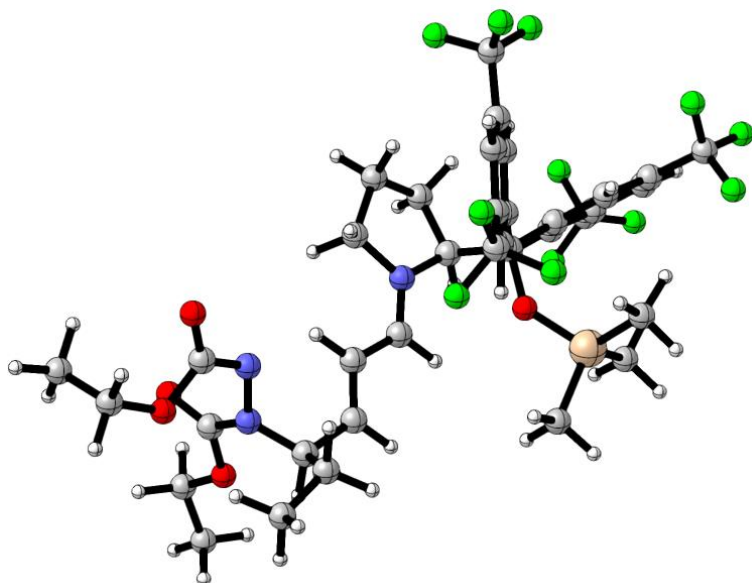
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.043171	-0.453672	1.516095
2	6	0	-3.611841	-0.900573	1.340658
3	6	0	-2.830542	-0.379705	0.350356
4	6	0	-1.513595	-0.847105	0.143329
5	7	0	-0.726901	-0.439368	-0.831101
6	6	0	0.636940	-0.969189	-1.055471

7	6	0	0.876894	-0.683258	-2.552207
8	6	0	-0.029431	0.511152	-2.923047
9	6	0	-1.177680	0.486968	-1.902248
10	1	0	-3.276673	0.374864	-0.297174
11	1	0	-1.085252	-1.582184	0.816374
12	1	0	0.596767	-2.041368	-0.853940
13	1	0	1.928645	-0.494312	-2.776026
14	1	0	0.583128	-1.570222	-3.122063
15	1	0	0.515192	1.455469	-2.867625
16	1	0	-0.411499	0.417453	-3.941992
17	1	0	-1.386835	1.469265	-1.470792
18	1	0	-2.110638	0.098258	-2.320829
19	6	0	1.677057	-0.390920	-0.012924
20	8	0	1.200846	-0.875086	1.235617
21	14	0	1.846136	-1.224698	2.778645
22	6	0	2.847473	0.199384	3.503538
23	1	0	3.036087	-0.018648	4.563038
24	1	0	3.824530	0.330064	3.027190
25	1	0	2.312748	1.154708	3.459603
26	6	0	0.281779	-1.496478	3.788262
27	1	0	-0.319699	-2.318820	3.382791
28	1	0	0.532628	-1.753286	4.824498
29	1	0	-0.346548	-0.598693	3.813864
30	6	0	2.870804	-2.804227	2.736300
31	1	0	3.107561	-3.109887	3.763329
32	1	0	2.319241	-3.627211	2.267269
33	1	0	3.818952	-2.683960	2.202794
34	6	0	3.091998	-0.949248	-0.282008
35	6	0	4.212159	-0.262872	0.201782
36	6	0	3.299394	-2.196777	-0.885882
37	6	0	5.492720	-0.808741	0.101400
38	1	0	4.092578	0.702268	0.678765
39	6	0	4.583142	-2.731151	-1.005846
40	1	0	2.469427	-2.782150	-1.261063
41	6	0	5.690678	-2.044983	-0.508260
42	1	0	6.683800	-2.471359	-0.582840
43	6	0	1.646329	1.148590	-0.022716
44	6	0	2.325776	1.894176	-0.994513
45	6	0	0.886884	1.837147	0.925826
46	6	0	2.236169	3.286643	-1.017720
47	1	0	2.940533	1.398283	-1.737841
48	6	0	0.829212	3.232519	0.922143
49	1	0	0.341103	1.282447	1.677897
50	6	0	1.495342	3.969707	-0.053136
51	1	0	1.442344	5.051327	-0.061508
52	6	0	-5.804152	-1.158539	2.650385
53	1	0	-5.206265	-1.028479	3.564312
54	1	0	-5.860074	-2.231245	2.453162
55	6	0	-7.206761	-0.580988	2.860219
56	1	0	-7.740968	-1.133031	3.641370
57	1	0	-7.161299	0.472093	3.163168
58	1	0	-7.788424	-0.631984	1.935218
59	1	0	-3.217149	-1.681476	1.993027
60	7	0	-5.695320	-0.460242	0.197663
61	7	0	-5.484684	0.769785	-0.495286
62	6	0	-6.593064	1.318789	-1.019689
63	8	0	-7.792996	0.665699	-0.727852
64	8	0	-6.590599	2.356322	-1.692571

65	6	0	-5.800656	-1.602030	-0.565948
66	8	0	-6.039455	-1.638370	-1.759961
67	8	0	-5.637003	-2.739589	0.188739
68	6	0	-8.956120	1.197399	-1.366366
69	1	0	-9.794901	0.887358	-0.732504
70	1	0	-8.901479	2.289879	-1.375535
71	6	0	-5.849174	-3.974543	-0.520282
72	1	0	-6.859152	-3.978302	-0.942259
73	1	0	-5.144255	-4.037139	-1.356150
74	1	0	-5.018507	0.616387	1.757541
75	6	0	0.081305	3.916590	2.037472
76	6	0	2.899141	4.033365	-2.145790
77	6	0	4.777199	-4.044857	-1.721499
78	6	0	6.661078	-0.020574	0.637460
79	6	0	-9.120805	0.659368	-2.783293
80	1	0	-10.061101	1.014860	-3.223700
81	1	0	-8.291565	1.001051	-3.409053
82	1	0	-9.127263	-0.436063	-2.782130
83	6	0	-5.651062	-5.110911	0.467176
84	1	0	-6.368142	-5.043581	1.291891
85	1	0	-5.798283	-6.071845	-0.037883
86	1	0	-4.639451	-5.095990	0.887368
87	9	0	-0.107958	5.227515	1.799999
88	9	0	-1.128217	3.351897	2.240352
89	9	0	0.761148	3.809644	3.206205
90	9	0	3.062133	5.340496	-1.867941
91	9	0	4.113868	3.517892	-2.436613
92	9	0	2.158707	3.949744	-3.278014
93	9	0	6.349139	0.578256	1.811315
94	9	0	7.029797	0.959639	-0.215601
95	9	0	7.740201	-0.798434	0.849403
96	9	0	4.949168	-3.859611	-3.049756
97	9	0	5.861381	-4.705383	-1.267842
98	9	0	3.708157	-4.857743	-1.572022

INT 2



HF (B3LYP/6-31G(d)) = -3424.5221815 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.746302 (Hartree/Particle)

Thermal correction = 0.641406 Hartrees

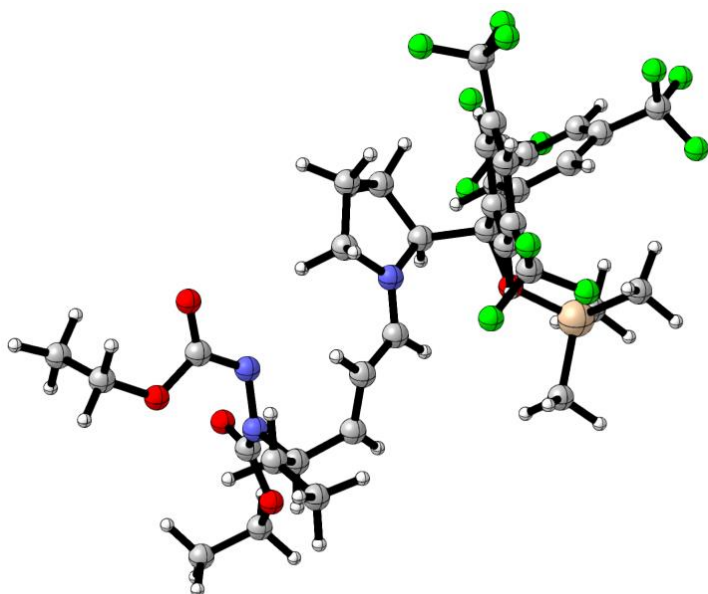
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.945196	-1.159401	-1.389494
2	6	0	3.472854	-1.389394	-1.186872
3	6	0	2.758030	-0.898006	-0.138420
4	6	0	1.380844	-1.207922	-0.016811
5	7	0	0.612169	-0.787070	0.960518
6	6	0	-0.810841	-1.181726	1.113537
7	6	0	-1.080714	-0.921365	2.610297
8	6	0	-0.078445	0.165228	3.052096
9	6	0	1.124006	0.005971	2.112174
10	1	0	3.279196	-0.249807	0.566874
11	1	0	0.892996	-1.824507	-0.764679
12	1	0	-0.865966	-2.245665	0.877268
13	1	0	-2.117672	-0.640033	2.804787
14	1	0	-0.894282	-1.849297	3.160133
15	1	0	-0.509108	1.164191	2.961783
16	1	0	0.220162	0.033361	4.094487
17	1	0	1.523913	0.956407	1.751731
18	1	0	1.944153	-0.553551	2.571122
19	6	0	-1.748060	-0.472763	0.054906
20	8	0	-1.277491	-0.965108	-1.193444
21	14	0	-1.912941	-1.211603	-2.762255
22	6	0	-2.769655	0.313139	-3.467173
23	1	0	-2.923141	0.150323	-4.542179
24	1	0	-3.756837	0.494510	-3.029713
25	1	0	-2.171173	1.224617	-3.360399
26	6	0	-0.350620	-1.592427	-3.738614

27	1	0	0.170295	-2.469826	-3.336374
28	1	0	-0.594783	-1.808269	-4.785703
29	1	0	0.349644	-0.749113	-3.730914
30	6	0	-3.073272	-2.694392	-2.793812
31	1	0	-3.299961	-2.952611	-3.836104
32	1	0	-2.615039	-3.575062	-2.329182
33	1	0	-4.025586	-2.501888	-2.289762
34	6	0	-3.218392	-0.903126	0.257347
35	6	0	-4.254201	-0.091216	-0.217078
36	6	0	-3.559976	-2.156970	0.784358
37	6	0	-5.582850	-0.520343	-0.182712
38	1	0	-4.032947	0.885509	-0.630961
39	6	0	-4.889903	-2.573804	0.839868
40	1	0	-2.801152	-2.838739	1.147265
41	6	0	-5.913981	-1.761892	0.350627
42	1	0	-6.944341	-2.094650	0.377795
43	6	0	-1.570792	1.055797	0.112590
44	6	0	-2.202909	1.838243	1.087389
45	6	0	-0.732251	1.694411	-0.803661
46	6	0	-1.988844	3.216098	1.145702
47	1	0	-2.879414	1.384938	1.803641
48	6	0	-0.552280	3.078673	-0.767777
49	1	0	-0.223721	1.110614	-1.559784
50	6	0	-1.169967	3.850998	0.211786
51	1	0	-1.022022	4.923180	0.245907
52	6	0	5.178755	-0.108716	-2.504364
53	1	0	4.837325	0.858127	-2.124343
54	1	0	4.546241	-0.370214	-3.363864
55	6	0	6.647040	-0.030696	-2.930489
56	1	0	6.779839	0.739463	-3.698925
57	1	0	7.277345	0.220773	-2.073537
58	1	0	6.991765	-0.985317	-3.347760
59	1	0	2.970119	-2.000310	-1.940529
60	7	0	5.621987	-0.813088	-0.140808
61	7	0	5.253599	0.450566	0.403735
62	6	0	6.275861	1.273961	0.678462
63	8	0	7.550780	0.809584	0.327554
64	8	0	6.142410	2.388145	1.199500
65	6	0	6.075179	-1.785025	0.711637
66	8	0	6.409476	-1.618798	1.873137
67	8	0	6.151101	-3.014472	0.090974
68	6	0	8.642990	1.625859	0.756057
69	1	0	9.470127	1.370090	0.083821
70	1	0	8.387757	2.681049	0.621264
71	6	0	6.735949	-4.058703	0.887134
72	1	0	6.139333	-4.202767	1.794473
73	1	0	7.740218	-3.755777	1.200933
74	1	0	5.367953	-2.106740	-1.737496
75	6	0	6.771713	-5.315544	0.035355
76	1	0	7.374907	-5.160342	-0.865293
77	1	0	7.211705	-6.140738	0.606120
78	1	0	5.762605	-5.610917	-0.272351
79	6	0	9.019633	1.348993	2.207187
80	1	0	9.910722	1.923475	2.491110
81	1	0	8.194452	1.636434	2.864542
82	1	0	9.227211	0.283748	2.355243
83	6	0	0.268923	3.716398	-1.859013
84	6	0	-2.612283	3.995096	2.274534

85	6	0	-6.636157	0.384228	-0.769578
86	6	0	-5.226800	-3.898608	1.477632
87	9	0	1.437607	3.068674	-2.043257
88	9	0	0.544066	5.008614	-1.605911
89	9	0	-0.394398	3.666827	-3.042318
90	9	0	-2.627266	5.319468	2.034619
91	9	0	-3.884789	3.602225	2.505471
92	9	0	-1.929200	3.800151	3.428709
93	9	0	-4.225033	-4.793069	1.328061
94	9	0	-5.440867	-3.764056	2.805817
95	9	0	-6.342222	-4.439290	0.947494
96	9	0	-6.416150	0.584203	-2.092289
97	9	0	-6.620330	1.601443	-0.185437
98	9	0	-7.876844	-0.120325	-0.636913

INT 3



HF (B3LYP/6-31G(d)) = -3424.5226601 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.746505 (Hartree/Particle)

Thermal correction = 0.640735 Hartrees

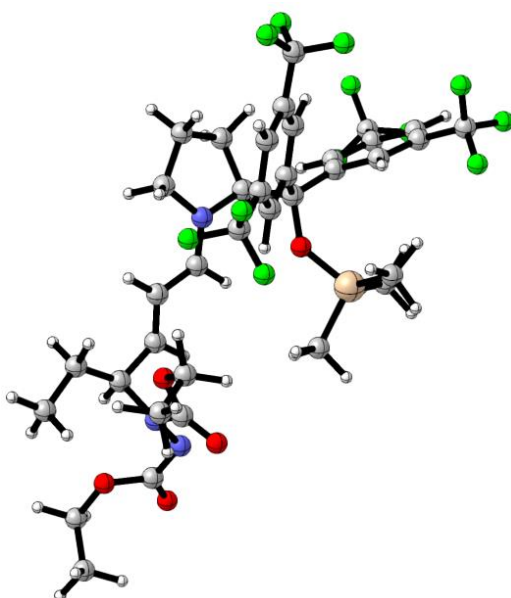
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.355407	0.168718	1.443619
2	6	0	-3.903013	-0.088539	1.718868
3	6	0	-2.949973	0.491293	0.926267
4	6	0	-1.738865	-0.178928	0.655320
5	7	0	-0.988598	0.065609	-0.397975
6	6	0	0.208044	-0.734703	-0.738355
7	6	0	0.306190	-0.579896	-2.270742

8	6	0	-0.398733	0.747733	-2.620199
9	6	0	-1.425682	0.965028	-1.500245
10	1	0	-3.206307	1.353847	0.328044
11	1	0	-1.406222	-0.985321	1.300627
12	1	0	-0.008584	-1.766552	-0.455564
13	1	0	1.336980	-0.614776	-2.630146
14	1	0	-0.224839	-1.417638	-2.732896
15	1	0	0.314104	1.574323	-2.661871
16	1	0	-0.893515	0.691865	-3.592353
17	1	0	-1.446548	1.998853	-1.143821
18	1	0	-2.445880	0.674681	-1.785262
19	6	0	1.457291	-0.320159	0.134762
20	8	0	1.039929	-0.595201	1.465810
21	14	0	1.756294	-1.016368	2.955414
22	6	0	3.098769	0.195862	3.493266
23	1	0	3.302867	0.033321	4.559770
24	1	0	4.046722	0.055574	2.963636
25	1	0	2.790030	1.240959	3.378187
26	6	0	0.286081	-0.914766	4.125074
27	1	0	-0.498620	-1.627262	3.844444
28	1	0	0.594501	-1.153049	5.150144
29	1	0	-0.157833	0.087351	4.137340
30	6	0	2.424681	-2.776907	2.916824
31	1	0	2.688213	-3.087053	3.936158
32	1	0	1.672427	-3.481516	2.543655
33	1	0	3.323168	-2.881651	2.300449
34	6	0	2.690161	-1.182243	-0.213626
35	6	0	3.965864	-0.730753	0.141492
36	6	0	2.580589	-2.465766	-0.767374
37	6	0	5.092778	-1.536881	-0.030087
38	1	0	4.090940	0.257785	0.567608
39	6	0	3.710776	-3.261261	-0.958739
40	1	0	1.619019	-2.874833	-1.050243
41	6	0	4.976408	-2.807422	-0.585181
42	1	0	5.850149	-3.433269	-0.720447
43	6	0	1.744825	1.184986	-0.016115
44	6	0	2.464658	1.694842	-1.104904
45	6	0	1.244004	2.086408	0.925047
46	6	0	2.670413	3.067677	-1.243930
47	1	0	2.881671	1.025782	-1.849406
48	6	0	1.476963	3.458080	0.798134
49	1	0	0.675794	1.714609	1.768089
50	6	0	2.186141	3.961809	-0.288244
51	1	0	2.363996	5.025369	-0.388021
52	6	0	-5.792299	1.621854	1.248107
53	1	0	-6.832939	1.607307	0.909937
54	1	0	-5.219583	2.091032	0.441957
55	6	0	-5.656959	2.440773	2.537080
56	1	0	-5.996918	3.469859	2.379070
57	1	0	-6.258756	2.012393	3.348036
58	1	0	-4.616929	2.482149	2.882023
59	1	0	-3.659037	-0.973397	2.304469
60	7	0	-5.532220	-0.659578	0.196717
61	7	0	-4.801624	-0.281399	-0.933601
62	6	0	-5.462377	0.451620	-1.845267
63	8	0	-6.833387	0.582628	-1.654033
64	8	0	-4.906093	0.974098	-2.821514
65	6	0	-5.869061	-1.998831	0.292349

66	8	0	-5.873049	-2.782811	-0.638583
67	8	0	-6.243774	-2.340465	1.566034
68	6	0	-7.539185	1.312653	-2.665609
69	1	0	-8.437284	1.691219	-2.164957
70	1	0	-6.931195	2.159203	-2.997137
71	6	0	-6.768335	-3.675758	1.725184
72	1	0	-6.178980	-4.362739	1.113466
73	1	0	-6.606903	-3.904258	2.782332
74	1	0	-5.975857	-0.286207	2.212610
75	6	0	0.979546	4.366346	1.891776
76	6	0	3.360866	3.580421	-2.480865
77	6	0	3.572325	-4.609734	-1.620653
78	6	0	6.425191	-1.003807	0.429535
79	6	0	-7.911121	0.426613	-3.848118
80	1	0	-8.517910	0.987317	-4.570129
81	1	0	-7.005753	0.076759	-4.351699
82	1	0	-8.486229	-0.443927	-3.514291
83	6	0	-8.244153	-3.746845	1.362228
84	1	0	-8.387358	-3.522740	0.301592
85	1	0	-8.627887	-4.755077	1.557432
86	1	0	-8.826859	-3.035043	1.956474
87	9	0	6.424895	-0.790062	1.768840
88	9	0	6.707525	0.182605	-0.150970
89	9	0	7.437892	-1.847099	0.155215
90	9	0	4.489826	-5.485732	-1.160698
91	9	0	3.744680	-4.520518	-2.958624
92	9	0	2.351230	-5.147182	-1.413184
93	9	0	4.356266	2.756961	-2.875313
94	9	0	3.890097	4.806280	-2.296667
95	9	0	2.492136	3.669589	-3.516402
96	9	0	1.131261	5.669232	1.587491
97	9	0	-0.330480	4.154181	2.150645
98	9	0	1.644641	4.139340	3.050459

INT 4



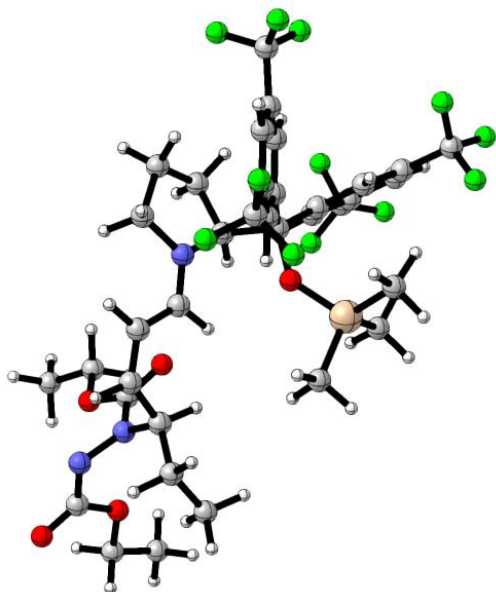
HF (B3LYP/6-31G(d)) = -3424.5175898 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.746603 (Hartree/Particle)
 Thermal correction = 0.642832 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.225297	-0.534755	1.272430
2	6	0	3.784622	-0.890719	1.287190
3	6	0	2.728335	-0.161325	1.778779
4	6	0	1.423320	-0.639202	1.566917
5	7	0	0.310484	-0.129797	2.075019
6	6	0	-1.017414	-0.743731	1.869474
7	6	0	-1.805557	-0.277989	3.109932
8	6	0	-1.155977	1.050923	3.552498
9	6	0	0.299953	0.970113	3.063667
10	1	0	2.893524	0.755591	2.334768
11	1	0	1.285419	-1.516554	0.944748
12	1	0	-0.866611	-1.824632	1.867563
13	1	0	-2.874498	-0.172025	2.913008
14	1	0	-1.696244	-1.033099	3.894978
15	1	0	-1.664116	1.903891	3.099479
16	1	0	-1.203107	1.179945	4.636401
17	1	0	0.645230	1.897681	2.596106
18	1	0	0.996534	0.714056	3.869337
19	6	0	-1.627155	-0.403172	0.447443
20	8	0	-0.647081	-0.876131	-0.460468
21	14	0	-0.570892	-1.465730	-2.065829
22	6	0	-1.344184	-0.268872	-3.303168
23	1	0	-0.997469	-0.540583	-4.308627
24	1	0	-2.438161	-0.301519	-3.321691
25	1	0	-1.031668	0.766074	-3.123009
26	6	0	1.276954	-1.600771	-2.362003
27	1	0	1.759770	-2.288896	-1.658911
28	1	0	1.466965	-1.989877	-3.369783
29	1	0	1.791390	-0.636323	-2.287297
30	6	0	-1.368907	-3.168065	-2.192108
31	1	0	-1.153307	-3.590737	-3.181676
32	1	0	-0.956324	-3.858398	-1.447226
33	1	0	-2.456779	-3.148063	-2.073276
34	6	0	-2.962038	-1.150924	0.230495
35	6	0	-3.829319	-0.722791	-0.782775
36	6	0	-3.300234	-2.318214	0.927496
37	6	0	-4.983281	-1.440259	-1.099956
38	1	0	-3.600707	0.174232	-1.346084
39	6	0	-4.464079	-3.025983	0.620872
40	1	0	-2.664917	-2.710624	1.711099
41	6	0	-5.313267	-2.596972	-0.397838
42	1	0	-6.206235	-3.157670	-0.646094
43	6	0	-1.784067	1.122746	0.298992
44	6	0	-2.928742	1.804157	0.733613
45	6	0	-0.721347	1.872819	-0.213173
46	6	0	-3.004965	3.196243	0.655539
47	1	0	-3.773474	1.257946	1.138085

48	6	0	-0.798668	3.265740	-0.281383
49	1	0	0.169421	1.364504	-0.560863
50	6	0	-1.938855	3.939487	0.149976
51	1	0	-1.996873	5.019544	0.093890
52	6	0	5.647600	0.740521	2.013264
53	1	0	5.484329	0.535363	3.081158
54	1	0	5.000913	1.577297	1.743915
55	6	0	7.111711	1.128357	1.788595
56	1	0	7.366720	2.008863	2.389203
57	1	0	7.787616	0.313688	2.064279
58	1	0	7.295667	1.365016	0.737052
59	1	0	3.579059	-1.815814	0.750059
60	7	0	5.503029	-0.636984	-0.214414
61	7	0	5.627298	-1.935093	-0.719192
62	6	0	6.763012	-2.575204	-0.372777
63	8	0	7.686423	-1.825948	0.365304
64	8	0	7.002017	-3.750470	-0.660021
65	6	0	5.034511	0.291334	-1.132554
66	8	0	5.075702	0.153591	-2.340791
67	8	0	4.561984	1.419437	-0.521640
68	6	0	8.913603	-2.494935	0.686615
69	1	0	9.293756	-1.978223	1.574847
70	1	0	8.702111	-3.537117	0.940511
71	6	0	4.216972	2.510954	-1.402930
72	1	0	3.698162	2.110653	-2.276965
73	1	0	3.520495	3.115885	-0.819688
74	1	0	5.824885	-1.350205	1.678898
75	6	0	0.402608	4.030450	-0.771172
76	6	0	-4.275140	3.887698	1.081412
77	6	0	-4.829764	-4.239660	1.438270
78	6	0	-5.882875	-0.919845	-2.192286
79	6	0	9.916126	-2.417263	-0.457959
80	1	0	10.867810	-2.876634	-0.163050
81	1	0	9.527897	-2.951317	-1.329443
82	1	0	10.107253	-1.375493	-0.738185
83	6	0	5.442209	3.313358	-1.814559
84	1	0	6.127252	2.692704	-2.398459
85	1	0	5.138047	4.166473	-2.432359
86	1	0	5.972210	3.697114	-0.936125
87	9	0	-4.825764	3.286266	2.160662
88	9	0	-5.204853	3.864193	0.101293
89	9	0	-4.061236	5.180578	1.399643
90	9	0	0.108622	5.306314	-1.083137
91	9	0	1.373696	4.063455	0.179652
92	9	0	0.949389	3.452315	-1.862502
93	9	0	-5.556784	-5.122963	0.725583
94	9	0	-5.566650	-3.897581	2.520325
95	9	0	-3.733612	-4.882726	1.896528
96	9	0	-6.754772	-1.853489	-2.619007
97	9	0	-6.602074	0.144445	-1.771860
98	9	0	-5.165237	-0.507330	-3.263723

INT 5



HF (B3LYP/6-31G(d)) = -3424.5254643 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.746173 (Hartree/Particle)

Thermal correction = 0.639921 Hartrees

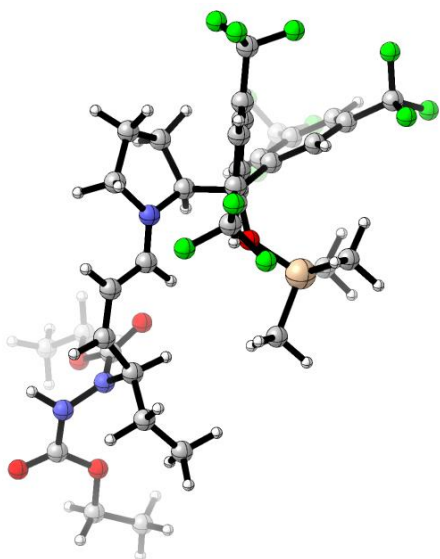
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.268864	-1.395350	0.841177
2	6	0	3.650896	-2.436926	-0.045783
3	6	0	2.465410	-2.376726	-0.722496
4	6	0	1.584852	-1.268896	-0.617855
5	7	0	0.534767	-1.073127	-1.388588
6	6	0	-0.283248	0.158535	-1.306237
7	6	0	-0.845482	0.294170	-2.735583
8	6	0	-0.877827	-1.131366	-3.327946
9	6	0	0.212429	-1.908039	-2.570802
10	1	0	2.228533	-3.170738	-1.423938
11	1	0	1.767204	-0.499933	0.115483
12	1	0	0.405238	0.970204	-1.066464
13	1	0	-1.824529	0.777047	-2.758234
14	1	0	-0.163086	0.925450	-3.312962
15	1	0	-1.853866	-1.598989	-3.185350
16	1	0	-0.676934	-1.120995	-4.401762
17	1	0	-0.117735	-2.899732	-2.248460
18	1	0	1.125200	-2.024747	-3.162942
19	6	0	-1.315869	0.106988	-0.109252
20	8	0	-0.495080	-0.028922	1.040872
21	14	0	-0.578455	0.381125	2.698316
22	6	0	-2.119191	-0.312249	3.539432
23	1	0	-1.976527	-0.246703	4.626036
24	1	0	-3.033468	0.242226	3.304730
25	1	0	-2.282983	-1.368558	3.297734
26	6	0	0.956216	-0.460610	3.384324

27	1	0	1.869383	-0.055494	2.933563
28	1	0	1.025749	-0.299761	4.466937
29	1	0	0.942940	-1.542948	3.211859
30	6	0	-0.454715	2.242758	2.950732
31	1	0	-0.311681	2.451212	4.018798
32	1	0	0.407087	2.659939	2.417309
33	1	0	-1.349844	2.783892	2.628367
34	6	0	-2.125979	1.419568	-0.026877
35	6	0	-3.347176	1.434510	0.655864
36	6	0	-1.629364	2.640292	-0.505905
37	6	0	-4.044946	2.625538	0.865309
38	1	0	-3.763173	0.511902	1.043138
39	6	0	-2.339275	3.826249	-0.315271
40	1	0	-0.679285	2.696028	-1.022050
41	6	0	-3.550788	3.831095	0.377163
42	1	0	-4.091778	4.755566	0.538471
43	6	0	-2.224309	-1.129565	-0.245896
44	6	0	-3.355224	-1.132086	-1.073058
45	6	0	-1.896203	-2.309000	0.426670
46	6	0	-4.127256	-2.284429	-1.224529
47	1	0	-3.653569	-0.231748	-1.598390
48	6	0	-2.684563	-3.454404	0.290817
49	1	0	-1.026726	-2.328088	1.071295
50	6	0	-3.802585	-3.455187	-0.538806
51	1	0	-4.414502	-4.342748	-0.642166
52	6	0	4.922424	-1.973848	2.097565
53	1	0	5.742716	-2.626845	1.786100
54	1	0	4.172464	-2.600158	2.600278
55	6	0	5.432960	-0.892189	3.054648
56	1	0	5.928599	-1.347240	3.919244
57	1	0	6.149036	-0.238605	2.549139
58	1	0	4.608090	-0.272920	3.430314
59	1	0	4.311079	-3.274287	-0.262378
60	7	0	5.241560	-0.769961	-0.085192
61	7	0	6.443207	-1.469050	-0.330203
62	6	0	7.557010	-0.793938	0.005167
63	8	0	7.362319	0.488602	0.541536
64	8	0	8.702837	-1.227084	-0.141937
65	6	0	4.735672	0.176077	-0.935379
66	8	0	3.600277	0.663291	-0.831301
67	8	0	5.609020	0.536190	-1.893708
68	6	0	8.560290	1.221745	0.801456
69	1	0	9.177976	0.687385	1.533157
70	1	0	9.152801	1.302423	-0.117574
71	6	0	5.182869	1.608170	-2.754637
72	1	0	4.913118	2.476047	-2.143612
73	1	0	4.286294	1.297025	-3.302947
74	1	0	3.553184	-0.623080	1.123561
75	6	0	6.335111	1.916660	-3.692726
76	1	0	6.598697	1.037938	-4.289654
77	1	0	6.053307	2.727997	-4.373086
78	1	0	7.221045	2.226394	-3.129833
79	6	0	8.159137	2.594600	1.318627
80	1	0	9.050863	3.199723	1.520152
81	1	0	7.542944	3.123244	0.582904
82	1	0	7.583702	2.512407	2.247544
83	6	0	-2.282641	-4.691162	1.052041
84	6	0	-5.271661	-2.268182	-2.203955

85	6	0	-5.335747	2.564786	1.640752
86	6	0	-1.818137	5.110826	-0.910008
87	9	0	-1.141815	-5.223919	0.555545
88	9	0	-3.228095	-5.649066	1.008791
89	9	0	-2.044655	-4.406267	2.352999
90	9	0	-6.171636	-3.238521	-1.954070
91	9	0	-5.924233	-1.086198	-2.192089
92	9	0	-4.821130	-2.453850	-3.469701
93	9	0	-0.471440	5.112338	-1.000975
94	9	0	-2.299944	5.300320	-2.160037
95	9	0	-2.182645	6.183249	-0.178045
96	9	0	-5.137596	2.030782	2.870690
97	9	0	-6.244158	1.780042	1.020432
98	9	0	-5.890727	3.779133	1.809904

INT 6



HF (B3LYP/6-31G(d)) = -3425.0118143 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.760859 (Hartree/Particle)

Thermal correction = 0.659876 Hartrees

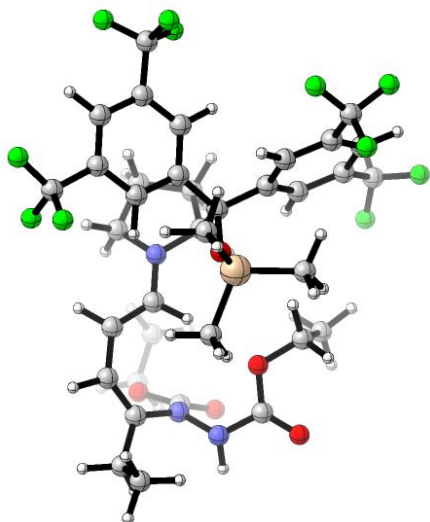
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.238875	-1.376655	0.341712
2	6	0	3.615724	-2.258863	-0.716419
3	6	0	2.411000	-2.132883	-1.327651
4	6	0	1.496349	-1.053783	-1.071196
5	7	0	0.386030	-0.877037	-1.732502
6	6	0	-0.514062	0.290044	-1.508602
7	6	0	-1.243461	0.421196	-2.859310
8	6	0	-1.257969	-0.988279	-3.486183
9	6	0	-0.037146	-1.708624	-2.897467

10	1	0	2.138223	-2.873477	-2.071790
11	1	0	1.729657	-0.305126	-0.324656
12	1	0	0.139349	1.139874	-1.311198
13	1	0	-2.246556	0.835357	-2.751272
14	1	0	-0.679508	1.112939	-3.492056
15	1	0	-2.173102	-1.524331	-3.234376
16	1	0	-1.196879	-0.942303	-4.575024
17	1	0	-0.259238	-2.722608	-2.556219
18	1	0	0.798490	-1.749278	-3.600538
19	6	0	-1.394254	0.127957	-0.199106
20	8	0	-0.433784	0.060369	0.843629
21	14	0	-0.374059	0.477030	2.511253
22	6	0	-1.705727	-0.405658	3.504482
23	1	0	-1.531549	-0.203067	4.568710
24	1	0	-2.718554	-0.060871	3.276989
25	1	0	-1.674065	-1.491667	3.369856
26	6	0	1.327415	-0.151411	2.996852
27	1	0	2.116764	0.404780	2.480143
28	1	0	1.481227	-0.013670	4.073249
29	1	0	1.448425	-1.218498	2.780605
30	6	0	-0.464871	2.337798	2.760075
31	1	0	-0.207179	2.563994	3.802206
32	1	0	0.253063	2.863868	2.121710
33	1	0	-1.459548	2.752041	2.572986
34	6	0	-2.300067	1.371553	-0.024062
35	6	0	-3.476699	1.287281	0.736280
36	6	0	-1.927916	2.627807	-0.516436
37	6	0	-4.254989	2.418204	0.982438
38	1	0	-3.792571	0.338649	1.150778
39	6	0	-2.715033	3.757721	-0.274106
40	1	0	-1.017450	2.762016	-1.086425
41	6	0	-3.886086	3.665495	0.473540
42	1	0	-4.491809	4.543827	0.664059
43	6	0	-2.196582	-1.190520	-0.249164
44	6	0	-3.424010	-1.296523	-0.918025
45	6	0	-1.662107	-2.342257	0.337030
46	6	0	-4.096495	-2.519504	-0.986391
47	1	0	-3.872137	-0.426127	-1.384436
48	6	0	-2.333838	-3.565262	0.256052
49	1	0	-0.720713	-2.279044	0.868173
50	6	0	-3.559159	-3.666838	-0.400406
51	1	0	-4.083152	-4.612740	-0.454334
52	6	0	4.874984	-2.230851	1.449695
53	1	0	5.750619	-2.747670	1.041729
54	1	0	4.149140	-3.012107	1.708375
55	6	0	5.244579	-1.436939	2.706808
56	1	0	5.709494	-2.097838	3.444608
57	1	0	5.950543	-0.636946	2.474780
58	1	0	4.356899	-0.992959	3.169250
59	1	0	4.238068	-3.094603	-1.035434
60	7	0	5.211569	-0.468386	-0.320597
61	7	0	6.400495	-1.011588	-0.790793
62	1	0	6.416576	-1.264781	-1.773687
63	6	0	7.650581	-0.567024	-0.356917
64	8	0	7.593121	0.129072	0.779967
65	8	0	8.659428	-0.849606	-0.977846
66	6	0	4.748774	0.739953	-0.825105
67	8	0	3.622685	1.168839	-0.593885

68	8	0	5.670721	1.356486	-1.568442
69	6	0	8.876238	0.589788	1.307650
70	1	0	9.488424	-0.288921	1.526280
71	1	0	9.373980	1.172746	0.529138
72	6	0	5.321301	2.678407	-2.083572
73	1	0	5.085218	3.322137	-1.232457
74	1	0	4.426032	2.577392	-2.702675
75	1	0	3.497059	-0.714751	0.785953
76	6	0	6.510873	3.183209	-2.873462
77	1	0	6.741305	2.518234	-3.710725
78	1	0	6.279719	4.174507	-3.275511
79	1	0	7.398068	3.268582	-2.239910
80	6	0	8.592252	1.413449	2.546755
81	1	0	9.538531	1.779863	2.956797
82	1	0	7.964219	2.278088	2.312196
83	1	0	8.096051	0.816512	3.317394
84	6	0	-1.686880	-4.776917	0.880476
85	6	0	-5.436012	-2.573244	-1.682293
86	6	0	-5.537634	2.301196	1.772100
87	6	0	-2.292093	5.078135	-0.872355
88	9	0	-0.513810	-5.083384	0.254502
89	9	0	-2.465637	-5.874982	0.821948
90	9	0	-1.376253	-4.565416	2.184153
91	9	0	-5.844565	-3.838265	-1.915584
92	9	0	-6.403313	-1.966471	-0.948989
93	9	0	-5.398904	-1.933409	-2.880338
94	9	0	-0.950677	5.262749	-0.781157
95	9	0	-2.600719	5.143663	-2.195615
96	9	0	-2.887174	6.130305	-0.273777
97	9	0	-5.596808	1.153618	2.486436
98	9	0	-6.623531	2.317757	0.956959
99	9	0	-5.685659	3.327656	2.642216

Dienamine D



HF (B3LYP/6-31G(d)) = -3424.5705765 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.747224 (Hartree/Particle)

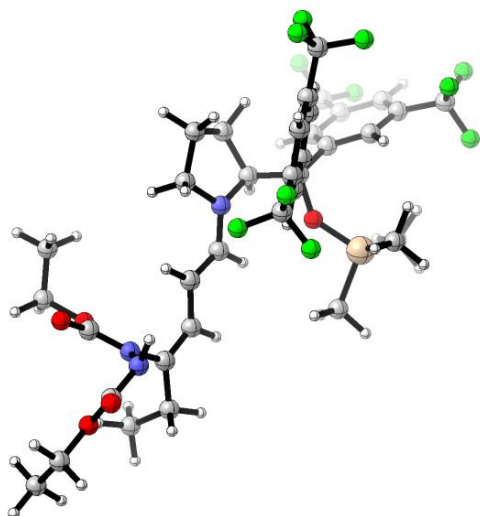
Thermal correction = 0.643515 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.225753	-1.323048	0.732326
2	6	0	4.312981	-2.257966	0.389455
3	6	0	3.088308	-2.219367	-0.394011
4	6	0	2.231006	-1.170534	-0.503694
5	7	0	1.085687	-1.172588	-1.262506
6	6	0	0.178309	-0.034897	-1.320864
7	6	0	-0.414701	-0.122145	-2.744886
8	6	0	-0.311414	-1.609407	-3.141318
9	6	0	0.886858	-2.144990	-2.340265
10	1	0	2.818508	-3.163977	-0.861383
11	1	0	2.413470	-0.247883	0.035457
12	1	0	0.766688	0.877963	-1.182090
13	1	0	-1.439702	0.253076	-2.807982
14	1	0	0.196938	0.491326	-3.415356
15	1	0	-1.223884	-2.146244	-2.871357
16	1	0	-0.166519	-1.735019	-4.217884
17	1	0	0.699184	-3.150599	-1.942952
18	1	0	1.804855	-2.200568	-2.943882
19	6	0	-0.879568	-0.024273	-0.133610
20	8	0	-0.072965	-0.004940	1.037727
21	14	0	-0.219824	0.028772	2.728203
22	6	0	-1.479362	-1.210663	3.399042
23	1	0	-1.483475	-1.135866	4.494590
24	1	0	-2.504991	-1.020873	3.062522
25	1	0	-1.229256	-2.244905	3.141005
26	6	0	1.510830	-0.434891	3.295352
27	1	0	2.255102	0.261520	2.894131
28	1	0	1.582291	-0.416415	4.389677
29	1	0	1.786678	-1.438624	2.953565
30	6	0	-0.659538	1.755211	3.354301
31	1	0	-0.471271	1.798520	4.435064
32	1	0	-0.038136	2.526282	2.884987
33	1	0	-1.708643	2.023559	3.196552
34	6	0	-1.752194	1.249670	-0.150603
35	6	0	-2.869554	1.324509	0.692547
36	6	0	-1.429485	2.387441	-0.899932
37	6	0	-3.629282	2.489519	0.790241
38	1	0	-3.158064	0.462906	1.284356
39	6	0	-2.195611	3.553200	-0.807095
40	1	0	-0.577286	2.392394	-1.566885
41	6	0	-3.299018	3.616738	0.039902
42	1	0	-3.887559	4.523036	0.115243
43	6	0	-1.714167	-1.311348	-0.197791
44	6	0	-2.966417	-1.378354	-0.821359
45	6	0	-1.154833	-2.496873	0.289949
46	6	0	-3.643247	-2.595094	-0.938788
47	1	0	-3.425122	-0.485662	-1.230037
48	6	0	-1.831278	-3.711213	0.165445
49	1	0	-0.179265	-2.470266	0.759039
50	6	0	-3.081113	-3.772870	-0.446375

51	1	0	-3.603662	-4.716808	-0.541224
52	6	0	6.397923	-1.658474	1.637957
53	1	0	7.269250	-1.057238	1.343343
54	1	0	6.677978	-2.704915	1.464334
55	6	0	6.129005	-1.471288	3.143608
56	1	0	7.012400	-1.749301	3.730901
57	1	0	5.870736	-0.434907	3.379038
58	1	0	5.294423	-2.105085	3.463554
59	1	0	4.569649	-3.259415	0.739553
60	6	0	-4.764075	2.539129	1.779025
61	6	0	-1.851597	4.732749	-1.679658
62	6	0	-1.158274	-4.950699	0.688718
63	6	0	-5.017139	-2.620502	-1.555772
64	9	0	-0.017412	-5.214857	0.005799
65	9	0	-1.942242	-6.043302	0.599730
66	9	0	-0.804818	-4.807951	1.988495
67	9	0	-5.300903	-3.821547	-2.103651
68	9	0	-5.980099	-2.366579	-0.639503
69	9	0	-5.146202	-1.688861	-2.527072
70	9	0	-5.436938	1.369159	1.825984
71	9	0	-4.307456	2.777465	3.033988
72	9	0	-5.651172	3.511638	1.488791
73	9	0	-0.514969	4.848528	-1.861376
74	9	0	-2.401474	4.615923	-2.910116
75	9	0	-2.293242	5.893871	-1.155218
76	7	0	5.181982	0.031395	0.234926
77	7	0	5.362979	1.049653	1.178638
78	1	0	6.324894	1.360583	1.283430
79	6	0	5.510749	0.399480	-1.068157
80	6	0	4.497605	2.133107	1.253396
81	8	0	5.596408	-0.665132	-1.882682
82	8	0	3.278942	1.859687	0.753975
83	8	0	4.827001	3.176739	1.783999
84	8	0	5.684845	1.559535	-1.404367
85	6	0	5.888910	-0.378004	-3.272265
86	1	0	6.336672	-1.303098	-3.642363
87	1	0	6.627239	0.425600	-3.319768
88	6	0	4.630734	-0.020091	-4.046989
89	1	0	4.198595	0.910579	-3.668759
90	1	0	4.876026	0.119060	-5.106141
91	1	0	3.885861	-0.818487	-3.966254
92	6	0	2.338420	2.965230	0.751188
93	1	0	1.363782	2.474525	0.740577
94	1	0	2.452815	3.525082	1.681944
95	6	0	2.538358	3.855739	-0.464478
96	1	0	1.740366	4.604442	-0.510585
97	1	0	3.501144	4.370943	-0.412537
98	1	0	2.509476	3.265835	-1.386794

Dienamine E



HF (B3LYP/6-31G(d)) = -3424.5821776 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.746779 (Hartree/Particle)

Thermal correction = 0.640447 Hartrees

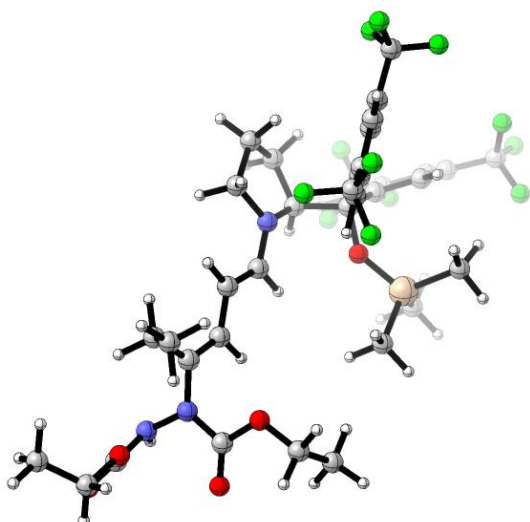
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.921342	-1.367143	0.955087
2	6	0	-3.587749	-1.528344	0.809601
3	6	0	-2.716727	-0.899619	-0.154772
4	6	0	-1.382572	-1.167056	-0.182916
5	7	0	-0.464783	-0.628267	-1.046511
6	6	0	0.919367	-1.093347	-1.113838
7	6	0	1.313778	-0.832742	-2.585029
8	6	0	0.381632	0.297461	-3.065218
9	6	0	-0.895335	0.114785	-2.233451
10	1	0	-3.147279	-0.185687	-0.850333
11	1	0	-0.957255	-1.859143	0.536680
12	1	0	0.934811	-2.162164	-0.877125
13	1	0	2.370692	-0.581965	-2.708344
14	1	0	1.129262	-1.744798	-3.163146
15	1	0	0.828171	1.276062	-2.872831
16	1	0	0.179569	0.234650	-4.137949
17	1	0	-1.352375	1.071500	-1.950870
18	1	0	-1.658713	-0.467784	-2.771187
19	6	0	1.848769	-0.421552	-0.017794
20	8	0	1.234624	-0.789220	1.212463
21	14	0	1.522439	-0.720663	2.881811
22	6	0	1.922183	1.023705	3.483498
23	1	0	2.027658	1.004802	4.576093
24	1	0	2.861313	1.415242	3.077231
25	1	0	1.128792	1.738553	3.239855
26	6	0	-0.123371	-1.286686	3.596682
27	1	0	-0.346767	-2.320544	3.307827
28	1	0	-0.104678	-1.245294	4.692622

29	1	0	-0.950014	-0.656108	3.250764
30	6	0	2.883613	-1.915337	3.413050
31	1	0	2.793839	-2.101220	4.491191
32	1	0	2.787042	-2.881524	2.904261
33	1	0	3.893076	-1.534969	3.230374
34	6	0	3.282138	-0.995390	-0.050276
35	6	0	4.298247	-0.346496	0.664026
36	6	0	3.603734	-2.204298	-0.680041
37	6	0	5.581730	-0.884938	0.752775
38	1	0	4.091170	0.593833	1.162754
39	6	0	4.894810	-2.734079	-0.605688
40	1	0	2.859675	-2.760283	-1.235789
41	6	0	5.893614	-2.083495	0.114397
42	1	0	6.890386	-2.501939	0.180024
43	6	0	1.817394	1.103565	-0.196724
44	6	0	2.771367	1.802246	-0.947605
45	6	0	0.733605	1.817720	0.323536
46	6	0	2.650510	3.178721	-1.154185
47	1	0	3.615974	1.281827	-1.383693
48	6	0	0.613940	3.192006	0.111490
49	1	0	-0.023478	1.293339	0.892213
50	6	0	1.570320	3.885855	-0.625895
51	1	0	1.475725	4.952570	-0.788222
52	6	0	-5.744083	-2.049443	2.018233
53	1	0	-6.330223	-1.293218	2.558749
54	1	0	-5.064806	-2.500376	2.751703
55	6	0	-6.703826	-3.122035	1.473693
56	1	0	-7.292598	-3.561325	2.287978
57	1	0	-7.399932	-2.689156	0.749409
58	1	0	-6.151688	-3.927067	0.976452
59	1	0	-3.110988	-2.223691	1.501070
60	7	0	-5.639867	-0.469238	0.083262
61	7	0	-6.033674	0.751011	0.626363
62	1	0	-5.443745	1.540318	0.383240
63	6	0	-7.367779	1.109216	0.753169
64	8	0	-8.186167	0.042916	0.754292
65	8	0	-7.713839	2.265237	0.908415
66	6	0	-5.970422	-0.694247	-1.240665
67	8	0	-6.519125	0.130646	-1.951886
68	8	0	-5.618054	-1.939700	-1.622429
69	6	0	-9.593626	0.351233	0.900640
70	1	0	-9.743539	0.860586	1.857577
71	1	0	-9.884864	1.040321	0.102624
72	6	0	-5.904187	-2.284018	-2.998860
73	1	0	-5.976886	-3.374066	-2.988314
74	1	0	-6.871995	-1.860153	-3.276071
75	6	0	-4.803459	-1.809337	-3.934637
76	1	0	-5.006307	-2.158058	-4.953782
77	1	0	-4.756034	-0.716678	-3.948698
78	1	0	-3.831416	-2.204298	-3.620830
79	6	0	-10.357113	-0.956611	0.827944
80	1	0	-10.048501	-1.637288	1.627785
81	1	0	-11.429500	-0.761343	0.936003
82	1	0	-10.192476	-1.452700	-0.133901
83	6	0	6.600460	-0.192603	1.618888
84	6	0	5.212416	-3.998038	-1.362728
85	6	0	-0.591992	3.891968	0.677648
86	6	0	3.730286	3.912133	-1.905920

87	9	0	-1.730340	3.471548	0.075809
88	9	0	-0.529039	5.230062	0.531152
89	9	0	-0.734968	3.632424	1.999259
90	9	0	3.257893	5.025012	-2.506837
91	9	0	4.732602	4.301665	-1.084224
92	9	0	4.288106	3.137371	-2.863390
93	9	0	6.559179	1.148290	1.463558
94	9	0	6.368838	-0.439494	2.932906
95	9	0	7.857941	-0.598825	1.354244
96	9	0	4.178283	-4.868250	-1.337252
97	9	0	5.473381	-3.740379	-2.665571
98	9	0	6.291628	-4.631380	-0.859213

Dienamine F



HF (B3LYP/6-31G(d)) = -3424.5809528 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.746884 (Hartree/Particle)

Thermal correction = 0.640566 Hartrees

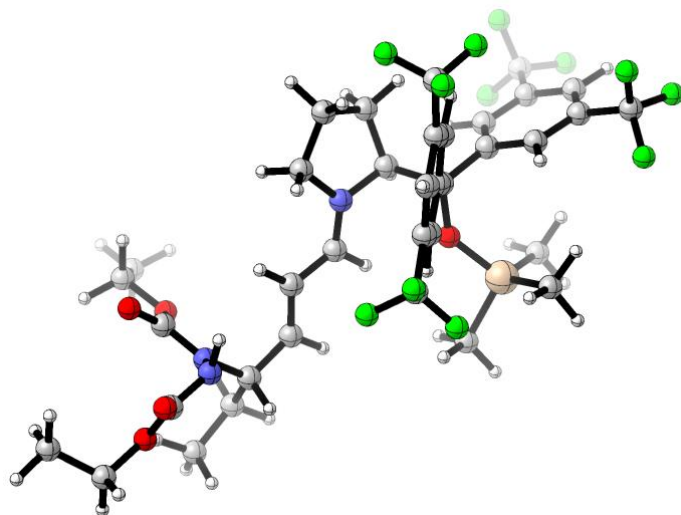
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.068668	-0.229892	-0.830784
2	6	0	-3.764932	-0.576144	-0.742820
3	6	0	-2.634511	0.111622	-1.322772
4	6	0	-1.367474	-0.366345	-1.189888
5	7	0	-0.232086	0.186999	-1.726385
6	6	0	1.055256	-0.507831	-1.719027
7	6	0	1.737764	-0.018683	-3.015793
8	6	0	1.088880	1.342784	-3.333880
9	6	0	-0.326560	1.231955	-2.750243
10	1	0	-2.810755	1.030074	-1.873553
11	1	0	-1.187694	-1.263505	-0.605934
12	1	0	0.863460	-1.585088	-1.752080

13	1	0	2.825872	0.045438	-2.930295
14	1	0	1.519337	-0.734945	-3.815303
15	1	0	1.639029	2.157057	-2.856383
16	1	0	1.068972	1.546514	-4.407973
17	1	0	-0.675074	2.175679	-2.312140
18	1	0	-1.062258	0.929755	-3.510871
19	6	0	1.868651	-0.281832	-0.375234
20	8	0	1.007060	-0.800651	0.633121
21	14	0	1.124518	-1.481533	2.181031
22	6	0	2.149209	-0.442102	3.380486
23	1	0	1.876704	-0.719695	4.407004
24	1	0	3.227274	-0.602871	3.280511
25	1	0	1.947760	0.629508	3.269295
26	6	0	-0.671700	-1.508362	2.739753
27	1	0	-1.291316	-2.104433	2.059959
28	1	0	-0.759605	-1.945609	3.741929
29	1	0	-1.093558	-0.497471	2.775029
30	6	0	1.796735	-3.241298	2.099635
31	1	0	1.724370	-3.708917	3.089929
32	1	0	1.217785	-3.856884	1.401302
33	1	0	2.847162	-3.280108	1.793642
34	6	0	3.196090	-1.069079	-0.365317
35	6	0	4.200430	-0.730843	0.550127
36	6	0	3.402830	-2.201828	-1.165085
37	6	0	5.356986	-1.502362	0.677534
38	1	0	4.085240	0.142984	1.180724
39	6	0	4.567743	-2.962209	-1.049805
40	1	0	2.658230	-2.518505	-1.883507
41	6	0	5.553079	-2.624551	-0.122416
42	1	0	6.449711	-3.223983	-0.023751
43	6	0	2.064759	1.226498	-0.156324
44	6	0	3.186615	1.921350	-0.623690
45	6	0	1.026874	1.960690	0.429712
46	6	0	3.271770	3.310680	-0.497274
47	1	0	4.004581	1.390297	-1.096816
48	6	0	1.107150	3.350068	0.535556
49	1	0	0.149368	1.440635	0.791650
50	6	0	2.230372	4.036946	0.077851
51	1	0	2.291823	5.114939	0.164359
52	6	0	-5.635170	0.943960	-1.588027
53	1	0	-6.507142	0.604604	-2.161964
54	1	0	-4.902673	1.294632	-2.322804
55	6	0	-6.059934	2.111333	-0.678811
56	1	0	-6.492662	2.925984	-1.271819
57	1	0	-6.812260	1.783044	0.044797
58	1	0	-5.203569	2.508836	-0.123385
59	1	0	-3.531380	-1.467451	-0.160306
60	7	0	-6.042356	-1.044687	-0.146509
61	7	0	-6.905012	-1.792034	-0.945809
62	1	0	-6.662490	-2.773968	-1.033383
63	6	0	-8.277657	-1.591022	-0.938397
64	8	0	-8.607184	-0.362783	-0.500950
65	8	0	-9.053808	-2.433590	-1.349445
66	6	0	-6.202891	-1.182502	1.221449
67	8	0	-7.007074	-1.945477	1.730631
68	8	0	-5.377188	-0.359431	1.900317
69	6	0	-10.022159	-0.048703	-0.503064
70	1	0	-10.125459	0.713604	0.272304

71	1	0	-10.579174	-0.940864	-0.209249
72	6	0	-5.484805	-0.411898	3.343836
73	1	0	-5.108444	0.560515	3.669968
74	1	0	-6.538776	-0.501612	3.616645
75	6	0	-10.474001	0.467729	-1.859649
76	1	0	-10.371391	-0.310338	-2.621319
77	1	0	-11.528145	0.763805	-1.809666
78	1	0	-9.885682	1.340782	-2.160894
79	6	0	-4.664056	-1.550643	3.928670
80	1	0	-4.705389	-1.511218	5.023384
81	1	0	-5.061454	-2.516767	3.605139
82	1	0	-3.616106	-1.474184	3.620727
83	6	0	4.524392	4.017187	-0.944316
84	6	0	-0.078229	4.104961	1.075681
85	6	0	6.362472	-1.113016	1.729289
86	6	0	4.783015	-4.131769	-1.976201
87	9	0	7.496916	-1.834667	1.647407
88	9	0	5.858605	-1.293085	2.976160
89	9	0	6.696891	0.192264	1.633328
90	9	0	5.582123	-5.068838	-1.424828
91	9	0	5.366780	-3.743766	-3.133833
92	9	0	3.617367	-4.730251	-2.306071
93	9	0	4.292669	5.312247	-1.246463
94	9	0	5.476355	3.998819	0.017139
95	9	0	5.063567	3.433684	-2.038975
96	9	0	0.247630	5.354264	1.469193
97	9	0	-1.048956	4.223607	0.137268
98	9	0	-0.633912	3.475232	2.133855

INT 7



HF (B3LYP/6-31G(d)) = -3425.008715 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761720 (Hartree/Particle)

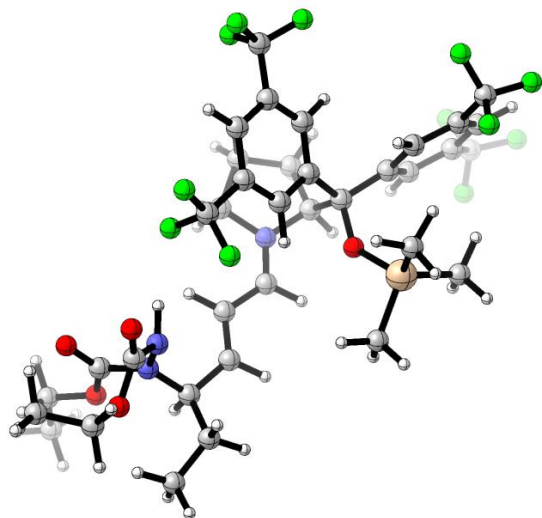
Thermal correction = 0.655961 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.789823	-1.347066	1.211410
2	6	0	-3.320327	-1.545291	0.970141
3	6	0	-2.606925	-1.096964	-0.089841
4	6	0	-1.202977	-1.359202	-0.149265
5	7	0	-0.402369	-0.965433	-1.100424
6	6	0	1.055232	-1.282510	-1.122894
7	6	0	1.429921	-1.075224	-2.603791
8	6	0	0.407462	-0.075624	-3.183094
9	6	0	-0.854176	-0.246917	-2.325525
10	1	0	-3.088168	-0.534520	-0.881950
11	1	0	-0.737356	-1.918379	0.654838
12	1	0	1.145579	-2.328617	-0.828722
13	1	0	2.459053	-0.733756	-2.724744
14	1	0	1.351213	-2.037719	-3.118612
15	1	0	0.774506	0.949889	-3.124477
16	1	0	0.195321	-0.285561	-4.233481
17	1	0	-1.311822	0.703021	-2.038895
18	1	0	-1.609446	-0.866291	-2.817484
19	6	0	1.850634	-0.466464	-0.021866
20	8	0	1.293170	-0.930389	1.199810
21	14	0	1.825000	-1.102605	2.824010
22	6	0	2.466662	0.513096	3.546332
23	1	0	2.566078	0.389223	4.632498
24	1	0	3.454232	0.793916	3.166224
25	1	0	1.781070	1.350327	3.375847
26	6	0	0.222591	-1.613334	3.670707
27	1	0	-0.171204	-2.550344	3.257594
28	1	0	0.394023	-1.777443	4.741185
29	1	0	-0.553058	-0.843854	3.577836
30	6	0	3.101607	-2.474163	2.984198
31	1	0	3.246172	-2.703219	4.047682
32	1	0	2.770816	-3.396249	2.492718
33	1	0	4.078204	-2.200992	2.573400
34	6	0	3.354806	-0.810249	-0.086705
35	6	0	4.294730	0.086080	0.435028
36	6	0	3.813826	-2.056813	-0.532469
37	6	0	5.645943	-0.254634	0.517561
38	1	0	3.978544	1.056095	0.799674
39	6	0	5.167702	-2.387187	-0.469134
40	1	0	3.131408	-2.802343	-0.920653
41	6	0	6.095487	-1.491100	0.060902
42	1	0	7.143490	-1.756790	0.128352
43	6	0	1.584461	1.043102	-0.178800
44	6	0	2.242259	1.811842	-1.148585
45	6	0	0.630216	1.671575	0.623951
46	6	0	1.933044	3.161519	-1.319514
47	1	0	3.010130	1.370560	-1.774851
48	6	0	0.347149	3.031088	0.472012
49	1	0	0.114559	1.102315	1.386576
50	6	0	0.987594	3.786632	-0.505939
51	1	0	0.763746	4.839091	-0.628543
52	6	0	-5.455314	-2.683791	1.645842
53	1	0	-4.876974	-3.047239	2.504819
54	1	0	-5.345225	-3.423207	0.850350

55	6	0	-6.924571	-2.537441	2.043402
56	1	0	-7.313659	-3.504499	2.378464
57	1	0	-7.048360	-1.820061	2.862319
58	1	0	-7.535455	-2.192633	1.205921
59	1	0	-2.799931	-2.094410	1.754854
60	7	0	-5.464990	-0.598135	0.141502
61	7	0	-5.634981	0.766040	0.362460
62	1	0	-5.028522	1.361834	-0.193828
63	6	0	-6.917211	1.326777	0.450959
64	8	0	-7.839051	0.423225	0.798880
65	8	0	-7.089788	2.516628	0.287075
66	6	0	-5.794919	-1.059402	-1.127558
67	8	0	-6.280405	-0.350249	-1.987102
68	8	0	-5.489815	-2.362017	-1.275254
69	6	0	-9.202861	0.918867	0.924534
70	1	0	-9.673398	0.214032	1.612820
71	1	0	-9.170234	1.908860	1.383671
72	6	0	-5.858062	-2.946550	-2.557085
73	1	0	-6.933432	-2.813671	-2.700633
74	1	0	-5.341285	-2.397189	-3.349323
75	1	0	-4.861531	-0.677668	2.079688
76	6	0	-0.672800	3.644657	1.396776
77	6	0	2.583247	3.909174	-2.455927
78	6	0	5.628744	-3.712731	-1.024344
79	6	0	6.611241	0.756036	1.086777
80	6	0	-9.903252	0.946049	-0.423063
81	1	0	-10.945801	1.254239	-0.286760
82	1	0	-9.419309	1.657902	-1.097347
83	1	0	-9.894075	-0.044463	-0.888758
84	6	0	-5.461718	-4.408771	-2.520689
85	1	0	-5.990080	-4.941017	-1.723637
86	1	0	-5.719774	-4.878867	-3.475153
87	1	0	-4.384253	-4.523141	-2.362788
88	9	0	-0.816375	4.965729	1.202948
89	9	0	-1.887879	3.068386	1.225452
90	9	0	-0.332897	3.448572	2.691475
91	9	0	2.463669	5.241559	-2.325482
92	9	0	3.895635	3.614699	-2.559617
93	9	0	2.008914	3.562109	-3.635791
94	9	0	6.093437	1.353436	2.185972
95	9	0	6.877637	1.735382	0.196544
96	9	0	7.782110	0.193829	1.437280
97	9	0	5.886774	-3.623331	-2.347899
98	9	0	6.753049	-4.144406	-0.423467
99	9	0	4.683698	-4.667739	-0.870919

INT 8



HF (B3LYP/6-31G(d)) = -3425.0133639 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761677 (Hartree/Particle)

Thermal correction = 0.658307 Hartrees

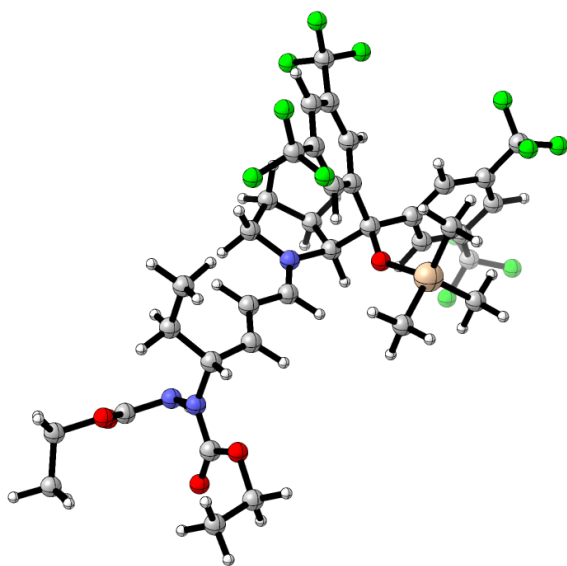
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.607087	-2.200794	-0.220856
2	6	0	3.116271	-2.303644	-0.034605
3	6	0	2.360605	-1.557157	0.806195
4	6	0	0.943967	-1.751427	0.840012
5	7	0	0.117796	-1.104526	1.614853
6	6	0	-1.362147	-1.252982	1.534490
7	6	0	-1.837103	-0.729976	2.902766
8	6	0	-0.753058	0.250541	3.402468
9	6	0	0.545215	-0.170336	2.694890
10	1	0	2.816543	-0.794984	1.429224
11	1	0	0.492502	-2.457677	0.152225
12	1	0	-1.565833	-2.317238	1.408525
13	1	0	-2.820648	-0.260101	2.844291
14	1	0	-1.926650	-1.578856	3.587425
15	1	0	-1.007447	1.281151	3.152330
16	1	0	-0.639265	0.196505	4.487144
17	1	0	1.084516	0.671582	2.252613
18	1	0	1.225823	-0.715264	3.354373
19	6	0	-1.929414	-0.548943	0.227127
20	8	0	-1.295981	-1.255675	-0.827063
21	14	0	-1.651798	-1.677653	-2.452735
22	6	0	-1.987405	-0.163647	-3.519750
23	1	0	-1.898899	-0.451773	-4.575121
24	1	0	-2.994168	0.244411	-3.383909
25	1	0	-1.262768	0.638242	-3.339985
26	6	0	-0.045586	-2.515467	-2.963225
27	1	0	0.132014	-3.426503	-2.377940
28	1	0	-0.088948	-2.811248	-4.018135

29	1	0	0.819179	-1.852849	-2.842292
30	6	0	-3.071321	-2.907758	-2.551175
31	1	0	-3.131505	-3.297666	-3.575311
32	1	0	-2.915964	-3.763511	-1.884178
33	1	0	-4.042633	-2.463383	-2.313941
34	6	0	-3.459869	-0.711429	0.141138
35	6	0	-4.192450	0.143842	-0.691631
36	6	0	-4.142281	-1.763562	0.764280
37	6	0	-5.556806	-0.053172	-0.905247
38	1	0	-3.698269	0.967528	-1.193719
39	6	0	-5.512255	-1.946271	0.565088
40	1	0	-3.626569	-2.469312	1.404275
41	6	0	-6.230357	-1.096420	-0.274010
42	1	0	-7.289511	-1.249340	-0.439399
43	6	0	-1.479539	0.924482	0.215013
44	6	0	-2.200800	1.931334	0.867927
45	6	0	-0.244364	1.255558	-0.350664
46	6	0	-1.688844	3.227264	0.964842
47	1	0	-3.168184	1.718002	1.308578
48	6	0	0.277359	2.543263	-0.223927
49	1	0	0.323648	0.499142	-0.877089
50	6	0	-0.440144	3.542516	0.431156
51	1	0	-0.034421	4.542831	0.526366
52	6	0	5.041084	-2.608883	-1.649038
53	1	0	4.793853	-1.793629	-2.337528
54	1	0	4.436432	-3.473016	-1.951793
55	6	0	6.525393	-2.967671	-1.744864
56	1	0	6.784555	-3.230930	-2.775501
57	1	0	7.154569	-2.126619	-1.444521
58	1	0	6.766598	-3.827189	-1.108424
59	1	0	2.625918	-3.073311	-0.629478
60	7	0	5.113402	-0.886390	0.188392
61	7	0	4.665811	0.215105	-0.533703
62	1	0	4.010779	0.812983	-0.040240
63	6	0	5.539343	0.994552	-1.302505
64	8	0	6.640804	0.323305	-1.659481
65	8	0	5.242610	2.124549	-1.631551
66	6	0	6.053991	-0.658292	1.187785
67	8	0	6.442018	0.450801	1.495414
68	8	0	6.456962	-1.812630	1.751595
69	6	0	7.617988	1.066372	-2.442821
70	1	0	8.147736	0.292627	-3.002097
71	1	0	7.082155	1.715604	-3.137807
72	6	0	7.467901	-1.682454	2.790655
73	1	0	7.059480	-1.064495	3.595304
74	1	0	8.331117	-1.162342	2.367292
75	1	0	5.047806	-2.925736	0.475857
76	6	0	7.816001	-3.080248	3.260772
77	1	0	8.216460	-3.682971	2.439582
78	1	0	8.577502	-3.020485	4.045146
79	1	0	6.938802	-3.588987	3.673401
80	6	0	8.553554	1.854298	-1.542222
81	1	0	9.323400	2.340690	-2.151544
82	1	0	8.006753	2.627710	-0.995801
83	1	0	9.047361	1.196096	-0.820682
84	6	0	1.694700	2.789408	-0.669782
85	6	0	-2.452680	4.251043	1.766815
86	6	0	-6.283403	0.899402	-1.822401

87	6	0	-6.211610	-3.061639	1.302999
88	9	0	2.551692	2.366647	0.316026
89	9	0	1.955272	4.083406	-0.889340
90	9	0	2.008398	2.092264	-1.776245
91	9	0	-2.105969	5.510103	1.445613
92	9	0	-3.784088	4.125997	1.593916
93	9	0	-2.209494	4.088542	3.091022
94	9	0	-5.462490	-4.187605	1.311724
95	9	0	-6.432489	-2.728628	2.594328
96	9	0	-7.401482	-3.362807	0.752774
97	9	0	-5.619121	1.042305	-2.994462
98	9	0	-6.376945	2.129326	-1.274015
99	9	0	-7.529189	0.480352	-2.106175

INT 9



HF (B3LYP/6-31G(d)) = -3425.0116478 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.762536 (Hartree/Particle)

Thermal correction = 0.659134 Hartrees

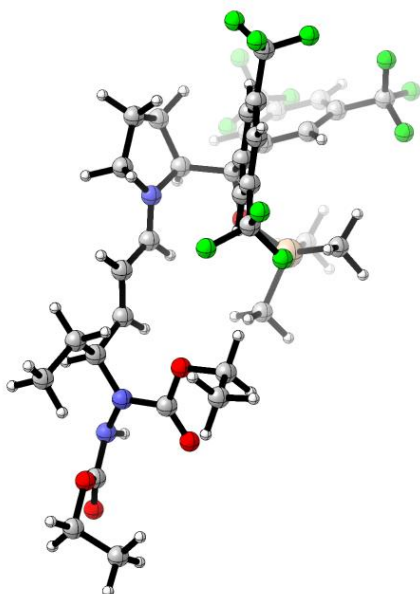
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.928688	0.302588	0.641223
2	6	0	-3.520843	-0.202805	0.428037
3	6	0	-2.627514	0.271676	-0.473295
4	6	0	-1.357269	-0.372657	-0.606554
5	7	0	-0.410748	-0.006741	-1.424971
6	6	0	0.907462	-0.696335	-1.503156
7	6	0	1.433316	-0.280685	-2.890048
8	6	0	0.758113	1.064592	-3.234876
9	6	0	-0.550956	1.084302	-2.430576
10	1	0	-2.856016	1.141624	-1.078368

11	1	0	-1.131641	-1.224321	0.025194
12	1	0	0.701402	-1.766279	-1.452232
13	1	0	2.522208	-0.214864	-2.913464
14	1	0	1.143471	-1.047094	-3.615265
15	1	0	1.389404	1.909867	-2.957125
16	1	0	0.557703	1.144715	-4.305256
17	1	0	-0.721808	2.030725	-1.910917
18	1	0	-1.424507	0.859482	-3.048484
19	6	0	1.801148	-0.370367	-0.235034
20	8	0	1.039578	-0.885937	0.846879
21	14	0	1.352015	-1.483656	2.426284
22	6	0	2.290478	-0.244960	3.489707
23	1	0	2.240408	-0.579785	4.533909
24	1	0	3.351868	-0.167869	3.232304
25	1	0	1.850335	0.757645	3.449094
26	6	0	-0.401310	-1.708526	3.073366
27	1	0	-0.953905	-2.451591	2.485399
28	1	0	-0.383089	-2.063109	4.110605
29	1	0	-0.966412	-0.768872	3.057464
30	6	0	2.237690	-3.141101	2.364642
31	1	0	2.260056	-3.573660	3.373141
32	1	0	1.717152	-3.853572	1.714478
33	1	0	3.273526	-3.060781	2.020855
34	6	0	3.157169	-1.101137	-0.325008
35	6	0	4.233764	-0.644365	0.442699
36	6	0	3.320992	-2.293882	-1.042947
37	6	0	5.429314	-1.362682	0.507243
38	1	0	4.144323	0.272526	1.013408
39	6	0	4.523540	-2.998615	-0.994056
40	1	0	2.518530	-2.707421	-1.640358
41	6	0	5.586396	-2.543214	-0.212631
42	1	0	6.512346	-3.103010	-0.157490
43	6	0	1.959630	1.154921	-0.084750
44	6	0	2.916645	1.877889	-0.808963
45	6	0	1.087124	1.862337	0.745846
46	6	0	2.986030	3.268263	-0.708115
47	1	0	3.626075	1.366241	-1.450288
48	6	0	1.166906	3.252301	0.853091
49	1	0	0.348559	1.324191	1.326010
50	6	0	2.112707	3.968849	0.124114
51	1	0	2.177369	5.046724	0.209547
52	6	0	-5.229594	1.730872	0.171005
53	1	0	-6.311731	1.868456	0.256097
54	1	0	-4.994760	1.836908	-0.894093
55	6	0	-4.505370	2.801453	0.997568
56	1	0	-4.804660	3.799641	0.662849
57	1	0	-4.761784	2.719687	2.060287
58	1	0	-3.414903	2.741195	0.914260
59	1	0	-3.257775	-1.082736	1.015746
60	7	0	-5.802997	-0.701354	-0.004907
61	7	0	-5.826443	-0.723848	-1.392476
62	1	0	-5.373297	-1.533552	-1.806185
63	6	0	-7.007836	-0.419175	-2.085747
64	8	0	-7.853232	0.306373	-1.346804
65	8	0	-7.153435	-0.750449	-3.244141
66	6	0	-6.436563	-1.752045	0.652650
67	8	0	-7.066566	-2.609548	0.065817
68	8	0	-6.244832	-1.680231	1.982728

69	6	0	-9.110173	0.670474	-1.987564
70	1	0	-9.419559	1.574255	-1.459029
71	1	0	-8.908677	0.911159	-3.033343
72	6	0	-6.938561	-2.681082	2.785021
73	1	0	-6.904928	-3.632569	2.251019
74	1	0	-6.334824	-2.750048	3.692048
75	1	0	-5.151449	0.231422	1.707606
76	6	0	0.173844	3.954655	1.742707
77	6	0	3.971914	4.007459	-1.577748
78	6	0	4.693619	-4.247153	-1.825173
79	6	0	6.540639	-0.825975	1.375182
80	6	0	-10.135315	-0.442085	-1.852916
81	1	0	-11.088683	-0.113475	-2.281277
82	1	0	-9.808627	-1.338101	-2.387840
83	1	0	-10.299034	-0.697742	-0.801366
84	6	0	-8.364244	-2.254612	3.086860
85	1	0	-8.954826	-2.193406	2.168393
86	1	0	-8.832970	-2.993448	3.746112
87	1	0	-8.384849	-1.283032	3.590630
88	9	0	6.081193	-0.528106	2.614398
89	9	0	7.055066	0.313317	0.865344
90	9	0	7.547578	-1.706496	1.512075
91	9	0	5.479809	-5.149796	-1.207790
92	9	0	5.263594	-3.966725	-3.017525
93	9	0	3.506552	-4.839976	-2.081887
94	9	0	5.150084	3.355391	-1.657271
95	9	0	4.214275	5.251234	-1.127976
96	9	0	3.496638	4.118406	-2.842936
97	9	0	0.506785	5.234645	1.975577
98	9	0	-1.062774	3.952957	1.179164
99	9	0	0.055174	3.329809	2.935247

INT 10



HF (B3LYP/6-31G(d)) = -3425.0097222 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761986 (Hartree/Particle)

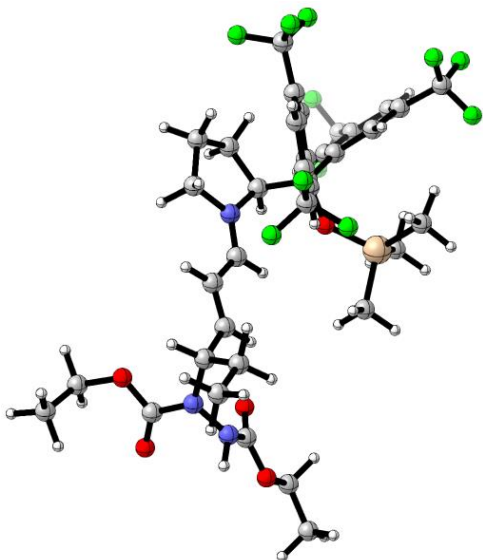
Thermal correction = 0.657244 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.872215	-0.734440	1.634391
2	6	0	3.404005	-1.045958	1.484145
3	6	0	2.365861	-0.399882	2.068731
4	6	0	1.035263	-0.865849	1.830592
5	7	0	-0.045834	-0.333316	2.329344
6	6	0	-1.416536	-0.832814	2.025361
7	6	0	-2.249382	-0.283053	3.198129
8	6	0	-1.521015	0.983780	3.695810
9	6	0	-0.046254	0.782729	3.315732
10	1	0	2.524344	0.470040	2.694555
11	1	0	0.882273	-1.717257	1.176946
12	1	0	-1.360409	-1.921843	2.041075
13	1	0	-3.282604	-0.080079	2.911802
14	1	0	-2.278160	-1.039479	3.988269
15	1	0	-1.918549	1.879996	3.217784
16	1	0	-1.632468	1.110696	4.774589
17	1	0	0.404682	1.667469	2.858539
18	1	0	0.567609	0.476393	4.167277
19	6	0	-1.851180	-0.449646	0.551193
20	8	0	-0.877034	-1.097639	-0.253789
21	14	0	-0.772839	-1.708250	-1.855659
22	6	0	-1.160204	-0.397045	-3.150641
23	1	0	-0.852656	-0.782982	-4.131261
24	1	0	-2.226808	-0.161682	-3.223528
25	1	0	-0.611227	0.536203	-2.982470
26	6	0	1.044439	-2.192063	-1.940482
27	1	0	1.280959	-2.995720	-1.232183
28	1	0	1.291407	-2.562465	-2.942511
29	1	0	1.707280	-1.343961	-1.731056
30	6	0	-1.853626	-3.230862	-2.080632
31	1	0	-1.590997	-3.715778	-3.029410
32	1	0	-1.691153	-3.963743	-1.282268
33	1	0	-2.922365	-2.998863	-2.117163
34	6	0	-3.257301	-1.004311	0.236382
35	6	0	-3.987216	-0.455167	-0.824934
36	6	0	-3.785544	-2.128607	0.883922
37	6	0	-5.197199	-1.016082	-1.234639
38	1	0	-3.609381	0.410604	-1.355081
39	6	0	-5.005300	-2.677129	0.484385
40	1	0	-3.258458	-2.609494	1.698399
41	6	0	-5.719380	-2.129491	-0.580745
42	1	0	-6.655697	-2.570666	-0.901154
43	6	0	-1.763753	1.076246	0.347773
44	6	0	-2.800621	1.943655	0.718729
45	6	0	-0.594126	1.632571	-0.173408
46	6	0	-2.663222	3.324981	0.568310
47	1	0	-3.729057	1.552811	1.120839
48	6	0	-0.464814	3.013711	-0.333785

49	1	0	0.217488	0.981173	-0.471104
50	6	0	-1.495465	3.872991	0.036268
51	1	0	-1.394882	4.944177	-0.087042
52	6	0	5.182760	0.682044	2.161800
53	1	0	4.621381	0.810097	3.095974
54	1	0	4.798538	1.419462	1.451120
55	6	0	6.666742	0.926792	2.442508
56	1	0	6.808836	1.938072	2.837184
57	1	0	7.054283	0.219712	3.185350
58	1	0	7.267158	0.820386	1.536932
59	1	0	3.185535	-1.906740	0.852325
60	7	0	5.594424	-1.117413	0.403223
61	7	0	6.379758	-2.264826	0.462703
62	1	0	5.945188	-3.093397	0.064549
63	6	0	7.740498	-2.230034	0.127840
64	8	0	8.262933	-1.004208	0.235525
65	8	0	8.334521	-3.248825	-0.158720
66	6	0	5.341726	-0.601771	-0.862092
67	8	0	5.868604	-1.019444	-1.873212
68	8	0	4.441510	0.402250	-0.797899
69	6	0	9.675035	-0.880823	-0.098197
70	1	0	10.001877	-0.006491	0.468279
71	1	0	10.196331	-1.767087	0.268407
72	6	0	4.213832	1.136256	-2.038592
73	1	0	4.192675	0.420277	-2.862059
74	1	0	3.224958	1.575731	-1.906431
75	1	0	5.249021	-1.453991	2.375346
76	6	0	0.822447	3.535057	-0.916049
77	6	0	-3.818915	4.215646	0.954950
78	6	0	-5.575301	-3.850566	1.243777
79	6	0	-5.939241	-0.375182	-2.381779
80	6	0	9.869431	-0.691160	-1.592722
81	1	0	10.932385	-0.531518	-1.805336
82	1	0	9.537282	-1.576014	-2.142495
83	1	0	9.310478	0.178324	-1.952735
84	6	0	5.273420	2.203937	-2.247931
85	1	0	6.262664	1.754053	-2.370762
86	1	0	5.041902	2.772972	-3.155134
87	1	0	5.298664	2.900871	-1.404111
88	9	0	-4.377035	3.805045	2.116988
89	9	0	-4.791459	4.193833	0.020096
90	9	0	-3.435198	5.496345	1.114247
91	9	0	0.813337	4.864538	-1.095446
92	9	0	1.876675	3.233719	-0.115685
93	9	0	1.080109	2.955451	-2.115782
94	9	0	-6.354304	-4.620097	0.460597
95	9	0	-6.332127	-3.437890	2.284317
96	9	0	-4.597813	-4.633695	1.752192
97	9	0	-6.848426	-1.206937	-2.921308
98	9	0	-6.589716	0.738832	-1.983919
99	9	0	-5.084683	-0.002890	-3.363822

INT 11



HF (B3LYP/6-31G(d)) = -3425.0201306 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761615 (Hartree/Particle)

Thermal correction = 0.657233 Hartrees

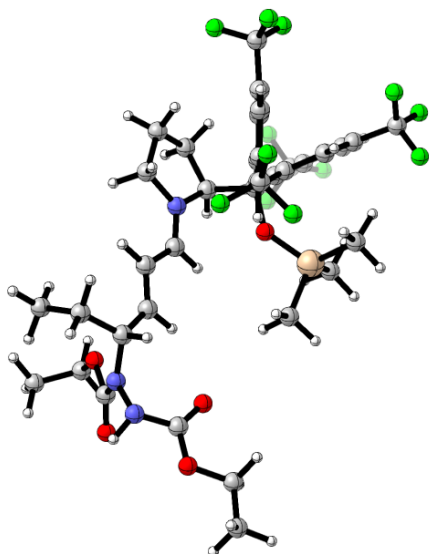
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.883908	1.067180	0.057997
2	6	0	-3.606503	0.333223	-0.240669
3	6	0	-2.611987	0.816269	-1.023620
4	6	0	-1.404131	0.064146	-1.144291
5	7	0	-0.340964	0.444317	-1.798034
6	6	0	0.929120	-0.331620	-1.809631
7	6	0	1.669582	0.230341	-3.038906
8	6	0	1.117918	1.651890	-3.284660
9	6	0	-0.273878	1.675093	-2.633174
10	1	0	-2.706638	1.779277	-1.515867
11	1	0	-1.327903	-0.887990	-0.631135
12	1	0	0.656982	-1.379436	-1.944036
13	1	0	2.752712	0.226145	-2.904830
14	1	0	1.451899	-0.412957	-3.896645
15	1	0	1.760207	2.411701	-2.837477
16	1	0	1.051361	1.870498	-4.352501
17	1	0	-0.431112	2.550864	-1.998044
18	1	0	-1.083146	1.625645	-3.366818
19	6	0	1.648855	-0.258989	-0.395618
20	8	0	0.739266	-0.918371	0.472036
21	14	0	0.830700	-1.824854	1.927104
22	6	0	1.785053	-0.926493	3.279925
23	1	0	1.563090	-1.412722	4.238790
24	1	0	2.870536	-0.968550	3.145333
25	1	0	1.487900	0.124078	3.373030
26	6	0	-0.988324	-1.957315	2.389876
27	1	0	-1.573062	-2.454644	1.606780

28	1	0	-1.102815	-2.547639	3.306930
29	1	0	-1.435980	-0.973969	2.576675
30	6	0	1.550384	-3.532496	1.609196
31	1	0	1.435705	-4.145641	2.512168
32	1	0	1.027178	-4.046903	0.794908
33	1	0	2.617010	-3.506688	1.365289
34	6	0	2.993899	-1.012250	-0.430695
35	6	0	3.988334	-0.699513	0.502132
36	6	0	3.215493	-2.097244	-1.290178
37	6	0	5.159567	-1.454726	0.586095
38	1	0	3.855022	0.134453	1.181129
39	6	0	4.397253	-2.834885	-1.220498
40	1	0	2.473508	-2.397917	-2.019399
41	6	0	5.376908	-2.525033	-0.276520
42	1	0	6.286998	-3.109093	-0.212788
43	6	0	1.795602	1.214376	0.031428
44	6	0	2.822855	2.031807	-0.456896
45	6	0	0.830762	1.792922	0.859529
46	6	0	2.863987	3.390940	-0.140991
47	1	0	3.604479	1.618202	-1.085148
48	6	0	0.880102	3.150701	1.181701
49	1	0	0.031275	1.180417	1.255949
50	6	0	1.893042	3.964270	0.680916
51	1	0	1.930601	5.018203	0.927493
52	6	0	-4.817176	1.711513	1.462439
53	1	0	-3.908317	2.324316	1.494596
54	1	0	-4.696504	0.924400	2.214198
55	6	0	-6.040814	2.574321	1.784716
56	1	0	-5.921944	3.040297	2.767985
57	1	0	-6.170144	3.373926	1.046659
58	1	0	-6.961577	1.983181	1.805020
59	1	0	-3.500815	-0.645555	0.222036
60	7	0	-6.038352	0.160354	-0.082569
61	7	0	-6.316659	-0.717747	0.954061
62	1	0	-7.243739	-0.603295	1.351277
63	6	0	-5.904173	-2.045394	0.817655
64	8	0	-6.628440	-2.817199	1.632868
65	8	0	-4.980953	-2.410012	0.112974
66	6	0	-6.682266	-0.095243	-1.291795
67	8	0	-7.558295	-0.928491	-1.410057
68	8	0	-6.220680	0.709756	-2.267080
69	6	0	-6.263915	-4.224956	1.672411
70	1	0	-6.338395	-4.626925	0.658433
71	1	0	-5.221657	-4.302268	1.996589
72	6	0	-6.895685	0.600904	-3.553802
73	1	0	-6.149904	0.954631	-4.268786
74	1	0	-7.108941	-0.452822	-3.742515
75	6	0	-8.157305	1.445714	-3.591546
76	1	0	-8.600399	1.395738	-4.592278
77	1	0	-8.893909	1.074873	-2.873377
78	1	0	-7.934963	2.493870	-3.366772
79	6	0	-7.214881	-4.911114	2.631749
80	1	0	-8.250947	-4.811208	2.294144
81	1	0	-6.971435	-5.977350	2.684511
82	1	0	-7.132266	-4.488556	3.637932
83	6	0	6.152981	-1.112787	1.668190
84	6	0	4.634739	-3.949842	-2.209462
85	6	0	-0.211620	3.703242	2.061059

86	6	0	3.926437	4.246506	-0.783399
87	9	0	-1.425818	3.556990	1.464499
88	9	0	-0.048513	5.009012	2.328782
89	9	0	-0.279736	3.041338	3.235933
90	9	0	3.597850	4.516697	-2.072662
91	9	0	4.084590	5.424045	-0.153979
92	9	0	5.120930	3.621148	-0.807846
93	9	0	6.417652	0.210914	1.689474
94	9	0	5.660131	-1.432762	2.889452
95	9	0	7.318064	-1.766445	1.516154
96	9	0	3.475390	-4.535413	-2.582913
97	9	0	5.224500	-3.487387	-3.334262
98	9	0	5.434691	-4.906041	-1.700927
99	1	0	-5.030541	1.859793	-0.678351

INT 12



HF (B3LYP/6-31G(d)) = -3425.0128402 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761544 (Hartree/Particle)

Thermal correction = 0.657237 Hartrees

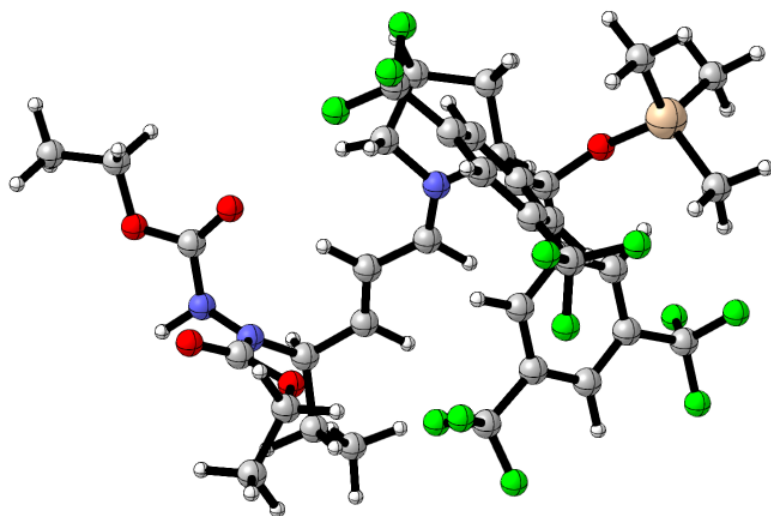
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.048961	1.007171	-0.830414
2	6	0	-3.725864	0.298695	-0.888204
3	6	0	-2.626533	0.697144	-1.576243
4	6	0	-1.412790	-0.033193	-1.403593
5	7	0	-0.276232	0.238510	-1.985917
6	6	0	0.960746	-0.563529	-1.774703
7	6	0	1.797952	-0.236955	-3.026843
8	6	0	1.336455	1.151226	-3.521377
9	6	0	-0.098403	1.317607	-2.996064

10	1	0	-2.651382	1.559065	-2.233429
11	1	0	-1.404205	-0.882618	-0.729261
12	1	0	0.652954	-1.609719	-1.758395
13	1	0	2.869772	-0.269914	-2.826281
14	1	0	1.591949	-0.996460	-3.787146
15	1	0	1.979248	1.945165	-3.138468
16	1	0	1.361308	1.211015	-4.611515
17	1	0	-0.269775	2.286859	-2.520023
18	1	0	-0.849548	1.173094	-3.777458
19	6	0	1.595102	-0.288424	-0.349487
20	8	0	0.588149	-0.724936	0.551056
21	14	0	0.538743	-1.374360	2.141928
22	6	0	1.383480	-0.249582	3.395335
23	1	0	1.085419	-0.569723	4.402156
24	1	0	2.476222	-0.303695	3.355242
25	1	0	1.084644	0.798922	3.286236
26	6	0	-1.312984	-1.443884	2.457521
27	1	0	-1.825826	-2.094146	1.738535
28	1	0	-1.508162	-1.853406	3.455963
29	1	0	-1.783303	-0.455162	2.414980
30	6	0	1.260689	-3.111014	2.200329
31	1	0	1.006721	-3.564083	3.167001
32	1	0	0.839979	-3.753452	1.418323
33	1	0	2.350655	-3.129498	2.107439
34	6	0	2.880004	-1.123502	-0.160566
35	6	0	3.822980	-0.728692	0.795433
36	6	0	3.085326	-2.343067	-0.819491
37	6	0	4.925218	-1.530777	1.094975
38	1	0	3.700908	0.208677	1.325602
39	6	0	4.201582	-3.131152	-0.536493
40	1	0	2.379769	-2.712797	-1.553247
41	6	0	5.128149	-2.735789	0.428031
42	1	0	5.984615	-3.357269	0.658451
43	6	0	1.845783	1.220267	-0.162557
44	6	0	2.968604	1.854394	-0.710705
45	6	0	0.914552	2.003609	0.522918
46	6	0	3.137673	3.234242	-0.592155
47	1	0	3.730376	1.278847	-1.225534
48	6	0	1.101503	3.380981	0.663512
49	1	0	0.045214	1.534313	0.965722
50	6	0	2.208226	4.010445	0.100252
51	1	0	2.351584	5.078687	0.205890
52	6	0	-5.363928	2.035565	-1.937139
53	1	0	-4.557035	2.779949	-1.937182
54	1	0	-6.261027	2.573454	-1.610165
55	6	0	-5.585972	1.492943	-3.351566
56	1	0	-5.794836	2.323053	-4.034306
57	1	0	-4.713069	0.953146	-3.732558
58	1	0	-6.438841	0.809804	-3.385204
59	1	0	-3.652833	-0.555666	-0.218388
60	7	0	-6.152123	0.061951	-0.566130
61	7	0	-6.873763	0.289920	0.599891
62	1	0	-7.880053	0.294513	0.471730
63	6	0	-6.407567	-0.364794	1.743087
64	8	0	-7.362119	-0.374102	2.676816
65	8	0	-5.272477	-0.788759	1.860669
66	6	0	-6.284405	-1.209378	-1.113219
67	8	0	-7.105582	-2.017823	-0.729476

68	8	0	-5.406951	-1.395567	-2.120083
69	6	0	-6.996061	-0.950165	3.961445
70	1	0	-6.667825	-1.979884	3.795247
71	1	0	-6.153182	-0.382320	4.366300
72	6	0	-5.487865	-2.676677	-2.811041
73	1	0	-4.487894	-2.809236	-3.229721
74	1	0	-5.677482	-3.454230	-2.068679
75	6	0	-6.553137	-2.663197	-3.893347
76	1	0	-6.542298	-3.621400	-4.424590
77	1	0	-7.546868	-2.526849	-3.458193
78	1	0	-6.367754	-1.866101	-4.620297
79	6	0	-8.218121	-0.875757	4.854114
80	1	0	-9.051194	-1.441408	4.425678
81	1	0	-7.979428	-1.302760	5.833715
82	1	0	-8.536986	0.161136	4.998843
83	6	0	5.858001	-1.077925	2.190380
84	6	0	4.420400	-4.402016	-1.320321
85	6	0	0.061245	4.163742	1.422977
86	6	0	4.303374	3.880020	-1.296790
87	9	0	-1.115209	4.188227	0.749225
88	9	0	0.431468	5.437822	1.637644
89	9	0	-0.193507	3.596732	2.623766
90	9	0	4.054264	3.977506	-2.627690
91	9	0	4.551300	5.120578	-0.841647
92	9	0	5.431586	3.152760	-1.163604
93	9	0	6.289899	0.183301	1.976542
94	9	0	5.222629	-1.075545	3.387306
95	9	0	6.936891	-1.872245	2.303765
96	9	0	3.248021	-5.010723	-1.609259
97	9	0	5.032698	-4.149686	-2.498884
98	9	0	5.186435	-5.281121	-0.648344
99	1	0	-4.981252	1.580015	0.105921

INT 13



HF (B3LYP/6-31G(d)) = -3425.0099615 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.761877 (Hartree/Particle)

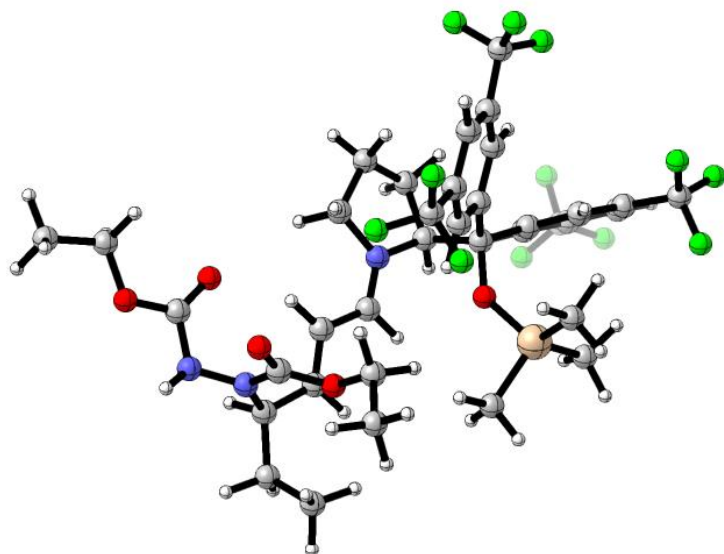
Thermal correction = 0.660003 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.529223	-2.034800	-0.429830
2	6	0	-3.103014	-1.851956	-0.878277
3	6	0	-2.518043	-0.655720	-1.121619
4	6	0	-1.166836	-0.612966	-1.574111
5	7	0	-0.503112	0.471697	-1.876249
6	6	0	0.912049	0.462801	-2.348935
7	6	0	1.027292	1.732296	-3.229353
8	6	0	-0.339585	2.463798	-3.153083
9	6	0	-1.111660	1.822926	-1.989326
10	1	0	-3.085710	0.258495	-0.982719
11	1	0	-0.623284	-1.546654	-1.681506
12	1	0	1.032336	-0.429640	-2.965816
13	1	0	1.858301	2.356864	-2.903095
14	1	0	1.251333	1.442119	-4.257440
15	1	0	-0.230141	3.541249	-3.003878
16	1	0	-0.897642	2.320243	-4.081889
17	1	0	-0.979923	2.351637	-1.041623
18	1	0	-2.180677	1.732767	-2.180203
19	6	0	2.044933	0.275399	-1.233908
20	8	0	3.197667	0.302643	-2.047936
21	14	0	4.861457	0.687988	-1.932930
22	6	0	5.466261	0.246688	-3.655537
23	1	0	6.537846	0.459086	-3.751580
24	1	0	5.318422	-0.816349	-3.877304
25	1	0	4.942149	0.826954	-4.423337
26	6	0	5.119192	2.521522	-1.591976
27	1	0	4.804345	2.818677	-0.586788
28	1	0	6.188688	2.751733	-1.680310
29	1	0	4.590049	3.150557	-2.317171
30	6	0	5.739130	-0.360788	-0.635032
31	1	0	6.820739	-0.298881	-0.812077
32	1	0	5.565345	-0.017203	0.389801
33	1	0	5.462053	-1.419408	-0.698606
34	6	0	2.137821	1.328166	-0.107898
35	6	0	2.879290	1.008487	1.039880
36	6	0	1.621054	2.623828	-0.193649
37	6	0	3.094822	1.944122	2.050912
38	1	0	3.303148	0.017555	1.152660
39	6	0	1.806606	3.550895	0.834809
40	1	0	1.084518	2.957540	-1.067088
41	6	0	2.548933	3.223853	1.965729
42	1	0	2.704842	3.946906	2.756594
43	6	0	1.865117	-1.138244	-0.633730
44	6	0	1.028611	-1.380013	0.464620
45	6	0	2.507539	-2.225628	-1.231596
46	6	0	0.844162	-2.678083	0.946923
47	1	0	0.527852	-0.557857	0.964587
48	6	0	2.340476	-3.518199	-0.729839
49	1	0	3.157703	-2.056678	-2.081449
50	6	0	1.505653	-3.756776	0.359619

51	1	0	1.383426	-4.759354	0.750666
52	6	0	-4.726315	-3.293284	0.458173
53	1	0	-5.732669	-3.224655	0.885759
54	1	0	-4.020372	-3.271036	1.291448
55	6	0	-4.593949	-4.605852	-0.321434
56	1	0	-4.777588	-5.455649	0.343387
57	1	0	-5.318578	-4.661424	-1.142220
58	1	0	-3.593351	-4.743311	-0.747846
59	1	0	-2.535624	-2.767970	-1.034407
60	7	0	-5.114060	-0.805854	0.132470
61	7	0	-6.155043	-0.212232	-0.563187
62	1	0	-7.066687	-0.304069	-0.123496
63	6	0	-5.918335	1.037619	-1.135156
64	8	0	-7.089565	1.615170	-1.416016
65	8	0	-4.817250	1.494996	-1.387089
66	6	0	-4.803710	-0.249377	1.369641
67	8	0	-5.406073	0.693808	1.843645
68	8	0	-3.758263	-0.883958	1.927099
69	6	0	-7.030255	2.910308	-2.074743
70	1	0	-6.456224	3.591839	-1.440984
71	1	0	-6.497882	2.791119	-3.023104
72	6	0	-3.367185	-0.441796	3.259893
73	1	0	-2.326475	-0.757821	3.336961
74	1	0	-3.425866	0.648122	3.291747
75	6	0	-4.228764	-1.080616	4.335275
76	1	0	-3.861009	-0.778678	5.322239
77	1	0	-5.269215	-0.756384	4.245622
78	1	0	-4.186588	-2.172842	4.274321
79	6	0	-8.456916	3.380043	-2.274730
80	1	0	-8.973690	3.481771	-1.315570
81	1	0	-8.452115	4.357182	-2.768697
82	1	0	-9.017441	2.679965	-2.901939
83	6	0	3.948883	1.535930	3.225515
84	6	0	1.139716	4.896947	0.703902
85	6	0	3.072047	-4.650226	-1.408355
86	6	0	-0.129779	-2.908986	2.073641
87	9	0	2.553595	-4.897637	-2.633065
88	9	0	3.007024	-5.793604	-0.701952
89	9	0	4.375688	-4.345764	-1.588182
90	9	0	-1.406538	-2.956686	1.605429
91	9	0	0.098533	-4.062971	2.721350
92	9	0	-0.091085	-1.906782	2.980946
93	9	0	3.465856	0.421611	3.817005
94	9	0	5.211164	1.249984	2.825729
95	9	0	4.025376	2.499075	4.160389
96	9	0	1.289637	5.399429	-0.543331
97	9	0	-0.193856	4.796478	0.921719
98	9	0	1.627391	5.796391	1.574599
99	1	0	-5.112542	-2.204559	-1.345717

INT 14



HF (B3LYP/6-31G(d)) = -3425.0150931 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.761849 (Hartree/Particle)
 Thermal correction = 0.658692 Hartrees

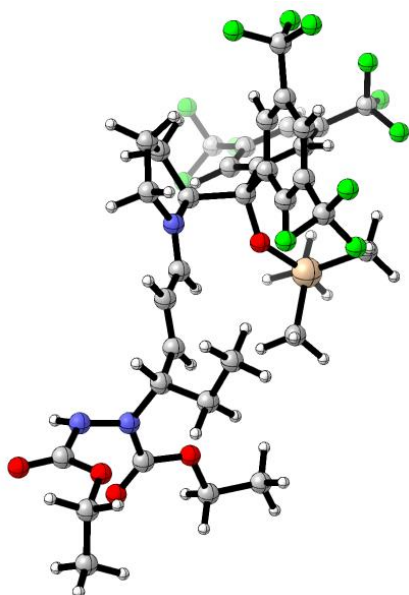
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.866916	-2.750848	-0.370372
2	6	0	-3.363347	-2.612248	-0.438644
3	6	0	-2.721209	-1.561761	-1.003685
4	6	0	-1.297968	-1.586558	-1.095831
5	7	0	-0.573023	-0.667439	-1.674176
6	6	0	0.908223	-0.751076	-1.781922
7	6	0	1.212256	0.154845	-2.990906
8	6	0	0.071135	1.192646	-3.045603
9	6	0	-1.142033	0.492505	-2.416845
10	1	0	-3.294617	-0.722051	-1.389979
11	1	0	-0.751022	-2.418655	-0.665833
12	1	0	1.141572	-1.797060	-1.982951
13	1	0	2.195929	0.622575	-2.921331
14	1	0	1.210608	-0.459634	-3.896859
15	1	0	0.329226	2.090288	-2.481686
16	1	0	-0.142455	1.499694	-4.071627
17	1	0	-1.702475	1.127786	-1.726710
18	1	0	-1.835998	0.101644	-3.165579
19	6	0	1.621621	-0.409429	-0.409959
20	8	0	1.058925	-1.345883	0.497204
21	14	0	1.422548	-2.000633	2.039166
22	6	0	2.966334	-3.075767	1.997538
23	1	0	2.941562	-3.764663	2.851482
24	1	0	3.017389	-3.683536	1.087195
25	1	0	3.890971	-2.496094	2.074044
26	6	0	1.571091	-0.672603	3.366388
27	1	0	0.684617	-0.032429	3.430678

28	1	0	1.689969	-1.169579	4.337943
29	1	0	2.444772	-0.025882	3.233350
30	6	0	-0.101982	-3.061065	2.351346
31	1	0	-0.036678	-3.540896	3.335245
32	1	0	-1.022453	-2.465377	2.334427
33	1	0	-0.197798	-3.858919	1.604940
34	6	0	3.145666	-0.637538	-0.529392
35	6	0	3.992609	-0.101151	0.448802
36	6	0	3.718619	-1.453414	-1.513031
37	6	0	5.358509	-0.384239	0.454633
38	1	0	3.591904	0.546089	1.220831
39	6	0	5.089527	-1.717700	-1.518024
40	1	0	3.119504	-1.905813	-2.292788
41	6	0	5.920430	-1.192646	-0.530521
42	1	0	6.981367	-1.411960	-0.526629
43	6	0	1.278456	1.028660	0.023511
44	6	0	2.030406	2.134748	-0.396710
45	6	0	0.146047	1.259655	0.807179
46	6	0	1.655963	3.429952	-0.037770
47	1	0	2.922254	1.997895	-0.997333
48	6	0	-0.219423	2.557065	1.173434
49	1	0	-0.451408	0.422421	1.145987
50	6	0	0.529265	3.653136	0.754944
51	1	0	0.247948	4.658607	1.043208
52	6	0	-5.352680	-3.995802	0.405385
53	1	0	-4.905345	-4.864123	-0.097904
54	1	0	-6.433257	-4.076172	0.238771
55	6	0	-5.056907	-4.066119	1.905365
56	1	0	-5.391138	-5.032048	2.298079
57	1	0	-3.986817	-3.969401	2.120100
58	1	0	-5.578425	-3.281742	2.459227
59	1	0	-2.782918	-3.454165	-0.063133
60	7	0	-5.546453	-1.488932	-0.023207
61	7	0	-6.559378	-1.073937	-0.874740
62	1	0	-7.478833	-1.028023	-0.446186
63	6	0	-6.263276	-0.022450	-1.742709
64	8	0	-7.402135	0.510193	-2.193174
65	8	0	-5.137489	0.302734	-2.076202
66	6	0	-5.266900	-0.640929	1.042110
67	8	0	-5.895130	0.378086	1.253882
68	8	0	-4.234695	-1.095870	1.776128
69	6	0	-7.272218	1.576181	-3.173812
70	1	0	-6.661523	2.371610	-2.737950
71	1	0	-6.747048	1.178822	-4.047491
72	6	0	-3.875375	-0.287273	2.936881
73	1	0	-2.811332	-0.489550	3.077701
74	1	0	-4.008159	0.761723	2.675135
75	6	0	-4.689561	-0.671115	4.159208
76	1	0	-4.352376	-0.081035	5.018697
77	1	0	-5.751148	-0.461341	3.999781
78	1	0	-4.566717	-1.731133	4.402385
79	6	0	-8.670907	2.049517	-3.513496
80	1	0	-9.181056	2.432526	-2.624442
81	1	0	-8.612845	2.856185	-4.251628
82	1	0	-9.269088	1.237018	-3.937485
83	6	0	6.198316	0.128155	1.597276
84	6	0	5.680897	-2.542096	-2.634942
85	6	0	-1.461537	2.731018	2.006637

86	6	0	2.439233	4.598511	-0.582881
87	9	0	-2.561651	2.342032	1.313642
88	9	0	-1.652778	4.000684	2.396256
89	9	0	-1.418644	1.957123	3.120313
90	9	0	2.002899	4.928852	-1.821362
91	9	0	2.316593	5.692868	0.191226
92	9	0	3.753055	4.310489	-0.691060
93	9	0	5.883356	1.402880	1.910156
94	9	0	5.988731	-0.613885	2.712141
95	9	0	7.514016	0.080929	1.322478
96	9	0	4.795604	-3.450928	-3.102560
97	9	0	6.038748	-1.765139	-3.681120
98	9	0	6.780796	-3.207668	-2.234688
99	1	0	-5.176862	-2.917410	-1.410142

INT 15



HF (B3LYP/6-31G(d)) = -3425.0116235 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761520 (Hartree/Particle)

Thermal correction = 0.656982 Hartrees

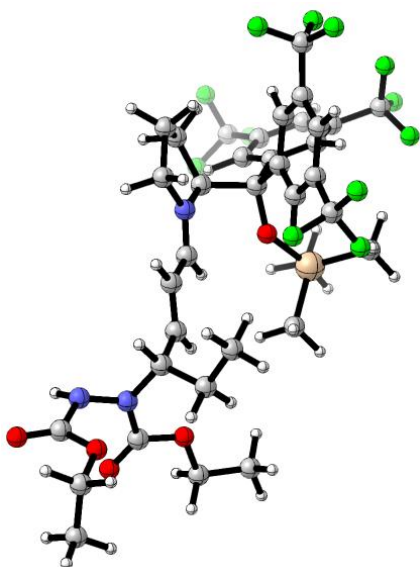
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.960395	0.237431	-0.293322
2	6	0	-3.558722	-0.297035	-0.384519
3	6	0	-2.582269	0.238051	-1.156747
4	6	0	-1.279638	-0.353894	-1.150490
5	7	0	-0.253215	0.071782	-1.832242
6	6	0	1.086075	-0.583108	-1.783615
7	6	0	1.762434	-0.082200	-3.074335

8	6	0	1.087615	1.257262	-3.441045
9	6	0	-0.309381	1.199563	-2.804422
10	1	0	-2.778866	1.114470	-1.766879
11	1	0	-1.102401	-1.221041	-0.524307
12	1	0	0.905100	-1.658159	-1.813669
13	1	0	2.843076	0.017800	-2.961762
14	1	0	1.590872	-0.820528	-3.863495
15	1	0	1.650528	2.107582	-3.052913
16	1	0	1.016299	1.381669	-4.523566
17	1	0	-0.578002	2.117438	-2.274779
18	1	0	-1.092742	0.972613	-3.532935
19	6	0	1.809084	-0.316941	-0.399642
20	8	0	0.945174	-0.930621	0.546199
21	14	0	1.108469	-1.646874	2.098466
22	6	0	2.048069	-3.272283	2.002058
23	1	0	1.946435	-3.803955	2.956744
24	1	0	1.647440	-3.925048	1.218166
25	1	0	3.117705	-3.135688	1.816325
26	6	0	1.891237	-0.477114	3.348728
27	1	0	1.422631	0.513306	3.347486
28	1	0	1.752647	-0.901427	4.351583
29	1	0	2.968771	-0.349052	3.203893
30	6	0	-0.695491	-1.963513	2.533324
31	1	0	-0.776265	-2.382948	3.543118
32	1	0	-1.287840	-1.041109	2.510437
33	1	0	-1.153783	-2.682487	1.843194
34	6	0	3.194537	-0.996802	-0.374532
35	6	0	4.168242	-0.544920	0.523844
36	6	0	3.477659	-2.144472	-1.127337
37	6	0	5.378487	-1.223358	0.676522
38	1	0	3.984153	0.334077	1.130096
39	6	0	4.695873	-2.809957	-0.987308
40	1	0	2.756754	-2.555851	-1.822876
41	6	0	5.655057	-2.358684	-0.080664
42	1	0	6.591524	-2.889448	0.041838
43	6	0	1.890537	1.197356	-0.131053
44	6	0	2.883088	1.997603	-0.712009
45	6	0	0.920863	1.818441	0.659109
46	6	0	2.889662	3.379061	-0.518023
47	1	0	3.669247	1.551652	-1.311396
48	6	0	0.943393	3.199498	0.868634
49	1	0	0.150444	1.220859	1.129170
50	6	0	1.922572	3.993481	0.278143
51	1	0	1.940349	5.064185	0.440571
52	6	0	-5.242487	0.952146	1.052025
53	1	0	-4.961406	0.303839	1.885850
54	1	0	-6.327923	1.089250	1.100423
55	6	0	-4.537549	2.308207	1.162704
56	1	0	-4.797946	2.788790	2.111029
57	1	0	-3.446285	2.221167	1.131530
58	1	0	-4.844455	2.984088	0.355589
59	1	0	-3.344914	-1.172789	0.226253
60	7	0	-5.914856	-0.848412	-0.619351
61	7	0	-6.608244	-0.720086	-1.815511
62	1	0	-6.465806	-1.488257	-2.464063
63	6	0	-7.940992	-0.287299	-1.819767
64	8	0	-8.236438	0.410304	-0.713890
65	8	0	-8.667836	-0.482302	-2.770830

66	6	0	-6.241052	-1.942552	0.169531
67	8	0	-7.106769	-2.742559	-0.122913
68	8	0	-5.450961	-2.012331	1.260923
69	6	0	-9.597809	0.921159	-0.626339
70	1	0	-9.509504	1.790023	0.029016
71	1	0	-9.909375	1.245947	-1.621022
72	6	0	-5.741608	-3.113768	2.169179
73	1	0	-6.795105	-3.056080	2.453885
74	1	0	-5.586077	-4.053410	1.631725
75	1	0	-5.114698	0.963051	-1.094997
76	6	0	-0.139728	3.802675	1.724934
77	6	0	3.912823	4.205359	-1.255139
78	6	0	4.991035	-4.008318	-1.856647
79	6	0	6.387204	-0.685173	1.661599
80	6	0	-10.539893	-0.124172	-0.054811
81	1	0	-11.539107	0.309863	0.062084
82	1	0	-10.615686	-0.985888	-0.723763
83	1	0	-10.195730	-0.466878	0.926115
84	6	0	-4.818895	-2.976434	3.363262
85	1	0	-4.993323	-2.033099	3.890598
86	1	0	-5.006837	-3.798014	4.062128
87	1	0	-3.767380	-3.019470	3.060480
88	9	0	0.085418	5.095885	2.007375
89	9	0	-1.344502	3.726298	1.101150
90	9	0	-0.268404	3.135425	2.893358
91	9	0	4.079597	5.420673	-0.704962
92	9	0	5.114143	3.592979	-1.289686
93	9	0	3.528069	4.391388	-2.542664
94	9	0	5.784812	-0.314526	2.816488
95	9	0	7.011052	0.409254	1.176226
96	9	0	7.332272	-1.593315	1.963932
97	9	0	5.585144	-3.639773	-3.012776
98	9	0	5.813701	-4.879013	-1.241866
99	9	0	3.859804	-4.670776	-2.186860

INT 16



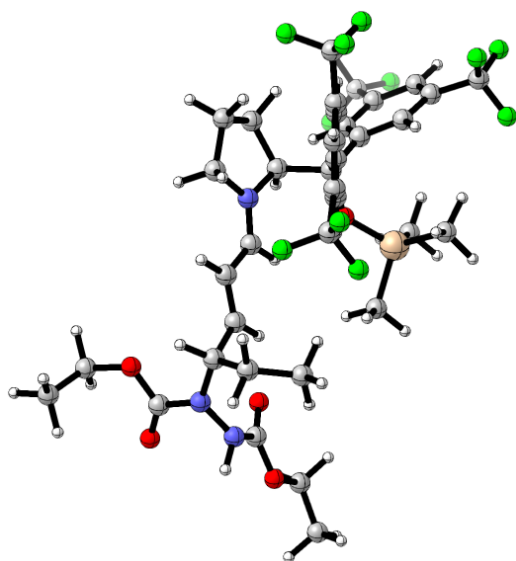
HF (B3LYP/6-31G(d)) = -3425.0116232 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.761511 (Hartree/Particle)
 Thermal correction = 0.656940 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.960516	0.237313	-0.294072
2	6	0	-3.558808	-0.297110	-0.384861
3	6	0	-2.582280	0.237793	-1.157137
4	6	0	-1.279616	-0.354083	-1.150605
5	7	0	-0.253168	0.071484	-1.832398
6	6	0	1.086161	-0.583354	-1.783640
7	6	0	1.762588	-0.082449	-3.074334
8	6	0	1.087800	1.257018	-3.441017
9	6	0	-0.309363	1.199058	-2.804834
10	1	0	-2.778871	1.113999	-1.767574
11	1	0	-1.102382	-1.221071	-0.524202
12	1	0	0.905234	-1.658415	-1.813675
13	1	0	2.843234	0.017511	-2.961741
14	1	0	1.591004	-0.820756	-3.863509
15	1	0	1.650505	2.107298	-3.052499
16	1	0	1.016821	1.381669	-4.523533
17	1	0	-0.578444	2.116974	-2.275500
18	1	0	-1.092408	0.971692	-3.533561
19	6	0	1.809103	-0.317105	-0.399651
20	8	0	0.945144	-0.930735	0.546196
21	14	0	1.108492	-1.646844	2.098538
22	6	0	1.891475	-0.477088	3.348674
23	1	0	1.752525	-0.901145	4.351590
24	1	0	2.969089	-0.349554	3.203991
25	1	0	1.423308	0.513538	3.347166
26	6	0	-0.695468	-1.963314	2.533495
27	1	0	-1.153815	-2.682408	1.843529
28	1	0	-0.776234	-2.382541	3.543378
29	1	0	-1.287780	-1.040893	2.510439
30	6	0	2.048059	-3.272287	2.002302
31	1	0	1.946685	-3.803691	2.957162
32	1	0	1.647280	-3.925282	1.218681
33	1	0	3.117645	-3.135679	1.816277
34	6	0	3.194575	-0.996922	-0.374482
35	6	0	4.168244	-0.544961	0.523891
36	6	0	3.477763	-2.144616	-1.127237
37	6	0	5.378549	-1.223291	0.676576
38	1	0	3.984063	0.334002	1.130166
39	6	0	4.696047	-2.809968	-0.987229
40	1	0	2.756842	-2.556113	-1.822700
41	6	0	5.655212	-2.358589	-0.080610
42	1	0	6.591745	-2.889240	0.041848
43	6	0	1.890536	1.197211	-0.131125
44	6	0	2.883221	1.997441	-0.711907
45	6	0	0.920716	1.818315	0.658830
46	6	0	2.889804	3.378887	-0.517894
47	1	0	3.669460	1.551470	-1.311170

48	6	0	0.943213	3.199384	0.868326
49	1	0	0.150209	1.220745	1.128762
50	6	0	1.922540	3.993329	0.278066
51	1	0	1.940324	5.064030	0.440535
52	6	0	-5.242637	0.953047	1.050754
53	1	0	-4.961328	0.305485	1.885082
54	1	0	-6.328102	1.089919	1.099126
55	6	0	-4.538035	2.309371	1.160282
56	1	0	-4.798430	2.790619	2.108272
57	1	0	-3.446752	2.222604	1.129058
58	1	0	-4.845229	2.984547	0.352686
59	1	0	-3.345037	-1.172676	0.226193
60	7	0	-5.914930	-0.848793	-0.619329
61	7	0	-6.608427	-0.721294	-1.815523
62	1	0	-6.466002	-1.489910	-2.463550
63	6	0	-7.941222	-0.288650	-1.819962
64	8	0	-8.236623	0.409756	-0.714575
65	8	0	-8.668134	-0.484419	-2.770813
66	6	0	-6.241123	-1.942337	0.170379
67	8	0	-7.106930	-2.742495	-0.121377
68	8	0	-5.450949	-2.011345	1.261762
69	6	0	-9.598047	0.920499	-0.627213
70	1	0	-9.509702	1.790268	0.026937
71	1	0	-9.910048	1.243856	-1.622221
72	6	0	-5.741587	-3.112065	2.170886
73	1	0	-6.795024	-3.054016	2.455745
74	1	0	-5.586286	-4.052129	1.634102
75	1	0	-5.114843	0.962351	-1.096268
76	6	0	-0.140133	3.802587	1.724309
77	6	0	3.913064	4.205325	-1.254723
78	6	0	4.991423	-4.008215	-1.856661
79	6	0	6.387136	-0.685070	1.661763
80	6	0	-10.539666	-0.124298	-0.053948
81	1	0	-11.538987	0.309588	0.062590
82	1	0	-10.615363	-0.986984	-0.721664
83	1	0	-10.195150	-0.465519	0.927373
84	6	0	-4.818629	-2.973956	3.364688
85	1	0	-4.992811	-2.030181	3.891322
86	1	0	-5.006552	-3.794963	4.064232
87	1	0	-3.767182	-3.017376	3.061726
88	9	0	0.085056	5.095741	2.006960
89	9	0	-1.344690	3.726404	1.100072
90	9	0	-0.269299	3.135228	2.892617
91	9	0	4.080795	5.419981	-0.703356
92	9	0	5.114023	3.592308	-1.290500
93	9	0	3.527749	4.392933	-2.541831
94	9	0	5.784638	-0.315010	2.816803
95	9	0	7.010563	0.409747	1.176735
96	9	0	7.332529	-1.592974	1.963755
97	9	0	5.585818	-3.639509	-3.012595
98	9	0	5.813960	-4.878978	-1.241790
99	9	0	3.860292	-4.670625	-2.187247

INT 17



HF (B3LYP/6-31G(d)) = -3425.0157765 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.761510 (Hartree/Particle)

Thermal correction = 0.657042 Hartrees

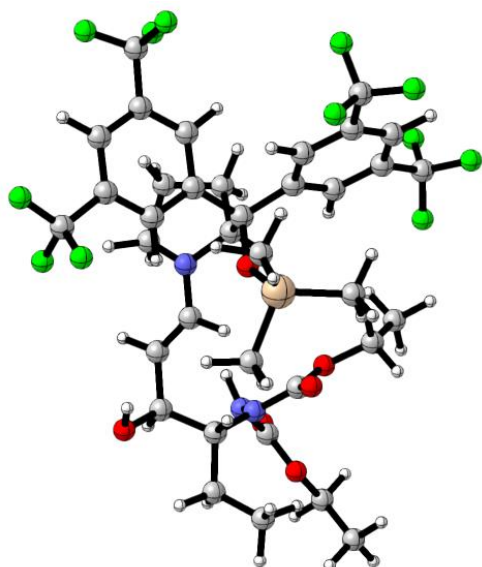
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.867670	1.158082	-0.162593
2	6	0	-3.589617	0.414111	-0.437719
3	6	0	-2.571994	0.895956	-1.191818
4	6	0	-1.369373	0.132475	-1.296019
5	7	0	-0.281927	0.523378	-1.902568
6	6	0	0.991924	-0.249934	-1.888557
7	6	0	1.796685	0.385831	-3.039823
8	6	0	1.250275	1.816717	-3.233510
9	6	0	-0.184422	1.785164	-2.687375
10	1	0	-2.642913	1.867960	-1.670005
11	1	0	-1.316703	-0.832660	-0.804253
12	1	0	0.733650	-1.289381	-2.098525
13	1	0	2.870297	0.379766	-2.844811
14	1	0	1.633312	-0.207286	-3.944400
15	1	0	1.849994	2.549400	-2.691631
16	1	0	1.259553	2.104838	-4.286782
17	1	0	-0.413839	2.632623	-2.035848
18	1	0	-0.934650	1.741571	-3.482209
19	6	0	1.639107	-0.257264	-0.435544
20	8	0	0.706517	-0.994983	0.341033
21	14	0	0.768649	-1.984273	1.744404
22	6	0	1.624470	-1.127569	3.187710
23	1	0	1.356381	-1.654868	4.112263
24	1	0	2.716305	-1.147972	3.113889
25	1	0	1.305262	-0.085905	3.303770
26	6	0	-1.060137	-2.227500	2.108714
27	1	0	-1.584929	-2.698770	1.269418

28	1	0	-1.184789	-2.883432	2.978739
29	1	0	-1.566112	-1.282453	2.338237
30	6	0	1.579501	-3.639521	1.370783
31	1	0	1.445381	-4.304864	2.233222
32	1	0	1.121746	-4.130573	0.504391
33	1	0	2.655199	-3.556646	1.187527
34	6	0	3.003277	-0.975393	-0.451451
35	6	0	3.942285	-0.704900	0.549458
36	6	0	3.292741	-1.997665	-1.365821
37	6	0	5.126720	-1.437982	0.642941
38	1	0	3.754449	0.078373	1.274131
39	6	0	4.488136	-2.711965	-1.285455
40	1	0	2.592730	-2.267298	-2.146976
41	6	0	5.413393	-2.442963	-0.276401
42	1	0	6.333871	-3.009532	-0.205995
43	6	0	1.718429	1.190935	0.085310
44	6	0	2.762846	2.055687	-0.263097
45	6	0	0.655250	1.707939	0.831439
46	6	0	2.727298	3.401967	0.107335
47	1	0	3.615097	1.691831	-0.826829
48	6	0	0.615990	3.056206	1.188628
49	1	0	-0.154301	1.053972	1.127706
50	6	0	1.651537	3.917051	0.829793
51	1	0	1.623928	4.963561	1.108228
52	6	0	-4.798839	1.958430	1.170763
53	1	0	-5.821605	2.281908	1.395859
54	1	0	-4.222558	2.864227	0.951519
55	6	0	-4.170119	1.272748	2.389881
56	1	0	-4.201501	1.956987	3.243994
57	1	0	-4.697307	0.358441	2.669997
58	1	0	-3.115606	1.030974	2.215550
59	1	0	-3.511156	-0.573268	0.013883
60	7	0	-6.020468	0.241193	-0.232836
61	7	0	-6.380187	-0.485738	0.890845
62	1	0	-7.329006	-0.315470	1.208507
63	6	0	-5.963063	-1.815356	0.969565
64	8	0	-6.729978	-2.466443	1.849063
65	8	0	-5.003550	-2.271550	0.374646
66	6	0	-6.599293	-0.169108	-1.432391
67	8	0	-7.484837	-0.998638	-1.490466
68	8	0	-6.064122	0.488959	-2.478858
69	6	0	-6.370608	-3.851153	2.111531
70	1	0	-6.413741	-4.401502	1.167691
71	1	0	-5.339742	-3.876826	2.476982
72	6	0	-6.670051	0.219268	-3.776107
73	1	0	-5.875374	0.452723	-4.487808
74	1	0	-6.906166	-0.844937	-3.831209
75	6	0	-7.900151	1.080918	-4.002996
76	1	0	-8.288147	0.905291	-5.012394
77	1	0	-8.687468	0.829755	-3.286688
78	1	0	-7.657533	2.144379	-3.908907
79	6	0	-7.354007	-4.387078	3.132129
80	1	0	-8.378646	-4.339814	2.750992
81	1	0	-7.116372	-5.433126	3.351848
82	1	0	-7.301369	-3.818461	4.065834
83	6	0	6.056072	-1.147404	1.794858
84	6	0	4.796666	-3.754516	-2.332119
85	6	0	-0.621670	3.574043	1.874508

86	6	0	3.826170	4.310463	-0.383019
87	9	0	-1.642176	3.692239	0.980067
88	9	0	-0.437666	4.780773	2.433576
89	9	0	-1.052639	2.727931	2.835672
90	9	0	3.636586	4.613668	-1.692530
91	9	0	3.871899	5.470218	0.295671
92	9	0	5.035956	3.722336	-0.289630
93	9	0	6.295350	0.176410	1.910068
94	9	0	5.505016	-1.548442	2.966336
95	9	0	7.239024	-1.773232	1.667042
96	9	0	3.672718	-4.370062	-2.761575
97	9	0	5.381445	-3.199124	-3.416884
98	9	0	5.632544	-4.700690	-1.864958
99	1	0	-5.029935	1.887157	-0.958872

EN-1



HF (B3LYP/6-31G(d)) = -3501.012727 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.775203 (Hartree/Particle)

Thermal correction = 0.668135 Hartrees

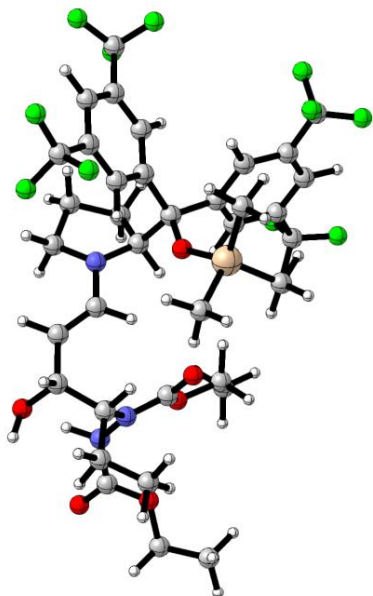
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.263191	-1.957085	0.792947
2	6	0	2.470771	-2.776129	-0.919150
3	6	0	1.587342	-1.783491	-0.666046
4	7	0	0.435089	-1.517631	-1.380800
5	6	0	-0.171758	-0.180061	-1.328484
6	6	0	-0.727127	0.033510	-2.755855
7	6	0	-0.906704	-1.381857	-3.334241
8	6	0	0.218460	-2.180308	-2.670964

9	1	0	2.279410	-3.483218	-1.722306
10	1	0	1.735482	-1.102497	0.164277
11	1	0	0.618194	0.542537	-1.103613
12	1	0	-1.648886	0.620653	-2.776863
13	1	0	0.016094	0.584320	-3.343026
14	1	0	-1.882696	-1.792224	-3.062223
15	1	0	-0.831895	-1.398160	-4.425096
16	1	0	-0.034793	-3.237111	-2.527690
17	1	0	1.143741	-2.141714	-3.268783
18	6	0	-1.213309	-0.017812	-0.149410
19	8	0	-0.456521	-0.292299	1.023994
20	14	0	-0.502750	0.091493	2.679219
21	6	0	-2.177538	-0.285276	3.471768
22	1	0	-2.056925	-0.262385	4.562927
23	1	0	-2.957390	0.441241	3.221576
24	1	0	-2.541182	-1.284897	3.206321
25	6	0	0.809367	-1.044806	3.400324
26	1	0	1.791139	-0.792835	2.985530
27	1	0	0.863947	-0.928141	4.489778
28	1	0	0.598365	-2.099830	3.189807
29	6	0	-0.008061	1.885145	2.974201
30	1	0	0.080351	2.070248	4.052555
31	1	0	0.970943	2.083185	2.523074
32	1	0	-0.728491	2.605546	2.573827
33	6	0	-1.753999	1.428698	-0.075903
34	6	0	-2.946443	1.703250	0.607317
35	6	0	-1.017364	2.520278	-0.552492
36	6	0	-3.374228	3.013878	0.823173
37	1	0	-3.544709	0.888635	0.996796
38	6	0	-1.448777	3.831678	-0.343656
39	1	0	-0.083505	2.373224	-1.078580
40	6	0	-2.629030	4.092496	0.348793
41	1	0	-2.952914	5.110492	0.527753
42	6	0	-2.331553	-1.063024	-0.291919
43	6	0	-3.483420	-0.841294	-1.056709
44	6	0	-2.166066	-2.318432	0.301216
45	6	0	-4.447030	-1.842191	-1.207074
46	1	0	-3.645646	0.115028	-1.542058
47	6	0	-3.134550	-3.313320	0.156231
48	1	0	-1.274193	-2.510602	0.883569
49	6	0	-4.283878	-3.085147	-0.597192
50	1	0	-5.035635	-3.856423	-0.707080
51	6	0	5.556592	-2.399885	1.495066
52	1	0	6.340901	-2.522932	0.736192
53	1	0	5.371008	-3.390392	1.921808
54	6	0	6.029973	-1.434365	2.584444
55	1	0	6.947928	-1.804892	3.055322
56	1	0	6.241475	-0.443179	2.172137
57	1	0	5.274438	-1.318915	3.370826
58	7	0	4.475893	-0.730319	-0.003143
59	7	0	5.091018	-0.873849	-1.236266
60	1	0	4.464855	-0.976138	-2.028807
61	6	0	6.302233	-0.283792	-1.554220
62	8	0	6.983650	0.109263	-0.465283
63	8	0	6.689351	-0.188861	-2.704266
64	6	0	3.905029	0.469817	0.356602
65	8	0	3.303368	0.652859	1.406082
66	8	0	4.088490	1.415053	-0.589280

67	6	0	8.283053	0.693876	-0.729481
68	1	0	8.903073	-0.047295	-1.242828
69	1	0	8.152813	1.547113	-1.401688
70	6	0	3.593828	2.736039	-0.259548
71	1	0	4.092640	3.080755	0.651277
72	1	0	2.522008	2.674100	-0.050862
73	1	0	3.524216	-1.684051	1.549843
74	6	0	3.883169	3.637845	-1.443781
75	1	0	3.401361	3.259139	-2.350991
76	1	0	3.492768	4.640582	-1.242212
77	1	0	4.959049	3.712336	-1.629848
78	6	0	8.876474	1.105326	0.603741
79	1	0	9.863592	1.551863	0.442997
80	1	0	8.241810	1.843337	1.104657
81	1	0	8.992250	0.241212	1.265339
82	6	0	-2.901132	-4.637131	0.834185
83	6	0	-5.691809	-1.537903	-1.997985
84	6	0	-4.672621	3.250754	1.550860
85	6	0	-0.626178	4.962862	-0.904464
86	9	0	-1.811252	-5.264532	0.335072
87	9	0	-3.947140	-5.477505	0.698976
88	9	0	-2.679373	-4.474422	2.160239
89	9	0	-6.368618	-2.655710	-2.332957
90	9	0	-6.542654	-0.747927	-1.302487
91	9	0	-5.400796	-0.878805	-3.143745
92	9	0	0.701799	4.721937	-0.771694
93	9	0	-0.856122	5.138882	-2.225434
94	9	0	-0.888597	6.134570	-0.293122
95	9	0	-4.861846	2.340828	2.535083
96	9	0	-5.734574	3.153778	0.719747
97	9	0	-4.717979	4.475288	2.114449
98	6	0	3.678293	-3.104076	-0.079085
99	1	0	4.478273	-3.452191	-0.742307
100	8	0	3.419600	-4.243981	0.767716
101	1	0	2.550895	-4.085938	1.172978

EN-2



HF (B3LYP/6-31G(d)) = -3501.0094542 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.775140 (Hartree/Particle)

Thermal correction = 0.667668 Hartrees

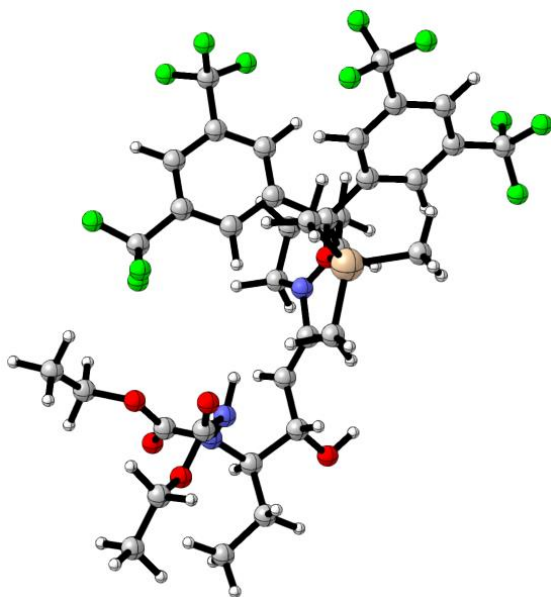
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.241756	-1.982220	0.695631
2	6	0	2.373255	-2.843587	-0.916560
3	6	0	1.510870	-1.836303	-0.674895
4	7	0	0.319667	-1.614481	-1.347723
5	6	0	-0.274224	-0.271334	-1.341134
6	6	0	-0.865958	-0.114431	-2.760757
7	6	0	-1.074939	-1.552412	-3.269285
8	6	0	0.059995	-2.332384	-2.599842
9	1	0	2.154577	-3.587373	-1.677640
10	1	0	1.696936	-1.108643	0.105563
11	1	0	0.526616	0.452500	-1.165044
12	1	0	-1.782530	0.481161	-2.783095
13	1	0	-0.133410	0.400909	-3.391967
14	1	0	-2.048036	-1.939496	-2.955124
15	1	0	-1.028458	-1.618791	-4.359971
16	1	0	-0.201546	-3.378600	-2.401501
17	1	0	0.967708	-2.332349	-3.224615
18	6	0	-1.286056	-0.047605	-0.145387
19	8	0	-0.508612	-0.288021	1.020625
20	14	0	-0.472741	0.187453	2.648144
21	6	0	-2.121746	-0.101354	3.528205
22	1	0	-1.954786	-0.043660	4.611829
23	1	0	-2.887402	0.641492	3.282060
24	1	0	-2.528229	-1.096821	3.314236
25	6	0	0.841459	-0.941490	3.377585
26	1	0	1.807195	-0.733364	2.905327

27	1	0	0.945626	-0.768968	4.456021
28	1	0	0.600162	-2.000460	3.229930
29	6	0	0.076628	1.981306	2.828052
30	1	0	0.242198	2.211356	3.888589
31	1	0	1.025681	2.133651	2.302062
32	1	0	-0.654469	2.700428	2.444668
33	6	0	-1.805408	1.408017	-0.117373
34	6	0	-2.970762	1.728398	0.592353
35	6	0	-1.071355	2.467613	-0.665079
36	6	0	-3.374805	3.053058	0.764169
37	1	0	-3.564564	0.939803	1.038246
38	6	0	-1.478413	3.792790	-0.499092
39	1	0	-0.157600	2.283691	-1.214151
40	6	0	-2.632036	4.099533	0.219209
41	1	0	-2.936780	5.128807	0.364345
42	6	0	-2.420137	-1.082055	-0.220168
43	6	0	-3.592281	-0.871061	-0.956713
44	6	0	-2.247739	-2.321528	0.404561
45	6	0	-4.568714	-1.866426	-1.050057
46	1	0	-3.758883	0.071517	-1.466712
47	6	0	-3.228183	-3.311472	0.314358
48	1	0	-1.339654	-2.505868	0.963884
49	6	0	-4.397419	-3.093633	-0.411054
50	1	0	-5.157682	-3.861500	-0.478682
51	6	0	5.459721	-2.458550	1.509711
52	1	0	6.313900	-2.621078	0.838783
53	1	0	5.213006	-3.439233	1.938093
54	6	0	5.860286	-1.500115	2.634972
55	1	0	6.725824	-1.888818	3.183115
56	1	0	6.124491	-0.517036	2.236398
57	1	0	5.040109	-1.369411	3.350414
58	7	0	4.550846	-0.771547	-0.091670
59	7	0	5.431149	-0.888400	-1.163671
60	1	0	5.240248	-1.689554	-1.759098
61	6	0	6.752811	-0.498888	-1.105507
62	8	0	7.003410	0.328495	-0.071498
63	8	0	7.567329	-0.835964	-1.947628
64	6	0	3.881082	0.410890	0.119232
65	8	0	3.101426	0.586292	1.049538
66	8	0	4.189895	1.349802	-0.793027
67	6	0	8.356118	0.839704	-0.005600
68	1	0	9.045572	-0.000433	0.124480
69	1	0	8.594456	1.324700	-0.956603
70	6	0	3.572251	2.641653	-0.587424
71	1	0	3.909366	3.045599	0.372485
72	1	0	2.486827	2.517754	-0.532918
73	1	0	3.464645	-1.672243	1.396339
74	6	0	3.975659	3.528470	-1.749598
75	1	0	3.660994	3.089725	-2.701931
76	1	0	3.494010	4.506392	-1.645371
77	1	0	5.060041	3.673782	-1.778078
78	6	0	8.420282	1.810583	1.157702
79	1	0	9.430983	2.225852	1.233649
80	1	0	7.717440	2.637675	1.015732
81	1	0	8.182041	1.311394	2.102404
82	6	0	-2.985563	-4.620080	1.017892
83	6	0	-5.835625	-1.574449	-1.809418
84	6	0	-4.645474	3.340811	1.521349

85	6	0	-0.661427	4.888799	-1.133310
86	9	0	-1.904496	-5.260345	0.515790
87	9	0	-4.034696	-5.462417	0.917220
88	9	0	-2.743664	-4.430453	2.336640
89	9	0	-6.512839	-2.699314	-2.121005
90	9	0	-6.675159	-0.788271	-1.095589
91	9	0	-5.580921	-0.918954	-2.965693
92	9	0	0.666537	4.626958	-1.054506
93	9	0	-0.950074	5.030193	-2.447070
94	9	0	-0.873949	6.083934	-0.547174
95	9	0	-4.823967	2.468521	2.541075
96	9	0	-5.734178	3.239487	0.725820
97	9	0	-4.649534	4.584313	2.044591
98	6	0	3.650094	-3.127414	-0.175788
99	1	0	3.489980	-3.970157	0.518713
100	8	0	4.589740	-3.569835	-1.187189
101	1	0	5.323050	-4.023728	-0.740537

EN-3



HF (B3LYP/6-31G(d)) = -3501.0161708 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.775088 (Hartree/Particle)

Thermal correction = 0.669430 Hartrees

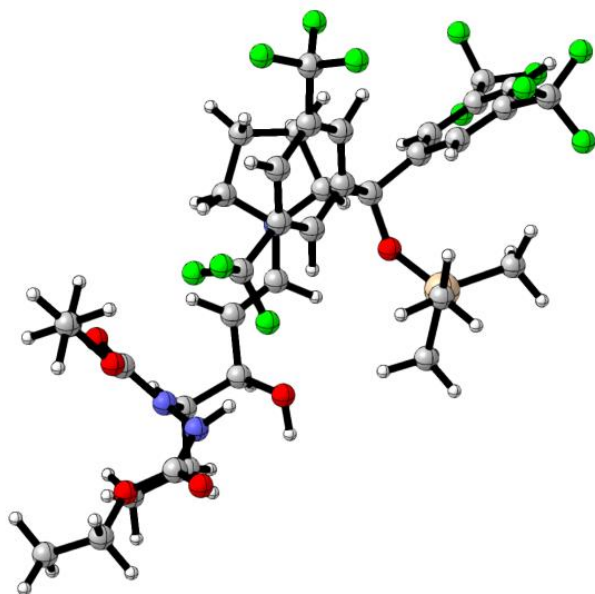
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.893847	-1.991841	-1.540170
2	6	0	-2.491437	-1.445412	-2.226441
3	6	0	-1.222635	-1.447856	-1.755991
4	7	0	-0.209589	-0.579887	-2.105372

5	6	0	1.196433	-0.892724	-1.826345
6	6	0	1.952160	-0.284306	-3.030758
7	6	0	1.023529	0.810804	-3.588990
8	6	0	-0.384091	0.297174	-3.268122
9	1	0	-2.824992	-0.711277	-2.956032
10	1	0	-0.925408	-2.188458	-1.018636
11	1	0	1.311194	-1.981506	-1.797913
12	1	0	2.941526	0.099458	-2.768264
13	1	0	2.100919	-1.067820	-3.782090
14	1	0	1.208105	1.768136	-3.095019
15	1	0	1.165564	0.962993	-4.662520
16	1	0	-1.089447	1.105547	-3.040013
17	1	0	-0.805544	-0.280691	-4.105458
18	6	0	1.666627	-0.401131	-0.394768
19	8	0	0.797727	-1.075244	0.512345
20	14	0	0.879435	-1.836347	2.028725
21	6	0	1.276334	-0.620874	3.417435
22	1	0	1.008442	-1.079418	4.378135
23	1	0	2.334319	-0.346384	3.473476
24	1	0	0.687043	0.298622	3.321968
25	6	0	-0.855575	-2.519176	2.263264
26	1	0	-1.155246	-3.153374	1.420419
27	1	0	-0.885571	-3.142705	3.166050
28	1	0	-1.613933	-1.738396	2.387549
29	6	0	2.104596	-3.273089	2.031711
30	1	0	1.966300	-3.857128	2.950828
31	1	0	1.930083	-3.949184	1.186416
32	1	0	3.150945	-2.955044	1.999967
33	6	0	3.132004	-0.790957	-0.107419
34	6	0	3.809127	-0.183307	0.959569
35	6	0	3.796846	-1.808294	-0.802777
36	6	0	5.092541	-0.586374	1.327982
37	1	0	3.327037	0.606766	1.523335
38	6	0	5.088482	-2.201440	-0.443172
39	1	0	3.320841	-2.323707	-1.627068
40	6	0	5.746049	-1.598596	0.626677
41	1	0	6.739888	-1.918524	0.915443
42	6	0	1.436748	1.113988	-0.287680
43	6	0	2.417855	2.051848	-0.634600
44	6	0	0.163071	1.582034	0.049689
45	6	0	2.131839	3.418903	-0.639304
46	1	0	3.414196	1.727741	-0.911543
47	6	0	-0.124943	2.948131	0.020789
48	1	0	-0.604221	0.870341	0.324374
49	6	0	0.854444	3.878144	-0.319882
50	1	0	0.628064	4.937169	-0.339739
51	6	0	-5.824542	-3.103431	-1.032123
52	1	0	-5.507122	-3.393820	-0.021522
53	1	0	-5.673421	-3.976607	-1.675060
54	6	0	-7.303686	-2.708095	-1.024586
55	1	0	-7.924299	-3.533810	-0.657150
56	1	0	-7.477710	-1.843245	-0.377623
57	1	0	-7.649875	-2.452874	-2.033279
58	7	0	-4.845981	-0.850886	-0.610407
59	7	0	-4.121025	-1.011349	0.559655
60	1	0	-3.160824	-0.685308	0.522259
61	6	0	-4.680559	-0.927416	1.821241
62	8	0	-6.015388	-1.063694	1.808186

63	8	0	-3.995462	-0.791584	2.820867
64	6	0	-5.296647	0.399672	-0.989830
65	8	0	-5.850651	0.631141	-2.051886
66	8	0	-5.067167	1.315399	-0.026272
67	6	0	-6.650967	-1.032844	3.110040
68	1	0	-6.266717	-1.865661	3.707066
69	1	0	-6.373549	-0.102118	3.613442
70	6	0	-5.556901	2.650976	-0.296619
71	1	0	-6.567288	2.580174	-0.707091
72	1	0	-4.911727	3.109124	-1.051592
73	1	0	-5.291486	-1.580826	-2.470738
74	6	0	-5.521778	3.416660	1.012332
75	1	0	-4.507397	3.444909	1.419059
76	1	0	-5.860098	4.445276	0.846316
77	1	0	-6.180186	2.952233	1.753676
78	6	0	-8.147496	-1.135181	2.889606
79	1	0	-8.661726	-1.113239	3.856480
80	1	0	-8.512598	-0.298221	2.285919
81	1	0	-8.407880	-2.069029	2.381683
82	6	0	-1.537960	3.389822	0.287243
83	6	0	3.225710	4.408313	-0.943370
84	6	0	5.785568	0.114875	2.467883
85	6	0	5.788909	-3.260328	-1.255792
86	9	0	-2.351069	3.066336	-0.751291
87	9	0	-1.639091	4.721667	0.470980
88	9	0	-2.052652	2.787477	1.383163
89	9	0	2.738185	5.543943	-1.488021
90	9	0	3.899353	4.764706	0.174886
91	9	0	4.136482	3.901724	-1.804458
92	9	0	4.924127	-4.194699	-1.710091
93	9	0	6.396077	-2.728270	-2.341917
94	9	0	6.740012	-3.896665	-0.541414
95	9	0	4.914898	0.443701	3.451112
96	9	0	6.369252	1.264903	2.062476
97	9	0	6.750706	-0.649965	3.017598
98	6	0	-3.471488	-2.517415	-1.846212
99	1	0	-3.092584	-3.056350	-0.962856
100	8	0	-3.666727	-3.453939	-2.927361
101	1	0	-2.780649	-3.667946	-3.259237

EN-4



HF (B3LYP/6-31G(d)) = -3501.0122542 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.775002 (Hartree/Particle)

Thermal correction = 0.670302 Hartrees

Coordinates from last standard orientation:

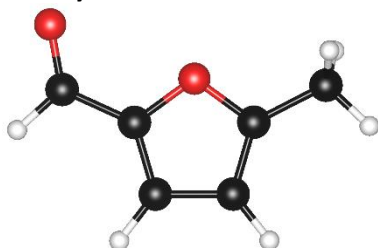
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.582775	-2.432813	-0.816746
2	6	0	-2.182474	-1.783586	-1.357716
3	6	0	-0.837845	-1.840558	-1.238026
4	7	0	0.066560	-1.028794	-1.881801
5	6	0	1.513396	-1.126563	-1.725372
6	6	0	2.050724	-0.400477	-2.981543
7	6	0	0.925779	0.554917	-3.426310
8	6	0	-0.364337	-0.121224	-2.942916
9	1	0	-2.659473	-1.072747	-2.023294
10	1	0	-0.381514	-2.545419	-0.551472
11	1	0	1.798170	-2.184632	-1.721446
12	1	0	2.992724	0.124249	-2.802432
13	1	0	2.241536	-1.147399	-3.759906
14	1	0	1.043402	1.535020	-2.956926
15	1	0	0.924916	0.709780	-4.508846
16	1	0	-1.097707	0.600998	-2.560767
17	1	0	-0.859585	-0.694107	-3.741492
18	6	0	2.040216	-0.573063	-0.325444
19	8	0	1.480599	-1.479494	0.622858
20	14	0	1.595595	-1.822684	2.281749
21	6	0	1.136462	-0.326421	3.337286
22	1	0	1.187127	-0.600501	4.398953
23	1	0	1.813798	0.522440	3.188687
24	1	0	0.117618	0.019928	3.131664
25	6	0	0.343112	-3.206958	2.498001
26	1	0	0.682554	-4.120367	1.994210

27	1	0	0.213287	-3.444916	3.561278
28	1	0	-0.633254	-2.935574	2.082046
29	6	0	3.301583	-2.461925	2.782352
30	1	0	3.202631	-3.005518	3.731220
31	1	0	3.697549	-3.166986	2.042215
32	1	0	4.046682	-1.675529	2.933207
33	6	0	3.577713	-0.643755	-0.218387
34	6	0	4.252320	0.102280	0.756446
35	6	0	4.335729	-1.533382	-0.992015
36	6	0	5.629094	-0.027356	0.946099
37	1	0	3.704605	0.794253	1.386407
38	6	0	5.714802	-1.653330	-0.810729
39	1	0	3.865912	-2.152818	-1.744777
40	6	0	6.374694	-0.903054	0.160905
41	1	0	7.443546	-1.003405	0.306963
42	6	0	1.474081	0.839062	-0.121066
43	6	0	2.169872	2.006404	-0.455669
44	6	0	0.138671	0.960390	0.282202
45	6	0	1.552237	3.258757	-0.368881
46	1	0	3.196640	1.957107	-0.798876
47	6	0	-0.483763	2.206534	0.330355
48	1	0	-0.429057	0.074189	0.532631
49	6	0	0.216855	3.369562	0.014819
50	1	0	-0.267756	4.337532	0.057823
51	6	0	-5.486004	-3.504088	-0.183242
52	1	0	-5.536267	-3.346915	0.902034
53	1	0	-5.006678	-4.480008	-0.336765
54	6	0	-6.901341	-3.538357	-0.768140
55	1	0	-7.505560	-4.309868	-0.277327
56	1	0	-7.403275	-2.576879	-0.632596
57	1	0	-6.876926	-3.764355	-1.840962
58	7	0	-5.002214	-1.073769	-0.416074
59	7	0	-5.004640	-0.767376	0.936772
60	1	0	-4.120952	-0.453330	1.321548
61	6	0	-6.121049	-0.343015	1.624989
62	8	0	-7.265951	-0.577620	0.955585
63	8	0	-6.047639	0.149104	2.737099
64	6	0	-5.147709	-0.070846	-1.356352
65	8	0	-5.057611	-0.249703	-2.561951
66	8	0	-5.426266	1.113480	-0.779742
67	6	0	-8.471671	-0.164782	1.640937
68	1	0	-8.548481	-0.715125	2.583861
69	1	0	-8.392623	0.899865	1.880295
70	6	0	-5.570366	2.231621	-1.685390
71	1	0	-6.426021	2.044580	-2.341790
72	1	0	-4.673883	2.296549	-2.307928
73	1	0	-4.716868	-2.456142	-1.901231
74	6	0	-5.761527	3.474930	-0.837861
75	1	0	-4.889656	3.645781	-0.199811
76	1	0	-5.892974	4.346533	-1.488358
77	1	0	-6.647159	3.383911	-0.200791
78	6	0	-9.641819	-0.452110	0.719948
79	1	0	-10.574207	-0.141502	1.203695
80	1	0	-9.542543	0.096742	-0.221989
81	1	0	-9.711836	-1.520701	0.492903
82	6	0	-1.961404	2.248091	0.605720
83	6	0	2.355348	4.499799	-0.655035
84	6	0	6.283870	0.723776	2.074714

85	6	0	6.506578	-2.562703	-1.714768
86	9	0	-2.660939	1.898962	-0.505390
87	9	0	-2.390887	3.474084	0.971400
88	9	0	-2.321176	1.380143	1.580428
89	9	0	1.574587	5.523398	-1.063313
90	9	0	3.022407	4.925779	0.442957
91	9	0	3.282469	4.286489	-1.616286
92	9	0	5.773469	-3.617036	-2.134809
93	9	0	6.929733	-1.911863	-2.823614
94	9	0	7.605688	-3.048800	-1.100061
95	9	0	6.114382	0.075421	3.254516
96	9	0	5.755464	1.956761	2.230052
97	9	0	7.611810	0.866569	1.889051
98	6	0	-3.074911	-2.684141	-0.545760
99	1	0	-2.892237	-3.741421	-0.803043
100	8	0	-2.744919	-2.503704	0.851480
101	1	0	-3.246075	-3.161517	1.362937

A.4.2: Energies and Reaction Coordinates for Chapter 3

Aldehyde A1



HF (M062X/6-31+G(d,p)) = -382.5277955 Hartrees

Imaginary Frequencies: none found

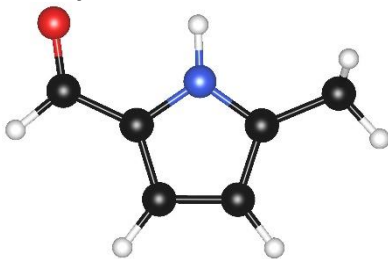
Zero-point correction = 0.108322 (Hartree/Particle)

Thermal correction = 0.076441 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.375744	-0.126055	-0.000039
2	6	0	1.299606	1.240881	-0.000011
3	1	0	2.137053	1.922463	0.000080
4	6	0	-0.088014	1.560053	0.000004
5	1	0	-0.543457	2.540475	0.000096
6	6	0	-0.754104	0.364370	-0.000024
7	8	0	0.137251	-0.661068	-0.000044
8	6	0	-2.181796	0.069935	0.000005
9	1	0	-2.818917	0.976375	0.000020
10	6	0	2.514381	-1.080950	0.000034
11	1	0	2.478849	-1.722943	-0.884593
12	1	0	3.457153	-0.532319	0.000007
13	1	0	2.478872	-1.722851	0.884728
14	8	0	-2.660308	-1.042757	0.000025

Aldehyde A2



HF (M062X/6-31+G(d,p)) = -362.6872371 Hartrees

Imaginary Frequencies: none found

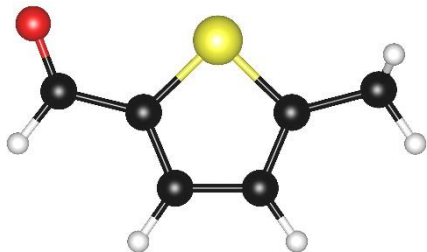
Zero-point correction = 0.121432 (Hartree/Particle)

Thermal correction = 0.089606 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.388959	-0.144738	-0.000005
2	6	0	-1.289247	1.241453	0.000009
3	6	0	0.083412	1.572549	0.000000
4	6	0	0.790787	0.379993	-0.000020
5	7	0	-0.125513	-0.644201	-0.000021
6	1	0	0.146813	-1.618146	-0.000017
7	1	0	-2.127298	1.923694	0.000026
8	1	0	0.520001	2.561822	-0.000006
9	6	0	-2.593252	-1.028401	0.000009
10	1	0	-2.616925	-1.670573	-0.886035
11	1	0	-2.617038	-1.670398	0.886175
12	1	0	-3.497466	-0.417921	-0.000107
13	6	0	2.211180	0.096703	0.000004
14	1	0	2.875750	0.980476	0.000014
15	8	0	2.663903	-1.035612	0.000014

Aldehyde A3



HF (M062X/6-31+G(d,p)) = -705.4955175 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.104736 (Hartree/Particle)

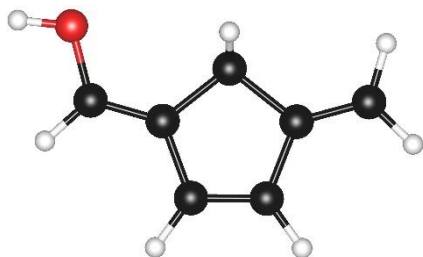
Thermal correction = 0.070700 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.904114	0.406018	0.000078
2	6	0	-0.180906	1.573719	0.000046
3	6	0	1.220542	1.346593	-0.000070
4	6	0	1.543305	0.011991	-0.000086
5	1	0	-0.646691	2.553622	0.000110
6	1	0	1.968404	2.131347	-0.000133
7	16	0	0.129805	-0.982765	-0.000004
8	6	0	2.913383	-0.593874	0.000039
9	1	0	3.072886	-1.218606	-0.883578
10	1	0	3.664247	0.199244	-0.001502
11	1	0	3.073792	-1.215983	0.885357
12	6	0	-2.359849	0.283404	0.000007
13	1	0	-2.896894	1.253285	-0.000024

14 8 0 -2.963349 -0.768221 -0.000030

Enol A4



HF (M062X/6-31+G(d,p)) = -346.5931717 Hartrees

Imaginary Frequencies: none found

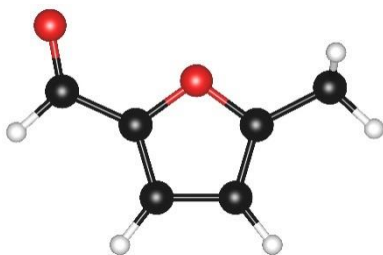
Zero-point correction = 0.131596 (Hartree/Particle)

Thermal correction = 0.099574 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.583220	-0.291727	-0.000109
2	6	0	1.439401	1.168394	0.000162
3	1	0	2.284272	1.847830	0.000309
4	6	0	0.138321	1.523998	0.000210
5	1	0	-0.240401	2.540783	0.000556
6	6	0	-0.719189	0.343465	-0.000336
7	6	0	-2.055285	0.336594	-0.000431
8	1	0	-2.644403	1.250420	-0.000299
9	6	0	2.732576	-0.977473	-0.000353
10	1	0	2.745972	-2.062922	-0.000708
11	1	0	3.689954	-0.465487	-0.000488
12	8	0	-2.740394	-0.846393	0.002435
13	1	0	-3.688099	-0.685655	-0.014639
14	6	0	0.177203	-0.877822	0.000056
15	1	0	-0.000924	-1.503524	-0.881060
16	1	0	-0.000702	-1.502873	0.881646

Enol A5



HF (M062X/6-31+G(d,p)) = -382.4882319 Hartrees

Imaginary Frequencies: none found

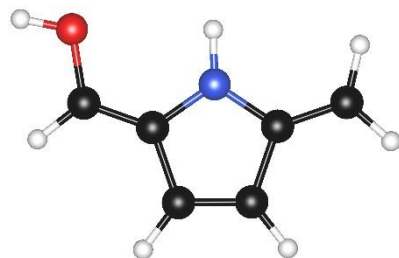
Zero-point correction = 0.107953 (Hartree/Particle)

Thermal correction = 0.076513 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.472947	-0.310612	0.000145
2	6	0	1.470349	1.150388	-0.000030
3	1	0	2.367223	1.753900	0.000023
4	6	0	0.190456	1.564747	-0.000096
5	1	0	-0.182181	2.580352	-0.000005
6	6	0	-0.652523	0.383111	0.000329
7	8	0	0.157017	-0.727622	0.000465
8	6	0	-1.989768	0.295686	-0.000219
9	1	0	-2.589699	1.199198	-0.000565
10	6	0	2.487729	-1.181719	-0.000218
11	1	0	2.304721	-2.248351	-0.000307
12	1	0	3.506223	-0.816782	-0.000947
13	8	0	-2.620485	-0.909123	-0.000267
14	1	0	-3.573680	-0.783965	0.000745

Enol A6



HF (M062X/6-31+G(d,p)) = -362.6370567 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.119909 (Hartree/Particle)

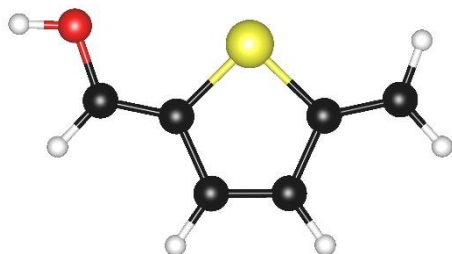
Thermal correction = 0.087709 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.503442	-0.316760	0.000030
2	6	0	-1.458566	1.152729	0.000066
3	1	0	-2.346119	1.771075	0.000128
4	6	0	-0.175706	1.562136	0.000020
5	1	0	0.192039	2.579752	0.000036
6	6	0	0.687264	0.385075	-0.000082
7	6	0	2.028144	0.325937	-0.000062
8	1	0	2.646147	1.215280	-0.000007
9	6	0	-2.589984	-1.111325	0.000050
10	1	0	-2.509377	-2.191917	0.000008
11	1	0	-3.578034	-0.670466	0.000122
12	8	0	2.637654	-0.904564	0.000145

13	1	0	3.593640	-0.806371	-0.001082
14	7	0	-0.168551	-0.711780	-0.000055
15	1	0	0.154075	-1.665137	-0.000119

Enol A7



HF (M062X/6-31+G(d,p)) = -705.4574365 Hartrees

Imaginary Frequencies: none found

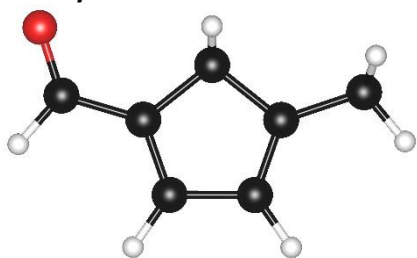
Zero-point correction = 0.104529 (Hartree/Particle)

Thermal correction = 0.071959 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.674854	-0.112802	0.000076
2	6	0	-1.373476	1.319149	0.000137
3	1	0	-2.174042	2.050523	0.000240
4	6	0	-0.061874	1.613624	0.000068
5	1	0	0.346517	2.618870	0.000107
6	6	0	0.809543	0.448104	-0.000078
7	6	0	2.149281	0.467685	-0.000068
8	1	0	2.700532	1.404107	-0.000018
9	6	0	-2.894566	-0.670051	0.000122
10	1	0	-3.039977	-1.744046	0.000063
11	1	0	-3.776512	-0.038367	0.000224
12	8	0	2.859943	-0.691066	0.000051
13	1	0	3.804831	-0.512421	-0.000865
14	16	0	-0.154076	-1.040274	-0.000106

Aldehyde A8



HF (M062X/6-31+G(d,p)) = -346.6127503 Hartrees

Imaginary Frequencies: none found

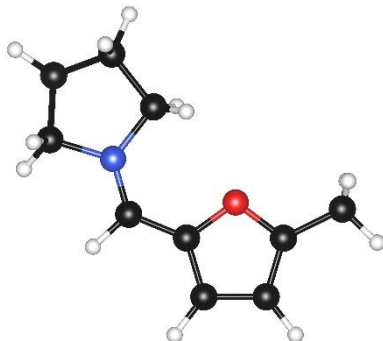
Zero-point correction = 0.130759 (Hartree/Particle)

Thermal correction = 0.098492 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.830027	0.295577	-0.000011
2	6	0	-0.159055	1.474461	-0.000091
3	6	0	1.275807	1.216431	-0.000142
4	6	0	1.489414	-0.120877	-0.000064
5	1	0	-0.616249	2.459337	-0.000163
6	1	0	2.045007	1.980624	-0.000259
7	6	0	2.798092	-0.841239	0.000002
8	1	0	2.887947	-1.487244	-0.880251
9	1	0	3.635476	-0.140054	-0.000817
10	1	0	2.888565	-1.485870	0.881209
11	6	0	-2.279187	0.140251	-0.000018
12	1	0	-2.856745	1.087657	0.000009
13	8	0	-2.850382	-0.933219	0.000156
14	6	0	0.161350	-0.829900	0.000102
15	1	0	0.040310	-1.478554	-0.877663
16	1	0	0.040379	-1.478373	0.878011

Iminium A9



HF (M062X/6-31+G(d,p)) = -519.028205 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.228589 (Hartree/Particle)

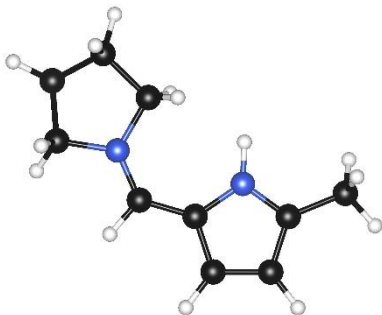
Thermal correction = 0.191270 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.071803	-1.678665	0.004074
2	6	0	3.184241	-0.819227	-0.030374
3	6	0	0.950806	-0.867405	0.026282
4	6	0	-0.408699	-1.239534	0.054838
5	6	0	2.686100	0.466379	-0.029158
6	6	0	3.336769	1.796960	-0.058705
7	7	0	-1.452144	-0.466013	0.073777

8	6	0	-1.443953	1.019389	0.063279
9	6	0	-2.842598	-0.991811	0.079932
10	6	0	-2.919511	1.387633	0.230088
11	1	0	-0.795916	1.386907	0.860248
12	6	0	-3.660028	0.202663	-0.399668
13	1	0	-2.903403	-1.874993	-0.558052
14	1	0	-3.169167	1.470108	1.292257
15	1	0	-4.702076	0.133023	-0.085526
16	1	0	-1.037387	1.348507	-0.898293
17	1	0	-3.150762	2.340271	-0.247802
18	1	0	-3.631665	0.264958	-1.491982
19	1	0	-0.599647	-2.311252	0.057511
20	1	0	2.072254	-2.760433	0.012738
21	1	0	4.228939	-1.091055	-0.053606
22	1	0	3.059039	2.378063	0.825286
23	1	0	-3.100152	-1.265023	1.108880
24	1	0	4.419962	1.679037	-0.078654
25	8	0	1.340123	0.443781	0.005360
26	1	0	3.024424	2.355435	-0.945855

Iminium A10



HF (M062X/6-31+G(d,p)) = -499.1821833 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.241203 (Hartree/Particle)

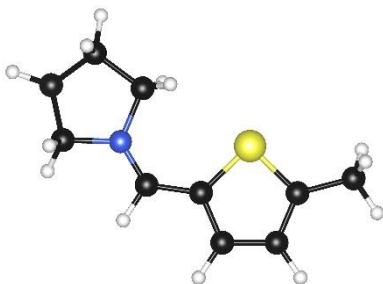
Thermal correction = 0.202793 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.996639	-1.668470	0.027647
2	6	0	3.172804	-0.930468	-0.010649
3	6	0	0.915231	-0.766556	0.026176
4	6	0	-0.432047	-1.151890	0.050023
5	6	0	2.819682	0.425304	-0.039192
6	6	0	3.687395	1.636511	-0.068385

7	7	0	-1.516532	-0.421401	0.068411
8	6	0	-1.567167	1.053771	0.082810
9	6	0	-2.881402	-1.005074	0.064175
10	6	0	-3.058864	1.369223	0.238010
11	1	0	-0.966175	1.434694	0.914624
12	6	0	-3.746083	0.159803	-0.405841
13	1	0	-2.905873	-1.878895	-0.588889
14	1	0	-3.317224	1.432134	1.299134
15	1	0	-4.785746	0.047346	-0.096183
16	1	0	-1.172792	1.427985	-0.870211
17	1	0	-3.322879	2.316372	-0.233682
18	1	0	-3.716760	0.234818	-1.497326
19	1	0	-0.597018	-2.227882	0.051474
20	1	0	1.899207	-2.745760	0.055098
21	1	0	4.185037	-1.306966	-0.019788
22	1	0	3.712983	2.117006	0.914987
23	1	0	-3.136363	-1.306299	1.086108
24	1	0	4.706845	1.356759	-0.334227
25	1	0	3.328477	2.366414	-0.799114
26	7	0	1.471294	0.509456	-0.014389
27	1	0	0.967823	1.382965	-0.048808

Iminium A11



HF (M062X/6-31+G(d,p)) = -841.9915834 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.225272 (Hartree/Particle)

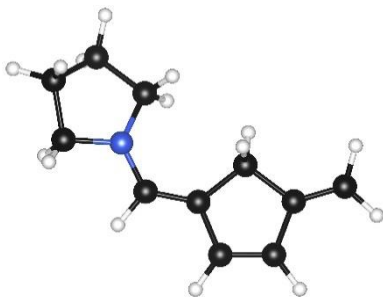
Thermal correction = 0.186669 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.720310	1.720016	0.020273
2	6	0	-2.995287	1.139557	-0.020358
3	6	0	-0.690694	0.782140	0.036786
4	6	0	0.669088	1.177416	0.061959
5	6	0	-2.956852	-0.242082	-0.037188
6	6	0	-4.116709	-1.185038	-0.063100

7	7	0	1.742356	0.444838	0.079098
8	6	0	1.791852	-1.035784	0.073044
9	6	0	3.112215	1.022841	0.079989
10	6	0	3.283625	-1.352559	0.214134
11	1	0	1.184190	-1.426914	0.893287
12	6	0	3.969756	-0.135808	-0.416371
13	1	0	3.135135	1.912600	-0.550918
14	1	0	3.550490	-1.433813	1.271986
15	1	0	5.011824	-0.028657	-0.112955
16	1	0	1.382776	-1.389160	-0.880286
17	1	0	3.541294	-2.292605	-0.274737
18	1	0	3.931750	-0.192626	-1.508670
19	1	0	0.841218	2.253715	0.063738
20	1	0	-1.536596	2.789280	0.036413
21	1	0	-3.923091	1.697979	-0.038656
22	1	0	-4.217720	-1.699675	0.897187
23	1	0	3.367293	1.296920	1.109261
24	1	0	-5.036174	-0.629560	-0.253372
25	1	0	-3.999595	-1.941921	-0.842529
26	16	0	-1.344337	-0.835852	-0.003653

Trienamine A12



HF (M062X/6-31+G(d,p)) = -482.7037554 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.238156 (Hartree/Particle)

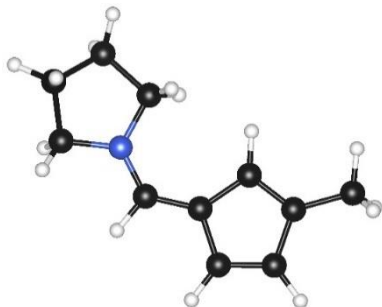
Thermal correction = 0.200257 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.986169	0.525401	0.090684
2	6	0	3.224370	-0.890424	-0.193906
3	6	0	2.053807	-1.560554	-0.274431
4	6	0	0.914644	-0.680760	-0.058783

5	1	0	4.213500	-1.317128	-0.313847
6	1	0	1.949128	-2.623620	-0.469634
7	6	0	-0.364344	-1.113596	0.005601
8	1	0	-0.551416	-2.184647	-0.079402
9	7	0	-1.496680	-0.356546	0.197985
10	6	0	3.910472	1.483933	0.237675
11	1	0	4.968826	1.258491	0.150892
12	1	0	3.634737	2.512362	0.450269
13	6	0	-2.799636	-1.009066	0.279490
14	1	0	-2.840244	-1.679950	1.143176
15	1	0	-3.011532	-1.600813	-0.627711
16	6	0	-3.763206	0.168656	0.390808
17	1	0	-3.774771	0.540132	1.420930
18	1	0	-4.784531	-0.093033	0.105329
19	6	0	-3.120024	1.201026	-0.542189
20	1	0	-3.449570	2.224287	-0.348606
21	1	0	-3.364983	0.958284	-1.581625
22	6	0	-1.613387	1.015036	-0.305882
23	1	0	-1.036162	1.127396	-1.231953
24	1	0	-1.225987	1.736727	0.423880
25	6	0	1.475178	0.711776	0.191346
26	1	0	1.191715	1.074725	1.186454
27	1	0	1.133799	1.454035	-0.536530

Fulvene trienamine A12'



HF (M062X/6-31+G(d,p)) = -482.720686 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.238397 (Hartree/Particle)

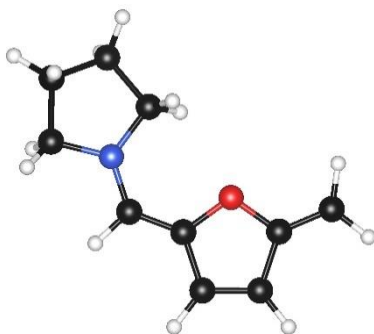
Thermal correction = 0.200207 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.868597	0.454201	0.031474
2	6	0	3.160927	-0.968990	-0.018590

3	6	0	1.985378	-1.658380	-0.047083
4	6	0	0.891804	-0.698183	-0.022925
5	1	0	4.158497	-1.393450	-0.029803
6	1	0	1.854234	-2.733793	-0.086343
7	6	0	-0.413795	-1.120447	-0.038348
8	1	0	-0.585430	-2.196641	-0.048984
9	7	0	-1.546153	-0.399018	-0.039632
10	6	0	-2.878625	-1.005029	-0.034747
11	1	0	-2.911636	-1.850111	0.658871
12	1	0	-3.142797	-1.367444	-1.038604
13	6	0	-3.780342	0.155887	0.382432
14	1	0	-3.772120	0.257793	1.472808
15	1	0	-4.813559	0.022393	0.055274
16	6	0	-3.089642	1.361604	-0.266138
17	1	0	-3.379903	2.315918	0.177781
18	1	0	-3.328913	1.396747	-1.334295
19	6	0	-1.599233	1.059706	-0.076607
20	1	0	-0.978014	1.437989	-0.895308
21	1	0	-1.209761	1.470557	0.864811
22	6	0	1.510593	0.620644	0.027420
23	1	0	1.006356	1.576379	0.073724
24	6	0	3.906864	1.533666	0.082882
25	1	0	3.443436	2.522744	0.135042
26	1	0	4.556985	1.418007	0.957441
27	1	0	4.550523	1.507961	-0.803617

Triamine A13



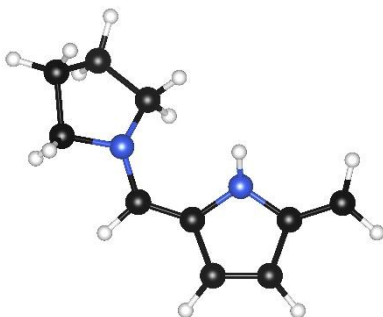
HF (M062X/6-31+G(d,p)) = -518.6058491 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.213928 (Hartree/Particle)
 Thermal correction = 0.175216 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	2.745192	0.599225	0.040828
2	6	0	3.244851	-0.767393	-0.035214
3	6	0	2.180404	-1.597980	-0.073379
4	6	0	0.984532	-0.797959	-0.023546
5	1	0	4.294025	-1.025899	-0.054817
6	1	0	2.185420	-2.678734	-0.130920
7	6	0	-0.308772	-1.201441	-0.026831
8	1	0	-0.476739	-2.274060	-0.063818
9	7	0	-1.434911	-0.439954	0.025448
10	6	0	3.391627	1.773288	0.099996
11	1	0	4.473192	1.788434	0.094450
12	1	0	2.848655	2.707707	0.154995
13	6	0	-2.766022	-1.033351	-0.003701
14	1	0	-2.841491	-1.852471	0.719833
15	1	0	-3.003213	-1.433705	-1.002591
16	6	0	-3.672495	0.147999	0.339848
17	1	0	-3.704936	0.284655	1.426068
18	1	0	-4.693889	0.013111	-0.022768
19	6	0	-2.944664	1.325690	-0.319117
20	1	0	-3.245953	2.296659	0.079918
21	1	0	-3.142050	1.325127	-1.396667
22	6	0	-1.464806	1.021085	-0.061154
23	1	0	-0.811203	1.375387	-0.863251
24	1	0	-1.109913	1.466989	0.876919
25	8	0	1.366674	0.533938	0.047267

Trienamine A14



HF (M062X/6-31+G(d,p)) = -498.7478339 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.226391 (Hartree/Particle)

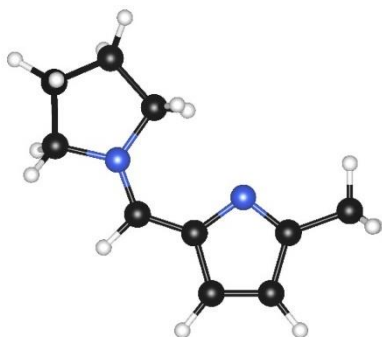
Thermal correction = 0.188996 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	2.829793	0.569448	0.106917
2	6	0	3.211752	-0.784762	-0.307677
3	6	0	2.107037	-1.555518	-0.376476
4	6	0	0.945933	-0.751857	-0.027353
5	7	0	1.431912	0.547781	0.184725
6	1	0	0.933279	1.196431	0.774274
7	1	0	4.233420	-1.077107	-0.509965
8	1	0	2.050578	-2.600391	-0.653932
9	6	0	-0.344221	-1.147847	0.055164
10	1	0	-0.573822	-2.205030	-0.063971
11	7	0	-1.413410	-0.299447	0.310760
12	6	0	3.632216	1.620059	0.364573
13	1	0	4.705196	1.513046	0.273203
14	1	0	3.236071	2.582317	0.667397
15	6	0	-2.721337	-0.909461	0.543053
16	1	0	-2.767170	-1.361328	1.538982
17	1	0	-2.924096	-1.699689	-0.201002
18	6	0	-3.695431	0.252046	0.366099
19	1	0	-3.725768	0.856623	1.279097
20	1	0	-4.710458	-0.081866	0.139434
21	6	0	-3.045561	1.042091	-0.774043
22	1	0	-3.403518	2.071489	-0.850872
23	1	0	-3.242905	0.540431	-1.727833
24	6	0	-1.550400	0.960462	-0.444271
25	1	0	-0.916551	0.939488	-1.336890
26	1	0	-1.242464	1.819290	0.167771

Fulvene trienamine A14'



HF (M062X/6-31+G(d,p)) = -498.7768887 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.227128 (Hartree/Particle)

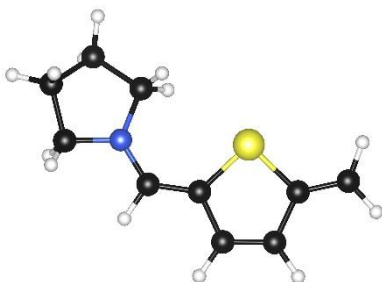
Thermal correction = 0.189429 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	2.692671	0.481895	0.026678
2	6	0	3.178172	-0.880804	0.015161
3	6	0	2.066997	-1.677579	-0.016139
4	6	0	0.942446	-0.777379	-0.024065
5	1	0	4.216558	-1.187257	0.029303
6	1	0	2.017508	-2.759682	-0.033153
7	6	0	-0.374391	-1.184693	-0.050228
8	1	0	-0.562355	-2.257509	-0.061540
9	7	0	-1.474110	-0.431614	-0.059064
10	6	0	-2.825811	-0.998428	-0.068463
11	1	0	-2.882023	-1.861841	0.600558
12	1	0	-3.095563	-1.323777	-1.082837
13	6	0	-3.695179	0.176488	0.376632
14	1	0	-3.685494	0.251199	1.469281
15	1	0	-4.731096	0.077308	0.045774
16	6	0	-2.968279	1.376841	-0.241176
17	1	0	-3.237668	2.327830	0.222601
18	1	0	-3.200938	1.442503	-1.309756
19	6	0	-1.488001	1.037726	-0.046131
20	1	0	-0.827573	1.425675	-0.823678
21	1	0	-1.093341	1.394171	0.912262
22	6	0	3.546325	1.711766	0.062109
23	1	0	4.179548	1.725047	0.955578
24	1	0	4.209354	1.754718	-0.808615
25	1	0	2.913381	2.600901	0.066281
26	7	0	1.378396	0.545287	0.003590

Trienamine A15



HF (M062X/6-31+G(d,p)) = -841.5716629 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.210916 (Hartree/Particle)

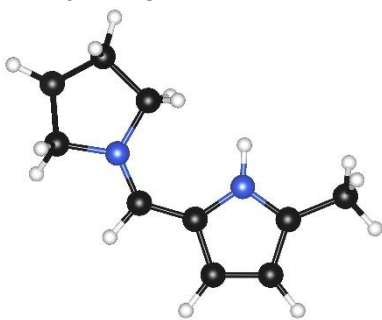
Thermal correction = 0.171406 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.055180	-0.346298	0.026575

2	6	0	-3.062135	1.102553	-0.150453
3	6	0	-1.838690	1.667574	-0.180820
4	6	0	-0.728078	0.749543	-0.036290
5	1	0	-3.997682	1.641832	-0.245034
6	1	0	-1.660578	2.731652	-0.303701
7	6	0	0.567522	1.153284	-0.002579
8	1	0	0.740098	2.227447	-0.059326
9	7	0	1.704859	0.414634	0.112913
10	6	0	-4.119293	-1.163239	0.090603
11	1	0	-5.118806	-0.750368	0.007663
12	1	0	-4.020571	-2.234036	0.224608
13	6	0	3.016371	1.056607	0.154104
14	1	0	3.068547	1.778395	0.975568
15	1	0	3.225683	1.588679	-0.787915
16	6	0	3.969654	-0.122597	0.336902
17	1	0	4.014637	-0.401804	1.394943
18	1	0	4.982564	0.100327	-0.005192
19	6	0	3.284907	-1.228782	-0.473454
20	1	0	3.625552	-2.232471	-0.210712
21	1	0	3.471005	-1.073842	-1.541617
22	6	0	1.796487	-1.019756	-0.170152
23	1	0	1.156534	-1.283277	-1.018283
24	1	0	1.476445	-1.610291	0.697772
25	16	0	-1.367927	-0.904876	0.157139

Iminium A16



HF (M062X/6-31+G(d,p)) = -483.1133476 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.251329 (Hartree/Particle)

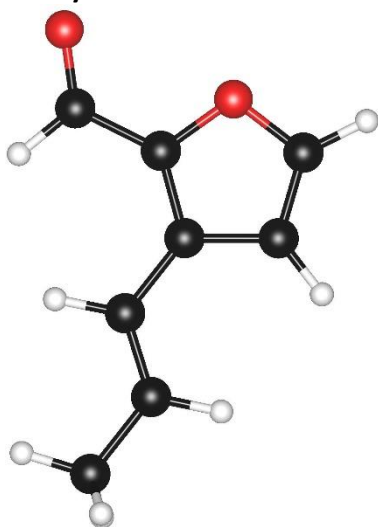
Thermal correction = 0.213321 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.886537	-1.632074	-0.005783
2	6	0	-3.159509	-0.975359	0.040865
3	6	0	-0.865688	-0.707269	-0.044241
4	6	0	0.482677	-1.130099	-0.070862
5	6	0	-2.963655	0.373338	0.031017
6	6	0	-3.997190	1.443894	0.064806
7	7	0	1.567462	-0.407366	-0.075299
8	6	0	1.632738	1.071582	-0.035825
9	6	0	2.929699	-0.999671	-0.086535
10	6	0	3.122754	1.374434	-0.211741
11	1	0	1.006168	1.492960	-0.824010
12	6	0	3.807807	0.148021	0.400483
13	1	0	2.949204	-1.888255	0.546478
14	1	0	3.366094	1.453901	-1.275577
15	1	0	4.843713	0.032365	0.079673
16	1	0	1.261928	1.406915	0.938833
17	1	0	3.403342	2.310643	0.272180
18	1	0	3.788641	0.200822	1.493555
19	1	0	0.651129	-2.206974	-0.082626
20	1	0	-1.745815	-2.709167	-0.007318
21	1	0	-4.118064	-1.477421	0.079215
22	1	0	-3.942072	2.060843	-0.838755
23	1	0	3.175415	-1.280860	-1.116285
24	1	0	-5.000507	1.022370	0.136176
25	1	0	-3.835386	2.110297	0.918710
26	6	0	-1.491390	0.666817	-0.030379
27	1	0	-1.264441	1.247653	-0.933811
28	1	0	-1.181829	1.273787	0.829821

Aldehyde B1



HF (M062X/6-31+G(d,p)) = -459.8920817 Hartrees

Imaginary Frequencies: none found

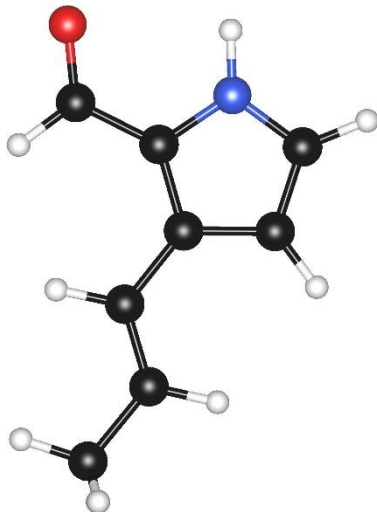
Zero-point correction = 0.142254 (Hartree/Particle)

Thermal correction = 0.107009 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.156592	0.332642	0.000118
2	6	0	-1.124296	-0.179309	-0.000104
3	6	0	-1.618166	-1.550818	-0.000173
4	1	0	-0.825187	-2.322712	-0.000582
5	6	0	1.401428	-0.432246	0.000331
6	6	0	2.623805	0.112161	-0.000054
7	6	0	3.899091	-0.671982	-0.000090
8	1	0	4.505492	-0.429055	0.878932
9	1	0	3.703921	-1.747239	0.001843
10	1	0	1.312386	-1.517116	0.000871
11	1	0	2.720925	1.197655	-0.000481
12	6	0	-1.349960	1.981493	0.000067
13	1	0	-1.942345	2.883819	0.000063
14	6	0	-0.008109	1.757558	0.000055
15	1	0	0.763585	2.512637	0.000161
16	1	0	4.503512	-0.431944	-0.881302
17	8	0	-2.036948	0.826516	-0.000184
18	8	0	-2.791127	-1.856896	0.000133

Aldehyde B2



HF (M062X/6-31+G(d,p)) = -440.0542266 Hartrees

Imaginary Frequencies: none found

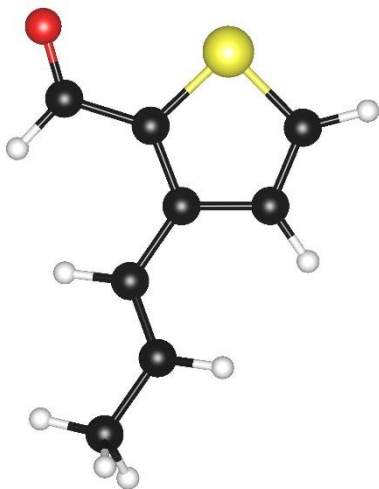
Zero-point correction = 0.155004 (Hartree/Particle)

Thermal correction = 0.119651 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.170557	0.344118	0.000294
2	6	0	-1.113486	-0.207302	0.000152
3	6	0	-1.593894	-1.574674	0.000029
4	1	0	-0.825434	-2.368153	0.000292
5	6	0	1.420573	-0.414254	0.000492
6	6	0	2.645751	0.123997	-0.000261
7	6	0	3.917927	-0.666789	-0.000212
8	1	0	4.526751	-0.429396	0.878934
9	1	0	3.716092	-1.741149	0.001731
10	1	0	1.332808	-1.500150	0.001360
11	1	0	2.747641	1.209094	-0.001064
12	6	0	-1.360946	2.008493	-0.000144
13	1	0	-1.894774	2.947372	-0.000345
14	6	0	-0.002751	1.754788	0.000230
15	1	0	0.773333	2.506068	0.000388
16	1	0	4.524921	-0.432292	-0.881427
17	8	0	-2.781778	-1.853912	-0.000277
18	7	0	-2.018887	0.823082	-0.000165
19	1	0	-3.017293	0.668069	0.000032

Aldehyde B3



HF (M062X/6-31+G(d,p)) = -782.8629443 Hartrees

Imaginary Frequencies: none found

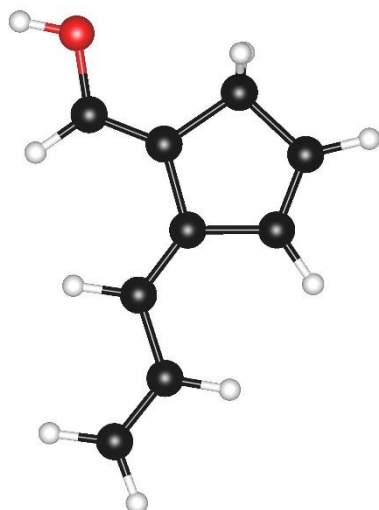
Zero-point correction = 0.138668 (Hartree/Particle)

Thermal correction = 0.102485 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.346814	-0.274220	-0.068014
2	6	0	0.863826	0.401062	-0.025519
3	6	0	1.101979	1.842626	-0.000699
4	1	0	0.199003	2.479863	-0.021404
5	6	0	-1.659162	0.379713	-0.125736
6	6	0	-2.827082	-0.232556	0.104243
7	6	0	-4.161055	0.443817	0.035167
8	1	0	-4.683485	0.373690	0.995173
9	1	0	-4.057680	1.500216	-0.225293
10	1	0	-1.674469	1.439573	-0.371163
11	1	0	-2.833113	-1.289184	0.370055
12	6	0	1.176432	-2.033636	-0.001317
13	1	0	1.591211	-3.032799	0.008566
14	6	0	-0.144064	-1.690428	-0.056519
15	1	0	-0.943562	-2.418934	-0.109864
16	1	0	-4.802421	-0.034604	-0.712885
17	8	0	2.207938	2.342223	0.044619
18	16	0	2.219791	-0.673368	0.033764

Enol B4

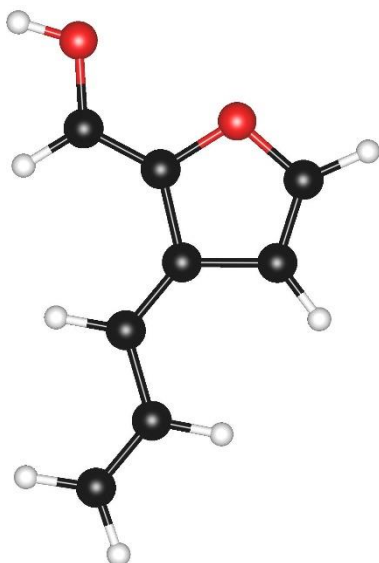


HF (M062X/6-31+G(d,p)) = -423.962005 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.165626 (Hartree/Particle)
 Thermal correction = 0.130196 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.338758	0.264310	0.000026
2	6	0	1.076592	-0.165825	-0.000039
3	6	0	1.534391	-1.419239	0.000128
4	1	0	0.882328	-2.289208	0.000318
5	6	0	-1.438569	-0.523758	-0.000098
6	6	0	-2.810125	-0.048347	0.000043
7	6	0	-3.881241	-0.855807	-0.000064
8	1	0	-4.890588	-0.460108	0.000061
9	1	0	-3.770003	-1.937185	-0.000278
10	1	0	-1.312150	-1.606048	-0.000320
11	1	0	-2.967748	1.028445	0.000260
12	6	0	0.965582	2.185159	0.000026
13	1	0	1.254164	3.230646	0.000034
14	6	0	-0.298314	1.735944	0.000162
15	1	0	-1.180390	2.364792	0.000314
16	6	0	1.967252	1.059445	-0.000187
17	1	0	2.623661	1.087570	-0.879163
18	1	0	2.624001	1.087530	0.878536
19	8	0	2.878252	-1.661293	-0.000064
20	1	0	3.049848	-2.607385	0.000770

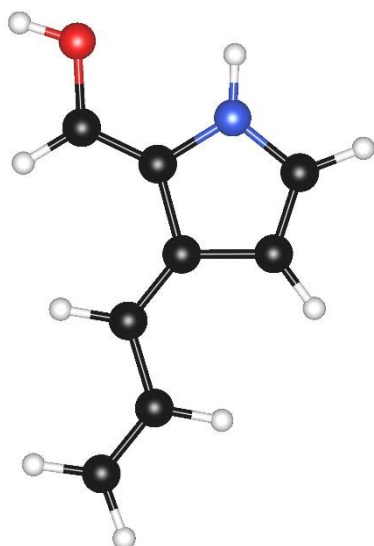
Enol B5



HF (M062X/6-31+G(d,p)) = -459.8540095 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.141517 (Hartree/Particle)
 Thermal correction = 0.106321 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.350825	0.264652	0.000063
2	6	0	1.063419	-0.144250	0.000032
3	6	0	1.621940	-1.360345	0.000087
4	1	0	0.999224	-2.248373	0.000162
5	6	0	-1.442305	-0.538923	0.000035
6	6	0	-2.809674	-0.060985	-0.000030
7	6	0	-3.887598	-0.860485	-0.000070
8	1	0	-4.893381	-0.456151	-0.000167
9	1	0	-3.785325	-1.942601	-0.000017
10	1	0	-1.305317	-1.619116	0.000057
11	1	0	-2.958075	1.017615	-0.000095
12	8	0	1.865207	0.986859	-0.000010
13	6	0	1.023095	2.057127	-0.000093
14	1	0	1.513580	3.020366	-0.000086
15	6	0	-0.277143	1.725747	0.000126
16	1	0	-1.105074	2.417643	0.000304
17	8	0	2.971270	-1.516077	-0.000282
18	1	0	3.197087	-2.450868	0.001281

Enol B6

HF (M062X/6-31+G(d,p)) = -440.0033034 Hartrees

Imaginary Frequencies: none found

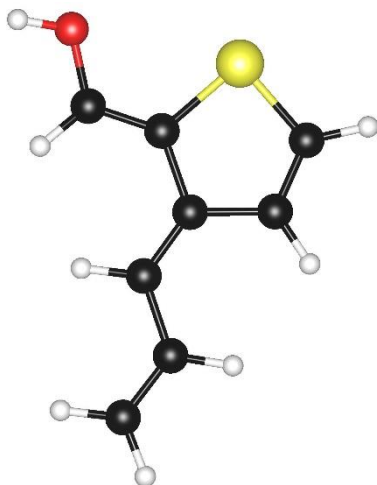
Zero-point correction = 0.152735 (Hartree/Particle)

Thermal correction = 0.116901 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.356701	0.274819	0.000033
2	6	0	1.056893	-0.169372	0.000443
3	6	0	1.584701	-1.402207	-0.000013
4	1	0	0.982242	-2.302049	-0.000626
5	6	0	-1.449809	-0.531306	0.000238
6	6	0	-2.816112	-0.055424	-0.000043
7	6	0	-3.896480	-0.853342	-0.000101
8	1	0	-4.901644	-0.447312	-0.000387
9	1	0	-3.796151	-1.935738	0.000098
10	1	0	-1.311820	-1.611526	0.000572
11	1	0	-2.963693	1.023366	-0.000291
12	6	0	1.018638	2.093959	-0.000152
13	1	0	1.447794	3.087094	-0.000358
14	6	0	-0.287204	1.735112	-0.000254
15	1	0	-1.124588	2.415147	-0.000395
16	8	0	2.951331	-1.529565	-0.001222
17	1	0	3.203512	-2.457111	0.005278
18	7	0	1.840591	0.989771	0.000898
19	1	0	2.846008	0.982824	-0.001299

Enol B7



HF (M062X/6-31+G(d,p)) = -782.8244225 Hartrees

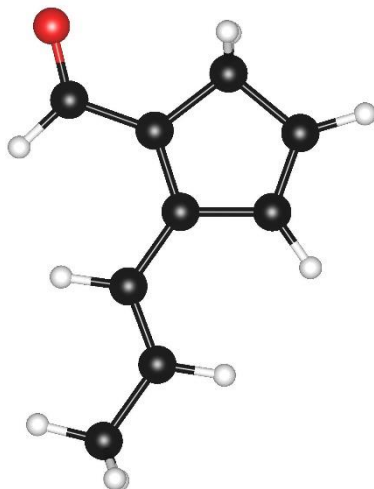
Imaginary Frequencies: none found

Zero-point correction = 0.138690 (Hartree/Particle)

Thermal correction = 0.102729 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.530561	-0.211753	-0.032191
2	6	0	-0.822248	0.384908	0.001438
3	6	0	-1.142555	1.682648	-0.077888
4	1	0	-0.389028	2.456814	-0.190392
5	6	0	1.689649	0.491100	0.040353
6	6	0	3.021498	-0.078152	-0.020263
7	6	0	4.145852	0.649812	0.062597
8	1	0	5.125339	0.187824	0.012848
9	1	0	4.109784	1.729618	0.182174
10	1	0	1.643536	1.572363	0.160605
11	1	0	3.106360	-1.156189	-0.140268
12	6	0	-0.862469	-2.109015	-0.042083
13	1	0	-1.179739	-3.144231	-0.054998
14	6	0	0.404393	-1.666396	-0.108656
15	1	0	1.253870	-2.333442	-0.179637
16	8	0	-2.442206	2.074794	-0.011325
17	1	0	-2.525648	3.015794	-0.192310
18	16	0	-2.087182	-0.861614	0.097046

Aldehyde B8

HF (M062X/6-31+G(d,p)) = -423.9821478 Hartrees

Imaginary Frequencies: none found

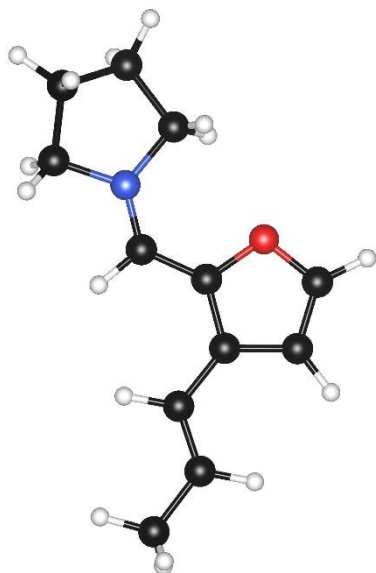
Zero-point correction = 0.165110 (Hartree/Particle)

Thermal correction = 0.129708 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.133036	0.304327	-0.000013
2	6	0	1.134397	-0.213557	-0.000130
3	6	0	1.520053	-1.617991	-0.000032
4	1	0	0.699936	-2.361707	-0.000108
5	6	0	-1.388875	-0.440435	0.000014
6	6	0	-2.604974	0.123106	0.000029
7	6	0	-3.890813	-0.642730	-0.000027
8	1	0	-4.492409	-0.391292	-0.880104
9	1	0	-3.712179	-1.720735	0.000317
10	1	0	-1.322556	-1.526616	0.000017
11	1	0	-2.690278	1.208923	0.000057
12	6	0	1.276827	2.122981	0.000026
13	1	0	1.662900	3.135474	0.000025
14	6	0	-0.022682	1.772252	0.000106
15	1	0	-0.863245	2.455336	0.000226
16	6	0	2.139477	0.898664	-0.000112
17	1	0	2.798702	0.850007	-0.876785
18	1	0	2.798726	0.849840	0.876538
19	1	0	-4.492823	-0.390780	0.879612
20	8	0	2.678874	-1.993520	0.000130

Iminium B9



HF (M062X/6-31+G(d,p)) = -596.3955132Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.262114 (Hartree/Particle)

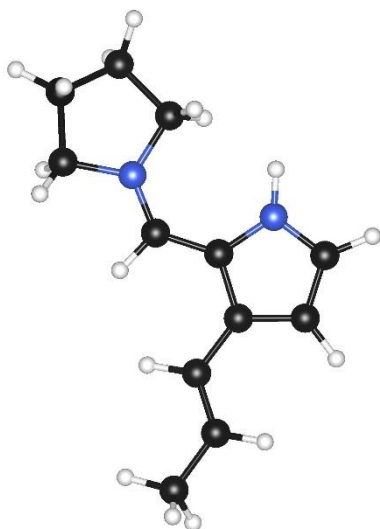
Thermal correction = 0.220898Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.767091	0.456765	0.001594
2	6	0	-0.369878	0.497308	0.012797
3	6	0	0.547701	-0.566714	0.037760
4	1	0	0.117143	-1.565920	0.036943
5	7	0	1.848244	-0.508273	0.055056
6	6	0	2.703466	-1.724094	0.048657
7	1	0	2.276199	-2.470158	-0.623574
8	1	0	2.738157	-2.126052	1.067099
9	6	0	4.063769	-1.185160	-0.383141
10	1	0	4.106791	-1.099269	-1.473419
11	1	0	4.878321	-1.832761	-0.056700
12	6	0	4.096202	0.200080	0.270102
13	1	0	4.837956	0.866227	-0.171957
14	1	0	4.313208	0.109886	1.338909
15	6	0	2.675307	0.725484	0.065657
16	1	0	2.327688	1.393829	0.854162
17	1	0	2.550528	1.226623	-0.899420
18	6	0	-2.603004	-0.729608	0.043893
19	6	0	-3.943392	-0.693308	-0.019969
20	6	0	-4.826074	-1.894202	0.024414
21	1	0	-5.443628	-1.944686	-0.878302
22	1	0	-4.251653	-2.818637	0.110616
23	1	0	-2.110727	-1.695563	0.135116
24	1	0	-4.442737	0.270897	-0.111794

25	6	0	-1.033801	2.567152	-0.072601
26	1	0	-0.861297	3.633093	-0.111323
27	6	0	-2.174581	1.821863	-0.053799
28	1	0	-3.181258	2.210601	-0.073046
29	1	0	-5.515101	-1.826764	0.872843
30	8	0	0.063870	1.796646	-0.031717

Iminium B10



HF (M062X/6-31+G(d,p)) = -576.5496683 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.275235 (Hartree/Particle)

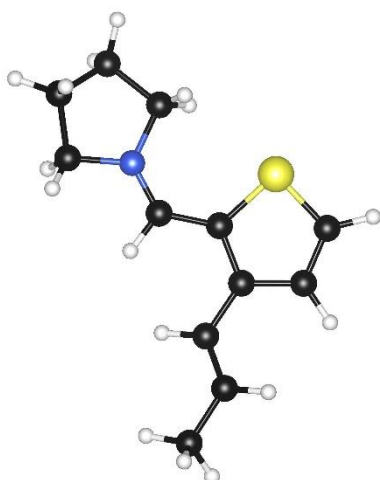
Thermal correction = 0.234419 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.778452	0.496202	0.043162
2	6	0	-0.360193	0.610650	0.009567
3	6	0	0.533384	-0.465978	0.012017
4	1	0	0.074008	-1.451744	-0.005576
5	7	0	1.843218	-0.473223	0.024678
6	6	0	2.636290	-1.728588	-0.010822
7	1	0	2.196220	-2.422490	-0.729016
8	1	0	2.622478	-2.179653	0.987558
9	6	0	4.033451	-1.242039	-0.384665
10	1	0	4.114336	-1.123409	-1.469718
11	1	0	4.807651	-1.936456	-0.056259
12	6	0	4.115499	0.118743	0.314865
13	1	0	4.897180	0.764373	-0.086969
14	1	0	4.298461	-0.014760	1.385210
15	6	0	2.720681	0.710802	0.095855
16	1	0	2.401271	1.356913	0.919241
17	1	0	2.662293	1.253061	-0.856490
18	6	0	-2.534708	-0.745728	0.141124

19	6	0	-3.854294	-0.832774	-0.082415
20	6	0	-4.651104	-2.090237	0.025967
21	1	0	-5.147303	-2.312452	-0.924298
22	1	0	-4.027996	-2.942501	0.305057
23	1	0	-1.998400	-1.651081	0.417971
24	1	0	-4.402327	0.064570	-0.368923
25	6	0	-1.212382	2.673713	-0.093938
26	1	0	-1.199752	3.752988	-0.156469
27	6	0	-2.288823	1.805059	-0.018979
28	1	0	-3.326287	2.101851	0.010389
29	1	0	-5.441494	-1.975098	0.774979
30	7	0	-0.063075	1.969610	-0.069076
31	1	0	0.852561	2.382215	-0.146331

Iminium B11



HF (M062X/6-31+G(d,p)) = -919.3607663 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.258647 (Hartree/Particle)

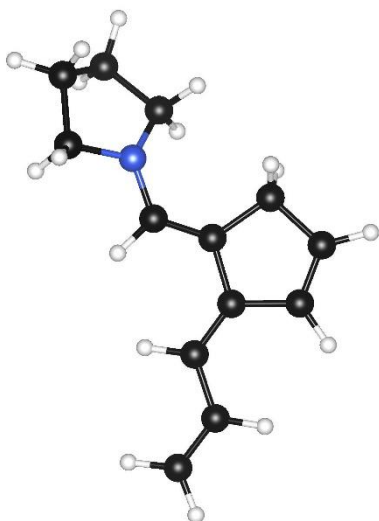
Thermal correction = 0.217046 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.762529	0.325871	0.097154
2	6	0	-0.362399	0.482490	0.069375
3	6	0	0.525181	-0.617074	0.047949
4	1	0	0.060778	-1.601353	0.015090
5	7	0	1.827730	-0.633629	0.044344
6	6	0	2.608753	-1.898288	-0.022249
7	1	0	2.141439	-2.581621	-0.733093
8	1	0	2.611871	-2.352525	0.974547
9	6	0	4.002220	-1.423292	-0.422398
10	1	0	4.059513	-1.291025	-1.507319
11	1	0	4.773986	-2.132585	-0.121044
12	6	0	4.114400	-0.073643	0.293345
13	1	0	4.895931	0.567676	-0.115426

14	1	0	4.316714	-0.222908	1.358200
15	6	0	2.725948	0.541229	0.105548
16	1	0	2.421669	1.194211	0.927459
17	1	0	2.646778	1.088526	-0.840788
18	6	0	-2.459654	-0.951221	0.235010
19	6	0	-3.727384	-1.149250	-0.159370
20	6	0	-4.467947	-2.435907	-0.009555
21	1	0	-4.798925	-2.803122	-0.986321
22	1	0	-3.856240	-3.204166	0.467855
23	1	0	-1.927002	-1.780202	0.695661
24	1	0	-4.268724	-0.331192	-0.634229
25	6	0	-1.550305	2.634189	-0.097167
26	1	0	-1.800906	3.685342	-0.166173
27	6	0	-2.418945	1.581290	0.002836
28	1	0	-3.493236	1.706542	0.042960
29	1	0	-5.370940	-2.283670	0.591047
30	16	0	0.089321	2.167444	-0.070106

Trienamine B12



HF (M062X/6-31+G(d,p)) = -560.0733681 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.271641 (Hartree/Particle)

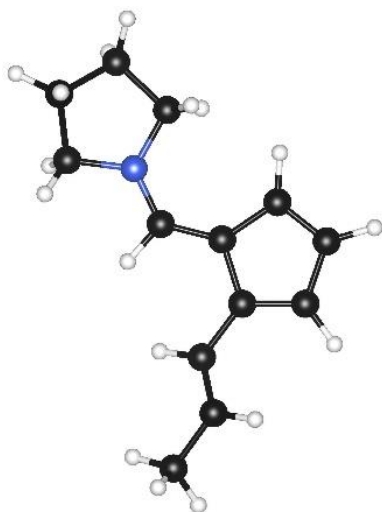
Thermal correction = 0.230718 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.844520	0.325597	-0.027217
2	6	0	-0.384984	0.529063	-0.058253
3	6	0	0.513622	-0.460181	-0.257109
4	1	0	0.150336	-1.471389	-0.447774
5	7	0	1.879807	-0.338735	-0.278135
6	6	0	2.712463	-1.494572	-0.604432
7	1	0	2.544915	-1.813400	-1.637772

8	1	0	2.485642	-2.345316	0.059507
9	6	0	4.129508	-0.980829	-0.362055
10	1	0	4.468233	-0.404485	-1.229743
11	1	0	4.844229	-1.787065	-0.183152
12	6	0	3.939353	-0.058403	0.846672
13	1	0	4.754011	0.656899	0.979887
14	1	0	3.861398	-0.659028	1.759360
15	6	0	2.597354	0.627234	0.559192
16	1	0	2.025501	0.825854	1.473207
17	1	0	2.740584	1.580634	0.034743
18	6	0	-2.512780	-0.842155	0.144514
19	6	0	-3.954495	-0.994414	0.100741
20	6	0	-4.596189	-2.159559	0.282093
21	1	0	-5.677556	-2.224829	0.237788
22	1	0	-4.049259	-3.078233	0.478606
23	1	0	-1.942082	-1.748912	0.341764
24	1	0	-4.546117	-0.102127	-0.097087
25	6	0	-1.486858	2.608780	-0.217529
26	1	0	-1.666828	3.674870	-0.304708
27	6	0	-2.437628	1.663904	-0.186653
28	1	0	-3.502871	1.853790	-0.242282
29	6	0	-0.104400	2.022009	-0.082396
30	1	0	0.542653	2.295941	-0.926624
31	1	0	0.385880	2.399097	0.825819

Fulvene trienamine B12'



HF (M062X/6-31+G(d,p)) = -560.0894673 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.272227 (Hartree/Particle)

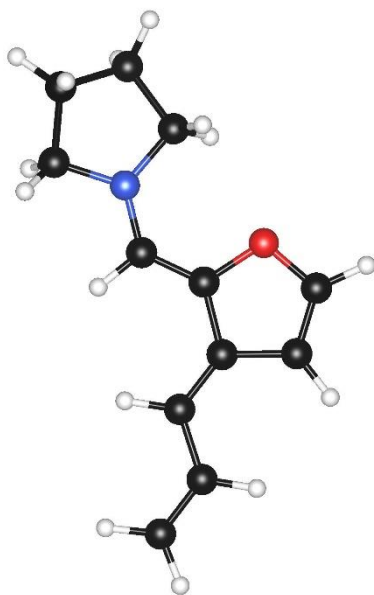
Thermal correction = 0.232627 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.795741	0.569478	0.117825

2	6	0	-0.336929	0.712185	0.067526
3	6	0	0.492483	-0.382459	0.096032
4	1	0	0.022265	-1.363529	0.148795
5	7	0	1.831082	-0.444608	0.060162
6	6	0	2.566638	-1.711555	0.081065
7	1	0	2.078433	-2.445710	-0.565879
8	1	0	2.606695	-2.116386	1.102150
9	6	0	3.958496	-1.308369	-0.402362
10	1	0	3.973413	-1.266496	-1.496576
11	1	0	4.733610	-2.002997	-0.072275
12	6	0	4.117621	0.100372	0.183151
13	1	0	4.889638	0.689904	-0.315059
14	1	0	4.372934	0.034983	1.246151
15	6	0	2.721901	0.712049	0.020124
16	1	0	2.466379	1.412312	0.822162
17	1	0	2.608139	1.234091	-0.939524
18	6	0	-2.525836	-0.692119	0.257233
19	6	0	-3.744172	-0.933834	-0.244963
20	6	0	-4.510629	-2.206380	-0.041179
21	1	0	-4.761658	-2.676445	-0.998742
22	1	0	-3.934690	-2.922641	0.552151
23	1	0	-2.048170	-1.489880	0.830228
24	1	0	-4.222762	-0.159312	-0.844524
25	6	0	-1.262310	2.789185	-0.100948
26	1	0	-1.394539	3.860487	-0.193786
27	6	0	-2.331758	1.829158	0.023122
28	1	0	-3.387865	2.066894	0.071237
29	6	0	-0.061485	2.134645	-0.071487
30	1	0	0.908067	2.602495	-0.157402
31	1	0	-5.457140	-2.019646	0.478915

Trienamine B13



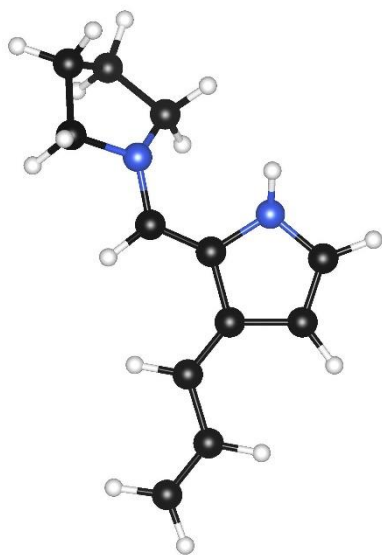
HF (M062X/6-31+G(d,p)) = -595.9714135 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.247927 (Hartree/Particle)

Thermal correction = 0.206796 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.865679	0.326327	0.003330
2	6	0	0.405487	0.417240	-0.010400
3	6	0	-0.517025	-0.572835	-0.020034
4	1	0	-0.128063	-1.587450	-0.020391
5	7	0	-1.872309	-0.484378	-0.020135
6	6	0	-2.722744	-1.670594	0.014291
7	1	0	-2.356519	-2.388546	0.755681
8	1	0	-2.745244	-2.169892	-0.966794
9	6	0	-4.095207	-1.098990	0.367440
10	1	0	-4.174565	-0.969978	1.452313
11	1	0	-4.914936	-1.739843	0.035520
12	6	0	-4.073739	0.268499	-0.325257
13	1	0	-4.818654	0.963760	0.067501
14	1	0	-4.256455	0.142972	-1.398100
15	6	0	-2.640477	0.758531	-0.095623
16	1	0	-2.272944	1.392860	-0.906557
17	1	0	-2.546720	1.324151	0.840538
18	6	0	2.637806	-0.793134	-0.048221
19	6	0	4.082137	-0.791347	-0.001103
20	6	0	4.852725	-1.891467	-0.055484
21	1	0	5.934057	-1.828115	-0.013245
22	1	0	4.414071	-2.882072	-0.143771
23	1	0	2.154955	-1.765665	-0.129787
24	1	0	4.571720	0.177748	0.088403
25	8	0	0.031441	1.766185	0.030357
26	6	0	1.184754	2.481773	0.088771
27	1	0	1.055982	3.554355	0.129784
28	6	0	2.292532	1.723508	0.081011
29	1	0	3.306382	2.091808	0.114660

Trienamine B14



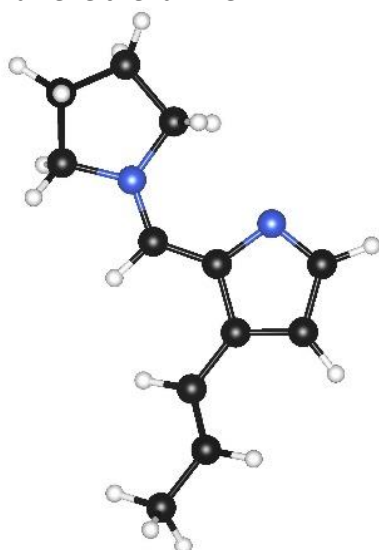
HF (M062X/6-31+G(d,p)) = -576.1149762 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.260139 (Hartree/Particle)
 Thermal correction = 0.219492 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.857374	0.329637	-0.069101
2	6	0	-0.394237	0.471413	-0.174996
3	6	0	0.540909	-0.484268	-0.367254
4	1	0	0.220975	-1.506911	-0.561141
5	7	0	1.905771	-0.250295	-0.374043
6	6	0	2.790119	-1.346045	-0.770950
7	1	0	2.758002	-1.498136	-1.854220
8	1	0	2.486219	-2.288115	-0.283660
9	6	0	4.161611	-0.901258	-0.268604
10	1	0	4.609212	-0.195962	-0.977415
11	1	0	4.850425	-1.738276	-0.135080
12	6	0	3.808419	-0.187359	1.040031
13	1	0	4.599550	0.471970	1.404727
14	1	0	3.595367	-0.929007	1.817740
15	6	0	2.526780	0.571898	0.681584
16	1	0	1.838440	0.682876	1.525516
17	1	0	2.765195	1.577550	0.308714
18	6	0	-2.547372	-0.830942	0.094632
19	6	0	-3.989503	-0.922797	0.156479
20	6	0	-4.674066	-2.068547	0.313091
21	1	0	-5.757423	-2.080904	0.351560
22	1	0	-4.161033	-3.022500	0.404668
23	1	0	-1.993463	-1.762776	0.196688
24	1	0	-4.548124	0.007819	0.065591
25	6	0	-1.311050	2.540073	-0.175460
26	1	0	-1.309558	3.621631	-0.215535
27	6	0	-2.367385	1.699652	-0.124698
28	1	0	-3.403651	1.998590	-0.074287

29	7	0	-0.102148	1.855207	-0.107269
30	1	0	0.703385	2.199012	-0.613207

Fulvene trienamine B14'



HF (M062X/6-31+G(d,p)) = -576.1430189 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.260901 (Hartree/Particle)
Thermal correction = 0.219145 Hartrees

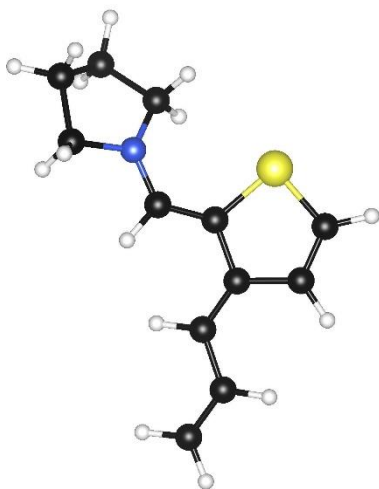
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.789362	0.552208	0.096862
2	6	0	-0.341784	0.632152	0.077758
3	6	0	0.504137	-0.458528	0.124022
4	1	0	0.050605	-1.446070	0.190651
5	7	0	1.833659	-0.472131	0.089602
6	6	0	2.615041	-1.712988	0.130982

7	1	0	2.131969	-2.486253	-0.472772
8	1	0	2.696542	-2.075106	1.164979
9	6	0	3.978599	-1.280416	-0.404470
10	1	0	3.961237	-1.272819	-1.499510
11	1	0	4.783643	-1.940981	-0.076028
12	6	0	4.104460	0.150419	0.133226
13	1	0	4.846266	0.746292	-0.402044
14	1	0	4.388768	0.126321	1.190923
15	6	0	2.690793	0.718239	-0.017802
16	1	0	2.412950	1.449492	0.742992
17	1	0	2.522357	1.193380	-0.990573
18	6	0	-2.592555	-0.666063	0.196777
19	6	0	-3.866376	-0.781219	-0.200290
20	6	0	-4.691431	-2.024430	-0.060991
21	1	0	-5.051206	-2.372133	-1.035724
22	1	0	-4.115368	-2.831574	0.400446
23	1	0	-2.115742	-1.544376	0.635521
24	1	0	-4.348931	0.080063	-0.662350
25	6	0	-1.027134	2.659903	-0.076715
26	1	0	-0.989100	3.741716	-0.157631
27	6	0	-2.213538	1.860388	0.000545
28	1	0	-3.233669	2.221598	0.013549
29	7	0	0.082299	1.951277	-0.032435
30	1	0	-5.577122	-1.841564	0.557992

Trienamine B15



HF (M062X/6-31+G(d,p)) = -918.9390192 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.245074 (Hartree/Particle)

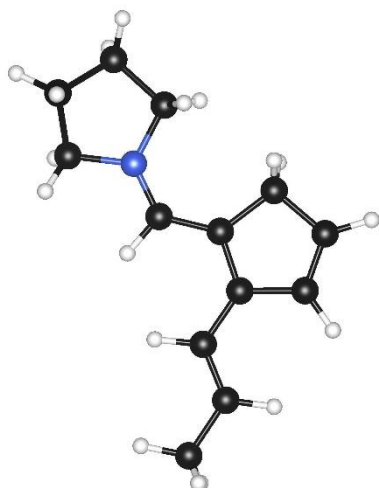
Thermal correction = 0.203768 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.844627	0.167030	-0.029628
2	6	0	-0.389359	0.382493	-0.051990

3	6	0	0.526010	-0.595573	-0.269111
4	1	0	0.145198	-1.590272	-0.503503
5	7	0	1.883339	-0.500346	-0.256770
6	6	0	2.712168	-1.645820	-0.633664
7	1	0	2.551584	-1.914156	-1.682370
8	1	0	2.466974	-2.521194	-0.011944
9	6	0	4.133697	-1.157112	-0.357793
10	1	0	4.502131	-0.583167	-1.214835
11	1	0	4.828206	-1.978773	-0.170488
12	6	0	3.941733	-0.234441	0.850376
13	1	0	4.772614	0.457444	1.004030
14	1	0	3.819960	-0.832512	1.760095
15	6	0	2.631196	0.488791	0.524880
16	1	0	2.061174	0.764655	1.418452
17	1	0	2.815915	1.399486	-0.059094
18	6	0	-2.451657	-1.036818	0.167918
19	6	0	-3.876687	-1.278189	0.081076
20	6	0	-4.454278	-2.471978	0.295324
21	1	0	-5.527436	-2.604531	0.217090
22	1	0	-3.861645	-3.345837	0.553623
23	1	0	-1.836144	-1.897092	0.424366
24	1	0	-4.514889	-0.436010	-0.180173
25	6	0	-1.699716	2.511015	-0.195085
26	1	0	-1.989306	3.552177	-0.261421
27	6	0	-2.524114	1.449401	-0.201789

Iminium B16



HF (M062X/6-31+G(d,p)) = -560.4863791 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.285357 (Hartree/Particle)

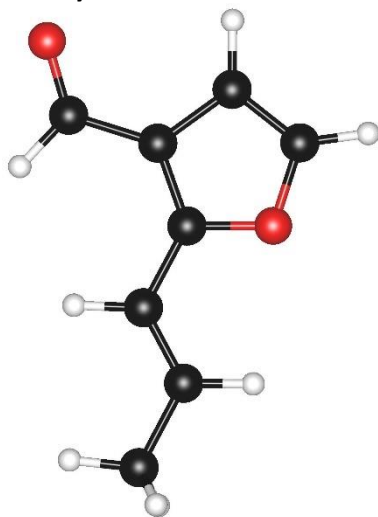
Thermal correction = 0.243778 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.739530	0.453729	-0.001317
2	6	0	-0.353124	0.631638	0.039042
3	6	0	0.536041	-0.456997	0.102536
4	1	0	0.100856	-1.452320	0.162249
5	7	0	1.844733	-0.456937	0.099348
6	6	0	2.638576	-1.708606	0.171844
7	1	0	2.139315	-2.494812	-0.397342
8	1	0	2.713674	-2.013614	1.221575
9	6	0	3.995921	-1.290757	-0.382248
10	1	0	3.977611	-1.305774	-1.476563
11	1	0	4.796095	-1.949315	-0.042291
12	6	0	4.137527	0.144339	0.136993
13	1	0	4.878942	0.728773	-0.409083
14	1	0	4.420559	0.137971	1.193950
15	6	0	2.729424	0.723059	-0.024641
16	1	0	2.479913	1.463064	0.737353
17	1	0	2.581340	1.162490	-1.016865
18	6	0	-2.465457	-0.799850	-0.002483
19	6	0	-3.808811	-0.885411	-0.017673
20	6	0	-4.570793	-2.165599	-0.020972
21	1	0	-5.215600	-2.217840	-0.904730
22	1	0	-3.911064	-3.035152	-0.012679
23	1	0	-1.900452	-1.728344	0.006884
24	1	0	-4.404100	0.025929	-0.028017
25	6	0	-1.411284	2.721100	-0.045676
26	1	0	-1.580467	3.791020	-0.076453
27	6	0	-2.364819	1.768662	-0.054149
28	1	0	-3.430666	1.947750	-0.096404
29	6	0	-0.050083	2.111690	0.017952
30	1	0	0.556740	2.418214	-0.843098
31	1	0	0.474775	2.452027	0.920113
32	1	0	-5.232129	-2.213497	0.850715

Aldehyde C1



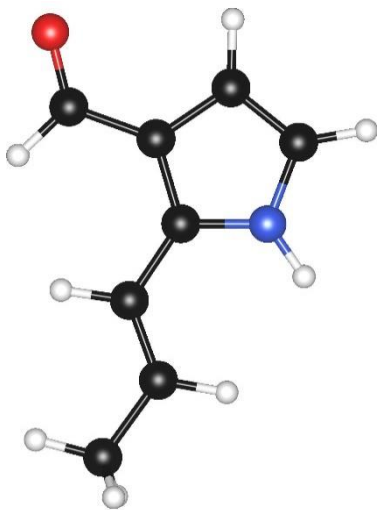
HF (M062X/6-31+G(d,p)) = -459.8997539 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.142096 (Hartree/Particle)

Thermal correction = 0.106772 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.806022	0.402470	-0.000384
2	6	0	-1.945642	-0.312131	0.000038
3	6	0	-3.243033	0.371508	-0.000186
4	1	0	-3.189623	1.481947	-0.000992
5	1	0	-1.959956	-1.398791	0.000649
6	1	0	-0.889709	1.490258	-0.000962
7	6	0	0.536826	-0.140667	-0.000173
8	6	0	1.700695	0.587561	-0.000012
9	6	0	0.939868	-1.527476	-0.000200
10	6	0	2.291320	-1.524967	0.000031
11	1	0	0.299992	-2.397277	-0.000370
12	1	0	3.038733	-2.302341	0.000082
13	6	0	2.003122	2.042417	0.000189
14	1	0	2.585516	2.314909	-0.884710
15	1	0	1.081021	2.624798	0.000013
16	1	0	2.585031	2.314730	0.885463
17	8	0	2.764021	-0.246351	0.000199
18	8	0	-4.315747	-0.193714	0.000427

Aldehyde C2



HF (M062X/6-31+G(d,p)) = -440.0527351 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.154786 (Hartree/Particle)

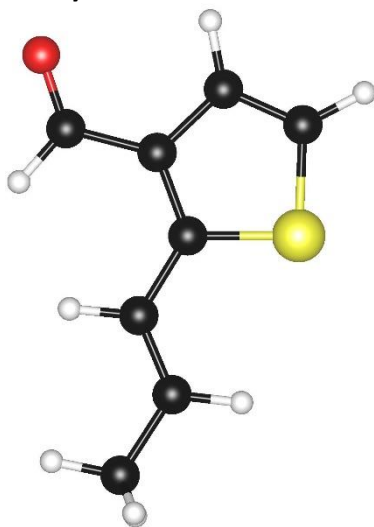
Thermal correction = 0.118401 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.806453	0.383111	-0.000368
2	6	0	-1.950248	-0.329496	0.000082
3	6	0	-3.241031	0.358683	-0.000175
4	1	0	-3.179161	1.469390	-0.000982
5	1	0	-1.967351	-1.415981	0.000729
6	1	0	-0.899120	1.470634	-0.000955
7	6	0	0.538075	-0.149235	-0.000173
8	6	0	1.703614	0.610340	-0.000011
9	6	0	0.933147	-1.528816	-0.000153
10	6	0	2.299178	-1.563585	0.000034
11	1	0	0.278540	-2.387971	-0.000312
12	1	0	2.988368	-2.393896	0.000033
13	6	0	1.926543	2.087293	0.000198
14	1	0	2.484613	2.405978	-0.886344
15	1	0	0.974723	2.619514	-0.000020
16	1	0	2.484075	2.405785	0.887149
17	8	0	-4.321519	-0.195059	0.000373
18	7	0	2.752514	-0.262048	0.000119
19	1	0	3.722917	0.011588	0.000291

Aldehyde C3



HF (M062X/6-31+G(d,p)) = -782.864751 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.138356 (Hartree/Particle)

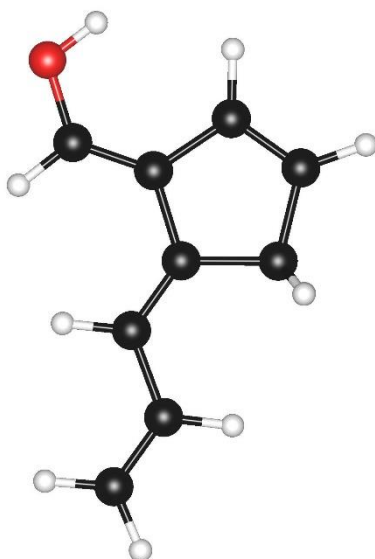
Thermal correction = 0.102913 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.122570	0.413475	-0.000143
2	6	0	-2.237350	-0.339552	0.000080
3	6	0	-3.556431	0.302756	-0.000062
4	1	0	-3.540218	1.414076	-0.000256

5	1	0	-2.223474	-1.425818	0.000363
6	1	0	-1.255161	1.495157	-0.000404
7	6	0	0.248157	-0.077147	-0.000081
8	6	0	1.357798	0.744430	0.000001
9	6	0	0.604945	-1.472177	-0.000100
10	6	0	1.946522	-1.675468	-0.000026
11	1	0	-0.116368	-2.280122	-0.000195
12	1	0	2.481138	-2.614697	-0.000022
13	6	0	1.439914	2.241439	0.000041
14	1	0	1.970802	2.605536	-0.884429
15	1	0	0.445847	2.690125	0.000016
16	1	0	1.970726	2.605494	0.884574
17	8	0	-4.609296	-0.298304	0.000127
18	16	0	2.815948	-0.183116	0.000068

Enol C4



HF (M062X/6-31+G(d,p)) = -423.9631305Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.165237 (Hartree/Particle)

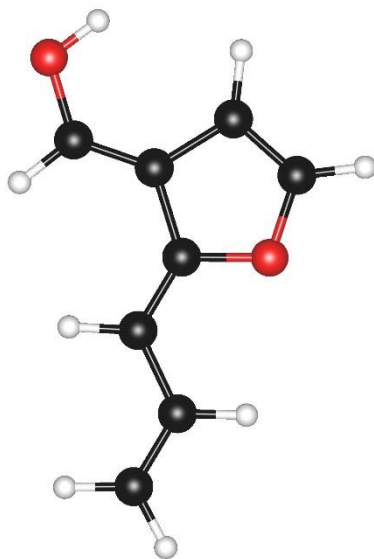
Thermal correction = 0.129479Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.656707	0.529157	-0.000313
2	6	0	-1.904970	-0.205457	-0.000317

3	6	0	-3.097111	0.413076	0.000091
4	1	0	-3.192027	1.495006	0.000384
5	1	0	-1.873206	-1.294198	-0.000726
6	1	0	-0.740816	1.615523	-0.000736
7	6	0	0.579237	-0.015994	0.000049
8	6	0	1.867806	0.726034	-0.000080
9	6	0	0.926677	-1.443364	0.000400
10	6	0	2.256356	-1.617983	0.000281
11	1	0	0.197518	-2.245675	0.000832
12	1	0	2.761187	-2.577652	0.000545
13	6	0	2.043536	2.050239	0.000386
14	1	0	3.039075	2.483475	0.000369
15	1	0	1.206007	2.741264	0.000859
16	6	0	2.991926	-0.302119	-0.000504
17	1	0	3.636920	-0.194995	0.880182
18	1	0	3.635635	-0.195509	-0.882217
19	8	0	-4.312699	-0.185443	0.000093
20	1	0	-4.209200	-1.145234	-0.000198

Enol C5



HF (M062X/6-31+G(d,p)) = -459.862049 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.141006 (Hartree/Particle)

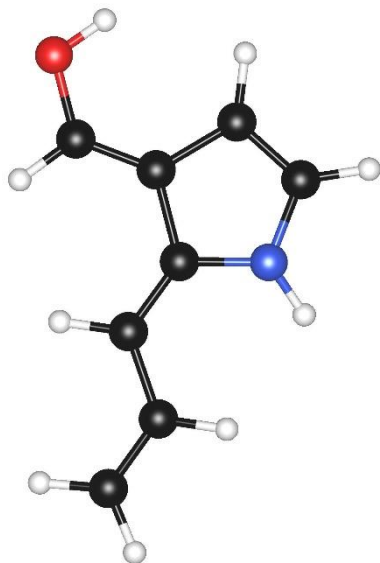
Thermal correction = 0.105386 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.645009	0.513107	-0.000311

2	6	0	-1.889148	-0.220402	-0.000467
3	6	0	-3.079553	0.397602	0.000399
4	1	0	-3.163770	1.483292	0.001584
5	1	0	-1.874770	-1.307130	-0.001285
6	1	0	-0.714583	1.600312	-0.000105
7	6	0	0.585610	-0.048214	-0.000259
8	6	0	1.872862	0.679530	0.000000
9	6	0	0.966719	-1.459056	-0.000134
10	8	0	2.891284	-0.263280	0.000422
11	6	0	2.306368	-1.498904	0.000336
12	1	0	0.308009	-2.314029	-0.000207
13	1	0	2.997658	-2.329425	0.000655
14	6	0	2.164720	1.982479	-0.000216
15	1	0	3.194700	2.315261	0.000010
16	1	0	1.373638	2.721001	-0.000711
17	8	0	-4.243545	-0.303973	-0.000742
18	1	0	-4.998215	0.291887	0.006533

Enol C6



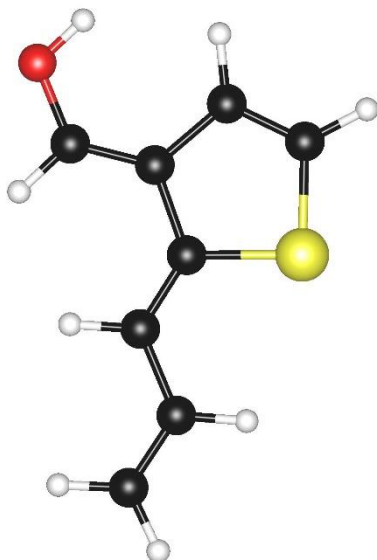
HF (M062X/6-31+G(d,p)) = -440.0059954 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.152594 (Hartree/Particle)
Thermal correction = 0.117225 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.644083	0.509298	-0.000447
2	6	0	-1.887949	-0.224226	-0.000632
3	6	0	-3.079773	0.391077	0.000796
4	1	0	-3.166834	1.476558	0.002498
5	1	0	-1.872166	-1.311002	-0.002011
6	1	0	-0.715933	1.596332	-0.000073
7	6	0	0.588202	-0.052594	-0.000392
8	6	0	1.872976	0.702316	-0.000040
9	6	0	0.954038	-1.468290	-0.000246
10	6	0	2.302438	-1.542486	0.000444
11	1	0	0.276967	-2.308476	-0.000384
12	1	0	2.936660	-2.418586	0.000876
13	6	0	2.093801	2.028942	-0.000369
14	1	0	3.098982	2.434458	-0.000048
15	1	0	1.267319	2.727208	-0.001050
16	8	0	-4.244667	-0.313004	-0.000929
17	1	0	-4.998621	0.283447	0.007505
18	7	0	2.868435	-0.279594	0.000626
19	1	0	3.854014	-0.082973	0.001054

Enol C7



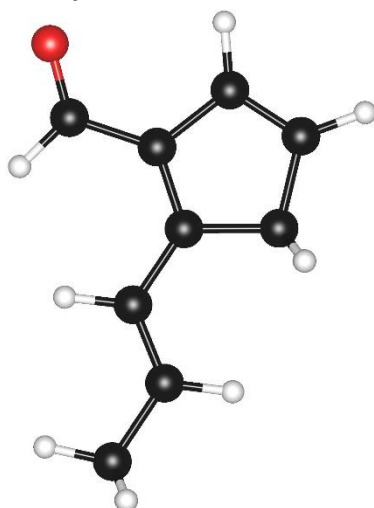
HF (M062X/6-31+G(d,p)) = -782.8262469 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.137839 (Hartree/Particle)
 Thermal correction = 0.101024 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.986210	0.518949	-0.000517
2	6	0	-2.208741	-0.249442	-0.001069
3	6	0	-3.412937	0.342563	0.001037
4	1	0	-3.521740	1.426144	0.003651
5	1	0	-2.174655	-1.335101	-0.003191
6	1	0	-1.101911	1.602027	0.000192
7	6	0	0.269851	0.009621	-0.000595
8	6	0	1.497249	0.848254	-0.000215
9	6	0	0.623468	-1.407149	-0.000604
10	6	0	1.945237	-1.640982	0.000265
11	1	0	-0.111655	-2.202411	-0.000881
12	1	0	2.431071	-2.608284	0.000724
13	6	0	1.594223	2.184578	-0.000719
14	1	0	2.555691	2.684925	-0.000362
15	1	0	0.708368	2.810237	-0.001564
16	8	0	-4.559402	-0.384678	-0.000762
17	1	0	-5.328577	0.192524	0.008869
18	16	0	2.942862	-0.195688	0.000822

Aldehyde C8



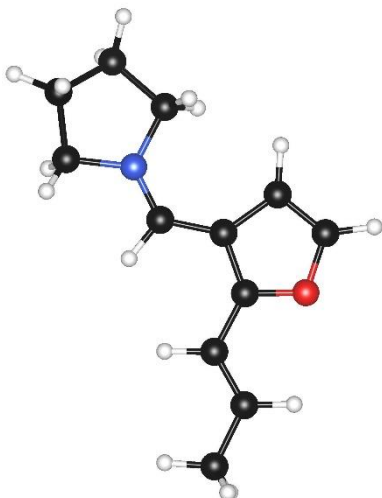
HF (M062X/6-31+G(d,p)) = -423.9812446 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.164541 (Hartree/Particle)
Thermal correction = 0.128672 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.809016	0.423497	-0.002025

2	6	0	-1.935255	-0.313468	0.000231
3	6	0	-3.246646	0.344971	-0.000648
4	1	0	-3.215960	1.456065	-0.003874
5	1	0	-1.932108	-1.399933	0.003048
6	1	0	-0.917563	1.508658	-0.004529
7	6	0	0.546942	-0.095455	-0.001192
8	6	0	1.689378	0.644532	-0.000237
9	6	0	0.908044	-1.528387	-0.000880
10	6	0	2.244217	-1.654121	0.000339
11	1	0	0.191576	-2.341389	-0.001835
12	1	0	2.806685	-2.579291	0.000563
13	6	0	1.858931	2.128941	0.000963
14	1	0	2.433405	2.452467	-0.874265
15	1	0	0.905118	2.659341	-0.008717
16	6	0	2.869788	-0.288211	0.000843
17	1	0	3.507257	-0.122816	0.880871
18	1	0	3.508437	-0.122969	-0.878363
19	1	0	2.415857	2.453168	0.887303
20	8	0	-4.307625	-0.242137	0.001929

Iminium C9



HF (M062X/6-31+G(d,p)) = -596.4039316 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.262326 (Hartree/Particle)

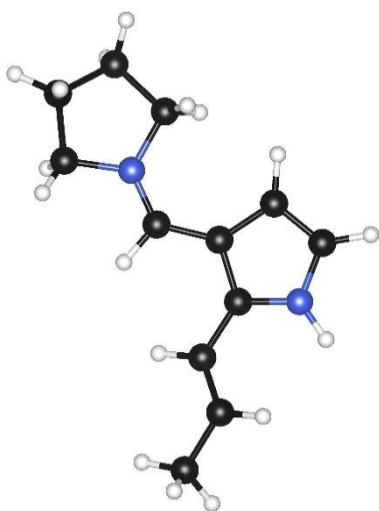
Thermal correction = 0.221163 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.029896	-0.553017	0.031467
2	6	0	0.200158	0.049768	0.040004
3	6	0	1.361853	-0.757862	0.068274
4	1	0	1.245447	-1.841659	0.081058
5	7	0	2.588481	-0.321630	0.075936
6	6	0	3.782286	-1.200811	0.081844
7	1	0	3.601432	-2.072076	-0.550068
8	1	0	3.966629	-1.528914	1.110752
9	6	0	4.888849	-0.273542	-0.412557
10	1	0	4.872621	-0.217486	-1.505503
11	1	0	5.876197	-0.615050	-0.099745
12	6	0	4.496086	1.074416	0.203239
13	1	0	4.971657	1.924742	-0.286613
14	1	0	4.763693	1.098937	1.263845
15	6	0	2.973928	1.108129	0.046074
16	1	0	2.461222	1.644850	0.847905
17	1	0	2.666812	1.525597	-0.919345
18	1	0	0.290263	1.130622	0.020182
19	1	0	-1.061948	-1.642572	0.051452
20	6	0	-2.281402	0.117197	-0.000771
21	6	0	-3.516982	-0.517815	-0.007806
22	6	0	-2.564809	1.536313	-0.033555
23	6	0	-3.907637	1.643132	-0.056993
24	1	0	-1.861789	2.355477	-0.039180
25	1	0	-4.593638	2.474543	-0.085026
26	6	0	-3.944101	-1.937853	0.015124
27	1	0	-4.539039	-2.164906	-0.873957
28	1	0	-3.086170	-2.609543	0.042844
29	1	0	-4.567148	-2.127484	0.893767
30	8	0	-4.484451	0.398500	-0.041248

Iminium C10

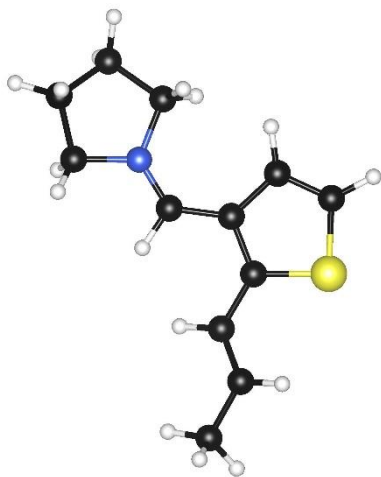


HF (M062X/6-31+G(d,p)) = -576.5659099 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.275330 (Hartree/Particle)
 Thermal correction = 0.233933 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.035455	-0.535357	0.009432
2	6	0	0.203500	0.064205	0.032468
3	6	0	1.356139	-0.744369	0.049630
4	1	0	1.235759	-1.827775	0.042462
5	7	0	2.590024	-0.315720	0.069404
6	6	0	3.776238	-1.201227	0.062986
7	1	0	3.595471	-2.057404	-0.589616
8	1	0	3.957019	-1.555251	1.084113
9	6	0	4.891058	-0.271163	-0.408106
10	1	0	4.880549	-0.195323	-1.499969
11	1	0	5.875369	-0.622668	-0.096520
12	6	0	4.501447	1.068234	0.228361
13	1	0	4.983188	1.924532	-0.244980
14	1	0	4.765011	1.073310	1.290326
15	6	0	2.979804	1.110337	0.066258
16	1	0	2.467651	1.636032	0.876139
17	1	0	2.677616	1.549605	-0.891395
18	1	0	0.295975	1.144962	0.034850
19	1	0	-1.062949	-1.626020	0.014032
20	6	0	-2.282589	0.125274	-0.016693
21	6	0	-3.525787	-0.539540	-0.012641
22	6	0	-2.558653	1.539827	-0.046432
23	6	0	-3.910376	1.683390	-0.058770
24	1	0	-1.840095	2.345704	-0.065101
25	1	0	-4.532599	2.564445	-0.085685
26	6	0	-3.860400	-1.992444	0.051421
27	1	0	-4.825478	-2.189400	-0.421248
28	1	0	-3.110914	-2.591754	-0.468367
29	1	0	-3.914111	-2.336304	1.089197
30	7	0	-4.474176	0.414444	-0.037273
31	1	0	-5.467959	0.229233	-0.040633

Iminium C11



HF (M062X/6-31+G(d,p)) = -919.3693188 Hartrees

Imaginary Frequencies: none found

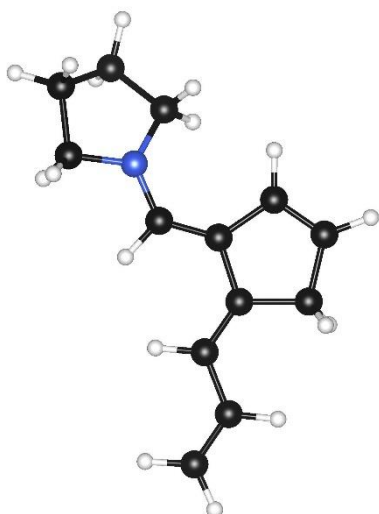
Zero-point correction = 0.258819 (Hartree/Particle)

Thermal correction = 0.216855 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.681402	0.586010	0.030573
2	6	0	-0.538678	-0.037826	0.041785
3	6	0	-1.711651	0.753549	0.065270
4	1	0	-1.610285	1.838874	0.072778
5	7	0	-2.932478	0.300491	0.074203
6	6	0	-4.137822	1.163495	0.075021
7	1	0	-3.967927	2.034468	-0.560378
8	1	0	-4.328005	1.493561	1.102262
9	6	0	-5.231274	0.219494	-0.416883
10	1	0	-5.212598	0.158847	-1.509553
11	1	0	-6.223598	0.549178	-0.107116
12	6	0	-4.821473	-1.120332	0.205438
13	1	0	-5.284942	-1.979206	-0.281133
14	1	0	-5.090234	-1.143583	1.265786
15	6	0	-3.298718	-1.134344	0.050627
16	1	0	-2.780293	-1.660532	0.855769
17	1	0	-2.984543	-1.552505	-0.912219
18	1	0	-0.616921	-1.119465	0.027975
19	1	0	0.686535	1.676649	0.045461
20	6	0	1.958413	-0.046933	0.002381
21	6	0	3.141810	0.694508	-0.001821
22	6	0	2.202870	-1.467387	-0.024019
23	6	0	3.524684	-1.764229	-0.046067
24	1	0	1.428233	-2.224437	-0.027574
25	1	0	3.994034	-2.737842	-0.070103
26	6	0	3.304046	2.184892	0.026275
27	1	0	4.357267	2.466097	-0.017915
28	1	0	2.801429	2.649040	-0.827348
29	1	0	2.887597	2.604384	0.947097
30	16	0	4.501872	-0.333897	-0.035918

Trienamine C12



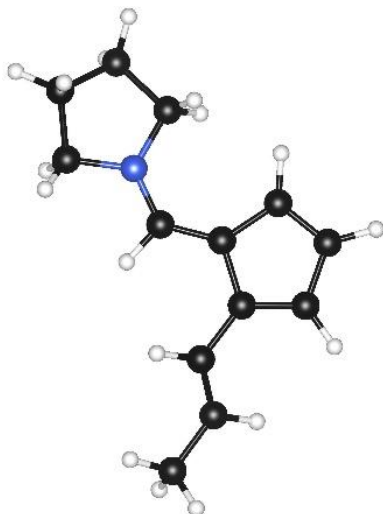
HF (M062X/6-31+G(d,p)) = -560.0783088 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.271150 (Hartree/Particle)
 Thermal correction = 0.228525 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.109614	0.654965	-0.030147
2	6	0	0.194354	0.042078	-0.036391
3	6	0	1.329504	0.791170	-0.058162
4	1	0	1.251764	1.877890	-0.070681
5	7	0	2.603294	0.322090	-0.059668
6	6	0	3.787258	1.171440	-0.066801
7	1	0	3.655207	2.024276	0.607247
8	1	0	3.994432	1.559157	-1.076091
9	6	0	4.891084	0.215756	0.389739
10	1	0	4.895083	0.153180	1.483190
11	1	0	5.883446	0.528765	0.057948
12	6	0	4.445490	-1.123153	-0.212183
13	1	0	4.904156	-1.987770	0.272022
14	1	0	4.700688	-1.154890	-1.276804
15	6	0	2.921539	-1.096137	-0.045336
16	1	0	2.399553	-1.619072	-0.857048
17	1	0	2.599093	-1.548608	0.905239
18	1	0	0.265368	-1.041768	-0.019968
19	1	0	-1.124153	1.745695	-0.049179
20	6	0	-2.302215	0.013080	-0.002919
21	6	0	-3.642997	0.649699	0.003076
22	6	0	-2.532552	-1.436011	0.030090
23	6	0	-3.843412	-1.720898	0.056732
24	1	0	-1.738083	-2.174152	0.033627
25	1	0	-4.268828	-2.717858	0.085384
26	6	0	-3.933289	1.955001	-0.024477
27	1	0	-4.962576	2.300515	-0.016659
28	1	0	-3.158830	2.715574	-0.056914
29	6	0	-4.681056	-0.466476	0.044625

30	1	0	-5.347050	-0.427585	-0.826149
31	1	0	-5.316884	-0.391048	0.935432

Fulvene trienamine C12'



HF (M062X/6-31+G(d,p)) = -560.0894486 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.272533 (Hartree/Particle)

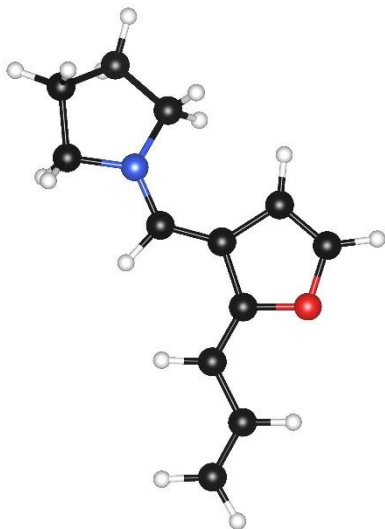
Thermal correction = 0.231392 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.795494	0.560098	-0.147086
2	6	0	-0.336870	0.705420	-0.090116
3	6	0	0.494497	-0.388127	-0.079518
4	1	0	0.028880	-1.370471	-0.145669
5	7	0	1.831237	-0.447230	0.002785
6	6	0	2.572624	-1.711030	-0.021933
7	1	0	2.155421	-2.383212	-0.776822
8	1	0	2.517439	-2.207966	0.956886
9	6	0	4.001041	-1.264448	-0.329892
10	1	0	4.120027	-1.121033	-1.409116
11	1	0	4.747053	-1.986876	0.007461
12	6	0	4.090551	0.082827	0.396651
13	1	0	4.900797	0.717215	0.031999
14	1	0	4.244982	-0.082206	1.468207
15	6	0	2.711514	0.707325	0.159907
16	1	0	2.374384	1.325978	0.998009
17	1	0	2.684937	1.320947	-0.750605
18	6	0	-2.525856	-0.706416	-0.224974
19	6	0	-3.749342	-0.920514	0.277028
20	6	0	-4.516144	-2.200881	0.133019
21	1	0	-5.457848	-2.039910	-0.404197
22	1	0	-3.936860	-2.948249	-0.417085
23	1	0	-2.043837	-1.534220	-0.749745

24	1	0	-4.232961	-0.115335	0.830282
25	6	0	-1.263345	2.788070	-0.036384
26	1	0	-1.395608	3.862998	-0.010343
27	6	0	-0.062468	2.133082	-0.021649
28	1	0	0.907381	2.606429	0.016307
29	6	0	-2.332084	1.822768	-0.115045
30	1	0	-3.388119	2.057488	-0.176693
31	1	0	-4.776464	-2.620009	1.111572

Trienamine C13



HF (M062X/6-31+G(d,p)) = -595.9798717 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.247648 (Hartree/Particle)

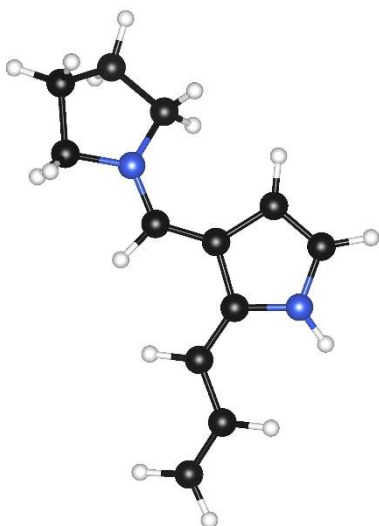
Thermal correction = 0.206087 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.115178	-0.643961	0.028256
2	6	0	0.187212	-0.037183	0.034621
3	6	0	1.321319	-0.790558	0.063178
4	1	0	1.239313	-1.876818	0.082184
5	7	0	2.594317	-0.325973	0.064005
6	6	0	3.776473	-1.179173	0.080529
7	1	0	3.640690	-2.039397	-0.583022
8	1	0	3.981581	-1.554622	1.094580
9	6	0	4.882784	-0.232015	-0.386978
10	1	0	4.886219	-0.180902	-1.480990
11	1	0	5.874183	-0.545041	-0.052602
12	6	0	4.442345	1.114474	0.201753
13	1	0	4.903504	1.972370	-0.291757
14	1	0	4.698564	1.156376	1.265731
15	6	0	2.918245	1.091612	0.036278
16	1	0	2.398502	1.623554	0.843330

17	1	0	2.596626	1.534926	-0.918625
18	1	0	0.258404	1.046751	0.012853
19	1	0	-1.144815	-1.733673	0.048872
20	6	0	-2.299560	0.016325	0.000168
21	6	0	-3.639086	-0.601527	-0.005936
22	6	0	-2.559533	1.453420	-0.030874
23	8	0	-4.575476	0.423566	-0.037251
24	6	0	-3.890727	1.608757	-0.051081
25	1	0	-1.829265	2.248655	-0.037067
26	1	0	-4.510986	2.493022	-0.075059
27	6	0	-4.045218	-1.875883	0.013156
28	1	0	-5.100450	-2.116394	0.004326
29	1	0	-3.322950	-2.681251	0.038809

Trienamine C14



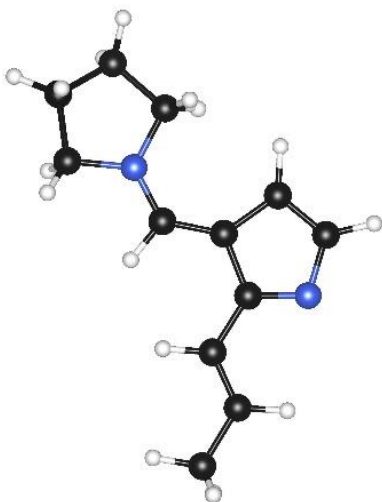
HF (M062X/6-31+G(d,p)) = -576.1231782 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.259749 (Hartree/Particle)
Thermal correction = 0.217801 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.117622	0.645405	-0.014131
2	6	0	0.186211	0.040611	-0.032851
3	6	0	1.320604	0.792825	-0.023717
4	1	0	1.240504	1.879120	0.000643
5	7	0	2.595041	0.326423	-0.035061
6	6	0	3.776555	1.178947	-0.025208
7	1	0	3.648554	2.008122	0.678447
8	1	0	3.972607	1.600951	-1.022952
9	6	0	4.887082	0.211623	0.388023
10	1	0	4.901311	0.111271	1.478547
11	1	0	5.875411	0.539098	0.058175

12	6	0	4.439896	-1.106993	-0.256025
13	1	0	4.904473	-1.986518	0.194616
14	1	0	4.686855	-1.101495	-1.323034
15	6	0	2.917233	-1.090523	-0.076233
16	1	0	2.390169	-1.584273	-0.902901
17	1	0	2.603359	-1.579228	0.859031
18	1	0	0.257517	-1.043383	-0.053094
19	1	0	-1.147533	1.735186	0.003080
20	6	0	-2.301567	-0.018587	-0.013628
21	6	0	-3.642504	0.619790	0.002428
22	6	0	-2.542703	-1.460490	0.004420
23	6	0	-3.876536	-1.653958	0.074055
24	1	0	-1.792646	-2.237183	-0.001203
25	1	0	-4.432069	-2.581096	0.116981
26	6	0	-3.985861	1.917739	-0.101508
27	1	0	-5.022070	2.233512	-0.061308
28	1	0	-3.229142	2.680534	-0.229680
29	7	0	-4.551134	-0.440159	0.138617
30	1	0	-5.529379	-0.336790	-0.073992

Fulvene trienamine C14'



HF (M062X/6-31+G(d,p)) = -576.1377698 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.261207 (Hartree/Particle)

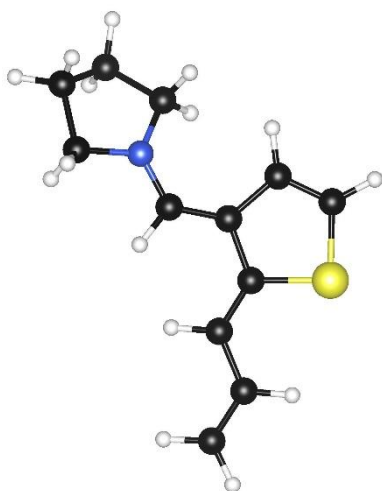
Thermal correction = 0.220211 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.768991	0.520421	-0.022940
2	6	0	-0.312468	0.653692	-0.025411
3	6	0	0.532663	-0.432109	-0.011580
4	1	0	0.086054	-1.424761	-0.029224
5	7	0	1.867430	-0.456605	0.018610
6	6	0	2.645620	-1.700682	0.006883

7	1	0	2.226152	-2.404954	-0.716374
8	1	0	2.630738	-2.167335	1.001336
9	6	0	4.051644	-1.222716	-0.354197
10	1	0	4.138716	-1.111996	-1.440255
11	1	0	4.826428	-1.912626	-0.014180
12	6	0	4.120830	0.149819	0.325581
13	1	0	4.904973	0.792812	-0.078411
14	1	0	4.301885	0.025305	1.398391
15	6	0	2.721564	0.728631	0.097859
16	1	0	2.386383	1.376494	0.913449
17	1	0	2.655348	1.294001	-0.840829
18	6	0	-2.530397	-0.731160	0.010468
19	6	0	-3.867743	-0.783402	0.027668
20	6	0	-4.667012	-2.049172	0.061559
21	1	0	-5.331168	-2.116717	-0.807495
22	1	0	-4.020354	-2.931477	0.068373
23	1	0	-1.974411	-1.668174	0.023590
24	1	0	-4.409334	0.161337	0.016814
25	6	0	-1.335649	2.641187	-0.070546
26	1	0	-1.583990	3.695145	-0.099472
27	6	0	-0.087719	2.085836	-0.057100
28	1	0	0.849709	2.619354	-0.086762
29	7	0	-2.352406	1.698960	-0.045650
30	1	0	-5.306348	-2.084965	0.950856

Trienamine C15



HF (M062X/6-31+G(d,p)) = -918.9445892 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.244232 (Hartree/Particle)

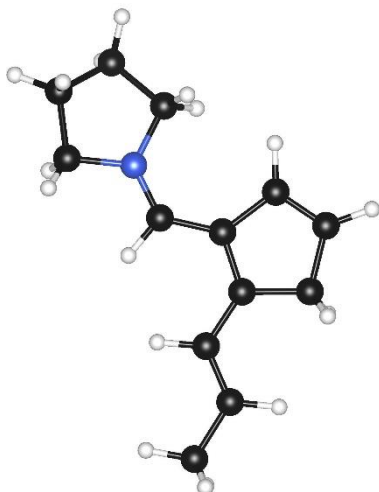
Thermal correction = 0.200726 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.740436	0.683344	-0.037885
2	6	0	0.547398	0.048767	-0.048990

3	6	0	1.692357	0.788243	-0.058939
4	1	0	1.623839	1.875642	-0.059017
5	7	0	2.957888	0.308802	-0.062584
6	6	0	4.150857	1.148229	-0.050330
7	1	0	4.018509	1.995909	0.629642
8	1	0	4.368689	1.541392	-1.054648
9	6	0	5.241505	0.178446	0.407392
10	1	0	5.234725	0.105091	1.500115
11	1	0	6.239378	0.486356	0.088029
12	6	0	4.790368	-1.150354	-0.212412
13	1	0	5.237992	-2.023656	0.266212
14	1	0	5.053420	-1.172964	-1.275271
15	6	0	3.265590	-1.113281	-0.056648
16	1	0	2.744835	-1.625276	-0.875539
17	1	0	2.933128	-1.567989	0.888939
18	1	0	0.606224	-1.035439	-0.045350
19	1	0	-0.729488	1.773411	-0.045245
20	6	0	-1.952550	0.067424	-0.017329
21	6	0	-3.242343	0.799549	-0.008205
22	6	0	-2.181262	-1.373105	0.008261
23	6	0	-3.476337	-1.725308	0.047238
24	1	0	-1.377290	-2.099335	0.000643
25	1	0	-3.876069	-2.730608	0.074935
26	6	0	-3.462669	2.122614	-0.043831
27	1	0	-4.466077	2.531933	-0.030974
28	1	0	-2.638204	2.825801	-0.088129
29	16	0	-4.592105	-0.368080	0.055863

Iminium C16



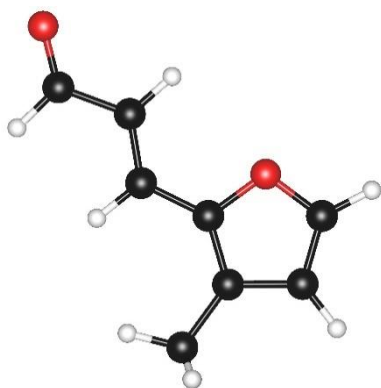
HF (M062X/6-31+G(d,p)) = -560.4866441 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.284901 (Hartree/Particle)
Thermal correction = 0.243456 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-1.028839	-0.593724	0.029855
2	6	0	0.194275	0.021660	0.040183
3	6	0	1.366295	-0.773820	0.064398
4	1	0	1.262495	-1.858939	0.071190
5	7	0	2.587056	-0.322542	0.074237
6	6	0	3.791755	-1.186755	0.074070
7	1	0	3.621171	-2.056177	-0.563209
8	1	0	3.980284	-1.518985	1.100891
9	6	0	4.886649	-0.242786	-0.414686
10	1	0	4.869153	-0.179658	-1.507234
11	1	0	5.878268	-0.574330	-0.104655
12	6	0	4.477620	1.096044	0.210229
13	1	0	4.942651	1.955517	-0.273784
14	1	0	4.744994	1.116615	1.270988
15	6	0	2.955231	1.112281	0.053190
16	1	0	2.435646	1.637717	0.857971
17	1	0	2.642880	1.531673	-0.909654
18	1	0	0.275447	1.103047	0.024627
19	1	0	-1.047607	-1.683068	0.046560
20	6	0	-2.290377	0.072602	-0.000969
21	6	0	-3.508027	-0.565760	-0.006145
22	6	0	-2.512724	1.532171	-0.033646
23	6	0	-3.831108	1.776366	-0.058116
24	1	0	-1.728677	2.279622	-0.038183
25	1	0	-4.306914	2.748222	-0.086281
26	6	0	-3.820659	-2.020982	0.020108
27	1	0	-4.419549	-2.292877	-0.855662
28	1	0	-2.932981	-2.654448	0.035185
29	6	0	-4.584474	0.477522	-0.043134
30	1	0	-5.251094	0.385197	0.825951
31	1	0	-5.223914	0.349565	-0.928072
32	1	0	-4.425354	-2.259822	0.901683

Aldehyde D1

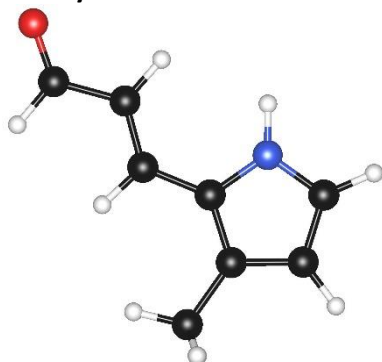


HF (M062X/6-31+G(d,p)) = -459.8979071 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.142232 (Hartree/Particle)
 Thermal correction = 0.107220 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.102481	0.233702	0.000662
2	6	0	1.220485	-0.152536	-0.000293
3	6	0	1.732705	-1.521036	-0.000535
4	1	0	0.973475	-2.327786	-0.001345
5	6	0	-1.344428	-0.515975	0.001103
6	6	0	-2.559712	0.047555	-0.000951
7	6	0	-3.843060	-0.720904	-0.000307
8	1	0	-4.445198	-0.469280	-0.879852
9	1	0	-3.664479	-1.798944	0.000203
10	1	0	-1.244975	-1.598792	0.003158
11	1	0	-2.629402	1.134185	-0.003093
12	6	0	1.104095	2.068347	0.000042
13	1	0	1.192255	3.143044	0.000020
14	6	0	1.999456	1.054762	-0.000831
15	1	0	3.076803	1.120251	-0.001701
16	1	0	-4.444698	-0.468471	0.879380
17	8	0	-0.172167	1.582452	0.000942
18	8	0	2.915149	-1.794664	0.000293

Aldehyde D2



HF (M062X/6-31+G(d,p)) = -440.0507199 Hartrees

Imaginary Frequencies: none found

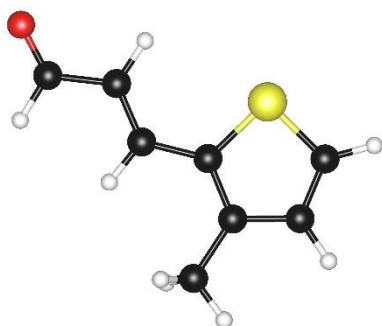
Zero-point correction = 0.154902 (Hartree/Particle)

Thermal correction = 0.118945 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.105054	0.294259	0.006244
2	6	0	1.210306	-0.174614	0.001134
3	6	0	1.629481	-1.571959	-0.000469
4	1	0	0.818978	-2.328335	0.002384
5	6	0	-1.360766	-0.443665	0.011096
6	6	0	-2.590663	0.086088	-0.010487
7	6	0	-3.854805	-0.717756	-0.002341
8	1	0	-4.460024	-0.505008	-0.890045
9	1	0	-3.639599	-1.788958	0.018323
10	1	0	-1.262397	-1.526477	0.033873
11	1	0	-2.717368	1.169269	-0.036964
12	6	0	1.284370	2.070152	-0.000962
13	1	0	1.532334	3.120735	-0.001999
14	6	0	2.079378	0.956498	-0.003712
15	1	0	3.158369	0.920876	-0.008570
16	1	0	-4.469122	-0.473160	0.870804
17	8	0	2.790153	-1.932376	-0.004543
18	7	0	-0.030214	1.656994	0.004617
19	1	0	-0.824369	2.277093	0.013190

Aldehyde D3

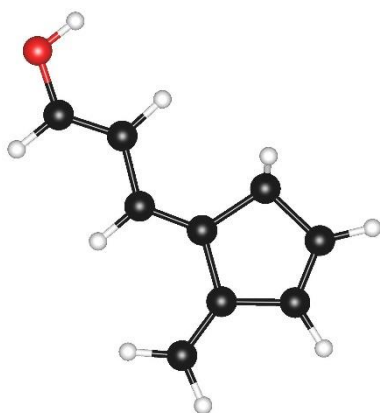


HF (M062X/6-31+G(d,p)) = -782.8633054 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.138643 (Hartree/Particle)
 Thermal correction = 0.102203 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.125050	-0.098312	0.005184
2	6	0	-1.157442	0.424254	0.001208
3	6	0	-1.481629	1.859008	-0.000075
4	1	0	-0.630460	2.565087	0.002036
5	6	0	1.392667	0.625986	0.010374
6	6	0	2.609713	0.066859	-0.010400
7	6	0	3.891835	0.838414	-0.002498
8	1	0	4.491419	0.604729	-0.888674
9	1	0	3.707890	1.915461	0.016113
10	1	0	1.321544	1.711153	0.033079
11	1	0	2.697905	-1.020084	-0.034860
12	6	0	-1.662947	-1.837838	-0.003394
13	1	0	-2.192573	-2.780246	-0.006459
14	6	0	-2.177586	-0.580968	-0.003807
15	1	0	-3.233527	-0.341085	-0.007702
16	1	0	4.497890	0.575842	0.871153
17	8	0	-2.619055	2.281731	-0.003641
18	16	0	0.065899	-1.829320	0.004056

Enol D4

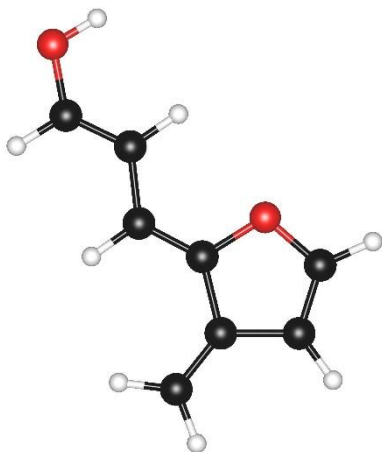


HF (M062X/6-31+G(d,p)) = -423.9608766 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.165335 (Hartree/Particle)
 Thermal correction = 0.129713 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.307748	0.235456	0.000003
2	6	0	-1.115973	-0.173308	0.000008
3	6	0	-1.581025	-1.434547	-0.000016
4	1	0	-0.927563	-2.299945	-0.000044
5	6	0	1.388492	-0.565664	0.000050
6	6	0	2.762105	-0.085795	0.000024
7	6	0	3.835796	-0.887779	-0.000023
8	1	0	4.843590	-0.487803	-0.000031
9	1	0	3.729165	-1.969592	-0.000042
10	1	0	1.256974	-1.647200	0.000096
11	1	0	2.910593	0.993208	0.000053
12	6	0	-1.117312	2.142470	0.000008
13	1	0	-1.458589	3.171293	0.000020
14	6	0	-1.911786	1.063957	0.000031
15	1	0	-2.996822	1.107156	0.000056
16	6	0	0.341184	1.758981	-0.000048
17	1	0	0.862999	2.154564	-0.881057
18	1	0	0.863107	2.154637	0.880862
19	8	0	-2.885229	-1.808447	-0.000021
20	1	0	-3.456991	-1.031371	0.000030

Enol D5



HF (M062X/6-31+G(d,p)) = -459.860336 Hartrees

Imaginary Frequencies: none found

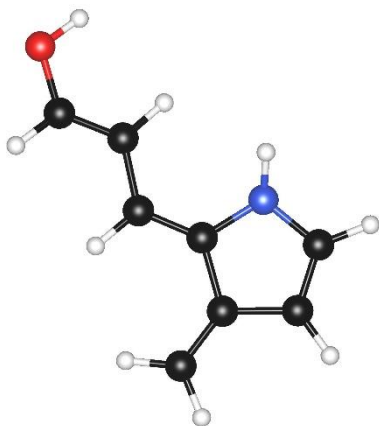
Zero-point correction = 0.141606 (Hartree/Particle)

Thermal correction = 0.106401 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.290035	0.179621	-0.000161
2	6	0	1.148336	-0.134971	0.000066
3	6	0	1.691412	-1.366053	-0.000500
4	1	0	1.092822	-2.269758	-0.001466
5	6	0	-1.385739	-0.600844	0.000143
6	6	0	-2.743917	-0.090076	-0.000095
7	6	0	-3.835039	-0.869159	0.000296
8	1	0	-4.832363	-0.444134	0.000123
9	1	0	-3.755690	-1.953254	0.000823
10	1	0	-1.241109	-1.677662	0.000632
11	1	0	-2.855529	0.991872	-0.000602
12	6	0	0.845586	2.094389	0.000045
13	1	0	0.884677	3.173895	-0.000063
14	6	0	1.815253	1.170643	0.000474
15	1	0	2.875187	1.380781	0.000739
16	8	0	-0.412649	1.561089	-0.000437
17	8	0	3.015761	-1.645232	-0.000046
18	1	0	3.531967	-0.829893	0.002076

Enol D6

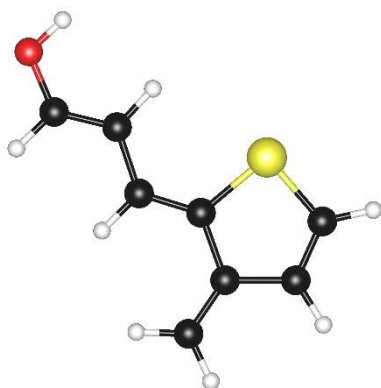


HF (M062X/6-31+G(d,p)) = -440.0055622 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.153962 (Hartree/Particle)
 Thermal correction = 0.118574 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.295607	0.228053	-0.009722
2	6	0	1.137291	-0.147054	0.014574
3	6	0	1.612468	-1.406036	-0.037870
4	1	0	0.969735	-2.276401	-0.105473
5	6	0	-1.395569	-0.564194	0.027833
6	6	0	-2.759008	-0.085899	-0.044847
7	6	0	-3.851887	-0.862197	0.039390
8	1	0	-4.849284	-0.444479	-0.034755
9	1	0	-3.768890	-1.936384	0.181251
10	1	0	-1.247622	-1.636430	0.117950
11	1	0	-2.910184	0.983763	-0.194886
12	6	0	0.997276	2.115899	0.019159
13	1	0	1.169402	3.183394	0.024359
14	6	0	1.893356	1.109258	0.058231
15	1	0	2.966441	1.234070	0.084774
16	8	0	2.920665	-1.753140	-0.019156
17	1	0	3.472399	-0.965558	0.062433
18	7	0	-0.297501	1.624841	-0.070725
19	1	0	-1.114722	2.182290	0.112180

Enol D7

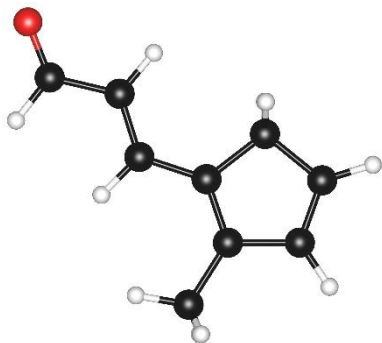


HF (M062X/6-31+G(d,p)) = -440.0055622 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.153962 (Hartree/Particle)
 Thermal correction = 0.118574 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.295607	0.228053	-0.009722
2	6	0	1.137291	-0.147054	0.014574
3	6	0	1.612468	-1.406036	-0.037870
4	1	0	0.969735	-2.276401	-0.105473
5	6	0	-1.395569	-0.564194	0.027833
6	6	0	-2.759008	-0.085899	-0.044847
7	6	0	-3.851887	-0.862197	0.039390
8	1	0	-4.849284	-0.444479	-0.034755
9	1	0	-3.768890	-1.936384	0.181251
10	1	0	-1.247622	-1.636430	0.117950
11	1	0	-2.910184	0.983763	-0.194886
12	6	0	0.997276	2.115899	0.019159
13	1	0	1.169402	3.183394	0.024359
14	6	0	1.893356	1.109258	0.058231
15	1	0	2.966441	1.234070	0.084774
16	8	0	2.920665	-1.753140	-0.019156
17	1	0	3.472399	-0.965558	0.062433
18	7	0	-0.297501	1.624841	-0.070725
19	1	0	-1.114722	2.182290	0.112180

Aldehyde D8

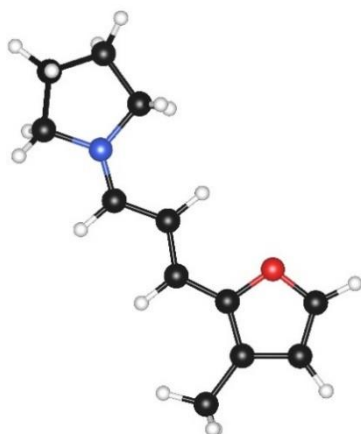


HF (M062X/6-31+G(d,p)) = -423.9805038 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.164887 (Hartree/Particle)
 Thermal correction = 0.129622 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.113819	0.281663	0.000145
2	6	0	1.162129	-0.209571	0.000027
3	6	0	1.559929	-1.621378	0.000172
4	1	0	0.744675	-2.369977	0.000730
5	6	0	-1.360488	-0.466393	0.000303
6	6	0	-2.579191	0.095678	-0.000359
7	6	0	-3.865027	-0.669881	-0.000171
8	1	0	-4.467677	-0.420157	-0.880152
9	1	0	-3.685433	-1.747835	0.000281
10	1	0	-1.292156	-1.552852	0.001034
11	1	0	-2.660568	1.182951	-0.001044
12	6	0	1.448470	2.062390	-0.000150
13	1	0	1.872773	3.058718	-0.000246
14	6	0	2.122967	0.900346	-0.000330
15	1	0	3.196217	0.756685	-0.000626
16	6	0	-0.030677	1.788382	0.000431
17	1	0	-0.527873	2.214458	0.881984
18	1	0	-0.528719	2.215069	-0.880316
19	1	0	-4.467837	-0.419462	0.879507
20	8	0	2.718855	-1.985626	-0.000195

Iminium D9



HF (M062X/6-31+G(d,p)) = -596.3965876 Hartrees

Imaginary Frequencies: none found

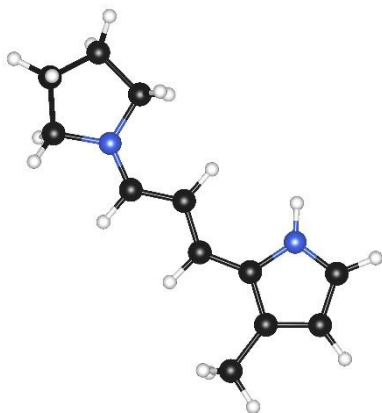
Zero-point correction = 0.262554 (Hartree/Particle)

Thermal correction = 0.221869 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.691202	0.394021	-0.012816
2	6	0	-0.303546	0.598035	-0.018739
3	6	0	0.596327	-0.494073	-0.007672
4	1	0	0.167257	-1.494035	-0.045647
5	7	0	1.895470	-0.464442	0.037045
6	6	0	2.734530	-1.691582	0.011388
7	1	0	2.310201	-2.411734	-0.689907
8	1	0	2.744049	-2.122550	1.018403
9	6	0	4.109605	-1.158707	-0.378783
10	1	0	4.173958	-1.038696	-1.464792
11	1	0	4.909639	-1.827159	-0.058654
12	6	0	4.149937	0.204240	0.320211
13	1	0	4.905457	0.875793	-0.088871
14	1	0	4.349195	0.076851	1.388487
15	6	0	2.736398	0.751832	0.113151
16	1	0	2.387552	1.384245	0.932558
17	1	0	2.641104	1.293913	-0.834105
18	6	0	-2.504530	-0.797624	0.028396
19	6	0	-3.848367	-0.761915	0.013660
20	6	0	-4.721951	-1.967653	0.057456
21	1	0	-5.372979	-1.992958	-0.822630
22	1	0	-4.143765	-2.892735	0.096878
23	1	0	-1.988991	-1.752404	0.077499
24	1	0	-4.342161	0.207859	-0.032419
25	6	0	-1.354447	2.565597	-0.078930
26	1	0	-1.731887	3.575213	-0.114552
27	6	0	-0.116032	2.035754	-0.062814
28	1	0	0.800813	2.600663	-0.093484
29	1	0	-5.380479	-1.923668	0.931391
30	8	0	-2.302198	1.578118	-0.045815

Iminium D10



HF (M062X/6-31+G(d,p)) = -576.5584271 Hartrees

Imaginary Frequencies: none found

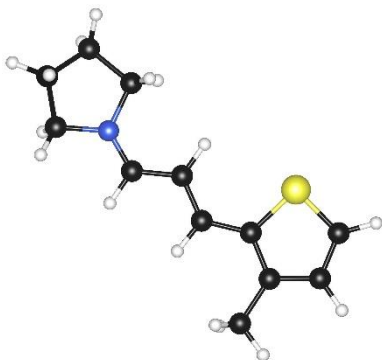
Zero-point correction = 0.275649 (Hartree/Particle)

Thermal correction = 0.235029 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.715324	0.467131	0.108580
2	6	0	-0.312458	0.656429	0.035958
3	6	0	0.560096	-0.454051	0.039368
4	1	0	0.104197	-1.443502	0.041747
5	7	0	1.862572	-0.460094	0.032756
6	6	0	2.665810	-1.709854	0.008394
7	1	0	2.218387	-2.421633	-0.687271
8	1	0	2.670585	-2.138165	1.016632
9	6	0	4.054053	-1.220157	-0.394833
10	1	0	4.118140	-1.121460	-1.483010
11	1	0	4.837344	-1.903678	-0.065053
12	6	0	4.133108	0.154659	0.277179
13	1	0	4.905748	0.797151	-0.146639
14	1	0	4.331238	0.042922	1.347542
15	6	0	2.733916	0.733427	0.062023
16	1	0	2.406191	1.402124	0.861499
17	1	0	2.646888	1.248840	-0.901202
18	6	0	-2.500605	-0.753312	0.250592
19	6	0	-3.759798	-0.889143	-0.190070
20	6	0	-4.588118	-2.119556	-0.018630
21	1	0	-4.913524	-2.501169	-0.991395
22	1	0	-4.039424	-2.905673	0.503848
23	1	0	-2.022684	-1.590694	0.753210
24	1	0	-4.229628	-0.063870	-0.727491
25	6	0	-1.304906	2.673837	-0.108544
26	1	0	-1.579106	3.714586	-0.187584
27	6	0	-0.083146	2.074954	-0.104125
28	1	0	0.855603	2.593148	-0.209052
29	1	0	-5.494926	-1.890597	0.550732
30	7	0	-2.269776	1.692125	0.025655
31	1	0	-3.260362	1.871282	0.119262

Iminium D11



HF (M062X/6-31+G(d,p)) = -919.3596831 Hartrees

Imaginary Frequencies: none found

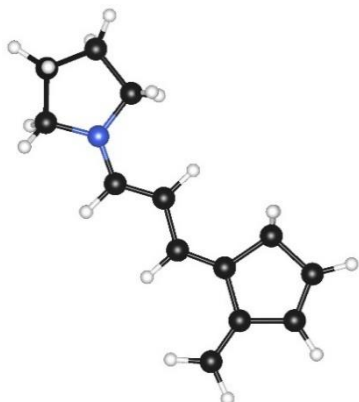
Zero-point correction = 0.258779 (Hartree/Particle)

Thermal correction = 0.216453 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.570318	0.231180	0.100240
2	6	0	-0.202107	0.550798	0.016608
3	6	0	0.744852	-0.512991	-0.002921
4	1	0	0.342243	-1.523576	-0.046115
5	7	0	2.043341	-0.458791	0.010814
6	6	0	2.891327	-1.682015	-0.046452
7	1	0	2.482309	-2.376714	-0.781534
8	1	0	2.881658	-2.149353	0.944114
9	6	0	4.272200	-1.134237	-0.389693
10	1	0	4.363483	-0.986638	-1.470345
11	1	0	5.066727	-1.807939	-0.066854
12	6	0	4.289813	0.211075	0.343229
13	1	0	5.054136	0.894363	-0.028494
14	1	0	4.458034	0.059879	1.413841
15	6	0	2.882025	0.758086	0.105113
16	1	0	2.511155	1.393444	0.912280
17	1	0	2.814315	1.296144	-0.846673
18	6	0	-2.191145	-1.079997	0.254689
19	6	0	-3.427289	-1.378756	-0.176790
20	6	0	-4.087777	-2.703986	0.003423
21	1	0	-4.362173	-3.129434	-0.967207
22	1	0	-3.444743	-3.411183	0.531381
23	1	0	-1.616459	-1.848198	0.767670
24	1	0	-4.001400	-0.616280	-0.704811
25	6	0	-1.142936	2.670485	-0.146636
26	1	0	-1.272210	3.738779	-0.252908
27	6	0	0.017578	1.970910	-0.128059
28	1	0	0.978034	2.451041	-0.241286
29	1	0	-5.017971	-2.587092	0.569381
30	16	0	-2.524866	1.650686	0.037209

Trienamine D12



HF (M062X/6-31+G(d,p)) = -560.073306 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.271512 (Hartree/Particle)

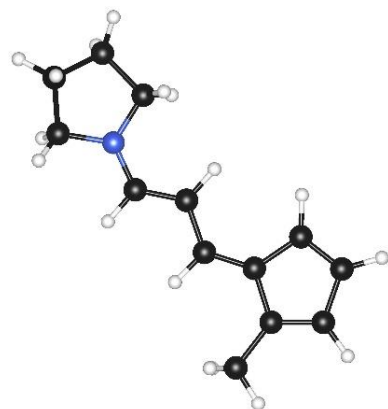
Thermal correction = 0.232085 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.827852	0.307121	-0.044236
2	6	0	-0.369781	0.541339	-0.108042
3	6	0	0.548475	-0.454960	-0.230683
4	1	0	0.179870	-1.471602	-0.363203
5	7	0	1.909509	-0.376128	-0.225989
6	6	0	2.729982	-1.574981	-0.389007
7	1	0	2.531914	-2.054097	-1.353162
8	1	0	2.518349	-2.304876	0.408446
9	6	0	4.157111	-1.040336	-0.275414
10	1	0	4.486988	-0.649786	-1.244033
11	1	0	4.866153	-1.806099	0.046405
12	6	0	4.003289	0.106225	0.730367
13	1	0	4.830875	0.818540	0.705944
14	1	0	3.929227	-0.298308	1.745606
15	6	0	2.668397	0.740677	0.327816
16	1	0	2.129762	1.175441	1.177995
17	1	0	2.815806	1.529372	-0.423448
18	6	0	-2.471286	-0.871883	0.084874
19	6	0	-3.916767	-1.014796	0.118382
20	6	0	-4.560359	-2.185751	0.240247
21	1	0	-5.643159	-2.239386	0.260034
22	1	0	-4.014014	-3.122157	0.321912
23	1	0	-1.897521	-1.793464	0.178189
24	1	0	-4.505457	-0.101732	0.036190
25	6	0	-1.361238	2.638861	-0.122039
26	1	0	-1.491799	3.714207	-0.155218
27	6	0	-0.181787	1.999846	-0.116530
28	1	0	0.779814	2.496022	-0.157334
29	6	0	-2.513519	1.666933	-0.106781
30	1	0	-3.177486	1.825417	0.752131

31 1 0 -3.133881 1.765635 -1.008252

Fulvene trienamine D12'



HF (M062X/6-31+G(d,p)) = -560.0912156 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.271813 (Hartree/Particle)

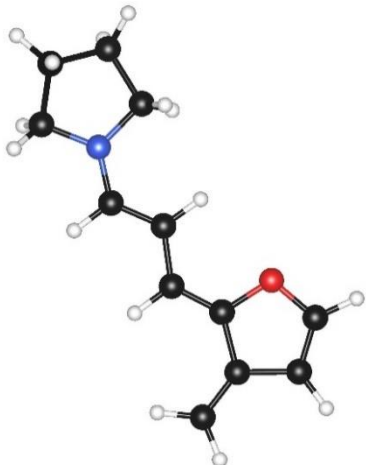
Thermal correction = 0.230195 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.132369	-0.547330	0.028544
2	6	0	0.172321	0.040776	0.036827
3	6	0	1.289492	-0.742770	0.061365
4	1	0	1.177782	-1.826743	0.073689
5	7	0	2.568300	-0.313685	0.067162
6	6	0	3.730101	-1.198576	0.066680
7	1	0	3.566911	-2.046889	-0.605195
8	1	0	3.927305	-1.588094	1.076092
9	6	0	4.858394	-0.275103	-0.395063
10	1	0	4.858583	-0.210690	-1.488324
11	1	0	5.842190	-0.618761	-0.068909
12	6	0	4.456515	1.075110	0.212129
13	1	0	4.940178	1.926107	-0.271335
14	1	0	4.714836	1.096440	1.276125
15	6	0	2.933025	1.097355	0.047304
16	1	0	2.426237	1.637058	0.856143
17	1	0	2.624809	1.551183	-0.906094
18	1	0	0.261487	1.122698	0.019997
19	1	0	-1.165068	-1.639215	0.048955
20	6	0	-2.324065	0.111288	-0.001303
21	6	0	-3.644430	-0.533435	-0.007354
22	6	0	-3.903273	1.753644	-0.060399
23	1	0	-4.407674	2.712233	-0.089997
24	6	0	-3.877234	-2.012989	0.024040
25	1	0	-4.948165	-2.230451	0.001535
26	1	0	-3.416804	-2.514614	-0.835080
27	6	0	-4.577746	0.455427	-0.042327
28	1	0	-5.652407	0.311020	-0.054757

29	6	0	-2.559581	1.554257	-0.035735
30	1	0	-1.791935	2.317623	-0.042166
31	1	0	-3.463250	-2.469034	0.930932

Trienamine D13



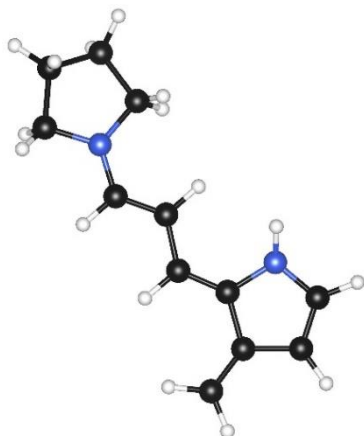
HF (M062X/6-31+G(d,p)) = -595.9750923 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.248397 (Hartree/Particle)
 Thermal correction = 0.207832 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.797682	0.277345	0.029812
2	6	0	0.348016	0.508579	0.077283
3	6	0	-0.566238	-0.498594	0.155267
4	1	0	-0.191104	-1.516858	0.243521
5	7	0	-1.920853	-0.416906	0.148842
6	6	0	-2.762880	-1.607594	0.255292
7	1	0	-2.510516	-2.181208	1.152461
8	1	0	-2.629705	-2.259802	-0.621717
9	6	0	-4.176118	-1.027483	0.296687
10	1	0	-4.423209	-0.723444	1.319425
11	1	0	-4.930561	-1.740239	-0.042727
12	6	0	-4.056776	0.204845	-0.607008
13	1	0	-4.855934	0.933379	-0.455248
14	1	0	-4.069347	-0.102875	-1.658021
15	6	0	-2.676749	0.765811	-0.249525
16	1	0	-2.186144	1.258137	-1.096906
17	1	0	-2.739684	1.486364	0.578314
18	6	0	2.536750	-0.849373	-0.074597
19	6	0	3.984544	-0.866065	-0.081179
20	6	0	4.732993	-1.975679	-0.191211
21	1	0	5.816026	-1.928216	-0.190079
22	1	0	4.277618	-2.958337	-0.285765
23	1	0	2.012351	-1.796474	-0.165483
24	1	0	4.476688	0.100107	0.011485

25	6	0	1.448436	2.473715	0.129376
26	1	0	1.810686	3.489859	0.175958
27	6	0	0.208780	1.966524	0.112985
28	1	0	-0.699600	2.545863	0.159158
29	8	0	2.422219	1.509987	0.089329

Trienamine D14



HF (M062X/6-31+G(d,p)) = -576.1195168 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.260292 (Hartree/Particle)

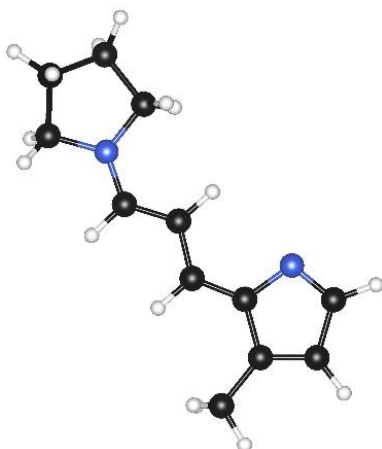
Thermal correction = 0.218647 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.810461	0.316915	-0.034383
2	6	0	-0.354818	0.552447	-0.068468
3	6	0	0.545656	-0.463681	-0.202131
4	1	0	0.157590	-1.469790	-0.355128
5	7	0	1.900709	-0.397330	-0.182714
6	6	0	2.729631	-1.584096	-0.388730
7	1	0	2.508527	-2.050918	-1.353832
8	1	0	2.547630	-2.326488	0.403448
9	6	0	4.153748	-1.033379	-0.309481
10	1	0	4.455489	-0.639631	-1.285961
11	1	0	4.878368	-1.792021	-0.006196
12	6	0	4.015744	0.112785	0.699461
13	1	0	4.835766	0.832526	0.651241
14	1	0	3.971940	-0.289704	1.717252
15	6	0	2.666019	0.734211	0.329715
16	1	0	2.147783	1.178683	1.186761
17	1	0	2.784754	1.509948	-0.439995
18	6	0	-2.499792	-0.849051	0.122349
19	6	0	-3.935742	-0.967312	0.036303
20	6	0	-4.643952	-2.089881	0.258505
21	1	0	-5.722863	-2.107526	0.156254
22	1	0	-4.153370	-3.017354	0.542018
23	1	0	-1.934629	-1.751935	0.333561

24	1	0	-4.492017	-0.074859	-0.255716
25	6	0	-1.404166	2.564316	-0.132656
26	1	0	-1.681360	3.607893	-0.185625
27	6	0	-0.177222	2.007402	-0.079641
28	1	0	0.752625	2.552505	-0.117696
29	7	0	-2.389412	1.579512	-0.170448
30	1	0	-3.343193	1.759356	0.096688

Fulvene trienamine D14'



HF (M062X/6-31+G(d,p)) = -576.1425105 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.260696 (Hartree/Particle)

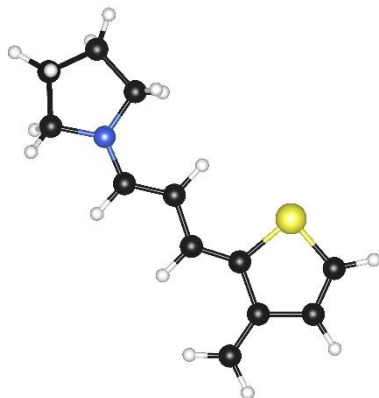
Thermal correction = 0.219094 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.141246	-0.596119	0.031325
2	6	0	0.149582	0.000656	0.039750
3	6	0	1.274935	-0.776097	0.066868
4	1	0	1.176179	-1.861574	0.081518
5	7	0	2.544636	-0.331557	0.072374
6	6	0	3.719892	-1.199588	0.072125
7	1	0	3.565533	-2.054286	-0.593545
8	1	0	3.925110	-1.579071	1.083541
9	6	0	4.833002	-0.262274	-0.398232
10	1	0	4.827619	-0.202290	-1.491732
11	1	0	5.822713	-0.591388	-0.075037
12	6	0	4.414475	1.084367	0.205665
13	1	0	4.885180	1.940083	-0.282071
14	1	0	4.675772	1.112860	1.268784
15	6	0	2.890633	1.086302	0.044767
16	1	0	2.376389	1.621970	0.850567
17	1	0	2.572978	1.528400	-0.910210
18	1	0	0.201975	1.084358	0.020312
19	1	0	-1.193510	-1.686367	0.051390
20	6	0	-2.322825	0.088962	0.000288
21	6	0	-3.664220	-0.481480	-0.010936

22	6	0	-3.659380	1.769595	-0.057142
23	1	0	-4.005512	2.798977	-0.084300
24	6	0	-4.001087	-1.940113	0.015772
25	1	0	-5.083429	-2.085694	-0.014318
26	1	0	-3.566988	-2.466631	-0.841201
27	6	0	-4.507846	0.589242	-0.047762
28	1	0	-5.590577	0.573713	-0.065994
29	7	0	-2.385025	1.489703	-0.029087
30	1	0	-3.622201	-2.420807	0.924356

Trienamine D15



HF (M062X/6-31+G(d,p)) = -918.9403592 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.244624 (Hartree/Particle)

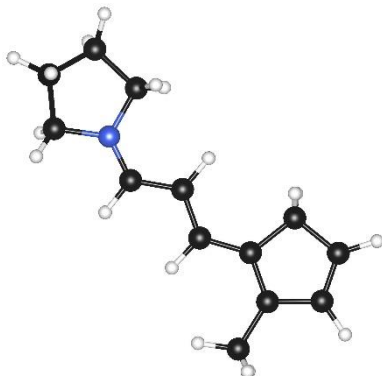
Thermal correction = 0.202883 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.640185	0.073354	-0.027715
2	6	0	-0.215382	0.446174	-0.092488
3	6	0	0.753541	-0.496227	-0.296318
4	1	0	0.435806	-1.510709	-0.534960
5	7	0	2.101909	-0.349431	-0.254567
6	6	0	2.987775	-1.471173	-0.575418
7	1	0	2.852962	-1.789304	-1.613814
8	1	0	2.770246	-2.328589	0.079401
9	6	0	4.383723	-0.909852	-0.304025
10	1	0	4.747470	-0.372512	-1.186433
11	1	0	5.105528	-1.690992	-0.056832
12	6	0	4.133857	0.074114	0.843850
13	1	0	4.934229	0.806313	0.969856
14	1	0	4.015208	-0.471934	1.785904
15	6	0	2.803341	0.720849	0.451116
16	1	0	2.209612	1.047790	1.311632
17	1	0	2.968527	1.587333	-0.204573
18	6	0	-2.174422	-1.162144	0.129944
19	6	0	-3.591008	-1.464054	0.139215
20	6	0	-4.103814	-2.696164	0.284062
21	1	0	-5.174302	-2.866426	0.288038

22	1	0	-3.460041	-3.564552	0.399687
23	1	0	-1.496624	-2.000586	0.278885
24	1	0	-4.277694	-0.625719	0.021012
25	6	0	-1.217676	2.570489	-0.095188
26	1	0	-1.347265	3.643870	-0.129701
27	6	0	-0.056286	1.897127	-0.062476
28	1	0	0.901303	2.400308	-0.087275
29	16	0	-2.642444	1.542923	-0.119138

Iminium D16



HF (M062X/6-31+G(d,p)) = -560.4807685 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.285113 (Hartree/Particle)

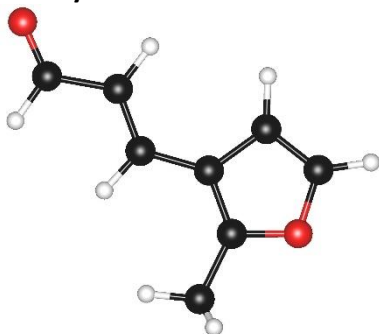
Thermal correction = 0.243995 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.717095	0.429196	-0.021872
2	6	0	-0.342112	0.639454	-0.059523
3	6	0	0.562277	-0.458225	-0.075570
4	1	0	0.131964	-1.454031	-0.157742
5	7	0	1.861905	-0.450077	-0.008842
6	6	0	2.667160	-1.700070	-0.062392
7	1	0	2.258924	-2.366730	-0.823707
8	1	0	2.608818	-2.186015	0.917625
9	6	0	4.077164	-1.196147	-0.349851
10	1	0	4.207686	-1.027708	-1.423401
11	1	0	4.836514	-1.905296	-0.018283
12	6	0	4.118772	0.130844	0.415012
13	1	0	4.918083	0.794256	0.082754
14	1	0	4.250001	-0.051274	1.486018
15	6	0	2.738931	0.734626	0.150346
16	1	0	2.367417	1.356224	0.966951
17	1	0	2.719172	1.305948	-0.783549
18	6	0	-2.433715	-0.822021	0.023850
19	6	0	-3.778781	-0.903923	0.048627
20	6	0	-4.548182	-2.178613	0.089844
21	1	0	-5.217818	-2.244224	-0.774511

22	1	0	-3.893102	-3.051794	0.095956
23	1	0	-1.869512	-1.751487	0.041870
24	1	0	-4.365164	0.014683	0.039430
25	6	0	-1.249778	2.748868	-0.081187
26	1	0	-1.380741	3.822763	-0.111097
27	6	0	-0.080904	2.092603	-0.100157
28	1	0	0.891155	2.559525	-0.160320
29	6	0	-2.387947	1.775526	-0.024451
30	1	0	-3.005094	1.910801	0.873480
31	1	0	-3.060828	1.879772	-0.885753
32	1	0	-5.185541	-2.207582	0.980119

Aldehyde E1



HF (M062X/6-31+G(d,p)) = -459.8995532 Hartrees

Imaginary Frequencies: none found

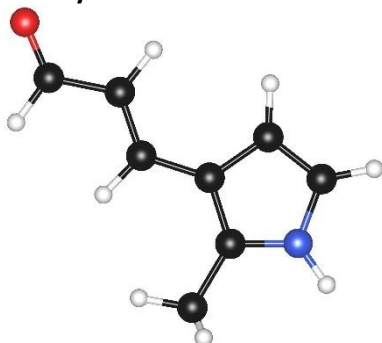
Zero-point correction = 0.142296 (Hartree/Particle)

Thermal correction = 0.107131 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.757427	0.479038	0.000182
2	6	0	1.879217	-0.265634	0.000242
3	6	0	3.190157	0.391113	0.000018
4	1	0	3.160620	1.502534	0.000196
5	1	0	1.854113	-1.351415	0.000341
6	1	0	0.844920	1.564908	0.000153
7	6	0	-0.585896	-0.033882	0.000150
8	6	0	-1.811344	0.587159	-0.000172
9	6	0	-2.075144	-1.632149	-0.000056
10	1	0	-2.366082	-2.671372	-0.000074
11	6	0	-2.095239	2.056040	0.000046
12	1	0	-2.671399	2.338803	0.885890
13	1	0	-1.176452	2.645768	-0.005341
14	6	0	-2.779071	-0.467913	-0.000346
15	1	0	-3.854673	-0.366105	-0.000679
16	1	0	-2.680602	2.337126	-0.880234
17	8	0	-0.749684	-1.388813	0.000298
18	8	0	4.250798	-0.196547	-0.000377

Aldehyde E2



HF (M062X/6-31+G(d,p)) = -440.0524551 Hartrees

Imaginary Frequencies: none found

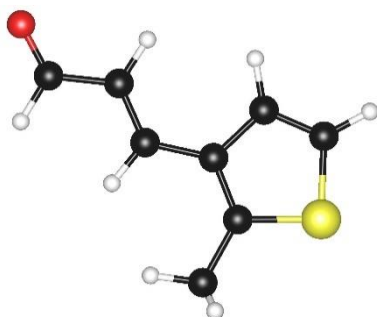
Zero-point correction = 0.154487 (Hartree/Particle)

Thermal correction = 0.119864 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.766700	0.423655	0.000034
2	6	0	1.907996	-0.297987	0.000017
3	6	0	3.205147	0.376714	0.000043
4	1	0	3.156322	1.487253	0.000432
5	1	0	1.932152	-1.385188	-0.000079
6	1	0	0.857839	1.509478	0.000201
7	6	0	-0.580048	-0.075399	-0.000051
8	6	0	-1.788044	0.620376	-0.000211
9	6	0	-2.231841	-1.593432	0.000077
10	1	0	-2.669754	-2.580565	0.000073
11	6	0	-1.976274	2.107023	0.000060
12	1	0	-2.529711	2.428712	0.887419
13	1	0	-1.024122	2.641650	-0.008778
14	6	0	-2.824018	-0.346691	-0.000049
15	1	0	-3.886814	-0.150321	-0.000192
16	1	0	-2.544729	2.426711	-0.878420
17	8	0	4.277124	-0.193160	-0.000104
18	7	0	-0.883114	-1.421716	0.000082
19	1	0	-0.204084	-2.165991	0.000082

Aldehyde E3

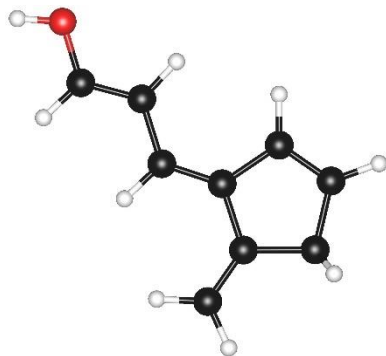


HF (M062X/6-31+G(d,p)) = -782.865599 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.138198 (Hartree/Particle)
 Thermal correction = 0.101369 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.926549	0.528431	0.004386
2	6	0	2.022446	-0.254338	-0.001684
3	6	0	3.356248	0.354682	0.000700
4	1	0	3.366117	1.466059	0.006957
5	1	0	1.975204	-1.340983	-0.008455
6	1	0	1.073545	1.609800	0.009277
7	6	0	-0.454458	0.101149	0.003767
8	6	0	-1.564857	0.924653	0.001802
9	6	0	-2.575878	-1.174312	-0.002870
10	1	0	-3.320406	-1.958495	-0.004191
11	6	0	-1.508831	2.428055	-0.002066
12	1	0	-0.923428	2.810688	0.839358
13	1	0	-1.060345	2.808791	-0.925064
14	6	0	-2.779074	0.177589	-0.002331
15	1	0	-3.762245	0.634147	-0.003921
16	1	0	-2.514497	2.845869	0.076027
17	8	0	4.394619	-0.271324	-0.003606
18	16	0	-0.907735	-1.576296	0.001789

Enol E4



HF (M062X/6-31+G(d,p)) = -423.9613425 Hartrees

Imaginary Frequencies: none found

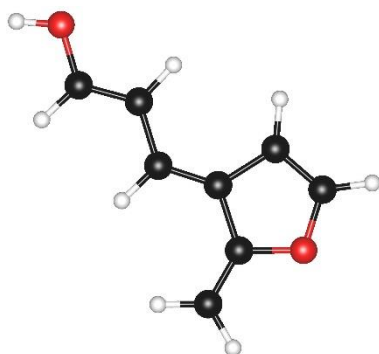
Zero-point correction = 0.164473 (Hartree/Particle)

Thermal correction = 0.127394 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.495803	-0.672379	0.000000
2	6	0	0.289802	-1.887812	0.000000
3	6	0	-0.278206	-3.101898	0.000000
4	1	0	-1.359432	-3.231789	0.000000
5	1	0	1.375079	-1.832658	0.000000
6	1	0	-1.578649	-0.797508	0.000000
7	6	0	0.000000	0.584507	0.000000
8	6	0	-0.792347	1.842581	0.000000
9	6	0	1.412743	0.987475	0.000000
10	6	0	1.534225	2.323023	0.000000
11	1	0	2.241479	0.288904	0.000000
12	1	0	2.473112	2.865432	0.000000
13	6	0	-2.122602	1.966041	0.000000
14	1	0	-2.595308	2.943513	0.000000
15	1	0	-2.779518	1.101496	0.000000
16	6	0	0.190523	3.006337	0.000000
17	1	0	0.057711	3.645802	0.881276
18	1	0	0.057711	3.645802	-0.881276
19	8	0	0.471436	-4.237600	0.000000
20	1	0	-0.093685	-5.015454	0.000000

Enol E5



HF (M062X/6-31+G(d,p)) = -459.8632432 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.142086 (Hartree/Particle)

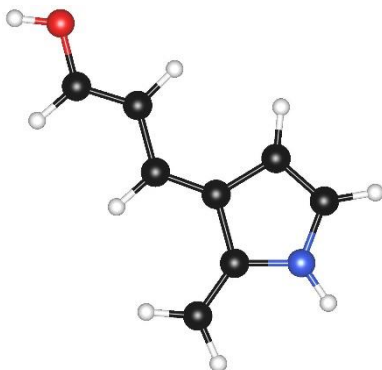
Thermal correction = 0.107406 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-0.600001	0.610946	-0.000201
2	6	0	-1.834554	-0.144729	-0.000349
3	6	0	-3.037133	0.451659	0.000217
4	1	0	-3.155020	1.531409	0.000775
5	1	0	-1.761903	-1.230844	-0.000899
6	1	0	-0.655176	1.696268	-0.000185
7	6	0	0.623157	0.057730	-0.000100
8	6	0	1.969529	0.663833	0.000030
9	6	0	2.107376	-1.589701	0.000130
10	1	0	2.362596	-2.639932	0.000176
11	6	0	2.285502	1.969956	-0.000039
12	1	0	3.321318	2.289499	0.000098
13	1	0	1.523122	2.741514	-0.000229
14	6	0	2.872117	-0.490595	0.000180
15	1	0	3.951270	-0.456522	0.000298
16	8	0	0.766127	-1.325243	-0.000058
17	8	0	-4.239556	-0.171850	0.000232
18	1	0	-4.114733	-1.129244	-0.000629

Enol E6



HF (M062X/6-31+G(d,p)) = -440.0057536 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.154170 (Hartree/Particle)

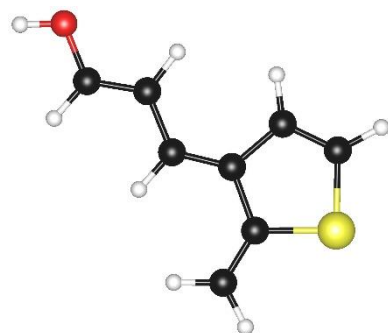
Thermal correction = 0.119075 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.610640	0.578955	-0.023314
2	6	0	-1.858502	-0.152608	0.070809
3	6	0	-3.056304	0.429598	-0.099515
4	1	0	-3.162545	1.482863	-0.341697
5	1	0	-1.824113	-1.213285	0.322858
6	1	0	-0.666976	1.658552	-0.133800
7	6	0	0.616551	0.021210	0.018802
8	6	0	1.942188	0.694943	-0.003443
9	6	0	2.253453	-1.559738	-0.041401
10	1	0	2.643959	-2.568572	-0.069135
11	6	0	2.180910	2.016548	0.067434
12	1	0	3.196208	2.396756	0.049875

13	1	0	1.377800	2.740901	0.150916
14	6	0	2.923287	-0.391938	-0.073716
15	1	0	3.995609	-0.266025	-0.104359
16	8	0	-4.266651	-0.174267	0.002308
17	1	0	-4.155069	-1.104405	0.234657
18	7	0	0.879156	-1.361374	0.096398
19	1	0	0.228594	-2.024853	-0.296514

Enol E7



HF (M062X/6-31+G(d,p)) = -782.8287946 Hartrees

Imaginary Frequencies: none found

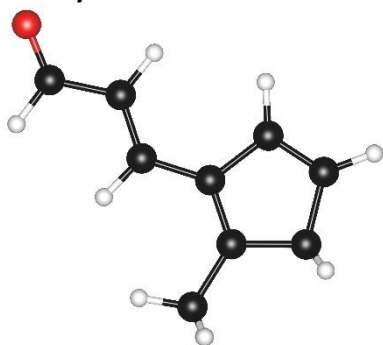
Zero-point correction = 0.138604 (Hartree/Particle)

Thermal correction = 0.102369 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.776382	0.695943	0.000325
2	6	0	-1.987905	-0.094670	0.000202
3	6	0	-3.206017	0.472105	0.000281
4	1	0	-3.346590	1.549220	0.000405
5	1	0	-1.901783	-1.181183	0.000088
6	1	0	-0.897243	1.778124	0.001081
7	6	0	0.479469	0.208589	-0.000337
8	6	0	1.741082	0.991546	0.000040
9	6	0	2.561326	-1.216600	0.000870
10	1	0	3.242414	-2.057930	0.001400
11	6	0	1.838727	2.333243	-0.000901
12	1	0	2.811264	2.813168	-0.000310
13	1	0	0.967491	2.978709	-0.002260
14	6	0	2.890008	0.082417	0.001290
15	1	0	3.911303	0.445293	0.002230
16	8	0	-4.392011	-0.175997	0.000280
17	1	0	-4.250600	-1.131271	0.000165
18	16	0	0.834874	-1.538850	-0.000979

Aldehyde E8



HF (M062X/6-31+G(d,p)) = -423.9849446 Hartrees

Imaginary Frequencies: none found

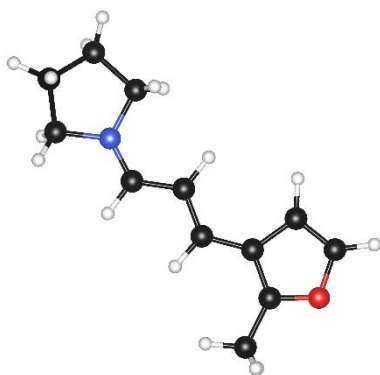
Zero-point correction = 0.164944 (Hartree/Particle)

Thermal correction = 0.129505 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.783936	0.448481	-0.000704
2	6	0	-1.911605	-0.292869	0.000066
3	6	0	-3.224794	0.354874	-0.000212
4	1	0	-3.200271	1.466582	-0.001543
5	1	0	-1.898095	-1.380196	0.001020
6	1	0	-0.894318	1.533762	-0.001640
7	6	0	0.562284	-0.070200	-0.000395
8	6	0	1.719611	0.652694	-0.000061
9	6	0	2.401169	-1.545595	0.000111
10	1	0	3.001699	-2.447050	0.000162
11	6	0	1.898859	2.137522	0.000340
12	1	0	2.471941	2.451439	-0.878529
13	1	0	0.949439	2.675010	-0.003794
14	6	0	2.854222	-0.277537	0.000309
15	1	0	3.892817	0.035867	0.000602
16	6	0	0.900997	-1.538314	-0.000290
17	1	0	0.493266	-2.051522	-0.881488
18	1	0	0.492892	-2.051432	0.880794
19	1	0	2.464499	2.451871	0.883906
20	8	0	-4.284339	-0.237333	0.000690

Iminium E9



HF (M062X/6-31+G(d,p)) = -596.4064371 Hartrees

Imaginary Frequencies: none found

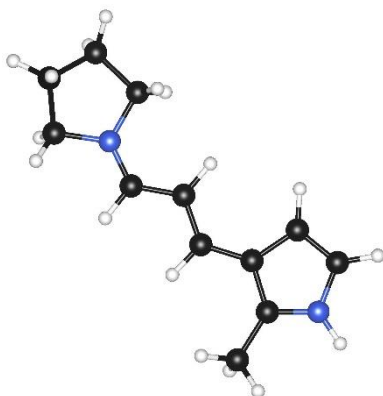
Zero-point correction = 0.262403 (Hartree/Particle)

Thermal correction = 0.221077 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.067826	0.654190	0.032542
2	6	0	-0.152866	0.026918	0.040890
3	6	0	-1.327905	0.810419	0.067953
4	1	0	-1.236381	1.896558	0.079228
5	7	0	-2.545869	0.346055	0.076087
6	6	0	-3.758645	1.197117	0.079817
7	1	0	-3.598347	2.070909	-0.554361
8	1	0	-3.951912	1.524111	1.107571
9	6	0	-4.843555	0.243520	-0.412981
10	1	0	-4.825364	0.185758	-1.505832
11	1	0	-5.838823	0.562574	-0.101462
12	6	0	-4.419460	-1.093802	0.205218
13	1	0	-4.874971	-1.956051	-0.282923
14	1	0	-4.686831	-1.122361	1.265827
15	6	0	-2.896776	-1.091897	0.048913
16	1	0	-2.371843	-1.615112	0.851841
17	1	0	-2.578526	-1.505002	-0.914828
18	1	0	-0.209130	-1.056038	0.021419
19	1	0	1.108211	1.741835	0.051912
20	6	0	2.313776	0.000439	0.000831
21	6	0	3.615183	0.486863	-0.010463
22	6	0	3.616160	-1.743616	-0.055159
23	1	0	3.800517	-2.807780	-0.079301
24	6	0	4.060073	1.911360	0.010020
25	1	0	4.651299	2.135352	-0.882142
26	1	0	3.220958	2.607947	0.045912
27	6	0	4.450553	-0.660083	-0.046819
28	1	0	5.530330	-0.681981	-0.064474
29	1	0	4.694615	2.096558	0.881095
30	8	0	2.330136	-1.368530	-0.027084

Iminium E10

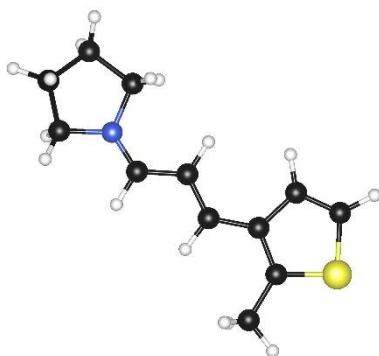


HF (M062X/6-31+G(d,p)) = -576.5614715 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.275266 (Hartree/Particle)
 Thermal correction = 0.234156 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.063741	0.531954	0.022623
2	6	0	-0.179461	-0.073439	0.035485
3	6	0	-1.328448	0.735181	0.059310
4	1	0	-1.203342	1.817893	0.064651
5	7	0	-2.566558	0.312474	0.071735
6	6	0	-3.746649	1.205778	0.072953
7	1	0	-3.560518	2.066517	-0.572170
8	1	0	-3.926611	1.552476	1.096807
9	6	0	-4.866957	0.287251	-0.407804
10	1	0	-4.856845	0.222767	-1.500395
11	1	0	-5.849282	0.641062	-0.092622
12	6	0	-4.485762	-1.061168	0.214579
13	1	0	-4.972166	-1.909584	-0.268081
14	1	0	-4.749920	-1.075860	1.276291
15	6	0	-2.963899	-1.109672	0.053650
16	1	0	-2.457301	-1.646752	0.860098
17	1	0	-2.663773	-1.542578	-0.907950
18	1	0	-0.286133	-1.153296	0.024581
19	1	0	1.092279	1.621442	0.038004
20	6	0	2.322472	-0.076296	-0.006220
21	6	0	3.591016	0.553678	-0.007728
22	6	0	3.877646	-1.680240	-0.058502
23	1	0	4.267890	-2.687957	-0.086817
24	6	0	3.840567	2.028901	0.029530
25	1	0	4.909072	2.232833	-0.051009
26	1	0	3.339551	2.541873	-0.796629
27	6	0	4.552078	-0.460558	-0.040059
28	1	0	5.624873	-0.334234	-0.049861
29	1	0	3.486756	2.467104	0.967841
30	7	0	2.552562	-1.446284	-0.037435
31	1	0	1.845373	-2.165257	-0.049742

Iminium E11



HF (M062X/6-31+G(d,p)) = -919.3709258 Hartrees

Imaginary Frequencies: none found

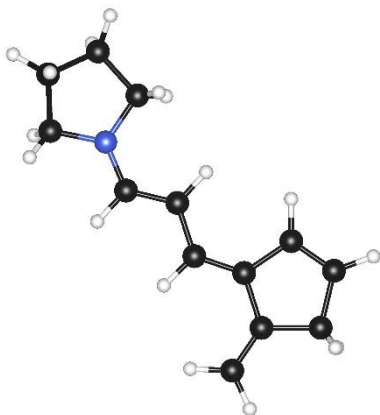
Zero-point correction = 0.258864 (Hartree/Particle)

Thermal correction = 0.216555 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.828413	0.722743	0.030469
2	6	0	-0.381840	0.073524	0.045192
3	6	0	-1.570133	0.836593	0.066215
4	1	0	-1.494818	1.923990	0.070199
5	7	0	-2.780878	0.353823	0.076442
6	6	0	-4.006571	1.186368	0.073891
7	1	0	-3.857996	2.060100	-0.563223
8	1	0	-4.207531	1.514082	1.099906
9	6	0	-5.075321	0.214367	-0.418196
10	1	0	-5.052519	0.151934	-1.510710
11	1	0	-6.076392	0.519664	-0.111547
12	6	0	-4.633374	-1.113586	0.207633
13	1	0	-5.073925	-1.984972	-0.278008
14	1	0	-4.903924	-1.141303	1.267437
15	6	0	-3.110138	-1.089293	0.056733
16	1	0	-2.581253	-1.600118	0.865157
17	1	0	-2.782501	-1.503622	-0.903357
18	1	0	-0.434289	-1.010866	0.035257
19	1	0	0.820470	1.813593	0.042148
20	6	0	2.113556	0.132595	0.001951
21	6	0	3.328102	0.827772	-0.007210
22	6	0	4.057398	-1.378007	-0.049961
23	1	0	4.706523	-2.243788	-0.072335
24	6	0	3.455068	2.323327	0.017167
25	1	0	4.504400	2.615087	-0.040565
26	1	0	2.934512	2.783516	-0.827822
27	6	0	4.430984	-0.055738	-0.036778
28	1	0	5.463943	0.270274	-0.048274
29	1	0	3.044001	2.741033	0.941357
30	16	0	2.365037	-1.591835	-0.026460

Trienamine E12



HF (M062X/6-31+G(d,p)) = -560.0793104 Hartrees

Imaginary Frequencies: none found

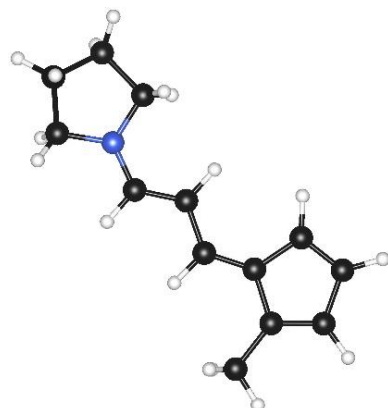
Zero-point correction = 0.271272 (Hartree/Particle)

Thermal correction = 0.228995 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.136738	0.696726	-0.029104
2	6	0	0.167393	0.076363	-0.037190
3	6	0	1.308037	0.815608	-0.063138
4	1	0	1.239352	1.902977	-0.079077
5	7	0	2.577405	0.335833	-0.064900
6	6	0	3.770153	1.172923	-0.077968
7	1	0	3.645493	2.033808	0.587092
8	1	0	3.983481	1.548100	-1.090637
9	6	0	4.862919	0.210121	0.390120
10	1	0	4.862953	0.156962	1.484076
11	1	0	5.859418	0.510124	0.058753
12	6	0	4.405446	-1.129324	-0.201819
13	1	0	4.853693	-1.994412	0.291185
14	1	0	4.663924	-1.172776	-1.265244
15	6	0	2.881134	-1.085339	-0.040540
16	1	0	2.356355	-1.608304	-0.850464
17	1	0	2.550140	-1.527861	0.911752
18	1	0	0.225229	-1.008859	-0.018606
19	1	0	-1.155075	1.787629	-0.047696
20	6	0	-2.312790	0.040429	-0.001203
21	6	0	-3.661898	0.651546	0.006906
22	6	0	-3.972939	-1.649129	0.052101
23	1	0	-4.449479	-2.623367	0.076834
24	6	0	-3.999286	1.951910	-0.011998
25	1	0	-5.040794	2.256152	-0.002774
26	1	0	-3.253020	2.739607	-0.038059
27	6	0	-4.614287	-0.473171	0.040408
28	1	0	-5.690105	-0.333774	0.053256
29	6	0	-2.475179	-1.469507	0.027641
30	1	0	-2.000185	-1.920410	0.910394
31	1	0	-2.025006	-1.951372	-0.851777

Fulvene trienaine E12'



HF (M062X/6-31+G(d,p)) = -560.0912156 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.271814 (Hartree/Particle)

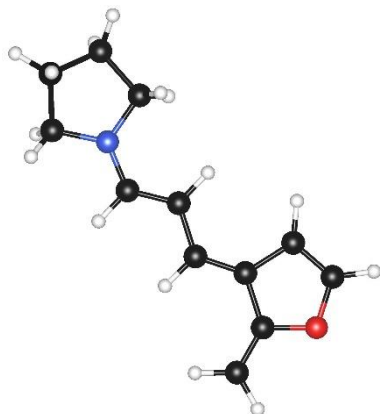
Thermal correction = 0.230197 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.132359	-0.547378	0.028635
2	6	0	0.172335	0.040713	0.037266
3	6	0	1.289509	-0.742835	0.061532
4	1	0	1.177812	-1.826813	0.073492
5	7	0	2.568307	-0.313723	0.067482
6	6	0	3.730157	-1.198531	0.066895
7	1	0	3.566748	-2.047108	-0.604591
8	1	0	3.927779	-1.587659	1.076379
9	6	0	4.858202	-0.275125	-0.395569
10	1	0	4.857839	-0.210908	-1.488841
11	1	0	5.842174	-0.618672	-0.069828
12	6	0	4.456555	1.075167	0.211609
13	1	0	4.939936	1.926112	-0.272227
14	1	0	4.715431	1.096672	1.275466
15	6	0	2.932965	1.097340	0.047589
16	1	0	2.426614	1.636964	0.856760
17	1	0	2.624160	1.551219	-0.905589
18	1	0	0.261489	1.122643	0.020912
19	1	0	-1.165092	-1.639267	0.048779
20	6	0	-2.324033	0.111284	-0.001140
21	6	0	-3.644396	-0.533426	-0.007600
22	6	0	-2.559540	1.554259	-0.035497
23	6	0	-3.903212	1.753678	-0.060509
24	1	0	-1.791888	2.317618	-0.041899
25	1	0	-4.407576	2.712287	-0.090149
26	6	0	-3.877273	-2.012959	0.023949
27	1	0	-4.948221	-2.230344	0.001328
28	1	0	-3.416797	-2.514809	-0.835018
29	6	0	-4.577702	0.455462	-0.042663

30	1	0	-5.652365	0.311090	-0.055304
31	1	0	-3.463442	-2.468855	0.930980

Trienamine E13



HF (M062X/6-31+G(d,p)) = -595.9781919 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.247817 (Hartree/Particle)

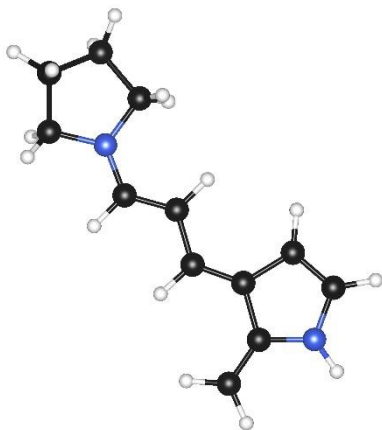
Thermal correction = 0.206159 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.150482	0.733600	-0.031192
2	6	0	0.145015	0.104943	-0.038036
3	6	0	1.289715	0.838323	-0.062832
4	1	0	1.230847	1.926266	-0.077863
5	7	0	2.554690	0.347002	-0.064257
6	6	0	3.754793	1.172983	-0.073757
7	1	0	3.638317	2.032315	0.594972
8	1	0	3.971803	1.550627	-1.084843
9	6	0	4.838766	0.198248	0.390306
10	1	0	4.838701	0.141168	1.484075
11	1	0	5.837897	0.490275	0.059652
12	6	0	4.368385	-1.134769	-0.206064
13	1	0	4.809116	-2.005723	0.283374
14	1	0	4.625508	-1.176680	-1.269901
15	6	0	2.844746	-1.077413	-0.043074
16	1	0	2.313894	-1.593396	-0.853213
17	1	0	2.510529	-1.518553	0.908490
18	1	0	0.182098	-0.979735	-0.019119
19	1	0	-1.197529	1.820382	-0.051851
20	6	0	-2.327768	0.082803	-0.001624
21	6	0	-3.715626	0.575124	0.007986
22	6	0	-3.665614	-1.682805	0.052640
23	1	0	-3.836389	-2.750030	0.076356
24	6	0	-4.147459	1.850305	-0.011207
25	1	0	-5.207588	2.075883	-0.000920
26	1	0	-3.457409	2.686584	-0.037509
27	6	0	-4.519508	-0.649704	0.043728

28	1	0	-5.597817	-0.704789	0.059733
29	8	0	-2.354323	-1.311679	0.027139

Trienamine E14



HF (M062X/6-31+G(d,p)) = -576.1207353Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.260177 (Hartree/Particle)

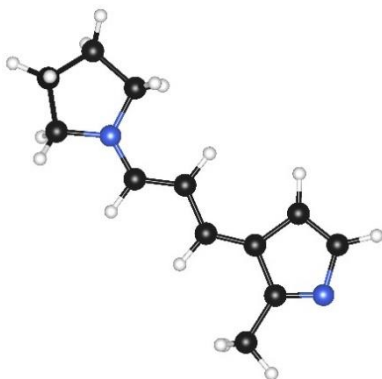
Thermal correction = 0.218584 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.147217	0.704635	0.000538
2	6	0	0.157289	0.087435	-0.027876
3	6	0	1.300043	0.816200	0.076473
4	1	0	1.234240	1.896341	0.202694
5	7	0	2.570531	0.332573	0.052214
6	6	0	3.760030	1.172207	0.072709
7	1	0	3.669969	1.948959	0.839082
8	1	0	3.921750	1.664292	-0.899426
9	6	0	4.872941	0.165574	0.365570
10	1	0	4.919365	-0.028533	1.442382
11	1	0	5.853775	0.512907	0.033718
12	6	0	4.392616	-1.087629	-0.378211
13	1	0	4.855253	-2.007940	-0.015540
14	1	0	4.618226	-0.993329	-1.445737
15	6	0	2.872512	-1.071650	-0.166665
16	1	0	2.325279	-1.455434	-1.038617
17	1	0	2.566831	-1.666880	0.707262
18	1	0	0.223198	-0.989559	-0.163161
19	1	0	-1.188341	1.791179	0.036667
20	6	0	-2.327818	0.048755	-0.013549
21	6	0	-3.701586	0.607826	-0.041564
22	6	0	-3.820803	-1.659093	0.155788
23	1	0	-4.127834	-2.692298	0.255218
24	6	0	-4.057402	1.896720	-0.206231
25	1	0	-5.102533	2.185589	-0.215440
26	1	0	-3.320302	2.681030	-0.340567

27	6	0	-4.587068	-0.551489	0.103963
28	1	0	-5.666641	-0.516261	0.122864
29	7	0	-2.469768	-1.358030	0.002327
30	1	0	-1.768801	-1.928817	0.451153

Fulvene trienamine E14'



HF (M062X/6-31+G(d,p)) = -576.138208 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.260572 (Hartree/Particle)

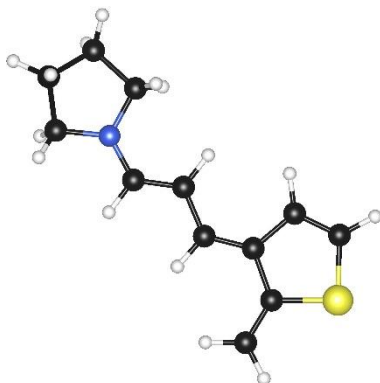
Thermal correction = 0.218975 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.124805	-0.524237	0.028073
2	6	0	0.175620	0.060634	0.036302
3	6	0	1.290971	-0.730905	0.062381
4	1	0	1.171225	-1.814051	0.075887
5	7	0	2.567785	-0.310860	0.068536
6	6	0	3.726049	-1.203421	0.071548
7	1	0	3.555573	-2.054312	-0.594643
8	1	0	3.919371	-1.586134	1.083716
9	6	0	4.858867	-0.288677	-0.395402
10	1	0	4.857910	-0.227913	-1.488803
11	1	0	5.840575	-0.637988	-0.069469
12	6	0	4.467005	1.065802	0.208823
13	1	0	4.955790	1.911993	-0.277577
14	1	0	4.726484	1.088455	1.272413
15	6	0	2.943780	1.099153	0.044938
16	1	0	2.440328	1.643503	0.852166
17	1	0	2.638320	1.549885	-0.910212
18	1	0	0.265994	1.142392	0.018550
19	1	0	-1.163657	-1.615865	0.048357
20	6	0	-2.315932	0.138575	-0.001676
21	6	0	-3.639592	-0.497214	-0.008892
22	6	0	-2.608376	1.562736	-0.036500
23	6	0	-3.962471	1.649657	-0.059915
24	1	0	-1.897223	2.377327	-0.043819
25	1	0	-4.573426	2.543143	-0.088285
26	6	0	-3.910320	-1.969375	0.024033

27	1	0	-4.988739	-2.130269	-0.013811
28	1	0	-3.449062	-2.481907	-0.827078
29	7	0	-4.594052	0.388297	-0.042770
30	1	0	-3.520363	-2.426689	0.939976

Trienamine E15



HF (M062X/6-31+G(d,p)) = -918.9451571 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.244509 (Hartree/Particle)

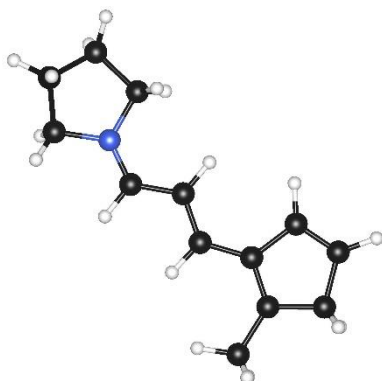
Thermal correction = 0.201144 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.904449	0.848680	-0.035707
2	6	0	0.374340	0.191099	-0.050000
3	6	0	1.538101	0.897517	-0.067011
4	1	0	1.503511	1.986538	-0.072611
5	7	0	2.787721	0.376503	-0.071522
6	6	0	4.009690	1.171801	-0.067592
7	1	0	3.907548	2.033227	0.600365
8	1	0	4.244949	1.543136	-1.076453
9	6	0	5.063311	0.168702	0.405691
10	1	0	5.049996	0.108963	1.499206
11	1	0	6.072905	0.436169	0.086552
12	6	0	4.565848	-1.150474	-0.199578
13	1	0	4.979063	-2.033600	0.291784
14	1	0	4.832449	-1.196168	-1.260854
15	6	0	3.042588	-1.055648	-0.051400
16	1	0	2.506793	-1.556347	-0.867592
17	1	0	2.688440	-1.488640	0.896372
18	1	0	0.400287	-0.895516	-0.042328
19	1	0	-0.896851	1.938833	-0.043648
20	6	0	-2.112719	0.244530	-0.011227
21	6	0	-3.440987	0.897337	0.008059
22	6	0	-4.035899	-1.383803	0.059527
23	1	0	-4.631724	-2.287372	0.086978
24	6	0	-3.680938	2.223209	-0.015189
25	1	0	-4.698562	2.597339	0.004997

26	1	0	-2.883016	2.956432	-0.055702
27	6	0	-4.492259	-0.122731	0.054293
28	1	0	-5.544707	0.136373	0.078043
29	16	0	-2.287805	-1.531013	0.012272

Iminium E16



HF (M062X/6-31+G(d,p)) = -560.4940946 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.285296 (Hartree/Particle)

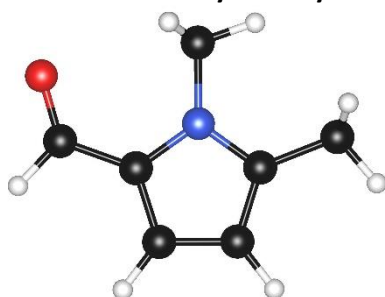
Thermal correction = 0.244124 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.050474	0.600880	0.029048
2	6	0	-0.181101	-0.017489	0.038623
3	6	0	-1.347808	0.772659	0.065486
4	1	0	-1.244281	1.857721	0.076372
5	7	0	-2.574357	0.324044	0.074431
6	6	0	-3.774617	1.191121	0.079290
7	1	0	-3.604868	2.061218	-0.557618
8	1	0	-3.963140	1.524223	1.106063
9	6	0	-4.873454	0.251832	-0.410438
10	1	0	-4.858669	0.193769	-1.503345
11	1	0	-5.863919	0.583290	-0.096478
12	6	0	-4.465252	-1.091247	0.206107
13	1	0	-4.932726	-1.947362	-0.281606
14	1	0	-4.731213	-1.116785	1.267176
15	6	0	-2.942703	-1.107640	0.047772
16	1	0	-2.424758	-1.638050	0.850893
17	1	0	-2.631318	-1.526845	-0.915908
18	1	0	-0.258488	-1.099964	0.021048
19	1	0	1.064196	1.690586	0.047219
20	6	0	2.299293	-0.054039	-0.001204
21	6	0	3.534538	0.569719	-0.007357
22	6	0	3.997449	-1.672574	-0.056040
23	1	0	4.517506	-2.622908	-0.082144
24	6	0	3.846733	2.026383	0.016253
25	1	0	4.441554	2.291085	-0.863977

26	1	0	2.960065	2.660142	0.036065
27	6	0	4.570681	-0.448767	-0.041525
28	1	0	5.632666	-0.233378	-0.052921
29	6	0	2.506428	-1.545173	-0.032106
30	1	0	2.055414	-2.012549	-0.917759
31	1	0	2.080605	-2.045493	0.848001
32	1	0	4.457908	2.259006	0.894444

Model A: N-Methyl Aldehyde

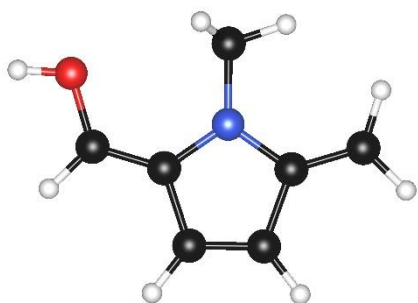


HF (M062X/6-31+G(d,p)) = -401.9760183 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.149452 (Hartree/Particle)
Thermal correction = 0.115336 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.431694	0.097266	0.000049
2	6	0	1.331592	1.485019	0.000243
3	6	0	-0.035549	1.807896	0.000246
4	6	0	-0.742589	0.611924	-0.000176
5	7	0	0.173284	-0.424027	-0.000049
6	1	0	2.170060	2.166626	0.000393
7	1	0	-0.481136	2.793490	0.000367
8	6	0	2.662441	-0.750927	0.000156
9	1	0	2.716414	-1.392257	0.886039
10	1	0	2.717117	-1.391562	-0.886195
11	1	0	3.540221	-0.102981	0.000718
12	6	0	-2.179749	0.439658	-0.000495
13	1	0	-2.737868	1.397026	-0.000637
14	8	0	-2.773108	-0.626205	-0.000456
15	6	0	-0.166760	-1.840676	0.000318
16	1	0	-0.753906	-2.087761	0.885908
17	1	0	-0.761887	-2.085904	-0.880354
18	1	0	0.756382	-2.419811	-0.004294

Model A: N-Methyl Enol

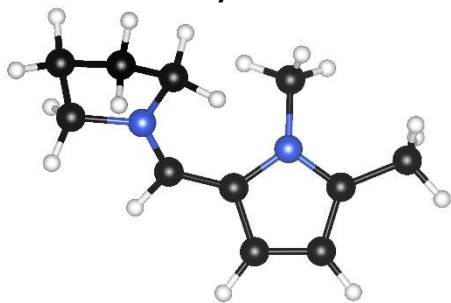


HF (M062X/6-31+G(d,p)) = -401.9241129 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.147610 (Hartree/Particle)
 Thermal correction = 0.114830 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.558034	-0.074061	-0.000042
2	6	0	1.513494	1.393769	-0.000060
3	1	0	2.401662	2.011126	-0.000108
4	6	0	0.231780	1.797207	-0.000024
5	1	0	-0.143980	2.812141	-0.000039
6	6	0	-0.628134	0.616561	0.000062
7	6	0	-1.973424	0.649482	0.000037
8	1	0	-2.485604	1.605266	-0.000013
9	6	0	2.670066	-0.837289	-0.000070
10	1	0	2.652371	-1.919093	-0.000048
11	1	0	3.636566	-0.350580	-0.000131
12	8	0	-2.744797	-0.485499	-0.000246
13	1	0	-3.675324	-0.244956	0.001157
14	7	0	0.225308	-0.488008	0.000052
15	6	0	-0.212921	-1.866870	0.000141
16	1	0	-0.811436	-2.087405	0.888161
17	1	0	-0.811305	-2.087584	-0.887924
18	1	0	0.664912	-2.511655	0.000278

Model A: N-Methyl Iminium



HF (M062X/6-31+G(d,p)) = -538.4674297 Hartrees
 Imaginary Frequencies: none found

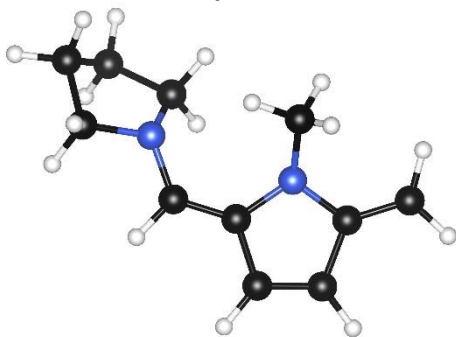
Zero-point correction = 0.270132 (Hartree/Particle)

Thermal correction = 0.231458 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.722837	1.857073	0.232348
2	6	0	-2.931929	1.229409	0.493860
3	6	0	-0.805995	0.868289	-0.176819
4	6	0	0.560658	1.139168	-0.361636
5	6	0	-2.773592	-0.128070	0.186240
6	6	0	-3.798586	-1.209555	0.187535
7	7	0	1.615022	0.367417	-0.267930
8	6	0	1.685857	-0.960140	0.375870
9	6	0	2.982235	0.907853	-0.513902
10	6	0	3.065431	-0.933008	1.030289
11	1	0	0.849155	-1.065871	1.071087
12	6	0	3.911550	-0.202457	-0.017598
13	1	0	3.101931	1.136695	-1.574624
14	1	0	3.026351	-0.362807	1.963721
15	1	0	4.840653	0.200515	0.386843
16	1	0	1.638069	-1.748339	-0.382025
17	1	0	3.430103	-1.936875	1.252589
18	1	0	4.165178	-0.879589	-0.838607
19	1	0	0.784982	2.183909	-0.578904
20	1	0	-1.483234	2.903547	0.368125
21	1	0	-3.845453	1.681422	0.851624
22	1	0	-3.434089	-2.111412	0.687288
23	1	0	3.094202	1.828920	0.067222
24	1	0	-4.692529	-0.863625	0.706803
25	1	0	-4.089087	-1.479715	-0.834051
26	7	0	-1.493089	-0.347597	-0.201778
27	6	0	-1.064931	-1.569150	-0.879793
28	1	0	-0.223923	-1.337833	-1.532687
29	1	0	-0.781418	-2.344591	-0.164033
30	1	0	-1.881588	-1.939556	-1.500783

Model A: N-Methyl Trienamine



HF (M062X/6-31+G(d,p)) = -538.036348 Hartrees

Imaginary Frequencies: none found

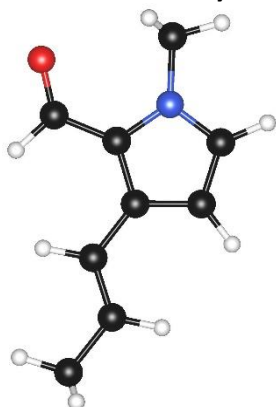
Zero-point correction = 0.255373 (Hartree/Particle)

Thermal correction = 0.216550 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.814713	-0.290995	0.174884
2	6	0	3.041271	1.135354	0.424505
3	6	0	1.890383	1.802036	0.213702
4	6	0	0.844891	0.846479	-0.130048
5	7	0	1.452245	-0.422839	-0.119433
6	1	0	3.998097	1.543542	0.721410
7	1	0	1.712587	2.864467	0.323323
8	6	0	-0.466044	1.151306	-0.287805
9	1	0	-0.729474	2.207776	-0.343159
10	7	0	-1.520895	0.247424	-0.353478
11	6	0	3.726602	-1.285042	0.158615
12	1	0	4.762619	-1.063211	0.379788
13	1	0	3.459920	-2.311244	-0.062630
14	6	0	-2.829785	0.783659	-0.728474
15	1	0	-2.902276	0.912720	-1.813030
16	1	0	-2.995164	1.768383	-0.257387
17	6	0	-3.818778	-0.241848	-0.177894
18	1	0	-3.900208	-1.091781	-0.864468
19	1	0	-4.816455	0.177492	-0.029747
20	6	0	-3.137271	-0.676126	1.123125
21	1	0	-3.519594	-1.618286	1.523197
22	1	0	-3.270119	0.099459	1.885641
23	6	0	-1.662979	-0.762671	0.716618
24	1	0	-0.972097	-0.540559	1.536400
25	1	0	-1.424492	-1.764457	0.336867
26	6	0	0.999916	-1.540788	-0.923578
27	1	0	0.959721	-2.459369	-0.327726
28	1	0	0.008023	-1.323316	-1.319312
29	1	0	1.691956	-1.701891	-1.760688

Model B: N-Methyl Aldehyde



HF (M062X/6-31+G(d,p)) = -479.3428132 Hartrees

Imaginary Frequencies: none found

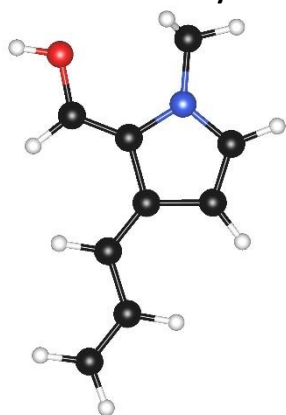
Zero-point correction = 0.183139 (Hartree/Particle)

Thermal correction = 0.145447 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.500004	-0.314085	-0.000219
2	6	0	-0.757848	0.307683	-0.000068
3	6	0	-1.070859	1.721983	0.000088
4	1	0	-0.190110	2.390109	-0.000160
5	6	0	1.794721	0.367839	-0.000532
6	6	0	2.983147	-0.247639	0.000319
7	6	0	4.303291	0.460140	0.000064
8	1	0	4.895763	0.185613	-0.879529
9	1	0	4.170264	1.545221	-0.001213
10	1	0	1.781120	1.456549	-0.001458
11	1	0	3.015861	-1.337018	0.001339
12	6	0	-1.112035	-1.885584	0.000171
13	1	0	-1.696717	-2.795127	0.000247
14	6	0	0.258648	-1.708013	0.000371
15	1	0	0.992808	-2.500095	0.000576
16	1	0	4.895047	0.187585	0.880756
17	8	0	-2.196907	2.193140	0.000602
18	7	0	-1.725914	-0.677391	-0.000303
19	6	0	-3.168718	-0.476452	-0.000478
20	1	0	-3.475004	0.082162	0.884505
21	1	0	-3.474061	0.086527	-0.882945
22	1	0	-3.640432	-1.460144	-0.003115

Model B: N-Methyl Enol



HF (M062X/6-31+G(d,p)) = -479.2896605 Hartrees

Imaginary Frequencies: none found

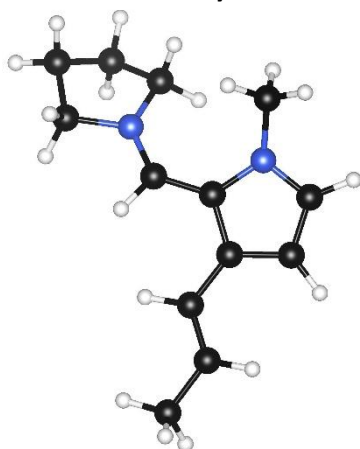
Zero-point correction = 0.181189 (Hartree/Particle)

Thermal correction = 0.144177 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.665774	0.250794	-0.000134
2	6	0	-0.712518	-0.310003	-0.000597
3	6	0	-1.049688	-1.610470	0.000066
4	1	0	-0.280281	-2.374202	0.001512
5	6	0	1.824424	-0.459271	-0.000076
6	6	0	3.144230	0.132753	0.000294
7	6	0	4.290461	-0.568111	0.000396
8	1	0	5.256317	-0.075753	0.000672
9	1	0	4.285298	-1.655134	0.000198
10	1	0	1.784728	-1.547289	-0.000295
11	1	0	3.198655	1.220269	0.000499
12	6	0	-0.852054	1.940021	-0.000964
13	1	0	-1.366095	2.893544	-0.001157
14	6	0	0.480328	1.696572	0.000109
15	1	0	1.256616	2.445374	0.000512
16	8	0	-2.353921	-2.034553	0.000206
17	1	0	-2.382784	-2.995300	-0.005005
18	7	0	-1.595456	0.782534	-0.001649
19	6	0	-3.041348	0.718901	0.001760
20	1	0	-3.415399	0.197518	-0.883308
21	1	0	-3.411580	0.200973	0.890545
22	1	0	-3.423565	1.741557	0.000595

Model B: N-Methyl Iminium



HF (M062X/6-31+G(d,p)) = -615.8341523 Hartrees

Imaginary Frequencies: none found

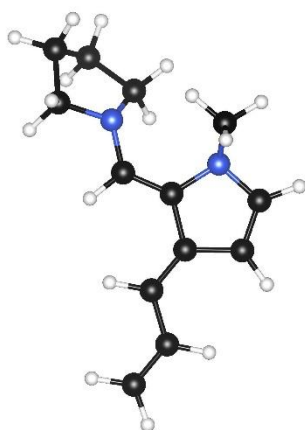
Zero-point correction = 0.303290 (Hartree/Particle)

Thermal correction = 0.260398 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.811152	0.364035	-0.055058
2	6	0	0.424778	0.574691	0.192680
3	6	0	-0.475122	-0.468409	0.463737
4	1	0	-0.015667	-1.378795	0.848089
5	7	0	-1.773729	-0.555436	0.304879
6	6	0	-2.507601	-1.790214	0.700901
7	1	0	-2.514532	-1.882130	1.788671
8	1	0	-1.983796	-2.650426	0.271200
9	6	0	-3.899165	-1.603635	0.092071
10	1	0	-4.567925	-1.124564	0.813260
11	1	0	-4.342873	-2.556578	-0.198661
12	6	0	-3.645054	-0.670443	-1.096586
13	1	0	-4.546884	-0.166905	-1.447642
14	1	0	-3.204823	-1.219390	-1.934975
15	6	0	-2.627727	0.315913	-0.525713
16	1	0	-2.006371	0.818940	-1.271267
17	1	0	-3.128453	1.059805	0.101330
18	6	0	2.493409	-0.925472	-0.071043
19	6	0	3.827825	-1.059563	-0.078744
20	6	0	4.547987	-2.367305	-0.090689
21	1	0	5.201782	-2.452928	0.783358
22	1	0	3.854933	-3.211368	-0.094141
23	1	0	1.886102	-1.827931	-0.079077
24	1	0	4.449264	-0.164388	-0.070942
25	6	0	1.344838	2.556787	-0.201384
26	1	0	1.390253	3.635623	-0.274126
27	6	0	2.361739	1.625499	-0.330809
28	1	0	3.382657	1.849249	-0.601424
29	1	0	5.191459	-2.439467	-0.973749
30	7	0	0.176317	1.946768	0.091327
31	6	0	-0.993990	2.675995	0.573483
32	1	0	-1.699127	2.881071	-0.233633
33	1	0	-1.482117	2.101848	1.362638
34	1	0	-0.660412	3.621739	1.000572

Model B: N-Methyl Trienamine



HF (M062X/6-31+G(d,p)) = -615.4020067 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.289129 (Hartree/Particle)

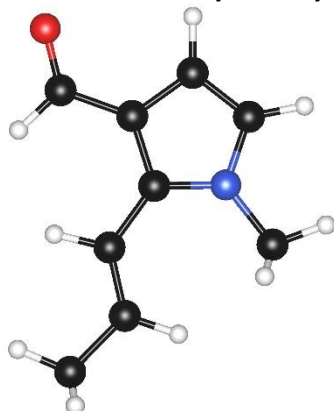
Thermal correction = 0.247231 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.897788	0.202946	-0.007825
2	6	0	-0.442985	0.390763	-0.174869
3	6	0	0.479549	-0.554031	-0.471925
4	1	0	0.135230	-1.529418	-0.816614
5	7	0	1.847247	-0.399223	-0.341899
6	6	0	2.712695	-1.449128	-0.877810
7	1	0	2.773134	-1.384303	-1.968628
8	1	0	2.321382	-2.447179	-0.615883
9	6	0	4.051327	-1.197903	-0.187636
10	1	0	4.593451	-0.397974	-0.703880
11	1	0	4.686034	-2.086560	-0.168391
12	6	0	3.614075	-0.729778	1.204473
13	1	0	4.398578	-0.201578	1.751431
14	1	0	3.303304	-1.593672	1.802239
15	6	0	2.403369	0.160634	0.905741
16	1	0	1.643656	0.139563	1.693492
17	1	0	2.706982	1.207031	0.767735
18	6	0	-2.579155	-0.972044	-0.050640
19	6	0	-4.008205	-1.098884	0.137461
20	6	0	-4.681783	-2.260097	0.081907
21	1	0	-5.755166	-2.300651	0.228662
22	1	0	-4.169636	-3.198498	-0.114929
23	1	0	-2.030163	-1.894819	-0.231439
24	1	0	-4.565397	-0.183962	0.333732
25	6	0	-1.360755	2.388840	0.326830
26	1	0	-1.365269	3.457920	0.504762
27	6	0	-2.406964	1.539061	0.297216
28	1	0	-3.433351	1.797873	0.512383
29	7	0	-0.136679	1.757691	0.087299
30	6	0	0.755272	2.449718	-0.842537
31	1	0	1.696030	1.906957	-0.933790
32	1	0	0.302668	2.525193	-1.841408

33 1 0 0.952645 3.454216 -0.459594

Model C: N-Methyl Aldehyde

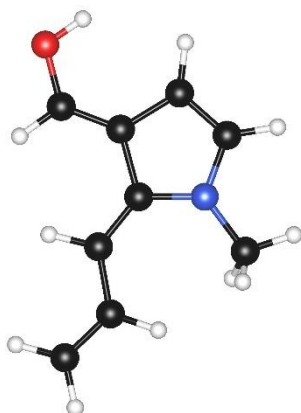


HF (M062X/6-31+G(d,p)) = -479.3380203 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.183041 (Hartree/Particle)
 Thermal correction = 0.147182 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.004769	0.102861	-0.000090
2	6	0	-1.333247	-0.317855	0.000070
3	6	0	-1.825738	-1.691553	-0.000113
4	1	0	-1.063766	-2.495822	-0.000332
5	6	0	1.182743	-0.754720	-0.000103
6	6	0	2.492186	-0.459614	0.000352
7	6	0	3.563452	-1.509072	0.000082
8	1	0	4.209845	-1.410275	0.879067
9	1	0	3.134293	-2.514402	0.002187
10	1	0	0.930484	-1.813388	-0.000438
11	1	0	2.842954	0.566860	0.000934
12	6	0	-1.317794	1.918362	0.000376
13	1	0	-1.524953	2.978692	0.000539
14	6	0	-2.158065	0.838715	0.000156
15	1	0	-3.237612	0.843382	0.000201
16	1	0	4.206820	-1.412755	-0.881421
17	8	0	-3.005916	-1.985007	-0.000108
18	7	0	-0.012853	1.473727	0.000065
19	6	0	1.126807	2.370713	-0.000467
20	1	0	1.737924	2.220838	0.893331
21	1	0	1.738232	2.219217	-0.893762
22	1	0	0.752395	3.394593	-0.001474

Model C: N-Methyl Enol

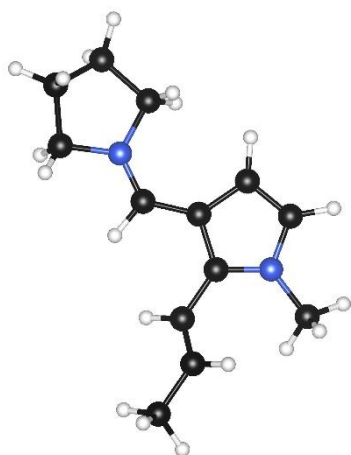


HF (M062X/6-31+G(d,p)) = -479.2920517 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.182672 (Hartree/Particle)
 Thermal correction = 0.144988 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.159835	0.040163	-0.012213
2	6	0	1.298875	-0.242662	0.016211
3	6	0	1.866239	-1.463406	-0.028807
4	1	0	1.296380	-2.382950	-0.093708
5	6	0	-1.158385	-0.882390	0.046348
6	6	0	-2.595569	-0.729682	-0.064629
7	6	0	-3.455470	-1.759700	0.020554
8	1	0	-4.524664	-1.611725	-0.078871
9	1	0	-3.105521	-2.774628	0.190247
10	1	0	-0.825869	-1.909834	0.175056
11	1	0	-3.010982	0.256766	-0.243185
12	6	0	1.011372	1.995784	-0.024243
13	1	0	1.109746	3.073488	-0.042324
14	6	0	1.974159	1.055352	0.036021
15	1	0	3.036306	1.252273	0.059505
16	8	0	3.198428	-1.706650	-0.007444
17	1	0	3.685999	-0.877570	0.071280
18	7	0	-0.256947	1.433880	-0.083770
19	6	0	-1.467712	2.207432	0.061001
20	1	0	-2.113882	2.110239	-0.816817
21	1	0	-2.023579	1.896136	0.952562
22	1	0	-1.194777	3.258501	0.170740

Model C: N-Methyl Iminium



HF (M062X/6-31+G(d,p)) = -615.8505083 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.303749 (Hartree/Particle)

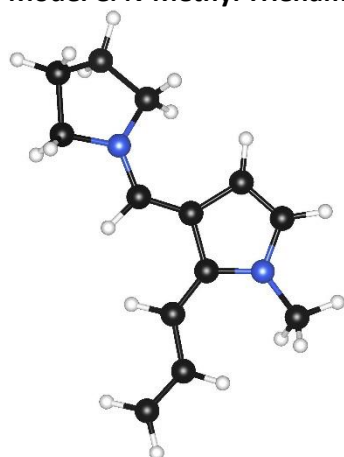
Thermal correction = 0.261707 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.492579	-0.248818	-0.134969
2	6	0	-0.106471	-0.545752	-0.044852
3	6	0	0.845996	0.492826	-0.079440
4	1	0	0.463237	1.512099	-0.122783
5	7	0	2.146619	0.402288	-0.055137
6	6	0	3.040332	1.587914	-0.057134
7	1	0	2.637574	2.353537	0.608060
8	1	0	3.094140	1.982647	-1.077527
9	6	0	4.380628	1.009326	0.386824
10	1	0	4.418118	0.939738	1.478511
11	1	0	5.219397	1.621265	0.052900
12	6	0	4.366642	-0.388276	-0.241140
13	1	0	5.083468	-1.072644	0.213990
14	1	0	4.586690	-0.325364	-1.311253
15	6	0	2.924294	-0.853118	-0.030418
16	1	0	2.556917	-1.523554	-0.811169
17	1	0	2.786596	-1.327467	0.947935
18	6	0	-2.129328	1.051907	-0.349932
19	6	0	-3.221478	1.480179	0.298362
20	6	0	-3.870678	2.807166	0.073872
21	1	0	-3.890354	3.385604	1.002847
22	1	0	-3.349563	3.385767	-0.691773
23	1	0	-1.659682	1.706290	-1.082344
24	1	0	-3.673048	0.839101	1.055645
25	6	0	-1.260697	-2.456948	0.177818
26	1	0	-1.621559	-3.467156	0.303241
27	6	0	0.007616	-1.966850	0.156851
28	1	0	0.899269	-2.557326	0.290046
29	1	0	-4.912018	2.675508	-0.237729
30	7	0	-2.158173	-1.415890	-0.007720
31	6	0	-3.599271	-1.629951	-0.112625

32	1	0	-4.072807	-1.560828	0.869113
33	1	0	-4.028311	-0.884851	-0.782080
34	1	0	-3.767221	-2.624777	-0.524930

Model C: N-Methyl Trienamine



HF (M062X/6-31+G(d,p)) = -615.405935 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.289306 (Hartree/Particle)

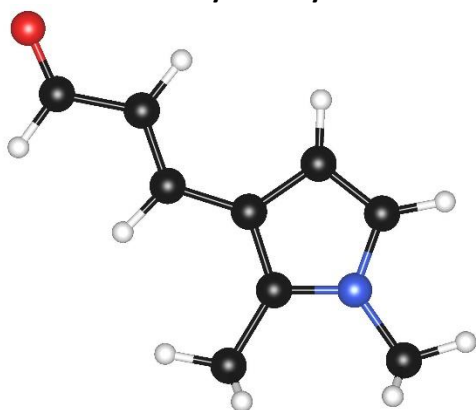
Thermal correction = 0.246842 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.567162	-0.122782	-0.027991
2	6	0	0.127385	-0.449763	-0.067520
3	6	0	-0.837610	0.504419	-0.211371
4	1	0	-0.519833	1.533954	-0.370908
5	7	0	-2.184581	0.342239	-0.198725
6	6	0	-3.089846	1.467203	-0.431620
7	1	0	-2.916051	1.910900	-1.416991
8	1	0	-2.937920	2.247837	0.329405
9	6	0	-4.476270	0.835159	-0.303145
10	1	0	-4.774784	0.393911	-1.260168
11	1	0	-5.238564	1.558725	-0.006503
12	6	0	-4.248853	-0.269003	0.735949
13	1	0	-5.025903	-1.036543	0.728860
14	1	0	-4.205196	0.166688	1.740033
15	6	0	-2.873235	-0.820769	0.351090
16	1	0	-2.311377	-1.216504	1.204505
17	1	0	-2.964215	-1.618272	-0.400048
18	6	0	2.120132	1.112444	0.177903
19	6	0	3.485308	1.547447	-0.016181
20	6	0	3.927816	2.795077	0.231856
21	1	0	4.956911	3.077054	0.041041
22	1	0	3.264640	3.560574	0.626503
23	1	0	1.425612	1.890951	0.483903
24	1	0	4.199350	0.837924	-0.425631

25	6	0	1.297422	-2.376852	-0.205840
26	1	0	1.645478	-3.397238	-0.296649
27	6	0	0.036558	-1.907051	-0.123599
28	1	0	-0.857354	-2.508527	-0.174329
29	7	0	2.230401	-1.340062	-0.191077
30	6	0	3.626202	-1.566946	0.112081
31	1	0	4.277572	-1.286390	-0.721068
32	1	0	3.916588	-0.992380	0.999055
33	1	0	3.771273	-2.629401	0.317926

Model D: N-Methyl Aldehyde



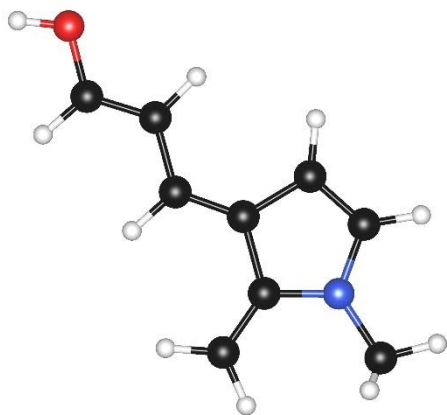
HF (M062X/6-31+G(d,p)) = -479.3435913 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.182803 (Hartree/Particle)
Thermal correction = 0.145068 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.237343	0.373788	-0.000219
2	6	0	-2.391076	-0.324071	-0.000067
3	6	0	-3.671192	0.381889	-0.000239
4	1	0	-3.592702	1.491658	-0.000539
5	1	0	-2.422672	-1.410171	0.000207
6	1	0	-1.318307	1.462318	-0.000473
7	6	0	0.100132	-0.173031	-0.000088
8	6	0	1.277036	0.573464	0.000027
9	6	0	0.481336	-1.553053	-0.000055
10	6	0	1.848317	-1.595298	0.000089
11	1	0	-0.179188	-2.407638	-0.000154
12	1	0	2.532608	-2.431051	0.000140
13	6	0	1.506464	2.048874	0.000099
14	1	0	2.067059	2.369716	-0.885015
15	1	0	0.555836	2.582972	-0.000075
16	1	0	2.066711	2.369679	0.885448
17	8	0	-4.760538	-0.154877	-0.000088
18	7	0	2.325105	-0.302266	0.000134
19	6	0	3.724815	0.074242	0.000312

20	1	0	3.969537	0.659716	-0.890337
21	1	0	3.969342	0.659608	0.891087
22	1	0	4.329408	-0.832747	0.000322

Model D: N-Methyl Enol



HF (M062X/6-31+G(d,p)) = -479.2982428 Hartrees

Imaginary Frequencies: none found

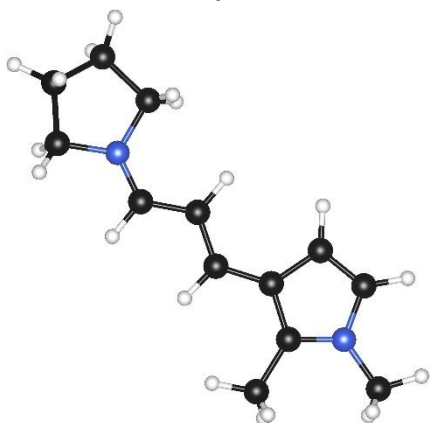
Zero-point correction = -479.2982428 (Hartree/Particle)

Thermal correction = 0.142483 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.090570	0.505750	-0.000676
2	6	0	-2.338077	-0.221732	-0.001024
3	6	0	-3.526821	0.399357	0.000769
4	1	0	-3.608443	1.485261	0.002905
5	1	0	-2.327176	-1.308579	-0.002772
6	1	0	-1.156611	1.593184	-0.000123
7	6	0	0.138366	-0.062725	-0.000690
8	6	0	1.428188	0.682719	-0.000196
9	6	0	0.498844	-1.478508	-0.000580
10	6	0	1.847996	-1.551346	0.000352
11	1	0	-0.178877	-2.318081	-0.000801
12	1	0	2.484832	-2.426992	0.000881
13	6	0	1.660634	2.010181	-0.000669
14	1	0	2.665863	2.413280	-0.000223
15	1	0	0.837221	2.712323	-0.001624
16	8	0	-4.695147	-0.298886	-0.000975
17	1	0	-5.446162	0.301249	0.008073
18	7	0	2.425921	-0.293256	0.000718
19	6	0	3.831279	0.007275	0.001354
20	1	0	4.107535	0.585968	-0.888955
21	1	0	4.106474	0.586872	0.891397
22	1	0	4.396040	-0.926431	0.002173

Model D: N-Methyl Iminium



HF (M062X/6-31+G(d,p)) = -615.8593694 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.303228 (Hartree/Particle)

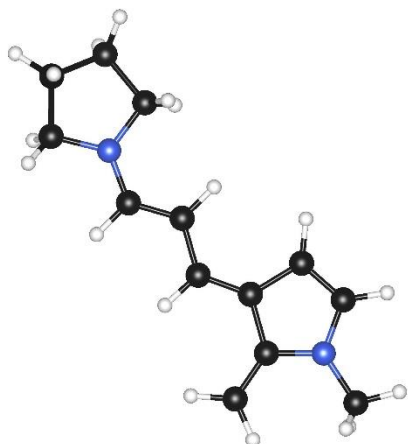
Thermal correction = 0.259681 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.591563	0.557354	0.033993
2	6	0	-0.646211	-0.050408	0.041316
3	6	0	-1.802418	0.748843	0.066576
4	1	0	-1.689921	1.833045	0.078085
5	7	0	-3.035160	0.311756	0.073286
6	6	0	-4.226609	1.188913	0.075746
7	1	0	-4.049491	2.056569	-0.562665
8	1	0	-4.415620	1.526221	1.101156
9	6	0	-5.333019	0.258954	-0.415332
10	1	0	-5.316765	0.200761	-1.508239
11	1	0	-6.321356	0.598334	-0.102947
12	6	0	-4.936635	-1.087835	0.201028
13	1	0	-5.410420	-1.939801	-0.287938
14	1	0	-5.204877	-1.111553	1.261609
15	6	0	-3.413888	-1.116112	0.045852
16	1	0	-2.902441	-1.650811	0.850440
17	1	0	-3.103464	-1.539360	-0.916483
18	1	0	-0.731896	-1.131527	0.023416
19	1	0	0.608179	1.647533	0.052860
20	6	0	1.839014	-0.096690	0.005331
21	6	0	3.090973	0.559984	0.002311
22	6	0	2.109311	-1.510249	-0.026016
23	6	0	3.460394	-1.653643	-0.046127
24	1	0	1.389006	-2.314664	-0.033371
25	1	0	4.080458	-2.537441	-0.070707
26	6	0	3.436662	2.009655	0.027837
27	1	0	4.019158	2.290736	-0.855454
28	1	0	2.539233	2.627704	0.045328
29	1	0	4.030660	2.257099	0.913572
30	7	0	4.043507	-0.390972	-0.028507
31	6	0	5.479133	-0.141465	-0.040817

32	1	0	5.757060	0.434129	-0.926473
33	1	0	5.777568	0.402998	0.857831
34	1	0	5.996883	-1.099280	-0.063655

Model D: N-Methyl Trienamine



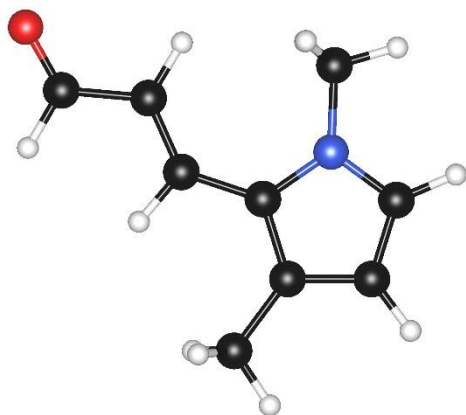
HF (M062X/6-31+G(d,p)) = -615.4153755 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.287821 (Hartree/Particle)
 Thermal correction = 0.243096 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.662053	0.669909	0.033299
2	6	0	-0.637146	0.055624	0.041815
3	6	0	-1.777819	0.798394	0.053959
4	1	0	-1.707435	1.885610	0.057001
5	7	0	-3.047713	0.319702	0.055991
6	6	0	-4.238308	1.159603	0.053140
7	1	0	-4.111028	2.007883	-0.627545
8	1	0	-4.450930	1.553964	1.058735
9	6	0	-5.333427	0.191473	-0.398118
10	1	0	-5.333920	0.119452	-1.491002
11	1	0	-6.329130	0.499521	-0.071704
12	6	0	-4.878924	-1.138639	0.216492
13	1	0	-5.329544	-2.011062	-0.261259
14	1	0	-5.136511	-1.163110	1.280736
15	6	0	-3.354805	-1.101092	0.053059
16	1	0	-2.830564	-1.612963	0.870314
17	1	0	-3.026350	-1.558912	-0.892852
18	1	0	-0.699494	-1.029057	0.034619
19	1	0	0.684827	1.759953	0.044206
20	6	0	1.849610	0.012669	0.011699
21	6	0	3.188139	0.657455	0.004070
22	6	0	2.098773	-1.426203	-0.018474
23	6	0	3.437427	-1.605628	-0.052625
24	1	0	1.356327	-2.209735	-0.022414

25	1	0	4.007544	-2.525530	-0.084085
26	6	0	3.526752	1.963752	0.046855
27	1	0	4.560050	2.287923	0.035751
28	1	0	2.761448	2.727299	0.096084
29	7	0	4.107752	-0.391723	-0.050156
30	6	0	5.531024	-0.199120	-0.038203
31	1	0	5.849122	0.403242	-0.898173
32	1	0	5.851048	0.311875	0.879266
33	1	0	6.024179	-1.171382	-0.090333

Model E: N-Methyl Aldehyde



HF (M062X/6-31+G(d,p)) = -479.3409082 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.183048 (Hartree/Particle)

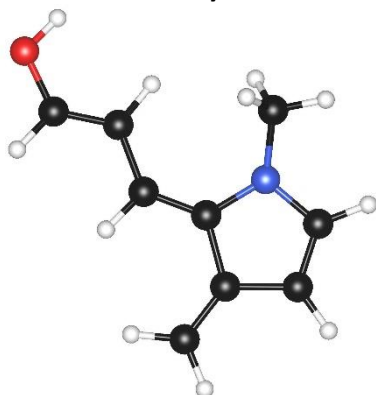
Thermal correction = 0.145284 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.791688	-0.532842	-0.007204
2	6	0	-1.951295	0.165128	0.004469
3	6	0	-3.219320	-0.564208	-0.003544
4	1	0	-3.124920	-1.672095	-0.020895
5	1	0	-2.026681	1.245417	0.021398
6	1	0	-0.895811	-1.619722	-0.020772
7	6	0	0.584007	-0.123074	-0.003392
8	6	0	1.689244	-0.982161	-0.001047
9	6	0	2.422988	1.143198	0.004610
10	1	0	2.992552	2.061840	0.005905
11	6	0	1.647132	-2.481870	0.001421
12	1	0	1.188209	-2.873517	0.915069
13	1	0	1.083990	-2.874545	-0.851246
14	6	0	2.843737	-0.174957	0.004604
15	1	0	3.869623	-0.514985	0.007255
16	1	0	2.660294	-2.885261	-0.058606
17	8	0	-4.314881	-0.040466	0.007696
18	7	0	1.065737	1.176498	-0.000114
19	6	0	0.281268	2.396632	-0.005899

20	1	0	-0.350796	2.443837	-0.896001
21	1	0	-0.342340	2.458971	0.889324
22	1	0	0.968335	3.243225	-0.016309

Model E: N-Methyl Enol

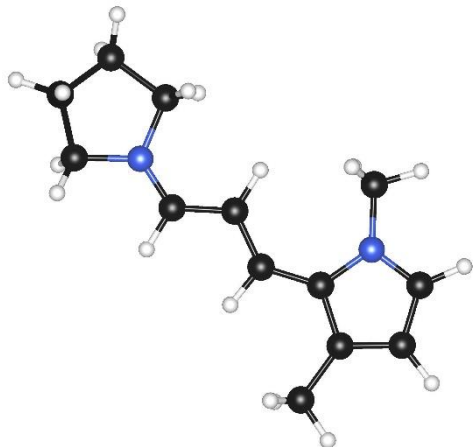


HF (M062X/6-31+G(d,p)) = -479.2919562 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.182499 (Hartree/Particle)
Thermal correction = 0.145346 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.650722	-0.670247	0.052774
2	6	0	-1.922200	0.017341	-0.071012
3	6	0	-3.088221	-0.635274	0.069235
4	1	0	-3.140505	-1.695965	0.296045
5	1	0	-1.950775	1.077018	-0.309168
6	1	0	-0.725667	-1.743903	0.211245
7	6	0	0.615579	-0.200784	-0.028870
8	6	0	1.852053	-1.037689	0.010848
9	6	0	2.440072	1.149802	-0.069816
10	1	0	2.949845	2.105021	-0.101534
11	6	0	1.927801	-2.380743	0.001774
12	1	0	2.891954	-2.876468	0.024558
13	1	0	1.045746	-3.010647	-0.032984
14	6	0	2.964145	-0.088152	0.011319
15	1	0	4.012730	-0.344923	0.033200
16	8	0	-4.329156	-0.096408	-0.046533
17	1	0	-4.263114	0.843554	-0.254789
18	7	0	1.051622	1.131192	-0.146231
19	6	0	0.246720	2.292357	0.158068
20	1	0	-0.437642	2.536068	-0.660513
21	1	0	-0.332165	2.136945	1.076987
22	1	0	0.910124	3.146549	0.306919

Model E: N-Methyl Iminium



HF (M062X/6-31+G(d,p)) = -615.8522084 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.303822 (Hartree/Particle)

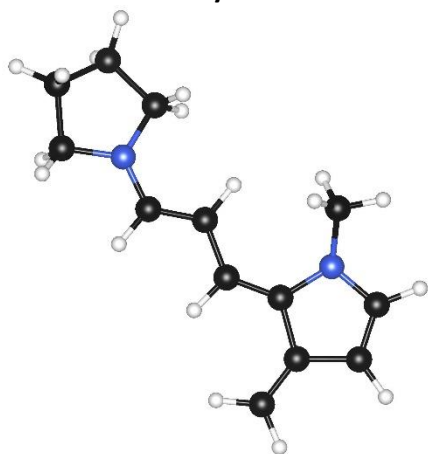
Thermal correction = 0.261010 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.912313	-0.629013	-0.029915
2	6	0	-0.325470	-0.003636	-0.043120
3	6	0	-1.474008	-0.811759	-0.064539
4	1	0	-1.352810	-1.894994	-0.069582
5	7	0	-2.712684	-0.386486	-0.074261
6	6	0	-3.894254	-1.276767	-0.071687
7	1	0	-3.708748	-2.137617	0.573559
8	1	0	-4.079265	-1.624277	-1.094441
9	6	0	-5.011037	-0.355596	0.412519
10	1	0	-4.997057	-0.291063	1.505092
11	1	0	-5.995407	-0.706767	0.100694
12	6	0	-4.628334	0.991971	-0.210827
13	1	0	-5.111085	1.841619	0.273405
14	1	0	-4.896119	1.007262	-1.271654
15	6	0	-3.105716	1.036007	-0.055372
16	1	0	-2.600691	1.571798	-0.863850
17	1	0	-2.800613	1.469582	0.904512
18	1	0	-0.436240	1.072017	-0.032773
19	1	0	0.889204	-1.719459	-0.043623
20	6	0	2.217478	-0.130222	-0.002254
21	6	0	3.395097	-0.929313	0.005450
22	6	0	3.969423	1.239841	0.049360
23	1	0	4.494198	2.185933	0.074371
24	6	0	3.445057	-2.425155	-0.020992
25	1	0	4.480479	-2.765610	0.022718
26	1	0	2.915427	-2.861089	0.831572
27	6	0	4.480217	-0.059878	0.037908
28	1	0	5.527207	-0.325807	0.051723
29	1	0	3.002345	-2.824303	-0.938821

30	7	0	2.627456	1.205963	0.025185
31	6	0	1.776571	2.385237	0.030739
32	1	0	1.168176	2.419166	-0.875949
33	1	0	1.138276	2.389356	0.917260
34	1	0	2.415293	3.267603	0.055697

Model E: N-Methyl Trienamine



HF (M062X/6-31+G(d,p)) = -615.4064184 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.288375 (Hartree/Particle)

Thermal correction = 0.244371 Hartrees

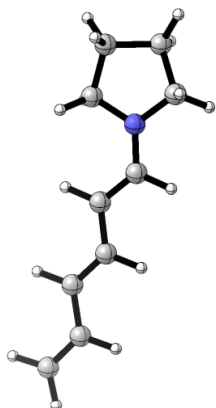
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.983478	-0.749614	0.055383
2	6	0	-0.319601	-0.129492	-0.019641
3	6	0	-1.453539	-0.867583	0.114654
4	1	0	-1.378514	-1.939621	0.293732
5	7	0	-2.730011	-0.396515	0.067125
6	6	0	-3.909902	-1.248274	0.090688
7	1	0	-3.823395	-2.003320	0.878825
8	1	0	-4.052955	-1.768045	-0.870443
9	6	0	-5.036554	-0.245236	0.338516
10	1	0	-5.094092	-0.013861	1.407378
11	1	0	-6.010725	-0.614410	0.010488
12	6	0	-4.562747	0.985403	-0.446422
13	1	0	-5.035148	1.913737	-0.118316
14	1	0	-4.783825	0.851722	-1.510614
15	6	0	-3.042462	0.991100	-0.229955
16	1	0	-2.497462	1.330742	-1.121794
17	1	0	-2.741321	1.635789	0.609516
18	1	0	-0.406193	0.934340	-0.203730
19	1	0	0.971560	-1.832115	0.173727
20	6	0	2.224807	-0.214390	-0.029231
21	6	0	3.501059	-0.982132	-0.053912
22	6	0	3.967503	1.238380	-0.046119

23	1	0	4.426997	2.219569	-0.040646
24	6	0	3.655318	-2.318715	-0.128969
25	1	0	4.647147	-2.756392	-0.151491
26	1	0	2.810611	-2.997097	-0.176384
27	6	0	4.558994	0.026925	-0.032513
28	1	0	5.620291	-0.172436	-0.046607
29	7	0	2.582712	1.150797	-0.100874
30	6	0	1.735167	2.236674	0.341226
31	1	0	0.987170	2.498917	-0.412855
32	1	0	1.223076	1.978317	1.276572
33	1	0	2.358735	3.115927	0.516642

A.4.3: Energies and Reaction Coordinates for Chapter 4

Trienamine A1



HF (M062X/6-31+G(d,p)) = -444.608138 Hartrees

Imaginary Frequencies: none found

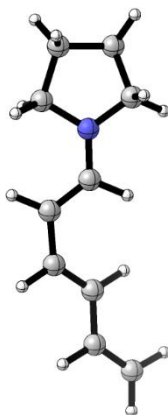
Zero-point correction = 0.230636 (Hartree/Particle)

Thermal correction = 0.191861 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.875507	-1.177912	0.112000
2	6	0	4.030011	-0.297005	-0.368866
3	6	0	3.648425	1.084352	0.178788
4	6	0	2.126460	1.128637	-0.000698
5	1	0	2.705899	-2.048162	-0.530627
6	1	0	5.002481	-0.647211	-0.016091
7	1	0	4.045547	-0.275861	-1.463769
8	1	0	3.897289	1.143171	1.243770
9	1	0	4.153954	1.905839	-0.332964
10	1	0	1.625960	1.705867	0.787401
11	1	0	1.834296	1.562205	-0.969529
12	7	0	1.736455	-0.270510	0.061133
13	6	0	0.440461	-0.674482	0.073310
14	1	0	0.309653	-1.755089	0.125339
15	6	0	-0.655970	0.125822	0.020919
16	1	0	-0.545807	1.206179	-0.035030
17	6	0	-1.992536	-0.419595	0.032201
18	1	0	-2.072757	-1.507716	0.089046
19	6	0	-3.135908	0.296928	-0.021422
20	6	0	-4.457819	-0.305359	-0.007683
21	1	0	-4.488470	-1.394103	0.051895
22	6	0	-5.611980	0.375414	-0.062595
23	1	0	-5.622437	1.460679	-0.122774
24	1	0	-6.570747	-0.130829	-0.048799
25	1	0	3.055006	-1.536797	1.137174
26	1	0	-3.084956	1.384594	-0.078696

Trienamine A2



HF (M062X/6-31+G(d,p)) = -444.6034316 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.230875 (Hartree/Particle)

Thermal correction = 0.192202 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.330603	1.308331	-0.385883
2	6	0	3.671255	0.993386	0.277214
3	6	0	3.798253	-0.521177	0.062418
4	6	0	2.359664	-1.036585	0.220990
5	1	0	1.852193	2.209185	0.011574
6	1	0	4.500361	1.558093	-0.154903
7	1	0	3.614407	1.221888	1.346658
8	1	0	4.152977	-0.720514	-0.954240
9	1	0	4.491111	-0.997487	0.759126
10	1	0	2.136540	-1.855738	-0.476339
11	1	0	2.149207	-1.399566	1.237480
12	7	0	1.539112	0.128782	-0.067181
13	6	0	0.188062	0.063029	-0.193337
14	1	0	-0.285746	1.018525	-0.415485
15	6	0	-0.576775	-1.051628	-0.066266
16	1	0	-0.097483	-2.016617	0.071317
17	6	0	-2.029053	-1.033006	-0.139705
18	1	0	-2.499673	-1.972146	-0.434823
19	6	0	-2.846408	0.009988	0.120025
20	6	0	-4.289437	-0.050346	-0.047204
21	1	0	-4.692623	-1.001832	-0.395620
22	6	0	-5.130655	0.965028	0.195575
23	1	0	-4.764505	1.928678	0.540523
24	1	0	-6.201042	0.861328	0.056557
25	1	0	2.451578	1.433273	-1.473638
26	1	0	-2.434128	0.949337	0.489111

Trienamine A3



HF (M062X/6-31+G(d,p)) = -444.6032643 Hartrees

Imaginary Frequencies: none found

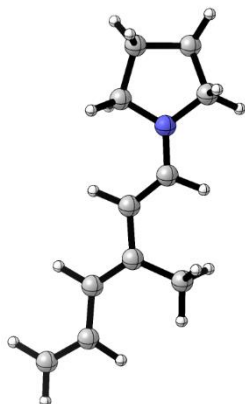
Zero-point correction = 0.230506 (Hartree/Particle)

Thermal correction = 0.191429 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.695662	1.277278	0.027202
2	6	0	-3.945691	0.471133	-0.329604
3	6	0	-3.665573	-0.887214	0.326765
4	6	0	-2.161373	-1.088400	0.101962
5	1	0	-2.481978	2.075779	-0.690877
6	1	0	-4.865976	0.939449	0.026283
7	1	0	-4.012188	0.357433	-1.416874
8	1	0	-3.875378	-0.830330	1.400168
9	1	0	-4.263149	-1.699605	-0.092039
10	1	0	-1.680726	-1.625507	0.930126
11	1	0	-1.949419	-1.644840	-0.823669
12	7	0	-1.646585	0.267202	0.000907
13	6	0	-0.318491	0.545524	-0.050157
14	1	0	-0.085080	1.608292	-0.108908
15	6	0	0.694718	-0.359487	-0.041043
16	1	0	0.479614	-1.423885	0.015486
17	6	0	2.078508	0.048906	-0.107234
18	1	0	2.265956	1.123528	-0.155404
19	6	0	3.137676	-0.787100	-0.134324
20	6	0	4.537779	-0.360823	-0.170069
21	1	0	5.235937	-1.062932	-0.625372
22	6	0	5.026142	0.790056	0.312774
23	1	0	4.393213	1.504656	0.832100
24	1	0	6.076942	1.039653	0.212551
25	1	0	-2.792335	1.729140	1.026623
26	1	0	2.952461	-1.860489	-0.154175

Trienamine B1



HF (M062X/6-31+G(d,p)) = -483.9049185 Hartrees

Imaginary Frequencies: none found

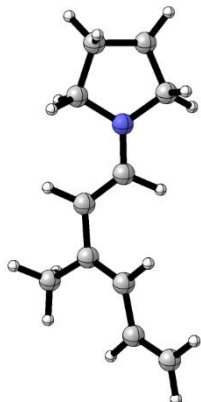
Zero-point correction = 0.259279 (Hartree/Particle)

Thermal correction = 0.218753 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.091533	1.048329	-0.077218
2	6	0	4.213811	0.116563	0.383638
3	6	0	3.788324	-1.235382	-0.203454
4	6	0	2.264453	-1.232314	-0.032614
5	1	0	2.949643	1.906156	0.588805
6	1	0	5.199420	0.443117	0.044652
7	1	0	4.223077	0.064708	1.477637
8	1	0	4.041176	-1.273327	-1.268473
9	1	0	4.262929	-2.087460	0.287656
10	1	0	1.750187	-1.769651	-0.840021
11	1	0	1.951786	-1.685723	0.920903
12	7	0	1.922856	0.179722	-0.054412
13	6	0	0.639163	0.631678	-0.054437
14	1	0	0.558237	1.716506	-0.075724
15	6	0	-0.475992	-0.141541	-0.023795
16	1	0	-0.371163	-1.223548	0.000473
17	6	0	-1.836181	0.379167	-0.015841
18	6	0	-2.879194	-0.488098	0.018341
19	6	0	-4.297174	-0.172777	0.032537
20	1	0	-4.593678	0.873588	0.013402
21	6	0	-5.265030	-1.102221	0.068608
22	1	0	-5.027117	-2.162801	0.088916
23	1	0	-6.314262	-0.828466	0.078391
24	1	0	3.288799	1.429837	-1.091272
25	1	0	-2.643220	-1.552699	0.038265
26	6	0	-2.011103	1.876467	-0.047882
27	1	0	-1.521293	2.339218	0.816247
28	1	0	-1.552314	2.297028	-0.949825
29	1	0	-3.057858	2.176238	-0.036443

Trienamine B2



HF (M062X/6-31+G(d,p)) = -483.9010804 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.258609 (Hartree/Particle)

Thermal correction = 0.217086 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.598183	-1.357675	0.424475
2	6	0	-3.985090	-0.715927	0.524159
3	6	0	-3.946805	0.350940	-0.577125
4	6	0	-2.519025	0.894798	-0.477044
5	1	0	-2.246663	-1.755553	1.382142
6	1	0	-4.792878	-1.440193	0.398250
7	1	0	-4.101139	-0.237181	1.502467
8	1	0	-4.096721	-0.116479	-1.556271
9	1	0	-4.702586	1.128969	-0.450870
10	1	0	-2.129633	1.261389	-1.434830
11	1	0	-2.446624	1.719340	0.251038
12	7	0	-1.754952	-0.253848	-0.023089
13	6	0	-0.404107	-0.222640	0.130159
14	1	0	0.027731	-1.155973	0.488470
15	6	0	0.404563	0.839919	-0.109332
16	1	0	-0.036868	1.798675	-0.373474
17	6	0	1.861465	0.790072	0.027957
18	6	0	2.569754	-0.339639	-0.213604
19	6	0	3.994460	-0.537504	0.003319
20	1	0	4.564838	0.285280	0.429373
21	6	0	4.640279	-1.679596	-0.277433
22	1	0	4.115950	-2.534615	-0.697203
23	1	0	5.703579	-1.790264	-0.095563
24	1	0	-2.594995	-2.177277	-0.309333
25	1	0	2.035984	-1.200468	-0.616015
26	6	0	2.494022	2.089520	0.463657
27	1	0	2.091226	2.914075	-0.134890
28	1	0	2.246805	2.305073	1.509362
29	1	0	3.578660	2.098520	0.353856

Trienamine B3



HF (M062X/6-31+G(d,p)) = -483.8998887 Hartrees

Imaginary Frequencies: none found

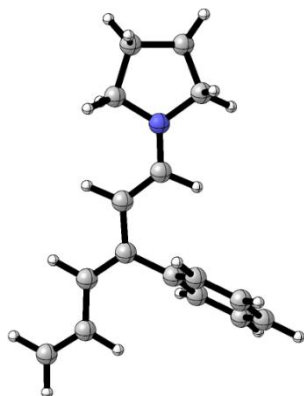
Zero-point correction = 0.259248 (Hartree/Particle)

Thermal correction = 0.218662 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.959374	1.177936	0.165760
2	6	0	-4.192472	0.374349	-0.250549
3	6	0	-3.867818	-1.030754	0.273314
4	6	0	-2.360465	-1.167713	0.020362
5	1	0	-2.775746	2.044281	-0.478624
6	1	0	-5.120235	0.782253	0.156775
7	1	0	-4.270472	0.360152	-1.342915
8	1	0	-4.069132	-1.081111	1.348727
9	1	0	-4.446246	-1.817489	-0.215576
10	1	0	-1.859393	-1.763950	0.794536
11	1	0	-2.142349	-1.634829	-0.952342
12	7	0	-1.884881	0.204549	0.036282
13	6	0	-0.563882	0.530425	-0.013846
14	1	0	-0.376274	1.601457	0.020967
15	6	0	0.467664	-0.346985	-0.099834
16	1	0	0.256571	-1.413647	-0.112363
17	6	0	1.874329	0.034895	-0.145943
18	6	0	2.819830	-0.938191	-0.152904
19	6	0	4.276036	-0.796358	-0.156193
20	1	0	4.812858	-1.566287	-0.711782
21	6	0	5.007009	0.128871	0.482599
22	1	0	4.551621	0.883555	1.116512
23	1	0	6.089738	0.131022	0.409122
24	1	0	-3.056183	1.536172	1.202849
25	1	0	2.461579	-1.967223	-0.185712
26	6	0	2.209905	1.503054	-0.219695
27	1	0	2.110696	1.987617	0.759199
28	1	0	3.231119	1.655877	-0.571045
29	1	0	1.531452	2.013147	-0.910716

Trienamine C1



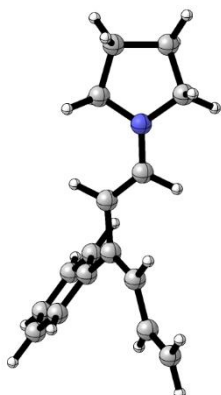
HF (M062X/6-31+G(d,p)) = -675.5786681 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.312563 (Hartree/Particle)
 Thermal correction = 0.265475 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.495907	1.194077	0.097238
2	6	0	4.836179	0.601562	0.535978
3	6	0	4.859476	-0.747209	-0.194671
4	6	0	3.404231	-1.222046	-0.106483
5	1	0	3.079208	1.898753	0.823914
6	1	0	5.684023	1.242394	0.284400
7	1	0	4.831331	0.441967	1.619517
8	1	0	5.136006	-0.595413	-1.243599
9	1	0	5.560225	-1.462800	0.240269
10	1	0	3.099692	-1.807723	-0.983448
11	1	0	3.221648	-1.839670	0.786586
12	7	0	2.646586	0.015432	-0.022071
13	6	0	1.289269	0.051616	-0.017811
14	1	0	0.866423	1.049580	0.081084
15	6	0	0.468444	-1.027988	-0.112814
16	1	0	0.897801	-2.023111	-0.199412
17	6	0	-0.983942	-0.954353	-0.072109
18	6	0	-1.742029	-2.079939	-0.043502
19	6	0	-3.194416	-2.131725	-0.052248
20	1	0	-3.724914	-1.184439	-0.133856
21	6	0	-3.901706	-3.269747	0.021414
22	1	0	-3.409922	-4.235888	0.104425
23	1	0	-4.985837	-3.264836	0.001212
24	1	0	3.594269	1.713577	-0.868240
25	1	0	-1.226576	-3.040758	-0.030966
26	6	0	-1.621765	0.395989	-0.045977
27	6	0	-1.571122	1.234030	-1.166024
28	6	0	-2.278843	0.844771	1.103858
29	6	0	-2.175142	2.489231	-1.139704
30	1	0	-1.063218	0.887158	-2.062219
31	6	0	-2.879029	2.102532	1.133776
32	1	0	-2.316918	0.195331	1.974253

33	6	0	-2.829313	2.927746	0.011547
34	1	0	-2.139470	3.123946	-2.020073
35	1	0	-3.387298	2.436597	2.033356
36	1	0	-3.299769	3.906032	0.032494

Trienamine C2



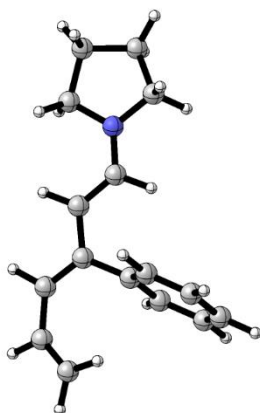
HF (M062X/6-31+G(d,p)) = -675.5752508 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.312253 (Hartree/Particle)
Thermal correction = 0.266195 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.017861	0.716569	0.729109
2	6	0	5.066943	-0.392828	0.606005
3	6	0	4.756023	-1.009632	-0.763387
4	6	0	3.226253	-0.992614	-0.803368
5	1	0	3.734833	0.914737	1.768310
6	1	0	6.088389	-0.015424	0.689966
7	1	0	4.910756	-1.138701	1.392834
8	1	0	5.154677	-0.373204	-1.560810
9	1	0	5.168749	-2.012847	-0.888508
10	1	0	2.820299	-0.915334	-1.819171
11	1	0	2.797876	-1.896121	-0.339223
12	7	0	2.886518	0.189975	-0.030310
13	6	0	1.605231	0.610928	0.137905
14	1	0	1.501706	1.505417	0.751031
15	6	0	0.495019	0.018102	-0.370501
16	1	0	0.578988	-0.930426	-0.895224
17	6	0	-0.848975	0.573038	-0.198394
18	6	0	-1.079962	1.911506	-0.159379
19	6	0	-2.323343	2.566074	0.220496
20	1	0	-3.130761	1.935614	0.587830
21	6	0	-2.506797	3.894251	0.169339
22	1	0	-1.724063	4.558503	-0.188926
23	1	0	-3.439123	4.349946	0.484443
24	1	0	4.381613	1.655631	0.287639

25	1	0	-0.251039	2.575807	-0.401642
26	6	0	-1.946046	-0.425741	-0.058460
27	6	0	-1.783397	-1.530285	0.787859
28	6	0	-3.135812	-0.313659	-0.789829
29	6	0	-2.791869	-2.480758	0.923363
30	1	0	-0.858617	-1.628704	1.349947
31	6	0	-4.143051	-1.267941	-0.661137
32	1	0	-3.257800	0.520851	-1.474922
33	6	0	-3.976563	-2.351851	0.199336
34	1	0	-2.653250	-3.322938	1.594765
35	1	0	-5.056473	-1.168460	-1.239966
36	1	0	-4.761474	-3.095136	0.300055

Trienamine C3



HF (M062X/6-31+G(d,p)) = -675.5728053 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.312537 (Hartree/Particle)

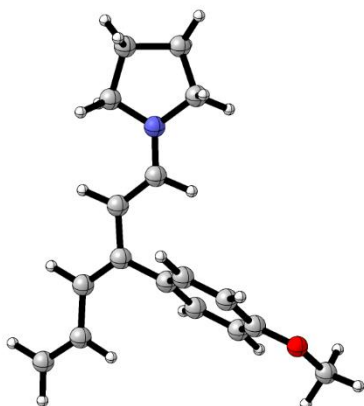
Thermal correction = 0.266906 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.420134	1.307704	-0.016991
2	6	0	-4.822624	0.838629	-0.409562
3	6	0	-4.908865	-0.543821	0.250018
4	6	0	-3.498605	-1.116241	0.063199
5	1	0	-2.991835	2.021769	-0.727611
6	1	0	-5.605005	1.524218	-0.076715
7	1	0	-4.887513	0.741249	-1.498593
8	1	0	-5.123790	-0.431312	1.318059
9	1	0	-5.680440	-1.182597	-0.184933
10	1	0	-3.193270	-1.758456	0.899686
11	1	0	-3.408473	-1.707007	-0.861132
12	7	0	-2.656897	0.066393	-0.011995
13	6	0	-1.299983	0.010827	-0.016475
14	1	0	-0.812032	0.982528	-0.065187
15	6	0	-0.552289	-1.123632	0.022175
16	1	0	-1.045205	-2.092032	0.060242

17	6	0	0.903003	-1.138750	-0.009629
18	6	0	1.583291	-2.311829	-0.063886
19	6	0	3.028143	-2.551520	-0.074232
20	1	0	3.303257	-3.540999	-0.439702
21	6	0	4.031801	-1.756214	0.328683
22	1	0	3.874571	-0.765127	0.740315
23	1	0	5.057375	-2.104476	0.258893
24	1	0	-3.427823	1.776312	0.979437
25	1	0	0.976324	-3.215038	-0.119852
26	6	0	1.609891	0.175616	-0.012572
27	6	0	1.672998	0.955573	1.146636
28	6	0	2.225873	0.639718	-1.178058
29	6	0	2.361969	2.167408	1.146904
30	1	0	1.193743	0.595592	2.053471
31	6	0	2.910085	1.853025	-1.180809
32	1	0	2.182288	0.028485	-2.075124
33	6	0	2.984616	2.617753	-0.016607
34	1	0	2.415212	2.757662	2.056874
35	1	0	3.390948	2.199602	-2.090659
36	1	0	3.524931	3.559400	-0.016270

Trienamine D1



HF (M062X/6-31+G(d,p)) = -790.0614728 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.345695 (Hartree/Particle)

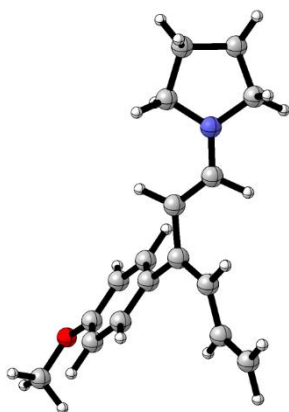
Thermal correction = 0.296674 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.499848	-1.891834	0.150681
2	6	0	-4.981290	-1.789796	0.514956
3	6	0	-5.414663	-0.508009	-0.208504
4	6	0	-4.204909	0.421324	-0.045849
5	1	0	-2.912154	-2.442897	0.891921
6	1	0	-5.552404	-2.669883	0.211459
7	1	0	-5.086511	-1.665220	1.598049
8	1	0	-5.578217	-0.719947	-1.270562

9	1	0	-6.332676	-0.074873	0.194141
10	1	0	-4.058044	1.074379	-0.916517
11	1	0	-4.290438	1.065104	0.842423
12	7	0	-3.086454	-0.495421	0.102502
13	6	0	-1.789423	-0.092063	0.078150
14	1	0	-1.067800	-0.902539	0.160676
15	6	0	-1.357638	1.192813	-0.022568
16	1	0	-2.083490	2.000464	-0.078874
17	6	0	0.045599	1.582645	-0.027861
18	6	0	0.402993	2.891670	0.029294
19	6	0	1.756195	3.414881	-0.050044
20	1	0	2.557303	2.696023	-0.212468
21	6	0	2.060031	4.718644	0.047354
22	1	0	1.288327	5.467448	0.208151
23	1	0	3.082786	5.069769	-0.033545
24	1	0	-3.368934	-2.382522	-0.826387
25	1	0	-0.392122	3.632681	0.117267
26	6	0	1.075413	0.505598	-0.104112
27	6	0	1.159321	-0.326667	-1.231522
28	6	0	1.975783	0.290117	0.937325
29	6	0	2.113242	-1.328409	-1.314913
30	1	0	0.466471	-0.171786	-2.054337
31	6	0	2.941460	-0.718659	0.873683
32	1	0	1.924090	0.923175	1.819219
33	6	0	3.009742	-1.531351	-0.258282
34	1	0	2.189477	-1.967728	-2.188379
35	1	0	3.622806	-0.853375	1.705302
36	8	0	3.906804	-2.541406	-0.426861
37	6	0	4.828043	-2.781599	0.615989
38	1	0	4.312993	-3.051339	1.546025
39	1	0	5.444818	-3.617564	0.287789
40	1	0	5.464172	-1.905999	0.793362

Trienamine D2



HF (M062X/6-31+G(d,p)) = -790.058389 Hartrees

Imaginary Frequencies: none found

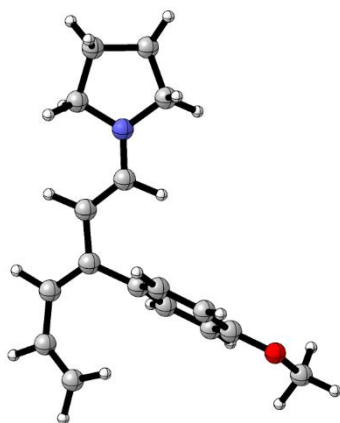
Zero-point correction = 0.345905 (Hartree/Particle)

Thermal correction = 0.297574 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.827653	0.110337	-0.675444
2	6	0	-5.620743	-1.195498	-0.571464
3	6	0	-5.155484	-1.772605	0.771676
4	6	0	-3.661917	-1.438660	0.786275
5	1	0	-4.621429	0.396896	-1.711998
6	1	0	-6.700086	-1.036972	-0.624460
7	1	0	-5.331790	-1.868946	-1.385603
8	1	0	-5.659280	-1.256617	1.596056
9	1	0	-5.347087	-2.843068	0.871127
10	1	0	-3.258416	-1.301737	1.796864
11	1	0	-3.065626	-2.222634	0.291350
12	7	0	-3.590393	-0.195059	0.038074
13	6	0	-2.427962	0.486278	-0.138555
14	1	0	-2.521943	1.393338	-0.734353
15	6	0	-1.210457	0.129966	0.344639
16	1	0	-1.087219	-0.822026	0.855189
17	6	0	-0.015545	0.959098	0.172585
18	6	0	-0.077530	2.317097	0.145222
19	6	0	0.993958	3.225699	-0.234635
20	1	0	1.908375	2.785488	-0.627981
21	6	0	0.898022	4.562009	-0.155587
22	1	0	0.001455	5.040953	0.230536
23	1	0	1.708447	5.208170	-0.474528
24	1	0	-5.364422	0.938446	-0.190368
25	1	0	-1.026699	2.787604	0.399718
26	6	0	1.269561	0.221827	0.035699
27	6	0	1.358702	-0.909597	-0.792282
28	6	0	2.408697	0.594826	0.751713
29	6	0	2.543191	-1.615961	-0.921929
30	1	0	0.480775	-1.222856	-1.350823
31	6	0	3.609435	-0.108748	0.639489
32	1	0	2.353452	1.444671	1.426450
33	6	0	3.678378	-1.217101	-0.206031
34	1	0	2.619094	-2.481859	-1.571493
35	1	0	4.467454	0.209638	1.219729
36	8	0	4.794119	-1.973999	-0.392599
37	6	0	5.967745	-1.592901	0.293667
38	1	0	5.827213	-1.645796	1.380079
39	1	0	6.737308	-2.303267	-0.007042
40	1	0	6.277839	-0.578422	0.015587

Trienamine D3



HF (M062X/6-31+G(d,p)) = -790.0554652 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.345900 (Hartree/Particle)

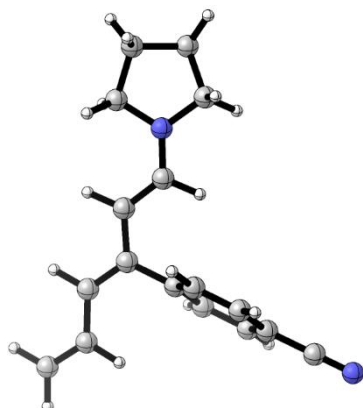
Thermal correction = 0.297126 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.531125	-1.837751	-0.005343
2	6	0	-4.998985	-1.776471	0.419296
3	6	0	-5.466728	-0.448465	-0.189624
4	6	0	-4.260370	0.476747	0.011103
5	1	0	-2.912005	-2.431569	0.674814
6	1	0	-5.575303	-2.637097	0.072714
7	1	0	-5.065220	-1.732658	1.511745
8	1	0	-5.658294	-0.579297	-1.260108
9	1	0	-6.375978	-0.057312	0.271648
10	1	0	-4.155160	1.212948	-0.796441
11	1	0	-4.315662	1.029825	0.961362
12	7	0	-3.129978	-0.436936	0.024761
13	6	0	-1.837478	-0.019582	0.024461
14	1	0	-1.106170	-0.825788	0.018500
15	6	0	-1.419213	1.273563	0.040085
16	1	0	-2.151447	2.077177	0.061266
17	6	0	-0.018705	1.670894	0.053658
18	6	0	0.327061	2.978005	0.174975
19	6	0	1.654126	3.598490	0.164689
20	1	0	1.664707	4.608683	0.574400
21	6	0	2.820182	3.127119	-0.305009
22	1	0	2.924260	2.149249	-0.762530
23	1	0	3.713176	3.741306	-0.245893
24	1	0	-3.432090	-2.260539	-1.017023
25	1	0	-0.494978	3.681237	0.305598
26	6	0	1.010024	0.595797	-0.047259
27	6	0	1.230045	-0.080659	-1.255011
28	6	0	1.787354	0.249687	1.055144
29	6	0	2.212115	-1.054909	-1.360527
30	1	0	0.632041	0.179638	-2.124436
31	6	0	2.777405	-0.731486	0.969382
32	1	0	1.631322	0.771401	1.995298

33	6	0	2.993755	-1.383211	-0.246432
34	1	0	2.398945	-1.573685	-2.295093
35	1	0	3.365624	-0.969839	1.847537
36	8	0	3.933470	-2.348716	-0.444370
37	6	0	4.777208	-2.674585	0.639882
38	1	0	4.203406	-3.078158	1.483020
39	1	0	5.462804	-3.436529	0.270485
40	1	0	5.348069	-1.799811	0.973950

Trienamine E1



HF (M062X/6-31+G(d,p)) = -767.796189 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.310970 (Hartree/Particle)

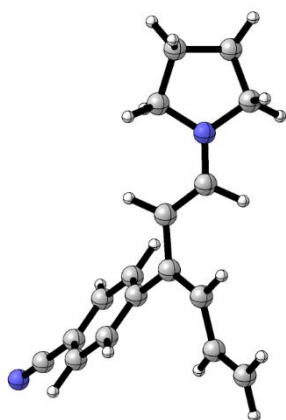
Thermal correction = 0.262390 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.440297	-1.807093	-0.126064
2	6	0	4.910053	-1.627494	-0.509789
3	6	0	5.298700	-0.346540	0.240475
4	6	0	4.047970	0.531389	0.116438
5	1	0	2.864401	-2.354131	-0.879288
6	1	0	5.523905	-2.488908	-0.238474
7	1	0	4.992580	-1.470415	-1.590555
8	1	0	5.486980	-0.576299	1.294588
9	1	0	6.190150	0.136483	-0.164743
10	1	0	3.893227	1.170470	0.995475
11	1	0	4.084030	1.183989	-0.769027
12	7	0	2.966687	-0.432068	-0.014747
13	6	0	1.657787	-0.078529	-0.021227
14	1	0	0.970559	-0.916256	-0.124806
15	6	0	1.176753	1.190213	0.077730
16	1	0	1.870654	2.022703	0.160908
17	6	0	-0.236432	1.531621	0.045326
18	6	0	-0.656134	2.821936	0.024757
19	6	0	-2.037673	3.272894	0.050873
20	1	0	-2.811870	2.511144	0.128532

21	6	0	-2.399655	4.563702	0.000085
22	1	0	-1.657681	5.354717	-0.075524
23	1	0	-3.441747	4.861457	0.032868
24	1	0	3.346403	-2.338323	0.833110
25	1	0	0.104600	3.602758	0.010653
26	6	0	-1.224930	0.412940	0.036292
27	6	0	-1.393729	-0.393164	1.168672
28	6	0	-1.989021	0.148645	-1.105637
29	6	0	-2.310722	-1.436930	1.168408
30	1	0	-0.803578	-0.186482	2.056832
31	6	0	-2.905776	-0.896969	-1.121740
32	1	0	-1.857559	0.773087	-1.984571
33	6	0	-3.066626	-1.692266	0.017625
34	1	0	-2.448876	-2.054921	2.049516
35	1	0	-3.496250	-1.103449	-2.008212
36	6	0	-4.010987	-2.779753	0.006077
37	7	0	-4.767998	-3.655823	-0.004837

Trienamine E2



HF (M062X/6-31+G(d,p)) = -767.7934736 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.311682 (Hartree/Particle)

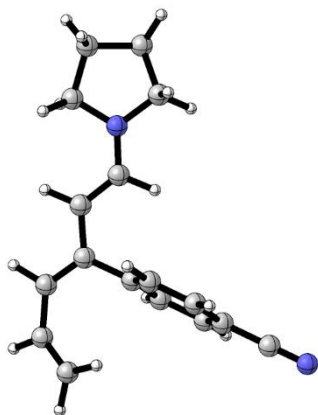
Thermal correction = 0.264173 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.651087	0.096191	-0.720459
2	6	0	-5.448381	-1.205622	-0.605481
3	6	0	-4.998998	-1.762948	0.751364
4	6	0	-3.504356	-1.433766	0.778016
5	1	0	-4.438254	0.371792	-1.758341
6	1	0	-6.526504	-1.044843	-0.671884
7	1	0	-5.152975	-1.891893	-1.406448
8	1	0	-5.510183	-1.233221	1.562228
9	1	0	-5.194622	-2.831078	0.865356
10	1	0	-3.113933	-1.274825	1.790502
11	1	0	-2.904261	-2.229649	0.308222

12	7	0	-3.417381	-0.207289	0.001681
13	6	0	-2.256517	0.473490	-0.163627
14	1	0	-2.340927	1.368994	-0.778124
15	6	0	-1.046378	0.128309	0.348968
16	1	0	-0.932011	-0.812978	0.880671
17	6	0	0.146913	0.959815	0.188579
18	6	0	0.091982	2.316274	0.125286
19	6	0	1.174962	3.215458	-0.245588
20	1	0	2.106625	2.771142	-0.590622
21	6	0	1.067617	4.552286	-0.212934
22	1	0	0.152798	5.036791	0.119555
23	1	0	1.887077	5.193472	-0.518068
24	1	0	-5.186047	0.930594	-0.244758
25	1	0	-0.864815	2.793191	0.334640
26	6	0	1.437437	0.222789	0.094707
27	6	0	1.541530	-0.909665	-0.725092
28	6	0	2.552714	0.609178	0.851574
29	6	0	2.730271	-1.621690	-0.814245
30	1	0	0.677347	-1.219568	-1.305144
31	6	0	3.745636	-0.099092	0.778145
32	1	0	2.470909	1.464005	1.516174
33	6	0	3.837845	-1.215810	-0.060259
34	1	0	2.809492	-2.489477	-1.460656
35	1	0	4.603855	0.199211	1.371061
36	6	0	5.070509	-1.955935	-0.138422
37	7	0	6.061128	-2.552316	-0.201330

Trienamine E3



HF (M062X/6-31+G(d,p)) = -767.7905 21 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.311268 (Hartree/Particle)

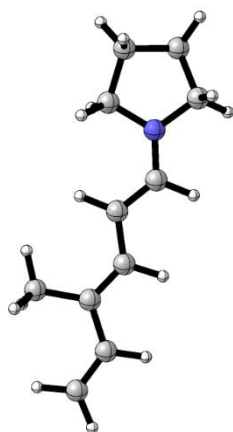
Thermal correction = 0.263092 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.449418	-1.778622	0.043938
2	6	0	-4.921135	-1.644571	0.438142

3	6	0	-5.336090	-0.340781	-0.256087
4	6	0	-4.102804	0.555821	-0.094639
5	1	0	-2.860723	-2.348444	0.769907
6	1	0	-5.519404	-2.505368	0.132274
7	1	0	-5.003183	-1.534697	1.524792
8	1	0	-5.520430	-0.528922	-1.319122
9	1	0	-6.236672	0.106736	0.169248
10	1	0	-3.961848	1.234825	-0.945586
11	1	0	-4.151023	1.169169	0.817880
12	7	0	-3.002679	-0.391118	-0.004382
13	6	0	-1.700470	-0.014000	0.013096
14	1	0	-0.997845	-0.842563	0.080687
15	6	0	-1.242926	1.266188	-0.034931
16	1	0	-1.951160	2.089045	-0.087338
17	6	0	0.165082	1.630654	0.012339
18	6	0	0.550468	2.929650	0.082121
19	6	0	1.899876	3.499421	0.106713
20	1	0	1.945706	4.502207	0.531134
21	6	0	3.049988	2.980141	-0.349058
22	1	0	3.112921	2.007736	-0.826034
23	1	0	3.973059	3.543831	-0.261527
24	1	0	-3.348197	-2.263530	-0.938720
25	1	0	-0.252252	3.663625	0.143565
26	6	0	1.163886	0.522695	0.010902
27	6	0	1.396127	-0.223900	-1.149649
28	6	0	1.878079	0.217471	1.174079
29	6	0	2.340915	-1.243222	-1.160140
30	1	0	0.839877	0.013468	-2.051953
31	6	0	2.821252	-0.802568	1.178868
32	1	0	1.697520	0.801069	2.071720
33	6	0	3.056713	-1.532545	0.007736
34	1	0	2.532600	-1.814207	-2.062637
35	1	0	3.379506	-1.038222	2.078802
36	6	0	4.033742	-2.590806	0.005624
37	7	0	4.817225	-3.443442	0.004181

Trienamine F1

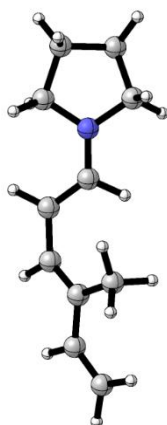


HF (M062X/6-31+G(d,p)) = -483.9070206 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.258910 (Hartree/Particle)
 Thermal correction = 0.217958 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.197815	-1.217577	0.096489
2	6	0	4.334523	-0.309107	-0.375161
3	6	0	3.930507	1.056673	0.195021
4	6	0	2.407149	1.076299	0.022336
5	1	0	3.041526	-2.081306	-0.558136
6	1	0	5.314471	-0.647114	-0.031260
7	1	0	4.345421	-0.271056	-1.469668
8	1	0	4.182967	1.103831	1.259723
9	1	0	4.419093	1.894736	-0.306224
10	1	0	1.899688	1.631407	0.821857
11	1	0	2.102774	1.520421	-0.937994
12	7	0	2.042267	-0.330365	0.062309
13	6	0	0.754199	-0.758180	0.066229
14	1	0	0.644034	-1.841844	0.099099
15	6	0	-0.357054	0.023997	0.027164
16	1	0	-0.249838	1.103419	-0.008175
17	6	0	-1.676461	-0.563803	0.028917
18	1	0	-1.696073	-1.655107	0.066045
19	6	0	-2.878608	0.062205	-0.008756
20	6	0	-4.093419	-0.750818	0.003484
21	1	0	-3.936562	-1.829134	0.042493
22	6	0	-5.352439	-0.288280	-0.028674
23	1	0	-5.576132	0.773577	-0.067501
24	1	0	-6.197294	-0.967907	-0.016301
25	1	0	3.387057	-1.587830	1.115814
26	6	0	-3.044557	1.555894	-0.062802
27	1	0	-3.614777	1.912397	0.803253
28	1	0	-2.088800	2.080568	-0.075502
29	1	0	-3.603353	1.849685	-0.959161

Trienamine F2



HF (M062X/6-31+G(d,p)) = -483.9015312 Hartrees

Imaginary Frequencies: none found

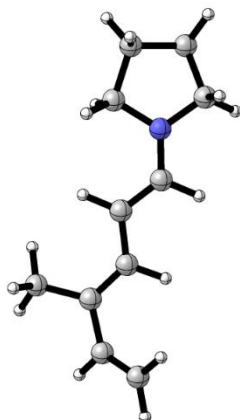
Zero-point correction = 0.259614 (Hartree/Particle)

Thermal correction = 0.219238 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.608357	1.280181	-0.354320
2	6	0	-4.013396	0.695092	-0.519999
3	6	0	-4.015316	-0.469253	0.478105
4	6	0	-2.604442	-1.047887	0.334660
5	1	0	-2.240313	1.762798	-1.265849
6	1	0	-4.799835	1.429169	-0.331398
7	1	0	-4.135681	0.312575	-1.539011
8	1	0	-4.157925	-0.088692	1.495237
9	1	0	-4.793888	-1.208597	0.278844
10	1	0	-2.231324	-1.502190	1.261070
11	1	0	-2.553998	-1.812721	-0.457123
12	7	0	-1.802678	0.109060	-0.025109
13	6	0	-0.452462	0.050734	-0.176088
14	1	0	0.002641	0.994490	-0.469302
15	6	0	0.318773	-1.057809	-0.026152
16	1	0	-0.168261	-2.011362	0.163141
17	6	0	1.762206	-1.090365	-0.202188
18	1	0	2.148370	-2.027329	-0.606461
19	6	0	2.687753	-0.137554	0.073078
20	6	0	4.081351	-0.403226	-0.292605
21	1	0	4.272809	-1.392576	-0.708835
22	6	0	5.108869	0.450634	-0.179150
23	1	0	4.986140	1.457908	0.206873
24	1	0	6.109072	0.160294	-0.481589
25	1	0	-2.582463	2.019156	0.460393
26	6	0	2.376973	1.166594	0.756454
27	1	0	2.312127	2.001468	0.046963
28	1	0	1.431340	1.106257	1.300279
29	1	0	3.168223	1.413084	1.471760

Trienamine F3



HF (M062X/6-31+G(d,p)) = -483.9012829 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.258764 (Hartree/Particle)

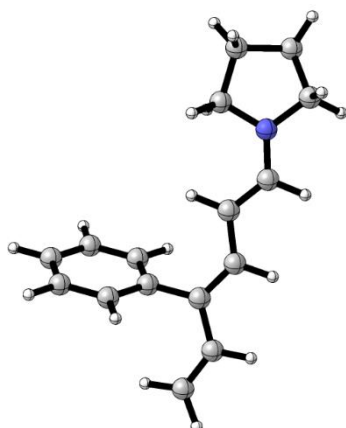
Thermal correction = 0.217450 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.034675	-1.294891	-0.051316
2	6	0	4.232895	-0.400530	-0.374272
3	6	0	3.894554	0.894417	0.376143
4	6	0	2.378126	1.028297	0.187851
5	1	0	2.847593	-2.053414	-0.818414
6	1	0	5.183704	-0.840867	-0.065930
7	1	0	4.271210	-0.211737	-1.452399
8	1	0	4.126543	0.777337	1.440145
9	1	0	4.440378	1.764187	0.004628
10	1	0	1.886249	1.489621	1.054398
11	1	0	2.119570	1.626846	-0.699160
12	7	0	1.933473	-0.343784	0.012104
13	6	0	0.621975	-0.686242	-0.073796
14	1	0	0.446453	-1.752254	-0.216605
15	6	0	-0.438506	0.160958	-0.004136
16	1	0	-0.267630	1.221835	0.151044
17	6	0	-1.795099	-0.328868	-0.113972
18	1	0	-1.901891	-1.410691	-0.206893
19	6	0	-2.930897	0.406101	-0.128214
20	6	0	-4.249472	-0.245059	-0.175730
21	1	0	-5.029418	0.304241	-0.706282
22	6	0	-4.573670	-1.418507	0.383194
23	1	0	-3.860042	-1.980197	0.979889
24	1	0	-5.565860	-1.841498	0.265435
25	1	0	3.176733	-1.807815	0.912548
26	6	0	-2.934918	1.914633	-0.100360
27	1	0	-3.081647	2.295351	0.918043
28	1	0	-2.006171	2.338458	-0.489314

29 1 0 -3.758064 2.305226 -0.708203

Trienamine G1



HF (M062X/6-31+G(d,p)) = -675.5798193 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.312824 (Hartree/Particle)

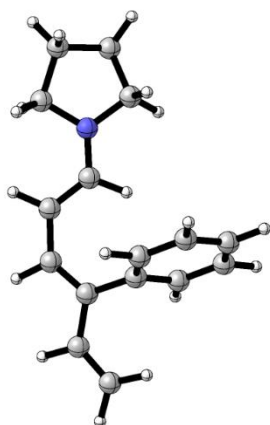
Thermal correction = 0.267344 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.417836	-0.944244	0.049829
2	6	0	5.235487	0.292449	-0.329244
3	6	0	4.473796	1.426079	0.370156
4	6	0	3.004542	1.024912	0.194856
5	1	0	4.494535	-1.749704	-0.688020
6	1	0	6.279889	0.218472	-0.018327
7	1	0	5.206913	0.434633	-1.414848
8	1	0	4.729054	1.443855	1.435042
9	1	0	4.689364	2.412035	-0.046727
10	1	0	2.376264	1.340529	1.037131
11	1	0	2.566391	1.444255	-0.723851
12	7	0	3.056890	-0.425884	0.107325
13	6	0	1.942969	-1.196403	0.042475
14	1	0	2.140753	-2.265326	-0.035722
15	6	0	0.657512	-0.751294	0.059883
16	1	0	0.447959	0.311426	0.135846
17	6	0	-0.450359	-1.671741	-0.009941
18	1	0	-0.188875	-2.731687	-0.033441
19	6	0	-1.773323	-1.366442	-0.030251
20	6	0	-2.763134	-2.444469	-0.065584
21	1	0	-2.347360	-3.450114	0.004667
22	6	0	-4.091791	-2.307851	-0.186516
23	1	0	-4.562898	-1.333116	-0.271742
24	1	0	-4.737148	-3.179114	-0.210168
25	6	0	-2.247021	0.045661	-0.033473
26	6	0	-3.024990	0.543274	1.019120

27	6	0	-1.925474	0.903576	-1.091625
28	6	0	-3.461232	1.866341	1.018627
29	1	0	-3.282513	-0.117294	1.842786
30	6	0	-2.361224	2.227522	-1.094939
31	1	0	-1.330017	0.519822	-1.916067
32	6	0	-3.130253	2.713366	-0.038959
33	1	0	-4.059501	2.236931	1.845790
34	1	0	-2.103861	2.877809	-1.925850
35	1	0	-3.471886	3.743955	-0.040704
36	1	0	4.734660	-1.340597	1.026445

Trienamine G2



HF (M062X/6-31+G(d,p)) = -675.5749487 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.312725 (Hartree/Particle)

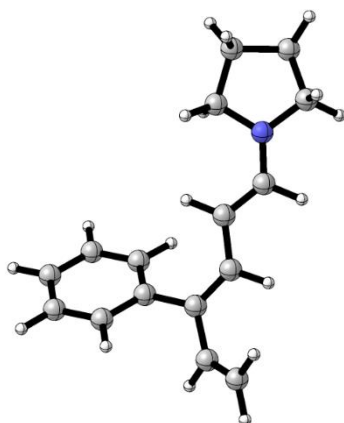
Thermal correction = 0.267070 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.959231	1.055219	-0.459132
2	6	0	-4.453080	0.766752	-0.614838
3	6	0	-4.690929	-0.338213	0.423095
4	6	0	-3.423441	-1.195070	0.324799
5	1	0	-2.499663	1.446893	-1.372038
6	1	0	-5.072293	1.651552	-0.451466
7	1	0	-4.652570	0.385541	-1.622159
8	1	0	-4.763811	0.102213	1.423205
9	1	0	-5.600514	-0.913959	0.239396
10	1	0	-3.136290	-1.637659	1.287424
11	1	0	-3.534067	-2.015839	-0.400294
12	7	0	-2.410987	-0.255782	-0.129603
13	6	0	-1.091330	-0.558139	-0.198236
14	1	0	-0.468821	0.266660	-0.534718
15	6	0	-0.545396	-1.772050	0.094500
16	1	0	-1.214966	-2.581825	0.370818
17	6	0	0.859518	-2.129345	0.014936

18	1	0	1.038624	-3.205109	-0.001106
19	6	0	1.976030	-1.357488	-0.032374
20	6	0	3.288451	-1.995012	-0.149723
21	1	0	3.267676	-3.082784	-0.220675
22	6	0	4.474994	-1.369784	-0.166996
23	1	0	4.553587	-0.288746	-0.097545
24	1	0	5.397744	-1.933818	-0.247477
25	6	0	1.927618	0.128288	0.065521
26	6	0	2.190731	0.932996	-1.048307
27	6	0	1.602486	0.742381	1.279973
28	6	0	2.104349	2.322027	-0.957426
29	1	0	2.453455	0.459709	-1.990959
30	6	0	1.516261	2.129419	1.373581
31	1	0	1.398155	0.117525	2.145122
32	6	0	1.761202	2.923569	0.252686
33	1	0	2.306310	2.933742	-1.831809
34	1	0	1.259694	2.592399	2.321967
35	1	0	1.693348	4.004864	0.324557
36	1	0	-2.778085	1.775810	0.352625

Trienamine G3



HF (M062X/6-31+G(d,p)) = -675.5761532 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.312972 (Hartree/Particle)

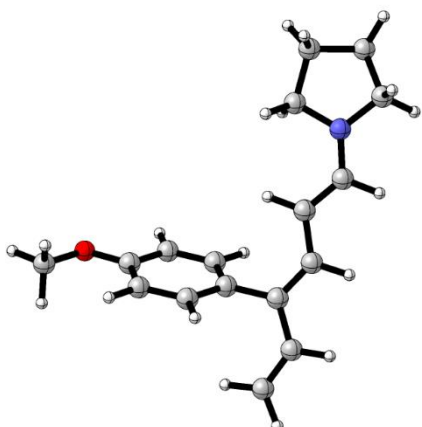
Thermal correction = 0.267605 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.370720	0.849444	-0.102588
2	6	0	-5.199391	-0.425891	-0.268116
3	6	0	-4.451554	-1.429247	0.619181
4	6	0	-2.977654	-1.079195	0.383853
5	1	0	-4.436166	1.517655	-0.967537
6	1	0	-6.244123	-0.289871	0.019854
7	1	0	-5.168297	-0.752294	-1.313177
8	1	0	-4.708621	-1.258738	1.670129

9	1	0	-4.677782	-2.470227	0.379541
10	1	0	-2.355544	-1.252930	1.270946
11	1	0	-2.541452	-1.654365	-0.447335
12	7	0	-3.014949	0.335561	0.048415
13	6	0	-1.894641	1.078053	-0.130245
14	1	0	-2.084244	2.117987	-0.395544
15	6	0	-0.611800	0.639776	-0.014030
16	1	0	-0.411144	-0.392146	0.256891
17	6	0	0.498622	1.540341	-0.208307
18	1	0	0.235698	2.587198	-0.367847
19	6	0	1.824708	1.246443	-0.190813
20	6	0	2.832170	2.321082	-0.253008
21	1	0	3.757511	2.071763	-0.773826
22	6	0	2.706224	3.542786	0.280623
23	1	0	1.834578	3.818869	0.867850
24	1	0	3.478248	4.293938	0.150498
25	6	0	2.348028	-0.141969	-0.116047
26	6	0	3.424450	-0.444951	0.729951
27	6	0	1.822070	-1.170224	-0.911873
28	6	0	3.941178	-1.736796	0.798728
29	1	0	3.848552	0.343450	1.346701
30	6	0	2.337711	-2.461787	-0.845195
31	1	0	1.014558	-0.941870	-1.602019
32	6	0	3.396991	-2.752319	0.014311
33	1	0	4.769997	-1.950828	1.467093
34	1	0	1.919728	-3.241179	-1.475755
35	1	0	3.800302	-3.758965	0.065679
36	1	0	-4.685497	1.410368	0.790409

Trienamine H1



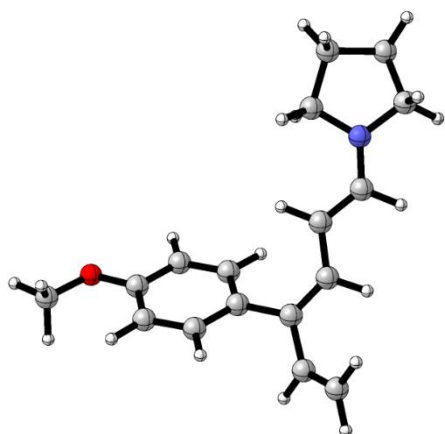
HF (M062X/6-31+G(d,p)) = -790.0624353 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.345419 (Hartree/Particle)
Thermal correction = 0.296139 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-5.094184	0.163087	0.182286
2	6	0	-5.600109	-1.204157	-0.280959
3	6	0	-4.547873	-2.162181	0.292861
4	6	0	-3.233009	-1.394572	0.112413
5	1	0	-5.408337	0.981720	-0.473542
6	1	0	-6.613370	-1.418629	0.065802
7	1	0	-5.591650	-1.248517	-1.375273
8	1	0	-4.737848	-2.327431	1.358732
9	1	0	-4.534568	-3.134889	-0.203193
10	1	0	-2.508159	-1.603393	0.909356
11	1	0	-2.746293	-1.621821	-0.848378
12	7	0	-3.646592	-0.000441	0.144084
13	6	0	-2.763165	1.027738	0.110879
14	1	0	-3.224629	2.015210	0.117590
15	6	0	-1.407748	0.922411	0.065358
16	1	0	-0.932290	-0.054074	0.062484
17	6	0	-0.571939	2.097351	0.037440
18	1	0	-1.094818	3.055269	0.077135
19	6	0	0.784379	2.139754	-0.012711
20	6	0	1.464761	3.436027	0.009083
21	1	0	0.806789	4.297136	0.131090
22	6	0	2.782989	3.650427	-0.114678
23	1	0	3.486226	2.834027	-0.248611
24	1	0	3.184286	4.657743	-0.090855
25	6	0	1.602893	0.898613	-0.096456
26	6	0	2.497282	0.559532	0.919048
27	6	0	1.504565	0.035559	-1.198064
28	6	0	3.270824	-0.601707	0.859413
29	1	0	2.591214	1.216238	1.780003
30	6	0	2.264384	-1.122488	-1.275796
31	1	0	0.820939	0.287099	-2.004806
32	6	0	3.152930	-1.446989	-0.245239
33	1	0	3.950095	-0.830600	1.672134
34	1	0	2.195551	-1.790093	-2.128573
35	1	0	-5.443350	0.385959	1.202151
36	8	0	3.857863	-2.601566	-0.410372
37	6	0	4.787146	-2.950679	0.592491
38	1	0	4.291238	-3.105670	1.558461
39	1	0	5.245778	-3.884152	0.267045
40	1	0	5.561678	-2.181873	0.701423

Trienamine H2



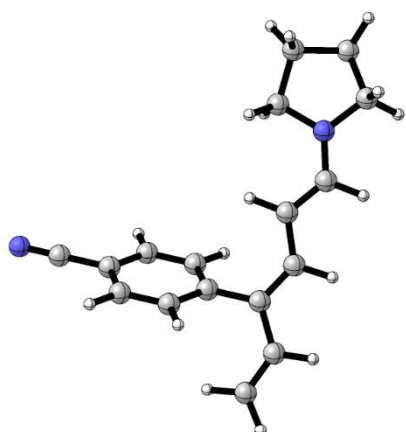
HF (M062X/6-31+G(d,p)) = -790.0588567 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.345870 (Hartree/Particle)
 Thermal correction = 0.296838 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.071365	-0.048510	-0.020360
2	6	0	-5.529298	-1.495179	-0.212123
3	6	0	-4.501248	-2.283406	0.609708
4	6	0	-3.188101	-1.534653	0.350783
5	1	0	-5.358980	0.605298	-0.850226
6	1	0	-6.558629	-1.658359	0.114735
7	1	0	-5.454584	-1.767862	-1.270245
8	1	0	-4.755889	-2.227988	1.673508
9	1	0	-4.443149	-3.337538	0.330714
10	1	0	-2.518174	-1.546854	1.220137
11	1	0	-2.632709	-1.951122	-0.503240
12	7	0	-3.621931	-0.178466	0.053144
13	6	0	-2.755155	0.853901	-0.099719
14	1	0	-3.231208	1.809972	-0.316809
15	6	0	-1.399431	0.785724	-0.014023
16	1	0	-0.914681	-0.160310	0.206893
17	6	0	-0.585214	1.967024	-0.174080
18	1	0	-1.129225	2.906402	-0.283327
19	6	0	0.770616	2.047825	-0.181974
20	6	0	1.441738	3.360300	-0.202620
21	1	0	2.385895	3.399681	-0.747472
22	6	0	0.998133	4.474628	0.393671
23	1	0	0.099200	4.471605	1.004181
24	1	0	1.529157	5.415399	0.292226
25	6	0	1.654579	0.854665	-0.184384
26	6	0	2.787771	0.805458	0.630921
27	6	0	1.418560	-0.240030	-1.034148
28	6	0	3.648788	-0.294319	0.632628
29	1	0	3.000380	1.642383	1.291448
30	6	0	2.262397	-1.338864	-1.047911
31	1	0	0.565456	-0.211364	-1.706303

32	6	0	3.382048	-1.375011	-0.208330
33	1	0	4.511899	-0.290684	1.287747
34	1	0	2.085335	-2.180019	-1.710452
35	1	0	-5.482516	0.373527	0.909567
36	8	0	4.151624	-2.496441	-0.290618
37	6	0	5.282510	-2.577025	0.549894
38	1	0	4.994967	-2.532769	1.607462
39	1	0	5.746987	-3.540375	0.340904
40	1	0	5.997035	-1.773402	0.333884

Trienamine I1



HF (M062X/6-31+G(d,p)) = -767.7985111 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.311429 (Hartree/Particle)

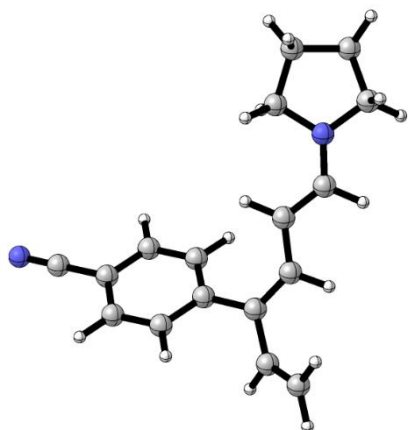
Thermal correction = 0.263132 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.955392	0.307561	-0.086482
2	6	0	5.506371	-1.065293	0.302361
3	6	0	4.512889	-2.026486	-0.363150
4	6	0	3.161628	-1.328457	-0.170677
5	1	0	5.213723	1.093190	0.630779
6	1	0	6.536676	-1.214128	-0.027628
7	1	0	5.471266	-1.181815	1.390775
8	1	0	4.736961	-2.112225	-1.431677
9	1	0	4.529166	-3.029551	0.067663
10	1	0	2.465989	-1.516636	-0.997744
11	1	0	2.664462	-1.635736	0.761849
12	7	0	3.513703	0.082525	-0.104409
13	6	0	2.588866	1.066455	-0.034658
14	1	0	3.006194	2.070870	0.034623
15	6	0	1.236212	0.902612	-0.037274
16	1	0	0.807409	-0.092012	-0.112749
17	6	0	0.357367	2.040717	0.034387
18	1	0	0.846897	3.016349	0.059482

19	6	0	-1.001884	2.044913	0.046759
20	6	0	-1.722082	3.319434	0.073753
21	1	0	-1.086187	4.202369	0.007492
22	6	0	-3.046773	3.494617	0.187122
23	1	0	-3.735642	2.659392	0.270944
24	1	0	-3.471518	4.492092	0.207194
25	6	0	-1.782202	0.779451	0.039040
26	6	0	-2.689727	0.506858	-0.994266
27	6	0	-1.630913	-0.162274	1.065305
28	6	0	-3.418012	-0.675570	-1.012847
29	1	0	-2.816570	1.234320	-1.790501
30	6	0	-2.355114	-1.348546	1.061077
31	1	0	-0.939389	0.048942	1.875944
32	6	0	-3.251563	-1.607918	0.018469
33	1	0	-4.113939	-0.885041	-1.818487
34	1	0	-2.237484	-2.072857	1.860341
35	1	0	5.320035	0.611825	-1.078787
36	6	0	-4.005764	-2.834430	0.008047
37	7	0	-4.611731	-3.821270	-0.000063

Trienamine I2



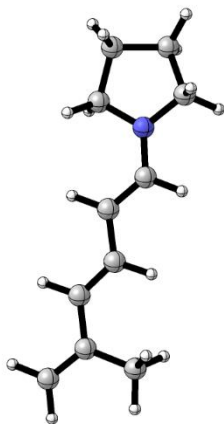
HF (M062X/6-31+G(d,p)) = -767.7952625 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.311916 (Hartree/Particle)
Thermal correction = 0.264172 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.920408	0.061161	0.125286
2	6	0	5.402821	-1.381024	0.288847
3	6	0	4.451641	-2.158823	-0.629411
4	6	0	3.104581	-1.458930	-0.416673
5	1	0	5.132793	0.687034	0.997799
6	1	0	6.455145	-1.505434	0.025002
7	1	0	5.266319	-1.699569	1.327796
8	1	0	4.766953	-2.047477	-1.672255

9	1	0	4.407499	-3.225467	-0.400861
10	1	0	2.478767	-1.460616	-1.317465
11	1	0	2.522945	-1.918400	0.396787
12	7	0	3.480686	-0.099643	-0.053746
13	6	0	2.575063	0.886893	0.131080
14	1	0	3.006022	1.845608	0.419261
15	6	0	1.223248	0.774020	-0.002227
16	1	0	0.785646	-0.174271	-0.298145
17	6	0	0.368637	1.915120	0.199361
18	1	0	0.881397	2.864879	0.358275
19	6	0	-0.991161	1.967220	0.184682
20	6	0	-1.690928	3.264195	0.237359
21	1	0	-2.644973	3.268660	0.766117
22	6	0	-1.254250	4.406596	-0.307408
23	1	0	-0.343960	4.440635	-0.899864
24	1	0	-1.802381	5.334292	-0.181502
25	6	0	-1.846096	0.759757	0.123407
26	6	0	-3.010032	0.757018	-0.662531
27	6	0	-1.555262	-0.387096	0.881027
28	6	0	-3.838949	-0.355944	-0.717741
29	1	0	-3.254734	1.638986	-1.247587
30	6	0	-2.375896	-1.504812	0.836289
31	1	0	-0.685262	-0.384009	1.530085
32	6	0	-3.521044	-1.495899	0.029380
33	1	0	-4.729729	-0.351730	-1.337149
34	1	0	-2.146519	-2.382640	1.431563
35	1	0	5.378072	0.531283	-0.757674
36	6	0	-4.372563	-2.654788	-0.021867
37	7	0	-5.054300	-3.590320	-0.062445

Trienamine J1



HF (M062X/6-31+G(d,p)) = -483.9080383 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.259268 (Hartree/Particle)

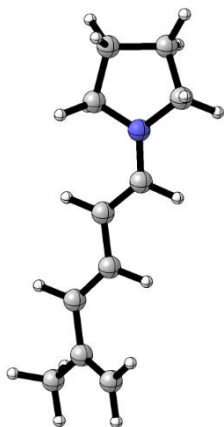
Thermal correction = 0.218766 Hartrees

Coordinates from last standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.226238	1.219779	-0.099309
2	6	0	4.433925	0.397472	0.353669
3	6	0	4.118722	-0.996404	-0.204865
4	6	0	2.602618	-1.123875	-0.009561
5	1	0	3.022526	2.075308	0.553211
6	1	0	5.380653	0.803075	-0.009761
7	1	0	4.467608	0.365419	1.447877
8	1	0	4.358829	-1.030986	-1.272897
9	1	0	4.672512	-1.795436	0.292376
10	1	0	2.124268	-1.709514	-0.805577
11	1	0	2.345139	-1.594733	0.951548
12	7	0	2.138748	0.253109	-0.034747
13	6	0	0.821218	0.584700	-0.047126
14	1	0	0.630334	1.657025	-0.082585
15	6	0	-0.227523	-0.277175	-0.010842
16	1	0	-0.055576	-1.350091	0.029975
17	6	0	-1.596169	0.188454	-0.017017
18	1	0	-1.733539	1.270037	-0.059187
19	6	0	-2.684675	-0.608538	0.025647
20	6	0	-4.072728	-0.147385	0.021023
21	6	0	-5.086691	-1.028319	0.067628
22	1	0	-4.900590	-2.097792	0.109395
23	1	0	-6.122159	-0.702614	0.064915
24	1	0	3.368655	1.595457	-1.124561
25	1	0	-2.539916	-1.688268	0.067640
26	6	0	-4.334641	1.336149	-0.038587
27	1	0	-3.878869	1.848149	0.815974
28	1	0	-3.906037	1.771598	-0.947954
29	1	0	-5.406845	1.542460	-0.031128

Trienamine J2



HF (M062X/6-31+G(d,p)) = -483.9035006 Hartrees

Imaginary Frequencies: none found

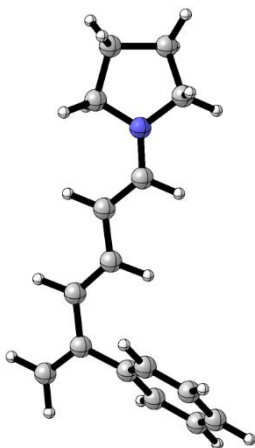
Zero-point correction = 0.258631 (Hartree/Particle)

Thermal correction = 0.217535 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.266404	1.200702	0.166259
2	6	0	4.446919	0.279088	0.477738
3	6	0	4.129755	-0.965906	-0.361240
4	6	0	2.607128	-1.100196	-0.235064
5	1	0	3.053016	1.909989	0.972754
6	1	0	5.410843	0.730251	0.232102
7	1	0	4.445024	0.024983	1.543073
8	1	0	4.399935	-0.786402	-1.407393
9	1	0	4.657998	-1.860020	-0.023754
10	1	0	2.145098	-1.509854	-1.142748
11	1	0	2.314974	-1.744299	0.608475
12	7	0	2.163581	0.263857	-0.000904
13	6	0	0.852076	0.612239	0.054897
14	1	0	0.678226	1.670612	0.247402
15	6	0	-0.211860	-0.217992	-0.097920
16	1	0	-0.059912	-1.277087	-0.291987
17	6	0	-1.569496	0.269339	-0.008398
18	6	0	-2.680907	-0.486028	-0.119462
19	6	0	-4.059818	0.022442	-0.043669
20	6	0	-4.409795	1.258684	-0.430941
21	1	0	-3.690817	1.940464	-0.874837
22	1	0	-5.430478	1.612816	-0.323350
23	1	0	3.448506	1.773446	-0.756225
24	1	0	-2.568357	-1.564517	-0.241160
25	1	0	-1.689770	1.337996	0.180108
26	6	0	-5.079514	-0.950781	0.495215
27	1	0	-5.103410	-1.857545	-0.120215
28	1	0	-4.819177	-1.260231	1.513351
29	1	0	-6.082126	-0.517142	0.506247

Trienamine K1

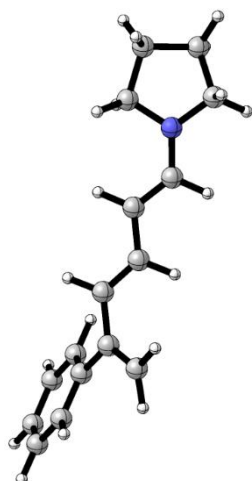


HF (M062X/6-31+G(d,p)) = -675.5792322 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.313032 (Hartree/Particle)
 Thermal correction = 0.267420 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.254305	-1.538521	0.157214
2	6	0	-5.608617	-0.965643	0.579593
3	6	0	-5.672269	0.353295	-0.201325
4	6	0	-4.230278	0.870246	-0.138464
5	1	0	-3.815086	-2.200184	0.910910
6	1	0	-6.439438	-1.638789	0.357204
7	1	0	-5.603660	-0.764745	1.656191
8	1	0	-5.950033	0.155612	-1.242198
9	1	0	-6.389631	1.065412	0.211593
10	1	0	-3.945681	1.434385	-1.035717
11	1	0	-4.059634	1.521268	0.733116
12	7	0	-3.438783	-0.343000	-0.017449
13	6	0	-2.081769	-0.332308	0.006455
14	1	0	-1.626534	-1.312612	0.143943
15	6	0	-1.284203	0.761110	-0.115657
16	1	0	-1.722140	1.746575	-0.255599
17	6	0	0.154833	0.660446	-0.053139
18	1	0	0.567922	-0.337717	0.097691
19	6	0	1.002517	1.707192	-0.154480
20	6	0	2.461328	1.643700	-0.053673
21	6	0	3.201966	2.764761	0.030426
22	1	0	2.734604	3.745364	0.032153
23	1	0	4.284680	2.721751	0.087700
24	1	0	-4.342484	-2.101019	-0.784702
25	1	0	0.585107	2.705348	-0.287460
26	6	0	3.139659	0.314938	-0.031151
27	6	0	2.950513	-0.611344	-1.064927
28	6	0	4.009187	-0.013369	1.013900
29	6	0	3.625328	-1.829221	-1.057800
30	1	0	2.280457	-0.361247	-1.883113
31	6	0	4.680875	-1.234744	1.025484
32	1	0	4.147346	0.696758	1.824255
33	6	0	4.492196	-2.145803	-0.011262
34	1	0	3.478404	-2.531960	-1.872559
35	1	0	5.349266	-1.474984	1.846868
36	1	0	5.016254	-3.096627	-0.005298

Trienamine K2



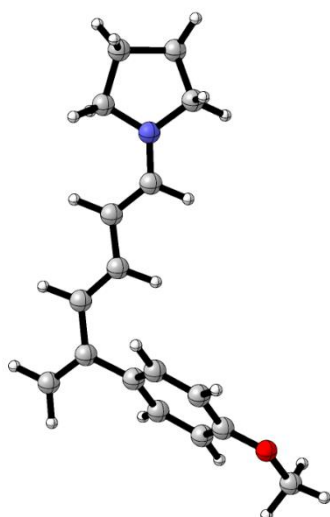
HF (M062X/6-31+G(d,p)) = -675.5769696 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.312708 (Hartree/Particle)
 Thermal correction = 0.267019 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.123746	0.653892	0.747788
2	6	0	6.140714	-0.467058	0.526959
3	6	0	5.708801	-1.047693	-0.825851
4	6	0	4.177093	-0.990916	-0.765314
5	1	0	4.962161	0.883367	1.806065
6	1	0	7.172115	-0.108039	0.532300
7	1	0	6.032237	-1.222324	1.312584
8	1	0	6.070735	-0.406542	-1.636687
9	1	0	6.083649	-2.058242	-1.000807
10	1	0	3.724736	-0.796201	-1.746503
11	1	0	3.741399	-1.923389	-0.376081
12	7	0	3.912506	0.108133	0.149352
13	6	0	2.669725	0.615424	0.349956
14	1	0	2.636396	1.458260	1.039909
15	6	0	1.515602	0.171432	-0.212403
16	1	0	1.526660	-0.670427	-0.900365
17	6	0	0.244774	0.792567	0.081898
18	6	0	-0.948871	0.396040	-0.405118
19	6	0	-2.226054	1.075393	-0.131817
20	6	0	-2.316652	2.408732	0.024265
21	1	0	-1.454070	3.050273	-0.124300
22	1	0	-3.250276	2.882786	0.310239
23	1	0	5.440348	1.577558	0.238938
24	1	0	-0.992680	-0.493458	-1.033769
25	1	0	0.264717	1.643000	0.766248
26	6	0	-3.437882	0.213938	-0.031059
27	6	0	-3.353606	-1.064297	0.536045
28	6	0	-4.682817	0.654799	-0.498594
29	6	0	-4.484682	-1.868432	0.654854
30	1	0	-2.393476	-1.418245	0.901610

31	6	0	-5.814089	-0.147690	-0.381556
32	1	0	-4.754943	1.626831	-0.977943
33	6	0	-5.720215	-1.412585	0.197969
34	1	0	-4.400496	-2.852465	1.106399
35	1	0	-6.768849	0.209968	-0.755315
36	1	0	-6.601432	-2.040901	0.283887

Trienamine L1



HF (M062X/6-31+G(d,p)) = -790.0621895 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.346018 (Hartree/Particle)

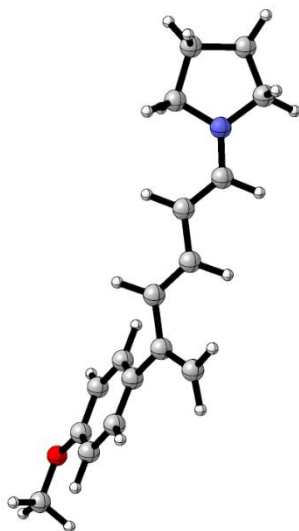
Thermal correction = 0.297168 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.665983	-1.899504	0.157816
2	6	0	-6.111425	-1.575766	0.539348
3	6	0	-6.374562	-0.269087	-0.220321
4	6	0	-5.044420	0.484495	-0.099880
5	1	0	-4.146170	-2.493190	0.916907
6	1	0	-6.806557	-2.375573	0.274598
7	1	0	-6.177612	-1.402960	1.618857
8	1	0	-6.582847	-0.487283	-1.273124
9	1	0	-7.215558	0.300742	0.180357
10	1	0	-4.828108	1.102776	-0.980615
11	1	0	-5.018248	1.140840	0.783542
12	7	0	-4.062414	-0.578716	0.035361
13	6	0	-2.725106	-0.346831	0.055563
14	1	0	-2.116201	-1.243822	0.166162
15	6	0	-2.114703	0.863147	-0.040065
16	1	0	-2.704900	1.770188	-0.147720
17	6	0	-0.676720	0.990745	0.004691
18	1	0	-0.109877	0.066247	0.122181

19	6	0	-0.006104	2.159910	-0.078710
20	6	0	1.447422	2.324975	-0.008770
21	6	0	1.996680	3.547870	0.118753
22	1	0	1.374837	4.435809	0.188915
23	1	0	3.072937	3.683412	0.142335
24	1	0	-4.624194	-2.447635	-0.795957
25	1	0	-0.577749	3.083049	-0.175952
26	6	0	2.328535	1.124541	-0.074101
27	6	0	2.227894	0.201281	-1.127943
28	6	0	3.311165	0.908631	0.890441
29	6	0	3.085851	-0.882910	-1.215625
30	1	0	1.473457	0.352245	-1.895149
31	6	0	4.181781	-0.182459	0.821625
32	1	0	3.394257	1.602795	1.722039
33	6	0	4.069426	-1.081385	-0.238404
34	1	0	3.021245	-1.591008	-2.035297
35	1	0	4.927534	-0.315765	1.596258
36	8	0	4.862038	-2.176041	-0.408295
37	6	0	5.867642	-2.410917	0.553981
38	1	0	5.435058	-2.567823	1.549520
39	1	0	6.384770	-3.315893	0.236201
40	1	0	6.580285	-1.578221	0.594384

Trienamine L2



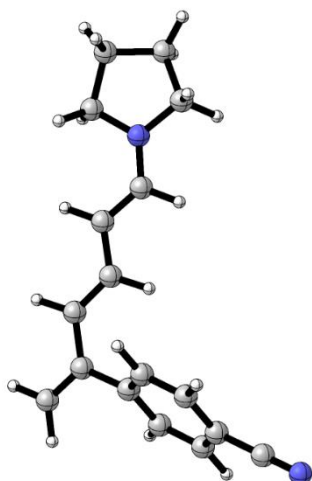
HF (M062X/6-31+G(d,p)) = -790.0596092 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.345443 (Hartree/Particle)
 Thermal correction = 0.295132 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.020466	0.347248	0.824112

2	6	0	6.931115	-0.853338	0.560938
3	6	0	6.495902	-1.304301	-0.839696
4	6	0	4.976348	-1.102103	-0.820092
5	1	0	5.833456	0.515834	1.889794
6	1	0	7.991585	-0.599039	0.621516
7	1	0	6.722380	-1.642019	1.291677
8	1	0	6.945835	-0.651938	-1.595748
9	1	0	6.778025	-2.333993	-1.068854
10	1	0	4.576108	-0.820776	-1.802753
11	1	0	4.441574	-2.005065	-0.487515
12	7	0	4.789779	-0.024773	0.137581
13	6	0	3.588515	0.568898	0.354930
14	1	0	3.611806	1.364957	1.098972
15	6	0	2.412475	0.260708	-0.250799
16	1	0	2.365675	-0.531896	-0.993719
17	6	0	1.191432	0.963728	0.071268
18	6	0	-0.024323	0.694418	-0.446546
19	6	0	-1.248620	1.449548	-0.130142
20	6	0	-1.237832	2.778345	0.082725
21	1	0	-0.331590	3.358879	-0.056673
22	1	0	-2.129500	3.307764	0.403693
23	1	0	6.450811	1.267816	0.400859
24	1	0	-0.132447	-0.147611	-1.130716
25	1	0	1.270126	1.763920	0.809875
26	6	0	-2.512854	0.668174	-0.050118
27	6	0	-2.510259	-0.641736	0.455992
28	6	0	-3.733885	1.200609	-0.466887
29	6	0	-3.681036	-1.375148	0.564330
30	1	0	-1.571829	-1.078757	0.786615
31	6	0	-4.923229	0.477238	-0.366018
32	1	0	-3.758437	2.196193	-0.900897
33	6	0	-4.897252	-0.817302	0.155377
34	1	0	-3.683656	-2.383473	0.965210
35	1	0	-5.848026	0.926042	-0.708833
36	8	0	-5.994101	-1.612254	0.295265
37	6	0	-7.243608	-1.076844	-0.084854
38	1	0	-7.261596	-0.828859	-1.153071
39	1	0	-7.979995	-1.853894	0.118057
40	1	0	-7.486082	-0.181495	0.500217

Trienamine M1



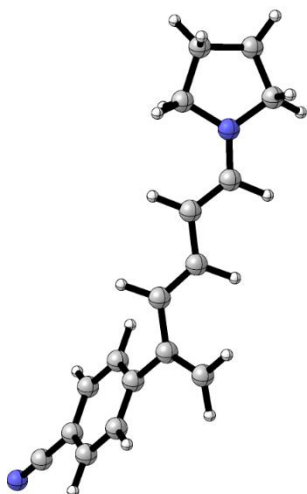
HF (M062X/6-31+G(d,p)) = -767.7976708 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.312049 (Hartree/Particle)
 Thermal correction = 0.264098 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.498309	-1.837333	0.285183
2	6	0	-5.959913	-1.472808	0.550954
3	6	0	-6.169672	-0.249214	-0.350312
4	6	0	-4.843937	0.511127	-0.228317
5	1	0	-4.024960	-2.352668	1.126967
6	1	0	-6.645057	-2.293839	0.329390
7	1	0	-6.085286	-1.191890	1.602132
8	1	0	-6.317562	-0.572240	-1.386377
9	1	0	-7.028513	0.358906	-0.059404
10	1	0	-4.573969	1.040773	-1.150812
11	1	0	-4.862514	1.248484	0.588531
12	7	0	-3.877534	-0.536158	0.063655
13	6	0	-2.543177	-0.310816	0.117868
14	1	0	-1.947892	-1.195260	0.343357
15	6	0	-1.916003	0.881406	-0.070650
16	1	0	-2.490252	1.778210	-0.289360
17	6	0	-0.480809	0.994817	0.015509
18	1	0	0.062179	0.073611	0.231657
19	6	0	0.217304	2.140983	-0.144510
20	6	0	1.670765	2.280605	-0.043887
21	6	0	2.258689	3.490510	0.014528
22	1	0	1.664707	4.399485	0.002283
23	1	0	3.337865	3.595069	0.056333
24	1	0	-4.408718	-2.476697	-0.605959
25	1	0	-0.328929	3.064208	-0.335292
26	6	0	2.523436	1.057660	-0.024479
27	6	0	2.399836	0.086264	-1.028185
28	6	0	3.487987	0.876663	0.973494
29	6	0	3.222815	-1.031396	-1.043039
30	1	0	1.657642	0.222690	-1.808829

31	6	0	4.315675	-0.240872	0.972809
32	1	0	3.578699	1.618035	1.761415
33	6	0	4.183280	-1.198764	-0.037301
34	1	0	3.131366	-1.775745	-1.827045
35	1	0	5.058913	-0.379707	1.750800
36	6	0	5.031190	-2.362657	-0.040265
37	7	0	5.710011	-3.300767	-0.041681

Trienamine M2



HF (M062X/6-31+G(d,p)) = -767.7952054 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.311110 (Hartree/Particle)

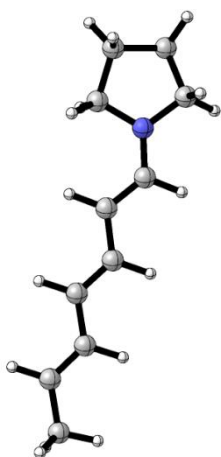
Thermal correction = 0.261387 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.812362	0.311271	-0.843635
2	6	0	-6.715855	-0.891302	-0.565980
3	6	0	-6.283593	-1.318503	0.842922
4	6	0	-4.765259	-1.108316	0.826104
5	1	0	-5.621917	0.466147	-1.910566
6	1	0	-7.777508	-0.644579	-0.634476
7	1	0	-6.499441	-1.689308	-1.284191
8	1	0	-6.740005	-0.657795	1.587631
9	1	0	-6.560383	-2.346281	1.086196
10	1	0	-4.369780	-0.810357	1.805452
11	1	0	-4.224466	-2.012142	0.506861
12	7	0	-4.580598	-0.042887	-0.146847
13	6	0	-3.384017	0.551663	-0.369792
14	1	0	-3.407996	1.335565	-1.126709
15	6	0	-2.207473	0.258557	0.245686
16	1	0	-2.159119	-0.520727	1.002154
17	6	0	-0.992224	0.963234	-0.084255
18	6	0	0.225006	0.710402	0.440783

19	6	0	1.441485	1.473033	0.120253
20	6	0	1.431902	2.794501	-0.132332
21	1	0	0.520262	3.374748	-0.034273
22	1	0	2.326741	3.317615	-0.454597
23	1	0	-6.248418	1.234570	-0.433522
24	1	0	0.337248	-0.118680	1.139509
25	1	0	-1.074932	1.751505	-0.835245
26	6	0	2.716985	0.705453	0.067780
27	6	0	2.726363	-0.608788	-0.419194
28	6	0	3.925419	1.269309	0.499802
29	6	0	3.908215	-1.334018	-0.498892
30	1	0	1.794722	-1.054523	-0.755085
31	6	0	5.113794	0.554906	0.427313
32	1	0	3.924811	2.271375	0.917303
33	6	0	5.107924	-0.751193	-0.075852
34	1	0	3.911416	-2.347144	-0.887068
35	1	0	6.045274	0.993882	0.769188
36	6	0	6.335554	-1.500157	-0.147069
37	7	0	7.322354	-2.103423	-0.204641

Trienamine N1



HF (M062X/6-31+G(d,p)) = -483.907329 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.258968 (Hartree/Particle)

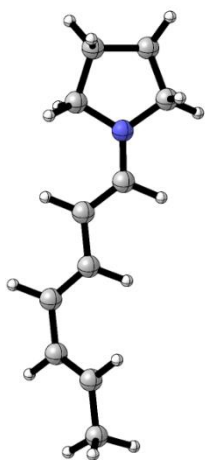
Thermal correction = 0.217859 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.499016	-1.194442	-0.113475
2	6	0	-4.665999	-0.328527	0.364516
3	6	0	-4.297569	1.058830	-0.177034
4	6	0	-2.776535	1.119436	0.007476
5	1	0	-3.323404	-2.065384	0.526831
6	1	0	-5.632805	-0.688588	0.005958
7	1	0	-4.686940	-0.311121	1.459401

8	1	0	-4.543639	1.118389	-1.242654
9	1	0	-4.813959	1.873048	0.335607
10	1	0	-2.280377	1.702337	-0.779528
11	1	0	-2.492094	1.557467	0.976748
12	7	0	-2.371328	-0.274754	-0.052497
13	6	0	-1.069163	-0.664246	-0.070689
14	1	0	-0.926790	-1.743255	-0.125283
15	6	0	0.017765	0.147704	-0.020272
16	1	0	-0.105355	1.226704	0.038248
17	6	0	1.362905	-0.380225	-0.036269
18	1	0	1.457423	-1.467098	-0.094084
19	6	0	2.495431	0.352435	0.013995
20	6	0	3.828843	-0.224911	-0.003925
21	1	0	3.884962	-1.314163	-0.062635
22	6	0	4.971335	0.477174	0.046217
23	1	0	4.911787	1.564759	0.104911
24	1	0	-3.669799	-1.552143	-1.140875
25	1	0	2.425292	1.439263	0.071844
26	6	0	6.343636	-0.125581	0.027201
27	1	0	6.924441	0.232429	-0.830713
28	1	0	6.908993	0.141409	0.927403
29	1	0	6.291760	-1.216667	-0.030147

Trienamine N2



HF (M062X/6-31+G(d,p)) = -483.902459 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.258718 (Hartree/Particle)

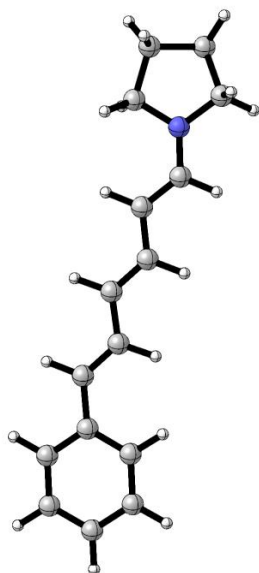
Thermal correction = 0.217335 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.214590	1.346359	-0.013213
2	6	0	-4.528055	0.606168	-0.269340
3	6	0	-4.292903	-0.738624	0.430673
4	6	0	-2.816560	-1.040935	0.141739

5	1	0	-2.997339	2.108163	-0.769141
6	1	0	-5.397989	1.144348	0.113619
7	1	0	-4.660574	0.453756	-1.345810
8	1	0	-4.442388	-0.623974	1.509577
9	1	0	-4.958937	-1.529674	0.079698
10	1	0	-2.324246	-1.556647	0.977099
11	1	0	-2.685781	-1.662426	-0.756758
12	7	0	-2.231387	0.273716	-0.066355
13	6	0	-0.888217	0.477990	-0.129416
14	1	0	-0.600150	1.524029	-0.231406
15	6	0	0.075893	-0.476642	-0.088968
16	1	0	-0.194514	-1.525746	0.006133
17	6	0	1.480963	-0.145104	-0.175574
18	1	0	1.725422	0.915618	-0.261553
19	6	0	2.492985	-1.037257	-0.175914
20	6	0	3.916039	-0.693314	-0.221725
21	1	0	4.572296	-1.421458	-0.701873
22	6	0	4.474137	0.415986	0.284585
23	1	0	3.842880	1.121322	0.826041
24	1	0	-3.226145	1.834425	0.974542
25	1	0	2.247834	-2.099100	-0.160320
26	6	0	5.930201	0.758564	0.176500
27	1	0	6.382112	0.889423	1.166148
28	1	0	6.480267	-0.026173	-0.350484
29	1	0	6.077601	1.698962	-0.367110

Trienamine O1



HF (M062X/6-31+G(d,p)) = -675.5835747 Hartrees

Imaginary Frequencies: none found

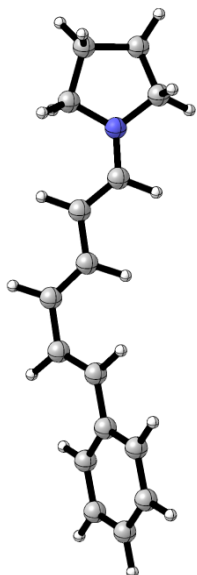
Zero-point correction = 0.312851 (Hartree/Particle)

Thermal correction = 0.266047 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.587635	1.255577	-0.023218
2	6	0	6.771347	0.394055	0.420379
3	6	0	6.451155	-0.966944	-0.211543
4	6	0	4.929894	-1.080956	-0.056015
5	1	0	5.377583	2.080436	0.665504
6	1	0	7.732632	0.801891	0.100391
7	1	0	6.776461	0.309524	1.512284
8	1	0	6.715576	-0.954820	-1.274259
9	1	0	6.982023	-1.796407	0.260149
10	1	0	4.461175	-1.628102	-0.884049
11	1	0	4.644707	-1.583908	0.880677
12	7	0	4.484726	0.303099	-0.037184
13	6	0	3.174113	0.653582	-0.038484
14	1	0	2.997245	1.728695	-0.023885
15	6	0	2.112736	-0.196246	-0.048702
16	1	0	2.271654	-1.271805	-0.060018
17	6	0	0.754053	0.284457	-0.038878
18	1	0	0.618821	1.368317	-0.025823
19	6	0	-0.351851	-0.494880	-0.043711
20	6	0	-1.699866	0.026559	-0.029892
21	1	0	-1.793244	1.112841	-0.016263
22	6	0	-2.806639	-0.743501	-0.025656
23	1	0	-2.672505	-1.825503	-0.026760
24	1	0	5.761968	1.678301	-1.024449
25	1	0	-0.237623	-1.579154	-0.056880
26	6	0	-4.200448	-0.288063	-0.007450
27	6	0	-5.223649	-1.243349	0.094466
28	6	0	-4.573157	1.064613	-0.087900
29	6	0	-6.564093	-0.869566	0.123835
30	1	0	-4.956461	-2.295512	0.154328
31	6	0	-5.910978	1.439633	-0.058330
32	1	0	-3.811251	1.832308	-0.181300
33	6	0	-6.916027	0.476200	0.048792
34	1	0	-7.333981	-1.630880	0.206597
35	1	0	-6.173511	2.491509	-0.122555
36	1	0	-7.959699	0.773553	0.070440

Trienamine O2



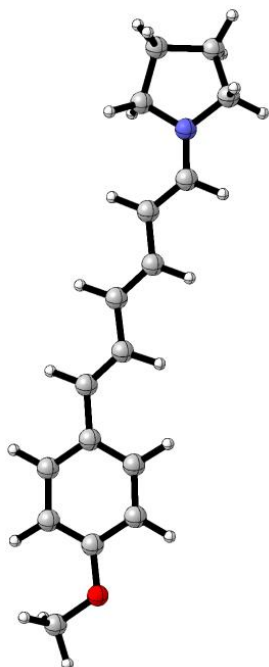
HF (M062X/6-31+G(d,p)) = -675.578578 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.313066 (Hartree/Particle)
 Thermal correction = 0.266419 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.078208	1.440549	0.467918
2	6	0	6.455194	0.781298	0.559160
3	6	0	6.377579	-0.305122	-0.521357
4	6	0	4.936989	-0.819247	-0.406810
5	1	0	4.761305	1.903303	1.408238
6	1	0	7.271947	1.488895	0.401196
7	1	0	6.579496	0.323014	1.545990
8	1	0	6.532712	0.142751	-1.508645
9	1	0	7.116736	-1.097858	-0.389476
10	1	0	4.521215	-1.124080	-1.376085
11	1	0	4.854538	-1.677528	0.276913
12	7	0	4.209733	0.320933	0.127829
13	6	0	2.856523	0.354164	0.219523
14	1	0	2.457572	1.288163	0.614183
15	6	0	1.998160	-0.643605	-0.121081
16	1	0	2.376991	-1.584995	-0.511895
17	6	0	0.571240	-0.492912	0.025960
18	1	0	0.222197	0.468023	0.408994
19	6	0	-0.349513	-1.444105	-0.249208
20	6	0	-1.791490	-1.265054	-0.134931
21	1	0	-2.371632	-2.171929	0.035025
22	6	0	-2.447329	-0.093700	-0.253506
23	1	0	-1.881822	0.793305	-0.537717
24	1	0	5.062789	2.211191	-0.318313
25	1	0	-0.001854	-2.428805	-0.559108
26	6	0	-3.892445	0.105984	-0.085531

27	6	0	-4.486724	1.269841	-0.596396
28	6	0	-4.718019	-0.819231	0.573715
29	6	0	-5.855283	1.493999	-0.477152
30	1	0	-3.861502	2.002301	-1.101106
31	6	0	-6.086103	-0.599370	0.689388
32	1	0	-4.280940	-1.708815	1.017145
33	6	0	-6.663997	0.557130	0.163341
34	1	0	-6.290044	2.401629	-0.884997
35	1	0	-6.704515	-1.327916	1.205337
36	1	0	-7.731258	0.729104	0.261308

Trienamine P1



HF (M062X/6-31+G(d,p)) = -790.0660455 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.345941 (Hartree/Particle)

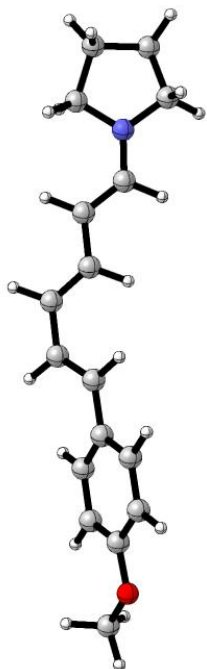
Thermal correction = 0.295586 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.604647	-1.280217	0.098879
2	6	0	7.804212	-0.454575	-0.369278
3	6	0	7.487949	0.940365	0.185824
4	6	0	5.969978	1.060426	0.002473
5	1	0	6.397662	-2.139201	-0.547925
6	1	0	8.756026	-0.854303	-0.012775
7	1	0	7.827580	-0.427393	-1.463875
8	1	0	7.736544	0.980657	1.251706
9	1	0	8.034043	1.739601	-0.319472

10	1	0	5.495754	1.650083	0.797862
11	1	0	5.702476	1.522330	-0.960252
12	7	0	5.511900	-0.318472	0.041899
13	6	0	4.196843	-0.656257	0.059542
14	1	0	4.010303	-1.729076	0.099944
15	6	0	3.143794	0.202215	0.023486
16	1	0	3.313076	1.275439	-0.021001
17	6	0	1.779182	-0.264610	0.036166
18	1	0	1.633049	-1.346278	0.079165
19	6	0	0.681834	0.525068	-0.001253
20	6	0	-0.673333	0.020074	0.011315
21	1	0	-0.779718	-1.064273	0.054476
22	6	0	-1.770322	0.802887	-0.025659
23	1	0	-1.621348	1.882530	-0.064410
24	1	0	6.758469	-1.650741	1.124243
25	1	0	0.808326	1.607417	-0.044239
26	6	0	-3.169929	0.368897	-0.017451
27	6	0	-4.185506	1.329340	-0.029618
28	6	0	-3.564857	-0.983360	0.001037
29	6	0	-5.538222	0.984852	-0.021955
30	1	0	-3.914567	2.382160	-0.044881
31	6	0	-4.899728	-1.344013	0.009006
32	1	0	-2.814645	-1.768159	0.007507
33	6	0	-5.899167	-0.361597	-0.002160
34	1	0	-6.286192	1.768950	-0.032057
35	1	0	-5.202302	-2.386103	0.022553
36	8	0	-7.182259	-0.817760	0.006152
37	6	0	-8.215791	0.142973	-0.002776
38	1	0	-8.172258	0.764334	-0.905540
39	1	0	-9.149968	-0.417783	0.006824
40	1	0	-8.167036	0.786395	0.884150

Trienamine P2



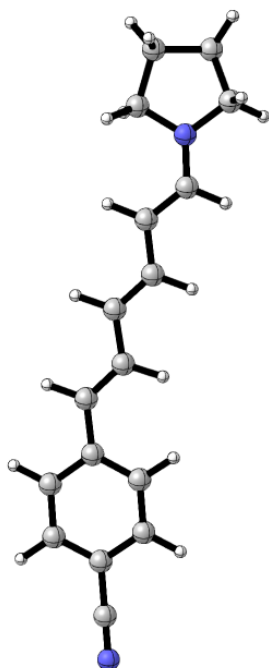
HF (M062X/6-31+G(d,p)) = -790.0608945 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.346132 (Hartree/Particle)
 Thermal correction = 0.296465 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.045584	1.452182	-0.560821
2	6	0	-7.429652	0.808555	-0.654591
3	6	0	-7.379538	-0.252612	0.452312
4	6	0	-5.943226	-0.785868	0.371350
5	1	0	-5.711859	1.891478	-1.506561
6	1	0	-8.239209	1.529907	-0.523855
7	1	0	-7.547143	0.328848	-1.632054
8	1	0	-7.543561	0.220482	1.426312
9	1	0	-8.125938	-1.039942	0.328798
10	1	0	-5.543302	-1.065107	1.355154
11	1	0	-5.862303	-1.666181	-0.283882
12	7	0	-5.196264	0.328771	-0.188461
13	6	0	-3.840051	0.348621	-0.251852
14	1	0	-3.425110	1.269054	-0.661644
15	6	0	-2.998276	-0.646939	0.131401
16	1	0	-3.394032	-1.574906	0.537471
17	6	0	-1.566063	-0.514302	0.010696
18	1	0	-1.198351	0.433042	-0.388391
19	6	0	-0.662344	-1.467858	0.329171
20	6	0	0.784622	-1.306799	0.246342
21	1	0	1.359702	-2.221041	0.098607
22	6	0	1.449344	-0.141090	0.369057
23	1	0	0.885185	0.752662	0.635237

24	1	0	-6.029994	2.239102	0.209489
25	1	0	-1.028366	-2.440688	0.655683
26	6	0	2.898244	0.045476	0.226050
27	6	0	3.507641	1.190186	0.769580
28	6	0	3.724896	-0.868032	-0.436419
29	6	0	4.873954	1.399055	0.681269
30	1	0	2.890145	1.924578	1.280809
31	6	0	5.102779	-0.677362	-0.531844
32	1	0	3.287099	-1.742712	-0.908387
33	6	0	5.683607	0.460776	0.032642
34	1	0	5.341306	2.280925	1.106844
35	1	0	5.702480	-1.410203	-1.058731
36	8	0	7.014416	0.747093	-0.007226
37	6	0	7.863819	-0.174348	-0.656540
38	1	0	8.872309	0.227454	-0.563283
39	1	0	7.817857	-1.160708	-0.179020
40	1	0	7.606576	-0.272044	-1.718376

Trienamine Q1



HF (M062X/6-31+G(d,p)) = -767.802988 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.311686 (Hartree/Particle)

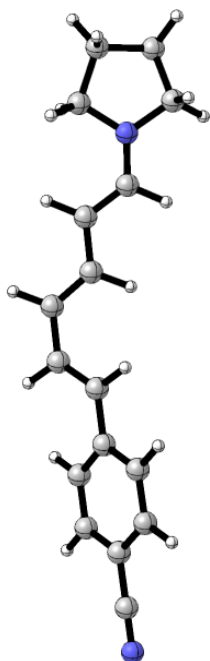
Thermal correction = 0.262273 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.332071	-1.363527	-0.044321
2	6	0	-7.539217	-0.558061	0.439039

3	6	0	-7.282471	0.827794	-0.167119
4	6	0	-5.764690	0.997902	-0.031272
5	1	0	-6.076684	-2.195180	0.620025
6	1	0	-8.489480	-0.995655	0.125957
7	1	0	-7.528418	-0.498268	1.532492
8	1	0	-7.562715	0.828613	-1.225785
9	1	0	-7.837024	1.625571	0.330860
10	1	0	-5.329931	1.584122	-0.850598
11	1	0	-5.484643	1.484670	0.915163
12	7	0	-5.264872	-0.368642	-0.055954
13	6	0	-3.945208	-0.665829	-0.065074
14	1	0	-3.723985	-1.732774	-0.072943
15	6	0	-2.917552	0.228216	-0.058678
16	1	0	-3.118853	1.296325	-0.048790
17	6	0	-1.545698	-0.200980	-0.058640
18	1	0	-1.370478	-1.279199	-0.067549
19	6	0	-0.465992	0.618152	-0.046802
20	6	0	0.892288	0.135639	-0.042423
21	1	0	1.012982	-0.947998	-0.051670
22	6	0	1.982347	0.932900	-0.022238
23	1	0	1.826600	2.011129	-0.004210
24	1	0	-6.506569	-1.767733	-1.052556
25	1	0	-0.615261	1.697710	-0.037749
26	6	0	3.378887	0.501593	-0.012075
27	6	0	4.389701	1.475037	0.074294
28	6	0	3.772942	-0.847903	-0.084680
29	6	0	5.732746	1.128879	0.094355
30	1	0	4.108481	2.522967	0.128794
31	6	0	5.110538	-1.206306	-0.065273
32	1	0	3.024970	-1.629756	-0.162013
33	6	0	6.102039	-0.218899	0.025238
34	1	0	6.499483	1.893372	0.164483
35	1	0	5.400585	-2.250384	-0.121882
36	6	0	7.490819	-0.590398	0.043604
37	7	0	8.609800	-0.890326	0.057434

Trienamine Q2



HF (M062X/6-31+G(d,p)) = -767.7977102 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.311612 (Hartree/Particle)
 Thermal correction = 0.261942 Hartrees

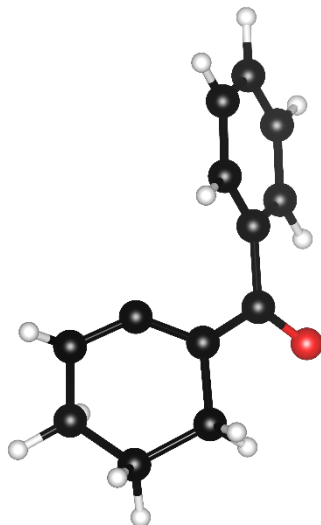
Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.823411	-1.527844	0.437351
2	6	0	-7.207539	-0.894053	0.588204
3	6	0	-7.176867	0.230623	-0.454216
4	6	0	-5.744915	0.768392	-0.351837
5	1	0	-5.470779	-2.010440	1.354434
6	1	0	-8.016658	-1.609556	0.427540
7	1	0	-7.312617	-0.472375	1.593381
8	1	0	-7.345295	-0.184555	-1.453554
9	1	0	-7.927218	1.003781	-0.277615
10	1	0	-5.360656	1.133127	-1.312522
11	1	0	-5.660326	1.588427	0.377005
12	7	0	-4.981074	-0.384840	0.101031
13	6	0	-3.630612	-0.386646	0.183870
14	1	0	-3.203944	-1.327043	0.531834
15	6	0	-2.799947	0.649650	-0.116668
16	1	0	-3.204924	1.598114	-0.460554
17	6	0	-1.372322	0.525108	0.009301
18	1	0	-0.998056	-0.446066	0.339089
19	6	0	-0.475231	1.512889	-0.222186
20	6	0	0.967300	1.362455	-0.127703
21	1	0	1.527114	2.281414	0.044674
22	6	0	1.653027	0.208366	-0.271074
23	1	0	1.111081	-0.690900	-0.560085

24	1	0	-5.818092	-2.274336	-0.370957
25	1	0	-0.847564	2.504425	-0.474339
26	6	0	3.101806	0.052589	-0.130860
27	6	0	3.717351	-1.103233	-0.641051
28	6	0	3.917883	1.009648	0.499068
29	6	0	5.088629	-1.293155	-0.553663
30	1	0	3.103360	-1.859072	-1.122789
31	6	0	5.289603	0.834123	0.588172
32	1	0	3.470537	1.893135	0.942320
33	6	0	5.885082	-0.319408	0.059564
34	1	0	5.549415	-2.188501	-0.957642
35	1	0	5.908967	1.578797	1.077359
36	6	0	7.307713	-0.505347	0.158322
37	7	0	8.453984	-0.652778	0.238234

A.4.4: Energies and Reaction Coordinates for Chapter 5

Allene 5.45a



HF (M062X/6-31+G(d,p)) = -577.5243274 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.213763 (Hartree/Particle)

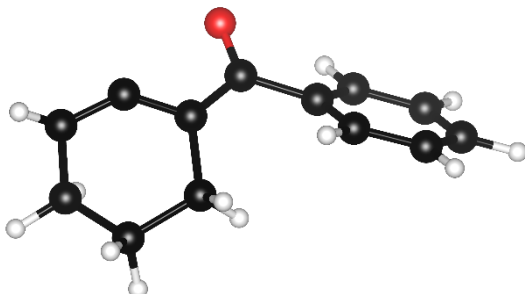
Thermal correction = 0.174502 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.916646	-1.404020	-0.633421
2	6	0	3.873501	-0.791467	0.173188
3	6	0	3.575416	0.409178	0.822053
4	6	0	2.323470	0.992572	0.661637
5	6	0	1.349229	0.370425	-0.129922
6	6	0	1.654259	-0.829833	-0.782724
7	1	0	3.151998	-2.327385	-1.152790
8	1	0	4.853041	-1.244002	0.292950
9	1	0	4.320043	0.887872	1.450093
10	1	0	2.079090	1.929079	1.153127
11	1	0	0.922769	-1.300938	-1.429464
12	6	0	0.022564	1.053057	-0.258690
13	6	0	-1.189574	0.236744	-0.481425
14	8	0	-0.055970	2.272197	-0.154195
15	6	0	-1.330518	-1.045267	-0.162128
16	6	0	-2.300580	-1.778813	0.336761
17	6	0	-2.543229	0.916733	-0.717797
18	6	0	-3.700185	0.197047	0.035767
19	1	0	-4.325692	0.949115	0.527569
20	6	0	-3.248847	-0.851271	1.096606
21	1	0	-4.113581	-1.391904	1.489234
22	1	0	-2.411777	1.937929	-0.345503
23	1	0	-2.778889	0.994108	-1.783124

24	1	0	-4.336817	-0.322989	-0.686831
25	1	0	-2.742120	-0.359827	1.930850
26	1	0	-2.583225	-2.779147	0.028019

Rotated Allene 5.45a



HF (M062X/6-31+G(d,p)) = -577.5186449 Hartrees

Imaginary Frequencies: none found

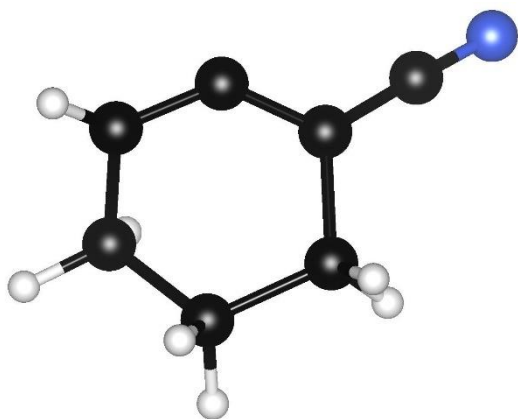
Zero-point correction = 0.214001 (Hartree/Particle)

Thermal correction = 0.175151 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.938213	1.355411	0.651715
2	6	0	-3.880396	0.747143	-0.177460
3	6	0	-3.561278	-0.431944	-0.853795
4	6	0	-2.301989	-1.003389	-0.697348
5	6	0	-1.346242	-0.384546	0.115340
6	6	0	-1.668876	0.797259	0.790031
7	1	0	-3.190935	2.262947	1.190325
8	1	0	-4.864970	1.189270	-0.294289
9	1	0	-4.295629	-0.905449	-1.497593
10	1	0	-2.042943	-1.928598	-1.202932
11	1	0	-0.940330	1.267486	1.444023
12	6	0	-0.017994	-1.050290	0.297540
13	6	0	1.198154	-0.213737	0.500854
14	8	0	0.058578	-2.271220	0.280739
15	6	0	2.382468	-0.757504	0.753283
16	6	0	3.624656	-0.522110	0.401282
17	6	0	1.346290	1.242397	0.025515
18	6	0	2.737289	1.504174	-0.633687
19	1	0	2.587263	2.055642	-1.567450
20	6	0	3.590579	0.235112	-0.927253
21	1	0	4.593573	0.521782	-1.252923
22	1	0	0.550726	1.404582	-0.710350
23	1	0	1.183383	1.969286	0.826696
24	1	0	3.328619	2.148480	0.024028
25	1	0	3.131994	-0.366064	-1.716124
26	1	0	4.503925	-0.557457	1.034572

Allene 5.45d



HF (M062X/6-31+G(d,p)) = -325.4744092 Hartrees

Imaginary Frequencies: none found

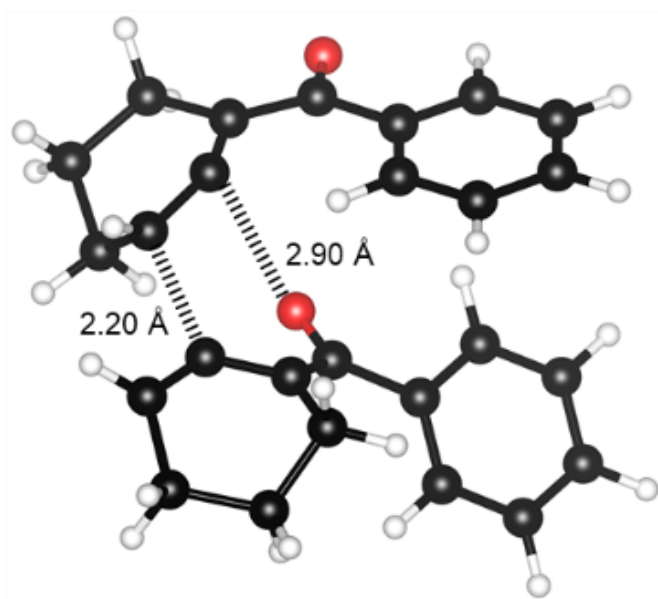
Zero-point correction = 0.121012 (Hartree/Particle)

Thermal correction = 0.089440 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.712299	-0.079119	-0.337109
2	6	0	-0.074341	-1.143408	-0.430077
3	6	0	-1.365865	-1.317030	-0.242597
4	6	0	-0.044181	1.259150	-0.400868
5	6	0	-1.528338	1.089029	0.033617
6	1	0	-1.793409	1.910360	0.706451
7	6	0	-1.869070	-0.261553	0.735070
8	1	0	-2.945647	-0.339458	0.901710
9	1	0	0.479443	1.934216	0.284517
10	1	0	0.013000	1.707397	-1.396226
11	1	0	-2.173991	1.174397	-0.845162
12	1	0	-1.362069	-0.334022	1.699930
13	1	0	-2.034078	-1.891843	-0.875021
14	6	0	2.079842	-0.113464	0.085427
15	7	0	3.193524	-0.108953	0.409003

Allene 5.45a: Diels-Alder Dimerization Transition State



HF (M062X/6-31+G(d,p)) = -1155.0452456 Hartrees

Imaginary Frequencies: 1 (-209.59 cm^{-1})

Zero-point correction = 0.428352 (Hartree/Particle)

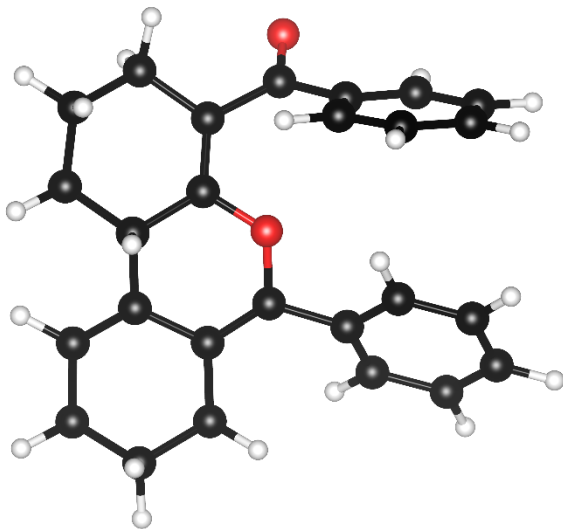
Thermal correction = 0.373832 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.408977	3.989827	0.801956
2	6	0	-1.350720	2.514566	1.276407
3	6	0	-0.380855	1.805938	0.343385
4	6	0	0.827028	2.432776	0.405763
5	6	0	1.138820	3.676340	0.739965
6	6	0	-0.017222	4.671273	0.706910
7	6	0	-0.663590	0.769541	-0.634117
8	6	0	2.713144	1.309476	0.369189
9	6	0	2.522135	0.004473	0.559396
10	6	0	2.831995	-1.142650	0.000710
11	6	0	4.073394	-0.999305	-0.900111
12	6	0	4.389405	0.482529	-1.231826
13	6	0	3.183256	1.448740	-1.087543
14	1	0	-1.885864	4.009145	-0.183754
15	1	0	-0.979627	2.471557	2.306411
16	1	0	2.093673	3.985469	1.153695
17	1	0	0.027117	5.312890	-0.179242
18	1	0	4.950814	-1.493607	-0.472813
19	1	0	5.188612	0.841174	-0.573793
20	1	0	2.365864	1.166876	-1.756013
21	1	0	3.805735	-1.553208	-1.806977
22	1	0	4.773939	0.535877	-2.255792
23	1	0	3.477572	2.482469	-1.294508
24	1	0	3.131983	1.939509	1.149789
25	1	0	0.139845	5.328242	1.570396
26	1	0	-2.048293	4.571190	1.474717

27	1	0	-2.345744	2.063378	1.265540
28	8	0	0.262813	0.220736	-1.243753
29	6	0	-2.066326	0.287071	-0.872097
30	6	0	-2.272776	-1.087193	-1.035545
31	6	0	-3.145532	1.164461	-1.015323
32	6	0	-3.546813	-1.579299	-1.302712
33	1	0	-1.425882	-1.761724	-0.939628
34	6	0	-4.417925	0.673643	-1.306275
35	1	0	-2.990916	2.236047	-0.927113
36	6	0	-4.622076	-0.699375	-1.439675
37	1	0	-3.700992	-2.649053	-1.408208
38	1	0	-5.246568	1.363761	-1.430144
39	1	0	-5.614696	-1.082602	-1.655888
40	6	0	1.984307	-2.353771	-0.100852
41	8	0	2.338353	-3.266999	-0.834382
42	6	0	0.708198	-2.475919	0.687638
43	6	0	0.021946	-3.693218	0.589611
44	6	0	0.161648	-1.451591	1.469345
45	6	0	-1.185668	-3.883389	1.254758
46	1	0	0.447379	-4.480872	-0.023250
47	6	0	-1.049472	-1.639164	2.131405
48	1	0	0.657902	-0.486291	1.555211
49	6	0	-1.724588	-2.854822	2.028042
50	1	0	-1.707435	-4.831120	1.166488
51	1	0	-1.469253	-0.827870	2.718581
52	1	0	-2.670904	-2.996869	2.540949

Allene 5.45a Dimerization cycloadduct: 5.48a



HF (M062X/6-31+G(d,p)) = -1155.2285749 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.437060 (Hartree/Particle)

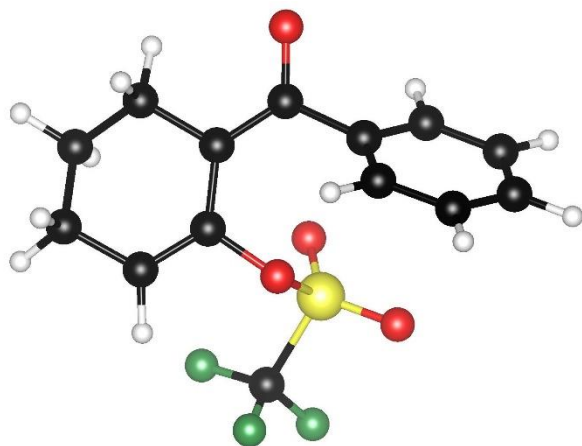
Thermal correction = 0.384690 Hartrees

Coordinates from last standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-4.175111	2.333655	-0.529226
2	6	0	-2.785487	2.396019	0.103072
3	6	0	-2.027607	1.095858	-0.081081
4	6	0	-2.818760	-0.135363	-0.234335
5	6	0	-4.159656	-0.118503	-0.125495
6	6	0	-4.954586	1.149002	0.034875
7	6	0	-0.679498	1.025973	-0.079423
8	6	0	-2.062490	-1.402137	-0.604454
9	6	0	-0.649792	-1.361095	-0.085258
10	6	0	0.020556	-2.409029	0.430817
11	6	0	-0.630656	-3.765819	0.579832
12	6	0	-1.832020	-3.903484	-0.351998
13	6	0	-2.763628	-2.704177	-0.204156
14	1	0	-4.705596	3.272443	-0.343847
15	1	0	-2.213062	3.228856	-0.315108
16	1	0	-4.715002	-1.049176	-0.202102
17	1	0	-5.186450	1.324185	1.095541
18	1	0	0.111441	-4.544134	0.370943
19	1	0	-1.483456	-3.970720	-1.390812
20	1	0	-3.094519	-2.621806	0.839402
21	1	0	-0.940398	-3.911248	1.622686
22	1	0	-2.372161	-4.829131	-0.131876
23	1	0	-3.657871	-2.841037	-0.818598
24	1	0	-1.959769	-1.386429	-1.703532
25	1	0	-5.917845	1.040014	-0.474329
26	1	0	-4.079508	2.216542	-1.615691
27	1	0	-2.910591	2.600185	1.176017
28	8	0	0.003766	-0.170583	-0.211705
29	6	0	0.304663	2.122572	0.071041
30	6	0	1.522171	2.044529	-0.623187
31	6	0	0.090600	3.204680	0.934626
32	6	0	2.479570	3.045291	-0.488799
33	1	0	1.719358	1.188469	-1.261161
34	6	0	1.052562	4.204496	1.069019
35	1	0	-0.812725	3.254198	1.531424
36	6	0	2.246250	4.133636	0.352754
37	1	0	3.414432	2.967368	-1.036221
38	1	0	0.872133	5.031791	1.748335
39	1	0	2.995328	4.911652	0.461760
40	6	0	1.401618	-2.272383	0.972356
41	8	0	1.698559	-2.839723	2.016216
42	6	0	2.446177	-1.513521	0.212910
43	6	0	3.467277	-0.870433	0.917150
44	6	0	2.448817	-1.500008	-1.185033
45	6	0	4.472348	-0.196590	0.227493
46	1	0	3.456840	-0.895445	2.002580
47	6	0	3.473962	-0.856321	-1.874413
48	1	0	1.650246	-1.997993	-1.728540
49	6	0	4.480287	-0.195046	-1.168086
50	1	0	5.251674	0.323149	0.775930
51	1	0	3.483089	-0.861304	-2.959868
52	1	0	5.270413	0.321197	-1.705025

5.51a conjugate base



HF (M062X/6-31+G(d,p)) = -1538.9291625 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.244850 (Hartree/Particle)

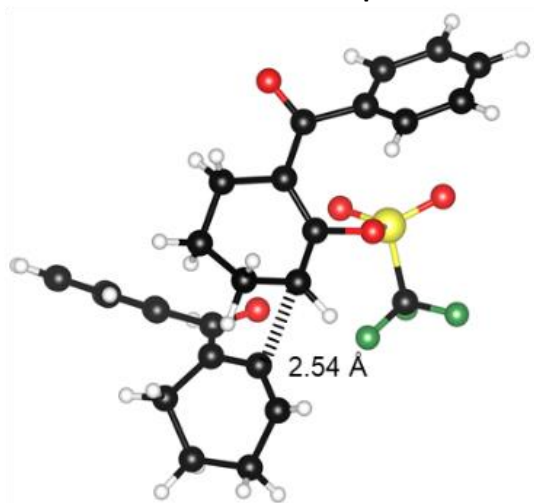
Thermal correction = 0.196083 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.721131	-1.038976	-0.735731
2	6	0	3.943764	-1.407952	0.591335
3	6	0	3.308345	-0.707934	1.617336
4	6	0	2.447843	0.346513	1.315597
5	6	0	2.216265	0.721731	-0.010856
6	6	0	2.872678	0.026484	-1.031639
7	1	0	4.210122	-1.580899	-1.540357
8	1	0	4.607671	-2.235219	0.824772
9	1	0	3.481890	-0.984985	2.653409
10	1	0	1.942715	0.884661	2.113952
11	1	0	2.707070	0.327025	-2.062814
12	6	0	1.384129	1.934986	-0.358861
13	6	0	0.033744	2.051919	-0.008154
14	8	0	2.023261	2.857142	-0.960432
15	6	0	-0.828503	1.072259	0.581854
16	6	0	-2.097730	1.248253	1.008634
17	6	0	-0.635541	3.391457	-0.268084
18	6	0	-2.158426	3.297294	-0.387623
19	1	0	-2.588947	4.298491	-0.499523
20	6	0	-2.764627	2.584979	0.825942
21	1	0	-3.843685	2.446761	0.692253
22	1	0	-0.385337	4.103075	0.535471
23	1	0	-0.208836	3.813039	-1.183664
24	1	0	-2.415664	2.727307	-1.289754
25	1	0	-2.641931	3.215485	1.719716
26	8	0	-0.311164	-0.259185	0.794165
27	16	0	-0.380386	-1.333955	-0.359980
28	8	0	-0.398021	-0.751250	-1.681160
29	8	0	0.528373	-2.394573	0.006448
30	6	0	-2.078816	-2.050679	-0.100250
31	9	0	-2.340492	-2.166718	1.197418

32	9	0	-3.008517	-1.298717	-0.671789
33	9	0	-2.103076	-3.259824	-0.655005
34	1	0	-2.635257	0.416794	1.451447

Transition State of nucleophilic attack of 5.45a by 5.51a conjugate base



HF (M062X/6-31+G(d,p)) = -2116.44527 Hartrees

Imaginary Frequencies: 1 (-246.41 cm^{-1})

Zero-point correction = 0.459692 (Hartree/Particle)

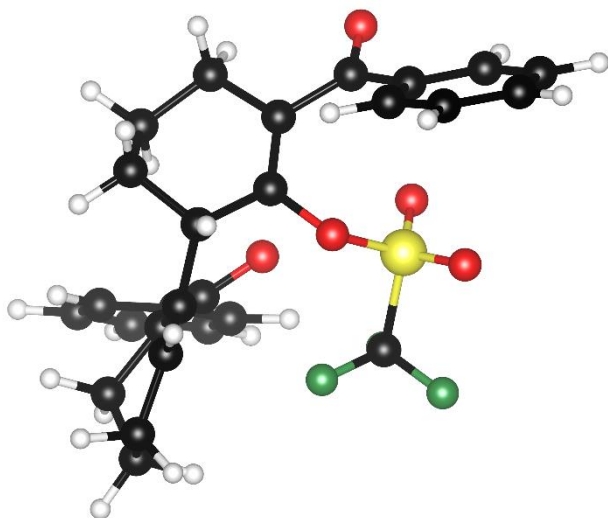
Thermal correction = 0.394413 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.640359	-0.100417	0.803922
2	6	0	-6.219205	-0.659760	-0.335307
3	6	0	-5.534005	-1.644960	-1.047737
4	6	0	-4.279292	-2.069178	-0.618163
5	6	0	-3.680756	-1.496181	0.508373
6	6	0	-4.375335	-0.512791	1.218847
7	1	0	-6.174263	0.658621	1.368371
8	1	0	-7.201208	-0.332392	-0.664066
9	1	0	-5.980202	-2.084304	-1.935240
10	1	0	-3.746818	-2.850992	-1.152216
11	1	0	-3.921123	-0.074791	2.104054
12	6	0	-2.375523	-2.067755	1.003499
13	6	0	-1.296912	-1.268322	1.468731
14	8	0	-2.332299	-3.324905	1.069345
15	6	0	-1.096146	0.121266	1.316782
16	6	0	-0.178767	0.892440	1.989220
17	6	0	-0.248668	-2.026168	2.266547
18	6	0	0.967440	-1.191729	2.664837
19	1	0	1.527100	-1.706728	3.454068
20	6	0	0.558357	0.213615	3.117731
21	1	0	1.435663	0.795745	3.414969
22	1	0	-0.726021	-2.437322	3.168277

23	1	0	0.071042	-2.899404	1.685624
24	1	0	1.637440	-1.085372	1.804743
25	1	0	-0.089814	0.128897	4.005912
26	8	0	-1.984964	0.873761	0.472576
27	16	0	-1.998516	0.763905	-1.112534
28	8	0	-1.215541	-0.340894	-1.605845
29	8	0	-3.353072	1.000299	-1.555392
30	6	0	-1.108110	2.339191	-1.541273
31	9	0	-0.054687	2.531888	-0.773266
32	9	0	-0.733207	2.272388	-2.815505
33	9	0	-1.945356	3.364396	-1.392129
34	6	0	4.743552	-2.511395	-2.674758
35	6	0	5.210253	-3.367872	-1.675915
36	6	0	4.872417	-3.132570	-0.343155
37	6	0	4.083499	-2.033507	-0.007244
38	6	0	3.613671	-1.171288	-1.003850
39	6	0	3.938693	-1.425495	-2.340288
40	1	0	5.000377	-2.696468	-3.713277
41	1	0	5.829033	-4.220948	-1.937008
42	1	0	5.219795	-3.806358	0.433904
43	1	0	3.814011	-1.857233	1.030988
44	1	0	3.550345	-0.762123	-3.107085
45	6	0	2.699943	-0.020196	-0.685743
46	6	0	2.880790	0.706179	0.569794
47	8	0	1.801949	0.264494	-1.479880
48	6	0	2.016167	1.658912	0.976592
49	6	0	2.176620	2.839513	1.540760
50	6	0	4.195800	0.889204	1.322891
51	6	0	4.643391	2.347617	1.033643
52	1	0	5.566347	2.569502	1.581252
53	6	0	3.579638	3.426958	1.373646
54	1	0	3.608323	4.226586	0.625722
55	1	0	4.061844	0.731603	2.399783
56	1	0	4.971348	0.201881	0.974897
57	1	0	4.886700	2.400746	-0.033198
58	1	0	3.816004	3.895891	2.336570
59	1	0	1.482208	3.301802	2.236470
60	1	0	-0.274125	1.968711	1.924405

Nucleophilic attack intermediate: 5.52a



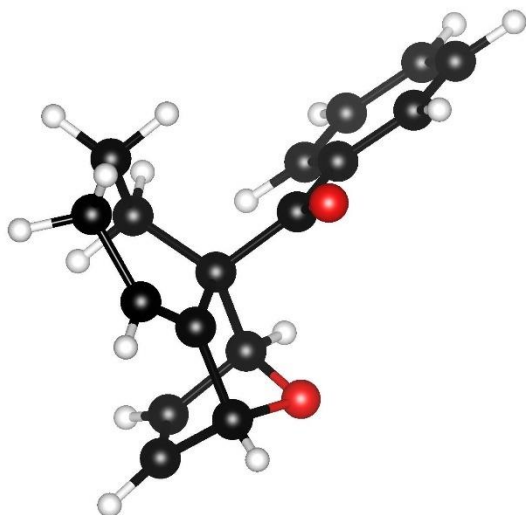
HF (M062X/6-31+G(d,p)) = -2116.542758 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.465089 (Hartree/Particle)
 Thermal correction = 0.404368 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.246041	-0.916701	-0.884904
2	6	0	-6.086492	-0.451381	0.125350
3	6	0	-5.775266	0.727893	0.805672
4	6	0	-4.628044	1.440277	0.471754
5	6	0	-3.772001	0.967797	-0.528270
6	6	0	-4.086864	-0.213185	-1.205815
7	1	0	-5.489866	-1.828645	-1.420621
8	1	0	-6.983292	-1.006427	0.383384
9	1	0	-6.427101	1.088134	1.595444
10	1	0	-4.371031	2.360113	0.988126
11	1	0	-3.428593	-0.577890	-1.989128
12	6	0	-2.573871	1.795433	-0.899557
13	6	0	-1.380702	1.149949	-1.505254
14	8	0	-2.648066	3.015618	-0.815829
15	6	0	-0.870348	-0.045797	-1.157693
16	6	0	0.036628	-0.893608	-2.005414
17	6	0	-0.661758	1.988942	-2.540676
18	6	0	0.676347	1.383299	-2.947388
19	1	0	1.070642	1.908979	-3.823523
20	6	0	0.494223	-0.099189	-3.252830
21	1	0	1.422556	-0.544718	-3.622476
22	1	0	-1.307030	2.117891	-3.421973
23	1	0	-0.525746	2.985157	-2.106625
24	1	0	1.395632	1.497183	-2.129774
25	1	0	-0.259580	-0.207598	-4.044336
26	8	0	-1.376261	-0.798916	-0.083962
27	16	0	-1.532904	-0.283533	1.425486
28	8	0	-1.494510	1.152159	1.548931
29	8	0	-2.657591	-1.042471	1.932010

30	6	0	-0.045520	-1.009654	2.338297
31	9	0	0.675735	-1.793338	1.568130
32	9	0	0.683390	-0.049892	2.873611
33	9	0	-0.547193	-1.746291	3.335464
34	6	0	4.457223	2.515595	1.926993
35	6	0	5.521924	2.724339	1.048059
36	6	0	5.507966	2.110882	-0.205029
37	6	0	4.445586	1.282859	-0.566948
38	6	0	3.379222	1.052857	0.311748
39	6	0	3.391988	1.697233	1.554434
40	1	0	4.455127	2.998022	2.900629
41	1	0	6.349318	3.367736	1.332758
42	1	0	6.320776	2.283847	-0.904946
43	1	0	4.430421	0.816517	-1.549260
44	1	0	2.544873	1.547627	2.216706
45	6	0	2.181891	0.214273	-0.071278
46	6	0	2.351280	-0.953693	-0.800026
47	8	0	1.045675	0.677314	0.307938
48	6	0	1.193748	-1.655161	-1.356985
49	6	0	1.218012	-2.992775	-1.566450
50	6	0	3.639267	-1.745652	-0.865117
51	6	0	3.399744	-3.159487	-0.312446
52	1	0	4.332319	-3.736414	-0.285382
53	6	0	2.352591	-3.894312	-1.152766
54	1	0	1.963859	-4.760419	-0.600115
55	1	0	4.005642	-1.840616	-1.902786
56	1	0	4.432118	-1.261780	-0.289105
57	1	0	3.042271	-3.065786	0.720369
58	1	0	2.828355	-4.310318	-2.054107
59	1	0	0.389467	-3.465184	-2.094341
60	1	0	-0.650440	-1.679011	-2.358994

Endo adduct 5.53a (Allene 5.45a with furan)

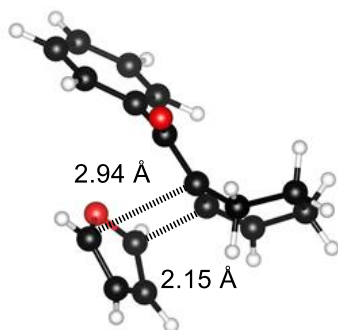


HF (M062X/6-31+G(d,p)) = -807.5321058 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.291267 (Hartree/Particle)
Thermal correction = 0.249445 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.744316	-0.016430	0.193466
2	6	0	2.064448	0.197928	-0.532158
3	6	0	2.796665	1.303582	-0.446941
4	6	0	0.788984	0.792254	1.501125
5	6	0	1.059702	2.265409	1.153428
6	1	0	0.229808	2.637257	0.540903
7	6	0	2.388021	2.477144	0.406490
8	1	0	3.196214	2.645128	1.131599
9	1	0	-0.138844	0.723484	2.073585
10	1	0	1.598710	0.389641	2.122253
11	1	0	1.057743	2.863130	2.069602
12	1	0	2.336174	3.391739	-0.195599
13	1	0	3.770123	1.351221	-0.933789
14	6	0	0.753256	-1.601546	0.204482
15	6	0	1.952361	-2.085323	1.003739
16	6	0	3.014221	-1.849695	0.228316
17	6	0	2.454955	-1.189670	-1.034908
18	8	0	1.178754	-1.832290	-1.144704
19	1	0	-0.201092	-2.091362	0.382166
20	1	0	1.922039	-2.453656	2.021067
21	1	0	4.066410	-1.962889	0.458288
22	1	0	3.026189	-1.258932	-1.958330
23	6	0	-0.437314	0.439319	-0.680974
24	6	0	-1.854107	0.137288	-0.256853
25	6	0	-2.201069	-0.508184	0.937556
26	6	0	-2.876224	0.542182	-1.126336
27	6	0	-3.538575	-0.739654	1.253264
28	1	0	-1.442369	-0.837320	1.638117
29	6	0	-4.210771	0.309362	-0.813334
30	1	0	-2.602815	1.041752	-2.049571
31	6	0	-4.545314	-0.333208	0.379574
32	1	0	-3.791233	-1.240317	2.182261
33	1	0	-4.990119	0.627570	-1.498416
34	1	0	-5.586374	-0.517341	0.626115
35	8	0	-0.250242	1.063085	-1.709028

Endo Transition State of trapping Allene 5.45a with furan

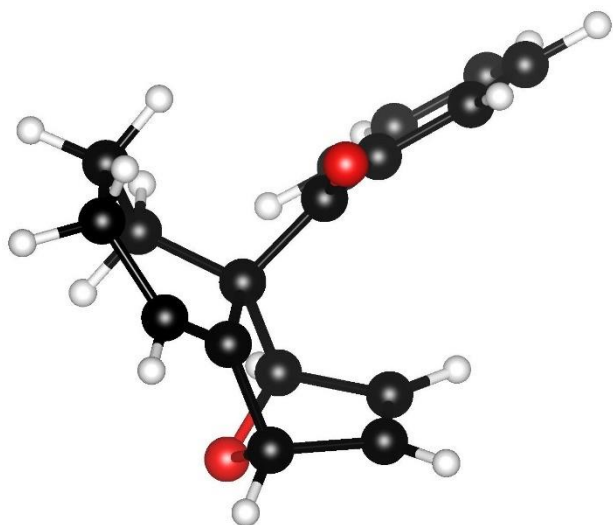


HF (M062X/6-31+G(d,p)) = -807.4666889 Hartrees
 Imaginary Frequencies: 1 (-220.31 cm⁻¹)
 Zero-point correction = 0.285996 (Hartree/Particle)
 Thermal correction = 0.241535 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.989966	-0.515253	0.535537
2	6	0	-1.254066	-0.060569	-0.721362
3	6	0	-2.239833	-0.376770	-1.552126
4	6	0	-2.278172	-1.018516	1.164126
5	6	0	-2.800859	-2.131188	0.221186
6	1	0	-2.095428	-2.966739	0.282896
7	6	0	-2.950852	-1.689098	-1.263207
8	1	0	-4.006746	-1.517553	-1.503228
9	1	0	-2.094216	-1.423717	2.161900
10	1	0	-3.009498	-0.205361	1.243877
11	1	0	-3.766021	-2.503961	0.580439
12	1	0	-2.614629	-2.490904	-1.929697
13	1	0	-2.633923	0.296161	-2.308495
14	6	0	-0.219918	2.277963	1.050942
15	6	0	-1.527127	2.644096	0.832123
16	6	0	-1.749188	2.479883	-0.548944
17	6	0	-0.568580	1.949829	-1.069992
18	8	0	0.394285	1.984629	-0.108913
19	1	0	0.397669	2.258588	1.936955
20	1	0	-2.234196	2.957563	1.585561
21	1	0	-2.663882	2.649465	-1.097685
22	1	0	-0.214520	1.860457	-2.086373
23	6	0	0.298114	-0.863824	1.120897
24	6	0	1.568583	-0.672664	0.339328
25	6	0	1.651450	-0.903164	-1.037048
26	6	0	2.715584	-0.288599	1.041313
27	6	0	2.865601	-0.737822	-1.702780
28	1	0	0.773650	-1.226245	-1.587462
29	6	0	3.922948	-0.104084	0.373654
30	1	0	2.643620	-0.131426	2.113499
31	6	0	3.999713	-0.327807	-1.002187
32	1	0	2.925877	-0.931562	-2.769366
33	1	0	4.804710	0.208857	0.924402
34	1	0	4.941813	-0.190112	-1.523956
35	8	0	0.378856	-1.311878	2.269909

Exo adduct: Allene 5.45a with furan



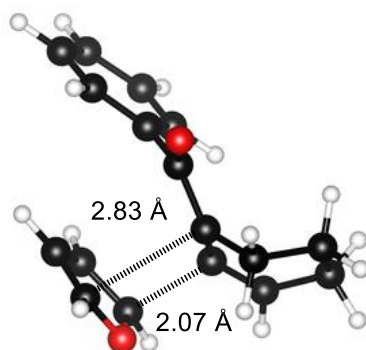
HF (M062X/6-31+G(d,p)) = -807.5325885 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.291333 (Hartree/Particle)
 Thermal correction = 0.249242 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.838630	-0.052633	0.355645
2	6	0	-2.151193	0.237645	-0.358007
3	6	0	-3.079196	-0.680728	-0.603491
4	6	0	-1.121712	-1.174373	1.377187
5	6	0	-1.662688	-2.411709	0.644161
6	1	0	-0.865080	-2.819513	0.015680
7	6	0	-2.909313	-2.128357	-0.222991
8	1	0	-3.815335	-2.420872	0.322748
9	1	0	-0.224614	-1.453200	1.939279
10	1	0	-1.857612	-0.788542	2.091871
11	1	0	-1.901065	-3.185925	1.379464
12	1	0	-2.888227	-2.759091	-1.119681
13	1	0	-4.044120	-0.378048	-1.008091
14	6	0	-2.313985	1.748206	-0.269832
15	6	0	-1.166800	2.422208	-1.010687
16	6	0	-0.082443	2.228745	-0.254468
17	6	0	-0.569368	1.399950	0.932745
18	8	0	-1.896048	1.903590	1.103572
19	1	0	-3.321494	2.130580	-0.424093
20	1	0	-1.239228	2.878972	-1.989525
21	1	0	0.947432	2.488633	-0.465774
22	1	0	-0.018400	1.463249	1.869085
23	6	0	0.257465	-0.517575	-0.611457
24	8	0	-0.028861	-1.036189	-1.675606
25	6	0	1.705526	-0.358902	-0.236617
26	6	0	2.144893	-0.153283	1.076292
27	6	0	2.648922	-0.421234	-1.270533
28	6	0	3.504850	-0.015134	1.349390
29	1	0	1.441218	-0.117029	1.899825

30	6	0	4.004244	-0.268656	-0.999919
31	1	0	2.298723	-0.581772	-2.285067
32	6	0	4.434950	-0.066275	0.312864
33	1	0	3.835314	0.132928	2.372383
34	1	0	4.725735	-0.307344	-1.809823
35	1	0	5.492908	0.050395	0.526302

Exo Transition State of trapping Allene 5.45a with furan



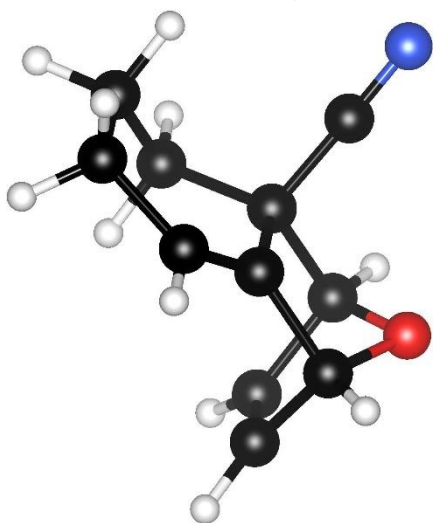
HF (M062X/6-31+G(d,p)) = -807.4635917 Hartrees
Imaginary Frequencies: 1 (-319.25 cm⁻¹)
Zero-point correction = 0.286041 (Hartree/Particle)
Thermal correction = 0.241415 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.092323	-0.337278	0.548023
2	6	0	-1.306412	0.042537	-0.752843
3	6	0	-2.243679	-0.363840	-1.599571
4	6	0	-2.410997	-0.764743	1.165323
5	6	0	-2.897282	-1.956451	0.301484
6	1	0	-2.194394	-2.781217	0.462435
7	6	0	-2.985924	-1.637520	-1.217318
8	1	0	-4.030666	-1.474147	-1.507326
9	1	0	-2.279055	-1.076668	2.203834
10	1	0	-3.136761	0.055300	1.130198
11	1	0	-3.875880	-2.301411	0.652747
12	1	0	-2.640009	-2.497999	-1.801054
13	1	0	-2.600397	0.221133	-2.442780
14	6	0	-0.895237	2.044823	-1.096767
15	6	0	0.470341	2.141729	-0.814780
16	6	0	0.568258	2.329408	0.568073
17	6	0	-0.729717	2.425768	1.034294
18	8	0	-1.601763	2.427548	0.018398
19	1	0	-1.416988	2.164738	-2.035589
20	1	0	1.271498	1.970181	-1.519535
21	1	0	1.461432	2.345675	1.174898
22	1	0	-1.136553	2.593297	2.020794
23	6	0	0.158322	-0.766746	1.159913
24	8	0	0.197884	-1.175243	2.326243

25	6	0	1.444826	-0.718135	0.380996
26	6	0	1.520275	-1.042911	-0.976744
27	6	0	2.615678	-0.381728	1.070218
28	6	0	2.748730	-1.013214	-1.638063
29	1	0	0.624241	-1.329582	-1.517095
30	6	0	3.836799	-0.328415	0.405972
31	1	0	2.550084	-0.152829	2.130083
32	6	0	3.905114	-0.643255	-0.953506
33	1	0	2.800068	-1.278798	-2.689532
34	1	0	4.735973	-0.047777	0.945751
35	1	0	4.857803	-0.608504	-1.473170

Endo adduct: 5.53d (Allene 5.45d with furan)



HF (M062X/6-31+G(d,p)) = -555.4920351 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.198464 (Hartree/Particle)

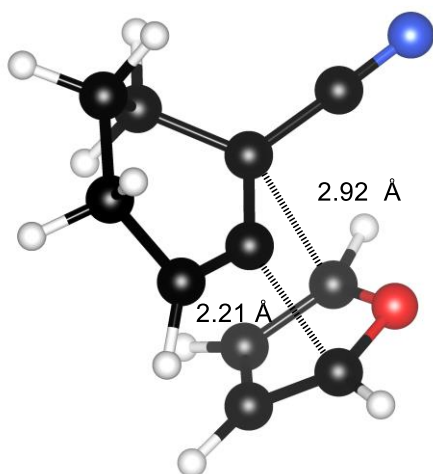
Thermal correction = 0.163567 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.122434	0.543609	0.311199
2	6	0	-0.051780	-0.546725	-0.745279
3	6	0	0.905111	-1.415976	-1.054729
4	6	0	1.113239	0.069920	1.379508
5	6	0	2.428059	-0.312516	0.683655
6	1	0	2.844607	0.586333	0.215062
7	6	0	2.252181	-1.415879	-0.375553
8	1	0	2.366044	-2.402543	0.093131
9	1	0	1.285944	0.847185	2.129983
10	1	0	0.670053	-0.800299	1.877263
11	1	0	3.157423	-0.639378	1.429877
12	1	0	3.054582	-1.348532	-1.118683
13	1	0	0.696183	-2.224677	-1.753464

14	6	0	0.618444	1.783889	-0.311558
15	7	0	1.020682	2.769897	-0.765506
16	6	0	-1.400994	0.789803	0.656298
17	6	0	-1.965114	-0.487714	1.250720
18	6	0	-2.080181	-1.335146	0.224665
19	6	0	-1.559891	-0.573047	-0.995827
20	8	0	-1.936802	0.771482	-0.670223
21	1	0	-1.611569	1.733655	1.156189
22	1	0	-2.138218	-0.666579	2.303752
23	1	0	-2.355350	-2.382410	0.232069
24	1	0	-1.909110	-0.865197	-1.983443

Endo Transition State of trapping Allene 5.45d with furan



HF (M062X/6-31+G(d,p)) = -555.418494 Hartrees

Imaginary Frequencies: 1 (-169.42 cm^{-1})

Zero-point correction = 0.193221 (Hartree/Particle)

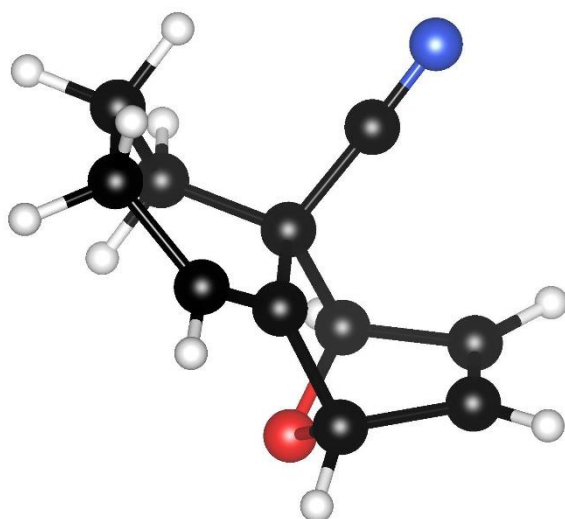
Thermal correction = 0.155483 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.539695	0.697469	0.133582
2	6	0	0.385088	-0.425921	-0.606588
3	6	0	1.188090	-1.468546	-0.757406
4	6	0	1.587837	0.479760	1.219605
5	6	0	2.867385	0.015495	0.480220
6	1	0	3.213239	0.854401	-0.132947
7	6	0	2.653311	-1.231781	-0.416619
8	1	0	2.977961	-2.136305	0.112179
9	1	0	1.784087	1.394911	1.784445
10	1	0	1.240030	-0.289834	1.917472
11	1	0	3.659881	-0.198317	1.205142
12	1	0	3.276085	-1.164027	-1.314694
13	1	0	0.841877	-2.476334	-0.969327
14	6	0	0.231129	2.007043	-0.326714
15	7	0	-0.016169	3.093479	-0.662655

16	6	0	-2.321745	0.448869	0.664644
17	6	0	-2.132070	-0.770165	1.265920
18	6	0	-1.792780	-1.666663	0.229928
19	6	0	-1.743159	-0.909500	-0.933529
20	8	0	-2.199450	0.346113	-0.673580
21	1	0	-2.603632	1.419784	1.043857
22	1	0	-2.200325	-0.974199	2.323979
23	1	0	-1.550517	-2.715999	0.313016
24	1	0	-1.706590	-1.193691	-1.974148

Exo adduct: Allene 5.45d with furan



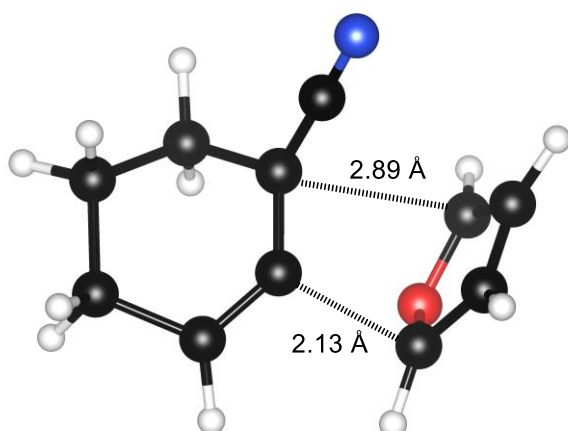
HF (M062X/6-31+G(d,p)) = -555.4903071 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.198513 (Hartree/Particle)
Thermal correction = 0.163509 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.080344	0.458595	0.366062
2	6	0	0.060630	-0.808984	-0.493622
3	6	0	1.167935	-1.435528	-0.878526
4	6	0	1.308637	0.385707	1.286924
5	6	0	2.566616	0.276320	0.413620
6	1	0	2.658542	1.198403	-0.170971
7	6	0	2.549868	-0.942589	-0.532883
8	1	0	3.067198	-1.786982	-0.060077
9	1	0	1.363644	1.270913	1.928349
10	1	0	1.188586	-0.497259	1.923993
11	1	0	3.452808	0.226597	1.052176
12	1	0	3.120344	-0.719123	-1.441439
13	1	0	1.089551	-2.405760	-1.366402
14	6	0	0.156165	1.694122	-0.431053
15	7	0	0.238730	2.683132	-1.027248

16	6	0	-1.350393	-1.358749	-0.316940
17	6	0	-2.350205	-0.366974	-0.893221
18	6	0	-2.363307	0.666332	-0.048239
19	6	0	-1.350138	0.311603	1.034257
20	8	0	-1.476820	-1.105695	1.100069
21	1	0	-1.478202	-2.415537	-0.543266
22	1	0	-2.854190	-0.472222	-1.845226
23	1	0	-2.875701	1.615019	-0.142226
24	1	0	-1.446043	0.770459	2.016995

Exo Transition State of trapping Allene 5.45d with furan



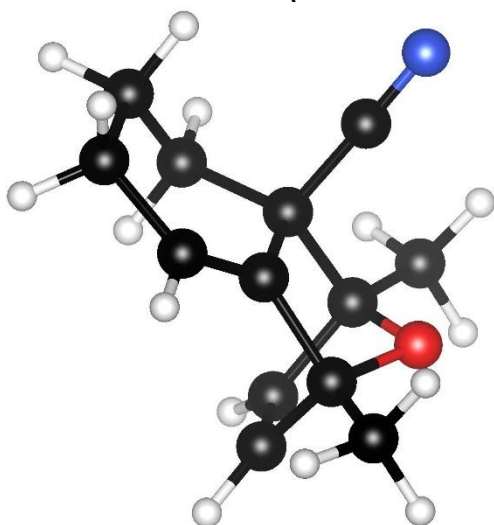
HF (M062X/6-31+G(d,p)) = -555.4154051 Hartrees
Imaginary Frequencies: 1 (-246.36 cm⁻¹)
Zero-point correction = 0.193484 (Hartree/Particle)
Thermal correction = 0.155726 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.478373	0.634822	0.197273
2	6	0	0.405666	-0.543898	-0.481896
3	6	0	1.330107	-1.467011	-0.694209
4	6	0	1.636093	0.604811	1.187270
5	6	0	2.895982	0.280338	0.346034
6	1	0	3.061289	1.121995	-0.335525
7	6	0	2.774783	-1.032077	-0.466335
8	1	0	3.244554	-1.857278	0.082756
9	1	0	1.755052	1.560838	1.703879
10	1	0	1.461049	-0.174161	1.936651
11	1	0	3.775234	0.220456	0.996419
12	1	0	3.322165	-0.942123	-1.410664
13	1	0	1.120331	-2.517750	-0.873675
14	6	0	0.063914	1.874413	-0.365107
15	7	0	-0.264594	2.903157	-0.799945
16	6	0	-1.538775	-1.417382	-0.429863
17	6	0	-2.266933	-0.388187	-1.021765

18	6	0	-2.616010	0.487962	0.016885
19	6	0	-2.147157	-0.089415	1.177807
20	8	0	-1.623006	-1.300206	0.929050
21	1	0	-1.273722	-2.397567	-0.798454
22	1	0	-2.421976	-0.257463	-2.082920
23	1	0	-3.102180	1.448784	-0.062147
24	1	0	-2.201854	0.207559	2.214332

Endo adduct: 5.54d (Allene 5.45d with furan)



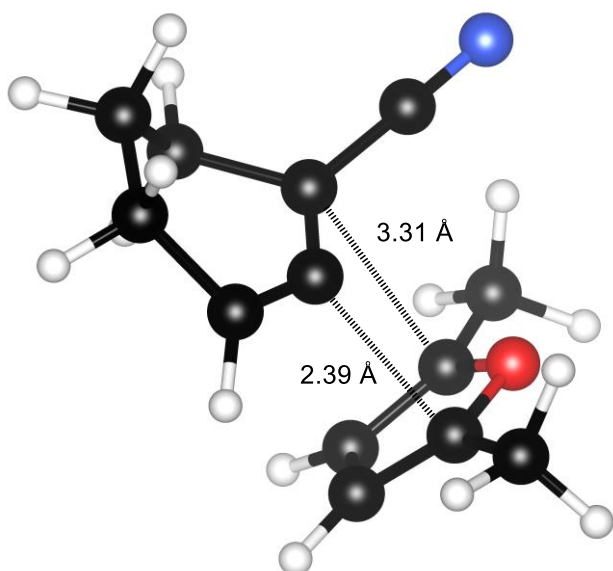
HF (M062X/6-31+G(d,p)) = -634.1012137 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.253023 (Hartree/Particle)
Thermal correction = 0.214982 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.418403	0.592198	-0.046332
2	6	0	-0.195981	-0.884169	0.267427
3	6	0	-1.163404	-1.793812	0.197707
4	6	0	-1.541297	0.738941	-1.078373
5	6	0	-2.796549	0.039542	-0.534916
6	1	0	-3.116469	0.562264	0.373539
7	6	0	-2.571399	-1.451770	-0.223425
8	1	0	-2.785681	-2.053661	-1.116886
9	1	0	-1.749698	1.793025	-1.287888
10	1	0	-1.202032	0.262096	-2.005429
11	1	0	-3.613807	0.139995	-1.254411
12	1	0	-3.288746	-1.785644	0.534652
13	1	0	-0.929984	-2.846941	0.350353
14	6	0	1.074820	1.003356	-0.402862
15	6	0	1.476607	0.195282	-1.630318
16	6	0	1.653566	-1.056277	-1.203771
17	6	0	1.328207	-1.040299	0.294957

18	8	0	1.744979	0.290369	0.646499
19	1	0	1.519339	0.587371	-2.639331
20	1	0	1.860960	-1.953532	-1.775657
21	6	0	1.397329	2.474279	-0.396894
22	1	0	0.812659	2.985485	-1.167384
23	1	0	1.167205	2.919518	0.573933
24	1	0	2.458472	2.620136	-0.611721
25	6	0	1.932069	-2.091193	1.185544
26	1	0	1.572600	-3.080781	0.890502
27	1	0	3.021219	-2.077401	1.098909
28	1	0	1.649509	-1.910956	2.225386
29	6	0	-0.786386	1.311323	1.186749
30	7	0	-1.095778	1.898811	2.135211

Endo Transition State of trapping Allene 5.45d with 2,5-Dimethylfuran



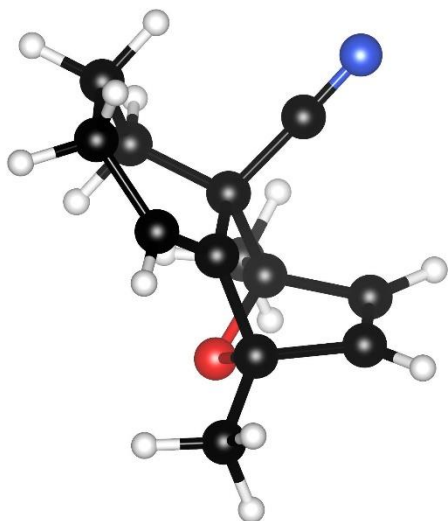
HF (M062X/6-31+G(d,p)) = -634.0288778 Hartrees
 Imaginary Frequencies: 1 (-96.31 cm⁻¹)
 Zero-point correction = 0.248618 (Hartree/Particle)
 Thermal correction = 0.207040 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.863545	0.779100	-0.104968
2	6	0	0.839061	-0.552644	-0.290249
3	6	0	1.737674	-1.486556	-0.035038
4	6	0	1.932726	1.147064	0.920702
5	6	0	3.252454	0.539265	0.377966
6	1	0	3.513172	1.088345	-0.532607
7	6	0	3.174795	-0.981137	0.064060
8	1	0	3.630025	-1.557754	0.877934
9	1	0	2.031182	2.229727	1.036272

10	1	0	1.674258	0.717525	1.894105
11	1	0	4.060238	0.711643	1.096907
12	1	0	3.754737	-1.209901	-0.835650
13	1	0	1.501093	-2.506439	0.254682
14	6	0	-2.072493	0.492387	0.630898
15	6	0	-1.705128	-0.341782	1.654286
16	6	0	-1.289477	-1.558190	1.054086
17	6	0	-1.398377	-1.383342	-0.311092
18	8	0	-1.945531	-0.157676	-0.554663
19	1	0	-1.713459	-0.089497	2.704858
20	1	0	-0.921650	-2.448726	1.544238
21	6	0	-2.632664	1.867448	0.585634
22	1	0	-2.637010	2.293453	1.590090
23	1	0	-2.037346	2.507286	-0.073233
24	1	0	-3.659277	1.853860	0.206717
25	6	0	-1.329702	-2.328417	-1.460813
26	1	0	-0.661218	-3.156097	-1.214634
27	1	0	-2.319562	-2.738112	-1.685747
28	1	0	-0.948828	-1.825186	-2.351998
29	6	0	0.376618	1.733172	-1.039017
30	7	0	-0.028043	2.547582	-1.764766

Exo adduct: Allene 5.45d with 2,5-Dimethylfuran



HF (M062X/6-31+G(d,p)) = -634.0999192 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.253326 (Hartree/Particle)

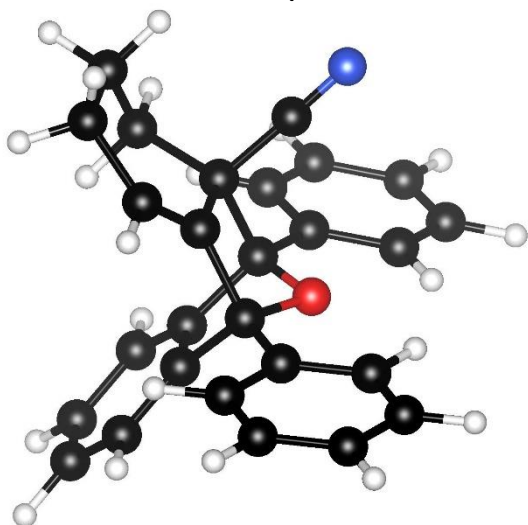
Thermal correction = 0.215371 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.418169	-0.574431	-0.044512
2	6	0	0.178000	0.894989	0.302860
3	6	0	1.150467	1.801296	0.304283

4	6	0	1.549954	-0.634885	-1.083603
5	6	0	2.804359	0.008671	-0.474720
6	1	0	3.123510	-0.602943	0.376172
7	6	0	2.584807	1.465701	-0.016204
8	1	0	2.891573	2.155956	-0.812339
9	1	0	1.758734	-1.669619	-1.374350
10	1	0	1.213276	-0.086082	-1.970144
11	1	0	3.620844	-0.023285	-1.201329
12	1	0	3.235052	1.692836	0.836248
13	1	0	0.902565	2.854356	0.429213
14	6	0	0.806128	-1.391792	1.117215
15	7	0	1.133444	-2.062063	2.002943
16	6	0	-1.330452	1.092958	0.135526
17	6	0	-2.034761	0.219486	1.169596
18	6	0	-1.880039	-1.040171	0.761320
19	6	0	-1.052405	-0.962318	-0.521327
20	8	0	-1.487176	0.287534	-1.058701
21	1	0	-2.482710	0.590534	2.083769
22	1	0	-2.164581	-1.959317	1.259572
23	6	0	-1.153839	-2.087112	-1.515418
24	1	0	-0.745150	-3.005486	-1.083123
25	1	0	-2.200573	-2.260511	-1.776276
26	1	0	-0.596108	-1.848628	-2.424499
27	6	0	-1.828650	2.498811	-0.063118
28	1	0	-2.902024	2.488250	-0.266205
29	1	0	-1.651192	3.088036	0.841039
30	1	0	-1.310351	2.972859	-0.900127

Endo adduct: 5.55d (Allene 5.45d with DPIBF)

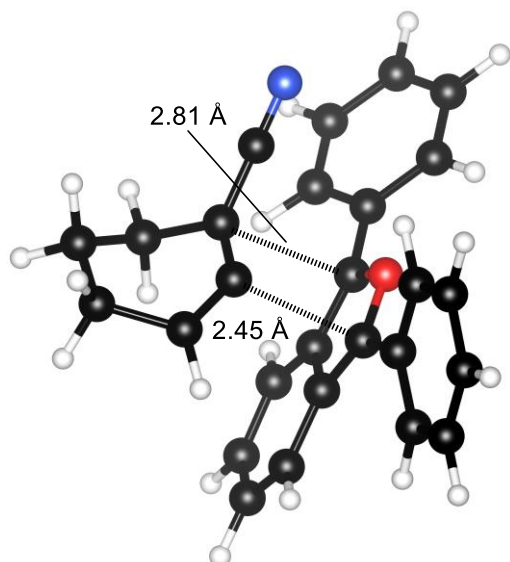


HF (M062X/6-31+G(d,p)) = -1171.047106 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.408415 (Hartree/Particle)
Thermal correction = 0.357823 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.715365	0.721605	1.117374
2	6	0	-0.803002	0.829933	0.998185
3	6	0	-1.506277	1.797889	1.575774
4	6	0	1.323683	2.117200	1.297870
5	6	0	0.659526	2.784551	2.511348
6	1	0	0.905033	2.198582	3.404090
7	6	0	-0.866596	2.905037	2.374210
8	1	0	-1.123301	3.843272	1.863949
9	1	0	2.405271	2.057524	1.450024
10	1	0	1.129529	2.686730	0.381014
11	1	0	1.091787	3.777250	2.662540
12	1	0	-1.327244	2.972580	3.365863
13	1	0	-2.579005	1.867475	1.406702
14	6	0	1.011374	-0.148158	-0.176738
15	6	0	0.574923	0.649201	-1.399622
16	6	0	-0.823548	0.609342	-1.389812
17	6	0	-1.180164	-0.163504	-0.115006
18	8	0	-0.073152	-1.082768	-0.058252
19	6	0	1.063570	-0.121666	2.277688
20	7	0	1.353831	-0.761019	3.197536
21	6	0	2.348274	-0.825566	-0.226780
22	6	0	3.512202	-0.052643	-0.300477
23	6	0	2.446380	-2.217390	-0.192457
24	6	0	4.761486	-0.667213	-0.343081
25	1	0	3.448033	1.031954	-0.323987
26	6	0	3.698566	-2.829703	-0.235019
27	1	0	1.542736	-2.814182	-0.130362
28	6	0	4.857068	-2.058362	-0.311473
29	1	0	5.658697	-0.059002	-0.399058
30	1	0	3.767187	-3.912625	-0.206481
31	1	0	5.830316	-2.537841	-0.344805
32	6	0	-2.505696	-0.857294	-0.026741
33	6	0	-3.690030	-0.126788	-0.174977
34	6	0	-2.572419	-2.230725	0.217800
35	6	0	-4.925429	-0.763382	-0.076672
36	1	0	-3.655582	0.941637	-0.367966
37	6	0	-3.810306	-2.865227	0.313315
38	1	0	-1.653188	-2.795164	0.331322
39	6	0	-4.988747	-2.134977	0.167459
40	1	0	-5.837941	-0.186945	-0.192241
41	1	0	-3.851898	-3.933164	0.503449
42	1	0	-5.951262	-2.630877	0.243792
43	6	0	1.269883	1.306113	-2.400393
44	6	0	0.526152	1.927290	-3.413047
45	1	0	1.042576	2.435756	-4.220763
46	6	0	-0.867326	1.884328	-3.405078
47	1	0	-1.421514	2.359172	-4.208580
48	6	0	-1.565155	1.225568	-2.383184
49	1	0	2.355079	1.326137	-2.422386
50	1	0	-2.649463	1.188239	-2.395651

Endo Transition State of trapping Allene 5.45d with DPIBF



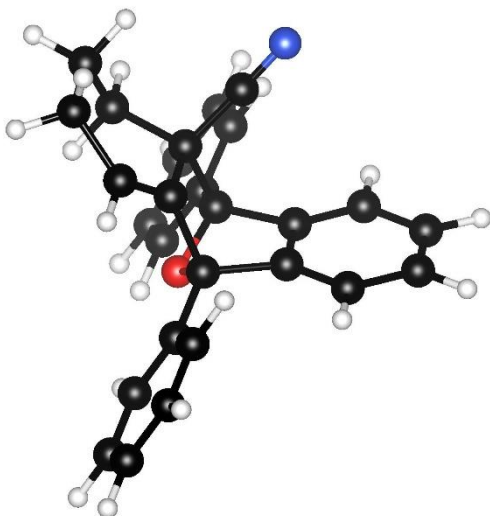
HF (M062X/6-31+G(d,p)) = -1170.957172 Hartrees
 Imaginary Frequencies: 1 (-129.44 cm^{-1})
 Zero-point correction = 0.403206 (Hartree/Particle)
 Thermal correction = 0.349084 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.529426	0.787636	1.632337
2	6	0	-0.788663	0.836032	1.364986
3	6	0	-1.670399	1.805664	1.510404
4	6	0	1.108377	2.195458	1.700199
5	6	0	0.255880	2.934250	2.766958
6	1	0	0.484299	2.481116	3.737123
7	6	0	-1.278695	2.883604	2.518033
8	1	0	-1.620444	3.827839	2.077663
9	1	0	2.163230	2.192053	1.988141
10	1	0	1.015844	2.675119	0.718777
11	1	0	0.569928	3.981577	2.822726
12	1	0	-1.809946	2.776967	3.468911
13	1	0	-2.524037	1.960884	0.854847
14	6	0	1.050894	-0.387296	-0.871837
15	6	0	0.571871	0.759906	-1.509089
16	6	0	-0.856640	0.711427	-1.404959
17	6	0	-1.156905	-0.458050	-0.688042
18	8	0	-0.000196	-1.136997	-0.482280
19	6	0	1.174688	-0.318118	2.257176
20	7	0	1.727283	-1.211846	2.754415
21	6	0	2.380015	-0.947438	-0.666085
22	6	0	3.498562	-0.106261	-0.573005
23	6	0	2.548243	-2.331927	-0.522720
24	6	0	4.764900	-0.644907	-0.367238
25	1	0	3.370682	0.970701	-0.621218
26	6	0	3.816675	-2.863669	-0.311675
27	1	0	1.682404	-2.983886	-0.577589

28	6	0	4.929170	-2.024929	-0.239789
29	1	0	5.622843	0.015609	-0.291205
30	1	0	3.936816	-3.936928	-0.202488
31	1	0	5.917022	-2.443327	-0.075488
32	6	0	-2.397761	-1.171567	-0.383902
33	6	0	-3.566742	-0.931769	-1.116257
34	6	0	-2.419497	-2.116174	0.653599
35	6	0	-4.742768	-1.612184	-0.803255
36	1	0	-3.553257	-0.240793	-1.952416
37	6	0	-3.590856	-2.802216	0.951542
38	1	0	-1.515006	-2.295343	1.228235
39	6	0	-4.759561	-2.547704	0.229264
40	1	0	-5.642428	-1.418264	-1.378826
41	1	0	-3.596694	-3.529901	1.757065
42	1	0	-5.674714	-3.079518	0.469087
43	6	0	-1.644908	1.775531	-1.926116
44	1	0	-2.725002	1.774093	-1.827714
45	6	0	-1.005968	2.816356	-2.546625
46	1	0	-1.588546	3.636635	-2.953816
47	6	0	0.418093	2.849437	-2.678592
48	1	0	0.877813	3.685313	-3.195863
49	6	0	1.205402	1.850041	-2.171604
50	1	0	2.282778	1.882162	-2.290880

Exo adduct: 5.56d (Allene 5.45d with DPIBF)



HF (M062X/6-31+G(d,p)) = -1171.0480176 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.407943 (Hartree/Particle)

Thermal correction = 0.356255 Hartrees

Coordinates from last standard orientation:

HF = -1171.0480176 hartrees

Zero-point correction=

0.407943 (Hartree/Particle)

Thermal correction to Gibbs Free Energy=

0.356255

Sum of electronic and zero-point Energies=

-1170.640075

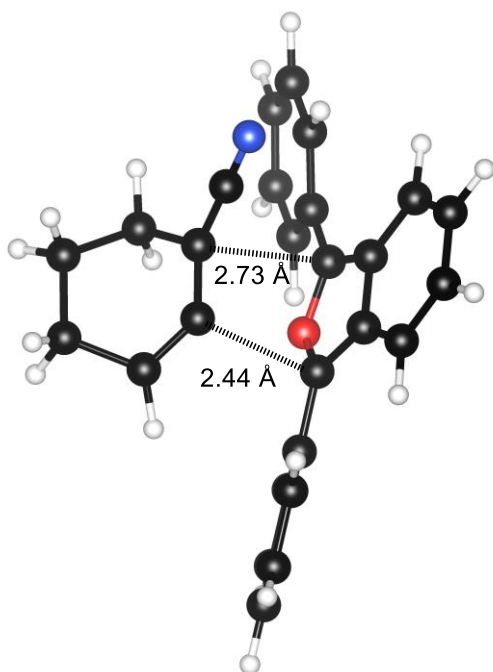
Sum of electronic and thermal Free Energies=

-1170.691762

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.753251	-0.973580	0.876964
2	6	0	0.773733	-1.050854	0.821487
3	6	0	1.445765	-2.156164	1.128279
4	6	0	-1.318091	-2.366469	0.552255
5	6	0	-0.762507	-3.370308	1.570277
6	1	0	-1.139927	-3.098760	2.562413
7	6	0	0.777566	-3.423296	1.593048
8	1	0	1.133274	-4.217978	0.924937
9	1	0	-2.411732	-2.354977	0.582692
10	1	0	-1.006363	-2.615691	-0.468461
11	1	0	-1.156855	-4.366367	1.351824
12	1	0	1.131491	-3.699198	2.592731
13	1	0	2.516588	-2.198883	0.938665
14	6	0	1.195354	0.117611	-0.074960
15	6	0	0.785093	1.433567	0.582699
16	6	0	-0.606712	1.481863	0.473674
17	6	0	-0.990761	0.174842	-0.209298
18	8	0	0.140306	-0.023835	-1.060937
19	6	0	-2.292598	0.117234	-0.948093
20	6	0	-3.492937	0.178838	-0.231065
21	6	0	-2.323608	0.008726	-2.338960
22	6	0	-4.712490	0.137363	-0.901794
23	1	0	-3.477468	0.251857	0.854455
24	6	0	-3.547246	-0.033935	-3.007867
25	1	0	-1.390951	-0.042261	-2.890765
26	6	0	-4.741883	0.031512	-2.293193
27	1	0	-5.638671	0.184490	-0.337916
28	1	0	-3.564711	-0.119236	-4.089897
29	1	0	-5.692397	-0.002284	-2.816234
30	6	0	2.562964	0.046796	-0.681355
31	6	0	3.686039	0.098619	0.151882
32	6	0	2.732361	-0.068463	-2.061398
33	6	0	4.966524	0.038119	-0.393441
34	1	0	3.558755	0.176645	1.229308
35	6	0	4.015934	-0.129766	-2.604438
36	1	0	1.859793	-0.107969	-2.704390
37	6	0	5.134006	-0.076217	-1.774002
38	1	0	5.832437	0.076693	0.259903
39	1	0	4.140596	-0.219295	-3.679145
40	1	0	6.131712	-0.125144	-2.198730
41	6	0	-1.336887	2.544303	0.975325
42	6	0	-0.628571	3.584812	1.590447
43	1	0	-1.168188	4.441670	1.981191
44	6	0	0.761357	3.538379	1.701512
45	1	0	1.286815	4.360455	2.177016
46	6	0	1.491112	2.452563	1.199324
47	1	0	-2.419252	2.581029	0.892108
48	1	0	2.573621	2.429628	1.279623
49	6	0	-1.247819	-0.556872	2.199582
50	7	0	-1.665100	-0.259870	3.237831

Exo Transition State of trapping Allene 5.45d with DPIBF



HF (M062X/6-31+G(d,p)) = -1170.9584057 Hartrees

Imaginary Frequencies: 1 (-154.26 cm^{-1})

Zero-point correction = 0.403658 (Hartree/Particle)

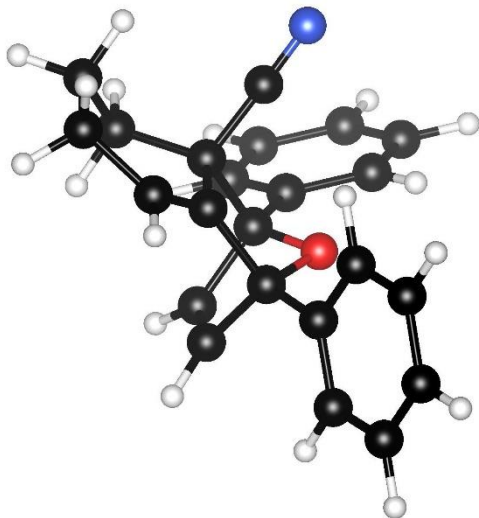
Thermal correction = 0.350470 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.677808	0.425308	-1.691976
2	6	0	0.663041	0.509464	-1.558384
3	6	0	1.483151	1.515417	-1.804655
4	6	0	-1.306299	1.812954	-1.684961
5	6	0	-0.608563	2.575861	-2.842342
6	1	0	-0.935761	2.116371	-3.780708
7	6	0	0.943805	2.569359	-2.770472
8	1	0	1.307643	3.529122	-2.385908
9	1	0	-2.387836	1.774711	-1.842798
10	1	0	-1.117067	2.296288	-0.720026
11	1	0	-0.958298	3.613137	-2.857114
12	1	0	1.366782	2.459721	-3.773913
13	1	0	2.405320	1.708275	-1.262416
14	6	0	1.220806	-0.474071	0.606932
15	6	0	0.759275	-1.770643	0.314790
16	6	0	-0.659433	-1.738644	0.488612
17	6	0	-0.973989	-0.434420	0.889989
18	8	0	0.170217	0.250372	1.077489
19	6	0	-2.221238	0.252869	1.199228
20	6	0	-3.421043	-0.162687	0.601913
21	6	0	-2.228105	1.364740	2.054603
22	6	0	-4.607997	0.509593	0.875887

23	1	0	-3.416267	-0.983185	-0.109327
24	6	0	-3.418692	2.035155	2.319821
25	1	0	-1.299811	1.695368	2.510160
26	6	0	-4.612592	1.607690	1.737510
27	1	0	-5.529324	0.183713	0.403503
28	1	0	-3.414329	2.893503	2.984153
29	1	0	-5.539480	2.131893	1.947073
30	6	0	2.556305	0.071944	0.828891
31	6	0	3.643397	-0.389974	0.072735
32	6	0	2.762306	1.085400	1.776401
33	6	0	4.915407	0.136355	0.278928
34	1	0	3.484947	-1.130870	-0.704543
35	6	0	4.035505	1.613291	1.971439
36	1	0	1.923257	1.450686	2.359871
37	6	0	5.117188	1.138814	1.228690
38	1	0	5.748103	-0.226244	-0.315533
39	1	0	4.183483	2.394722	2.710121
40	1	0	6.108725	1.551973	1.383371
41	6	0	-1.436431	-2.909134	0.268401
42	6	0	-0.787467	-4.055197	-0.109248
43	1	0	-1.355662	-4.964323	-0.276976
44	6	0	0.630523	-4.087619	-0.276579
45	1	0	1.102542	-5.022951	-0.560217
46	6	0	1.404814	-2.974560	-0.070548
47	1	0	-2.510971	-2.904415	0.412526
48	1	0	2.482408	-3.024218	-0.179411
49	6	0	-1.369173	-0.673579	-2.276903
50	7	0	-1.978613	-1.552624	-2.733431

Endo adduct: Allene 5.45d with 2,5-Diphenylfuran



HF (M062X/6-31+G(d,p)) = -1017.4404702 Hartrees

Imaginary Frequencies: none found

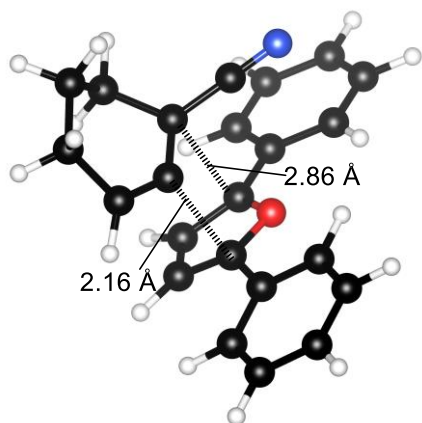
Zero-point correction = 0.359699 (Hartree/Particle)

Thermal correction = 0.311187 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.715747	1.149760	0.102901
2	6	0	-0.791148	1.237832	-0.095646
3	6	0	-1.454790	2.388445	-0.139020
4	6	0	1.391812	2.405716	-0.452145
5	6	0	0.752408	3.635114	0.211758
6	1	0	0.962038	3.594861	1.286681
7	6	0	-0.767101	3.724689	-0.016595
8	1	0	-0.972623	4.268483	-0.948604
9	1	0	2.470113	2.386574	-0.264990
10	1	0	1.225813	2.420519	-1.536103
11	1	0	1.229882	4.544297	-0.163626
12	1	0	-1.228934	4.319087	0.779504
13	1	0	-2.521987	2.386032	-0.358914
14	6	0	1.015372	1.011731	1.539604
15	7	0	1.264887	0.922157	2.666402
16	6	0	0.970876	-0.281081	-0.561586
17	6	0	0.561950	-0.171591	-2.025293
18	6	0	-0.770929	-0.123199	-2.030950
19	6	0	-1.200562	-0.166310	-0.560823
20	8	0	-0.145074	-0.973189	0.004455
21	1	0	1.248349	-0.069454	-2.856227
22	1	0	-1.438816	0.059746	-2.864343
23	6	0	-2.558283	-0.679712	-0.184738
24	6	0	-3.068382	-0.407559	1.088380
25	6	0	-3.297485	-1.470240	-1.066617
26	6	0	-4.306657	-0.915488	1.472262
27	1	0	-2.489750	0.204039	1.775484
28	6	0	-4.540949	-1.974242	-0.685328
29	1	0	-2.899928	-1.699425	-2.051285
30	6	0	-5.046943	-1.696461	0.583349
31	1	0	-4.695374	-0.701296	2.462872
32	1	0	-5.111216	-2.585402	-1.377733
33	1	0	-6.014729	-2.088129	0.880907
34	6	0	2.287502	-0.919747	-0.240075
35	6	0	2.380958	-1.913443	0.736041
36	6	0	3.441222	-0.487657	-0.901456
37	6	0	3.619867	-2.475401	1.041344
38	1	0	1.483119	-2.240065	1.250686
39	6	0	4.678679	-1.046590	-0.590278
40	1	0	3.374967	0.286367	-1.662615
41	6	0	4.769465	-2.043908	0.381034
42	1	0	3.687006	-3.250265	1.798602
43	1	0	5.569851	-0.706641	-1.108454
44	1	0	5.732836	-2.482879	0.620977

Endo Transition State of trapping Allene 5.45d with 2,5-Diphenylfuran



HF (M062X/6-31+G(d,p)) = -1017.3774224 Hartrees

Imaginary Frequencies: 1 (-213.61 cm⁻¹)

Zero-point correction = 0.355958 (Hartree/Particle)

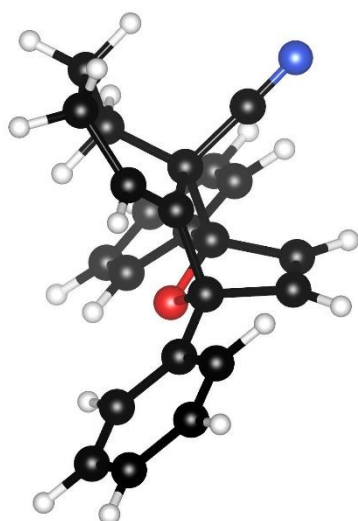
Thermal correction = 0.305401 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.279813	1.685929	-0.531600
2	6	0	0.960436	1.363043	-0.078191
3	6	0	1.956851	2.152042	0.297122
4	6	0	-0.656897	3.101764	-0.117906
5	6	0	0.475400	4.012998	-0.653437
6	1	0	0.431596	3.979870	-1.747247
7	6	0	1.890547	3.596408	-0.177215
8	1	0	2.189092	4.200796	0.688380
9	1	0	-1.621584	3.405179	-0.533197
10	1	0	-0.718040	3.160681	0.974868
11	1	0	0.290850	5.051321	-0.357924
12	1	0	2.628687	3.801068	-0.959855
13	1	0	2.727387	1.856692	1.005905
14	6	0	-0.879709	1.067451	-1.659828
15	7	0	-1.398355	0.566546	-2.574185
16	6	0	-1.175472	-0.574206	0.979577
17	6	0	-0.692677	-0.002251	2.147010
18	6	0	0.701597	-0.055272	2.070891
19	6	0	1.016764	-0.605861	0.818743
20	8	0	-0.144383	-1.049072	0.246552
21	1	0	-1.287753	0.422305	2.941892
22	1	0	1.409617	0.319027	2.796068
23	6	0	2.268936	-1.179495	0.303162
24	6	0	2.297460	-1.800898	-0.951051
25	6	0	3.447707	-1.078857	1.049772
26	6	0	3.491268	-2.317041	-1.446453
27	1	0	1.385246	-1.869441	-1.536063
28	6	0	4.642003	-1.587946	0.544427
29	1	0	3.435412	-0.613053	2.030991
30	6	0	4.667853	-2.209740	-0.703203
31	1	0	3.504198	-2.799424	-2.418804
32	1	0	5.551213	-1.506578	1.131728

33	1	0	5.598086	-2.609631	-1.093782
34	6	0	-2.527444	-0.846117	0.505685
35	6	0	-2.741038	-1.646584	-0.623842
36	6	0	-3.628371	-0.303137	1.185271
37	6	0	-4.038379	-1.905829	-1.058610
38	1	0	-1.892122	-2.059345	-1.158247
39	6	0	-4.920103	-0.564999	0.745436
40	1	0	-3.472011	0.331498	2.052673
41	6	0	-5.129575	-1.369434	-0.377472
42	1	0	-4.195638	-2.526014	-1.935405
43	1	0	-5.765474	-0.138230	1.275738
44	1	0	-6.139274	-1.571772	-0.720564

Exo adduct: Allene 5.45d with 2,5-Diphenylfuran



HF (M062X/6-31+G(d,p)) = -1017.4399581 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.360007 (Hartree/Particle)

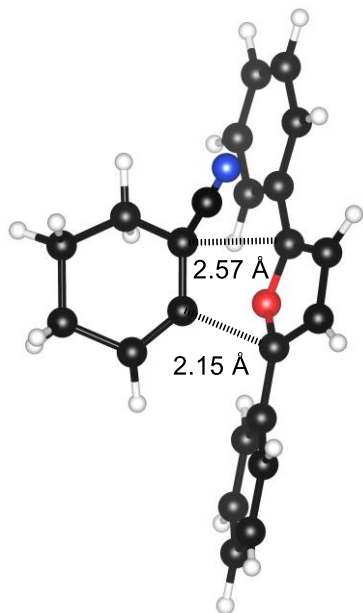
Thermal correction = 0.311723 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.742474	1.164158	0.090361
2	6	0	-0.782176	1.164728	0.028591
3	6	0	-1.471486	1.973718	-0.769661
4	6	0	1.276191	1.540362	-1.300056
5	6	0	0.726778	2.924729	-1.672011
6	1	0	1.133763	3.656667	-0.965694
7	6	0	-0.814233	2.992676	-1.664119
8	1	0	-1.200257	2.805513	-2.674139
9	1	0	2.370783	1.545596	-1.304587
10	1	0	0.933131	0.771716	-2.001967
11	1	0	1.096926	3.210860	-2.660183
12	1	0	-1.145334	4.004819	-1.405718

13	1	0	-2.545659	1.828778	-0.875921
14	6	0	1.289632	2.106587	1.079533
15	7	0	1.757180	2.850529	1.833537
16	6	0	-1.194447	-0.195090	0.613715
17	6	0	-0.753634	-0.240968	2.075033
18	6	0	0.574200	-0.348853	2.058232
19	6	0	0.968623	-0.344902	0.581402
20	8	0	-0.157639	-0.982149	-0.014382
21	1	0	-1.417307	-0.132997	2.923866
22	1	0	1.268721	-0.344099	2.889119
23	6	0	-2.572550	-0.670805	0.271272
24	6	0	-2.775561	-1.609732	-0.741196
25	6	0	-3.671459	-0.135056	0.948927
26	6	0	-4.069550	-2.016172	-1.066514
27	1	0	-1.919876	-2.022029	-1.265705
28	6	0	-4.963491	-0.538915	0.618948
29	1	0	-3.519195	0.605269	1.730616
30	6	0	-5.164878	-1.482491	-0.389199
31	1	0	-4.220330	-2.752175	-1.850038
32	1	0	-5.811640	-0.117261	1.149223
33	1	0	-6.171145	-1.799769	-0.644073
34	6	0	2.274620	-0.949705	0.170103
35	6	0	2.339185	-1.854713	-0.890544
36	6	0	3.448936	-0.562037	0.823263
37	6	0	3.570605	-2.373121	-1.290688
38	1	0	1.424773	-2.150518	-1.394687
39	6	0	4.677990	-1.077568	0.417906
40	1	0	3.405912	0.146472	1.647394
41	6	0	4.740865	-1.985565	-0.639776
42	1	0	3.614578	-3.079748	-2.113648
43	1	0	5.585085	-0.772053	0.929712
44	1	0	5.698131	-2.389144	-0.954421

Exo Transition State of trapping Allene 5.45d with 2,5-Diphenylfuran

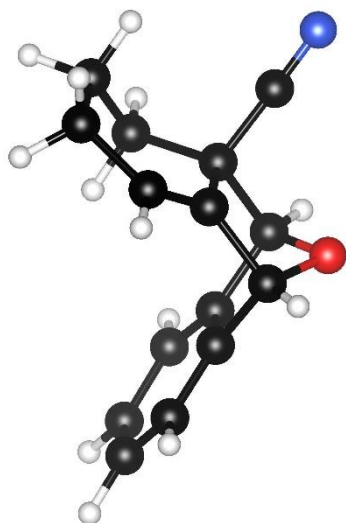


HF (M062X/6-31+G(d,p)) = -1017.3753822 Hartrees
Imaginary Frequencies: 1 (-310.39 cm⁻¹)
Zero-point correction = 0.356020 (Hartree/Particle)
Thermal correction = 0.305718 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.657641	1.600001	0.216615
2	6	0	-0.695420	1.399024	0.125836
3	6	0	-1.532380	1.818678	-0.810513
4	6	0	1.258404	1.860457	-1.154596
5	6	0	0.506475	3.097376	-1.706709
6	1	0	0.775820	3.952768	-1.077878
7	6	0	-1.033099	2.928005	-1.730022
8	1	0	-1.362721	2.643405	-2.736676
9	1	0	2.334650	2.049419	-1.104323
10	1	0	1.093153	0.983890	-1.792422
11	1	0	0.857713	3.324276	-2.718781
12	1	0	-1.520528	3.883633	-1.509652
13	1	0	-2.475014	1.330610	-1.045462
14	6	0	1.285074	2.170241	1.360574
15	7	0	1.836413	2.628393	2.277592
16	6	0	-1.167147	-0.574926	0.850264
17	6	0	-0.715287	-0.417105	2.176514
18	6	0	0.659281	-0.588906	2.151732
19	6	0	0.999512	-0.877170	0.825798
20	8	0	-0.125748	-1.072602	0.107455
21	1	0	-1.331289	-0.133644	3.018036
22	1	0	1.353943	-0.451868	2.967304
23	6	0	-2.525001	-0.842619	0.355390
24	6	0	-2.733384	-1.635831	-0.777890
25	6	0	-3.622271	-0.270250	1.009687
26	6	0	-4.027425	-1.860226	-1.242798
27	1	0	-1.883678	-2.076649	-1.289134
28	6	0	-4.912886	-0.499485	0.542200
29	1	0	-3.463715	0.370364	1.872990
30	6	0	-5.120076	-1.295116	-0.585699
31	1	0	-4.181713	-2.479478	-2.120982
32	1	0	-5.757105	-0.049290	1.054673
33	1	0	-6.126678	-1.470012	-0.951838
34	6	0	2.278246	-1.159603	0.182517
35	6	0	2.324399	-1.679589	-1.117819
36	6	0	3.474506	-0.876389	0.857239
37	6	0	3.552352	-1.920109	-1.728820
38	1	0	1.399436	-1.895742	-1.642984
39	6	0	4.697169	-1.117990	0.240119
40	1	0	3.446725	-0.453686	1.857450
41	6	0	4.740722	-1.641799	-1.053454
42	1	0	3.580932	-2.325237	-2.735387
43	1	0	5.618234	-0.892614	0.767948
44	1	0	5.696517	-1.828103	-1.532656

Endo adduct: Allene 5.45d with Isobenzofuran



HF (M062X/6-31+G(d,p)) = -709.1003513 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.246431 (Hartree/Particle)

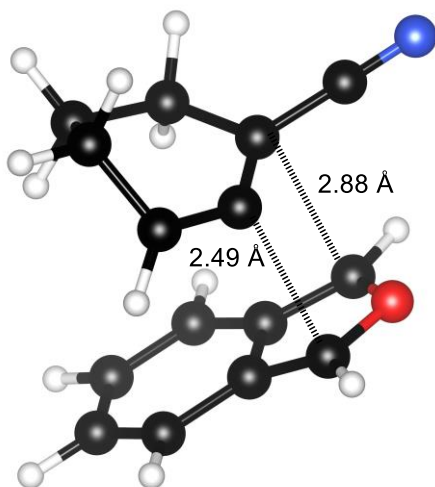
Thermal correction = 0.207962 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.143464	-0.457781	-0.344384
2	6	0	0.806996	0.251222	0.969315
3	6	0	1.206188	1.487608	1.248291
4	6	0	1.317803	0.578730	-1.458936
5	6	0	2.387736	1.588708	-1.018895
6	1	0	3.338431	1.057080	-0.896864
7	6	0	2.026839	2.313428	0.290071
8	1	0	1.435589	3.211834	0.067046
9	1	0	1.603087	0.098311	-2.399837
10	1	0	0.351190	1.074986	-1.603430
11	1	0	2.544158	2.326736	-1.810187
12	1	0	2.938018	2.674038	0.780249
13	1	0	0.851986	1.975975	2.155079
14	6	0	-0.044324	-1.489186	-0.376060
15	6	0	-1.351586	-0.731782	-0.466828
16	6	0	-1.538918	-0.184052	0.808653
17	6	0	-0.298424	-0.604280	1.585972
18	8	0	-0.036951	-1.894165	1.002055
19	6	0	2.382197	-1.244330	-0.197440
20	7	0	3.359539	-1.859050	-0.115752
21	6	0	-2.250026	-0.493682	-1.492509
22	6	0	-3.370599	0.298950	-1.205789
23	1	0	-4.106275	0.486412	-1.981409
24	6	0	-3.556496	0.844176	0.065246
25	1	0	-4.435878	1.449142	0.263248
26	6	0	-2.629066	0.619740	1.092662
27	1	0	-2.103224	-0.910630	-2.484508

28	1	0	-2.772187	1.057766	2.075831
29	1	0	-0.357359	-0.658599	2.670986
30	1	0	0.100600	-2.341201	-1.038603

Endo Transition State of trapping Allene 5.45d with Isobenzofuran



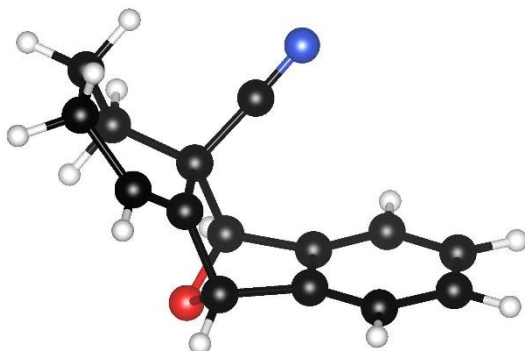
HF (M062X/6-31+G(d,p)) = -708.9967282 Hartrees
Imaginary Frequencies: 1 (-134.21 cm^{-1})
Zero-point correction = 0.240331 (Hartree/Particle)
Thermal correction = 0.198535 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.672902	-0.047281	0.212826
2	6	0	-1.167536	0.313551	-0.977104
3	6	0	-0.880766	1.508063	-1.461924
4	6	0	-1.425346	0.964531	1.339518
5	6	0	-1.172740	2.390369	0.777595
6	1	0	-1.681112	3.120877	1.415128
7	6	0	-1.624545	2.591084	-0.698480
8	1	0	-1.356959	3.592436	-1.044051
9	1	0	-2.321436	0.957880	1.969635
10	1	0	-0.582600	0.657858	1.969761
11	1	0	-0.101149	2.612747	0.825254
12	1	0	-2.708199	2.473441	-0.785192
13	1	0	-0.033255	1.735026	-2.102671
14	6	0	0.346629	-2.084050	0.462873
15	6	0	1.295887	-1.081845	0.529037
16	6	0	1.474174	-0.618715	-0.819851
17	6	0	0.580906	-1.351821	-1.592007
18	8	0	-0.012780	-2.285730	-0.817164
19	6	0	-2.629779	-1.091439	0.388866
20	7	0	-3.404586	-1.939801	0.563103
21	6	0	2.008922	-0.464747	1.601432
22	6	0	2.869312	0.553856	1.299191

23	1	0	3.426977	1.041234	2.092647
24	6	0	3.068083	0.996338	-0.053082
25	1	0	3.777355	1.797048	-0.237541
26	6	0	2.392603	0.434443	-1.101092
27	1	0	1.868840	-0.802164	2.623676
28	1	0	2.547708	0.776449	-2.119773
29	1	0	0.414338	-1.430688	-2.654861
30	1	0	-0.093584	-2.741720	1.196789

Exo adduct: Allene 5.45d with Isobenzofuran



HF (M062X/6-31+G(d,p)) = -709.0983945 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.246431 (Hartree/Particle)

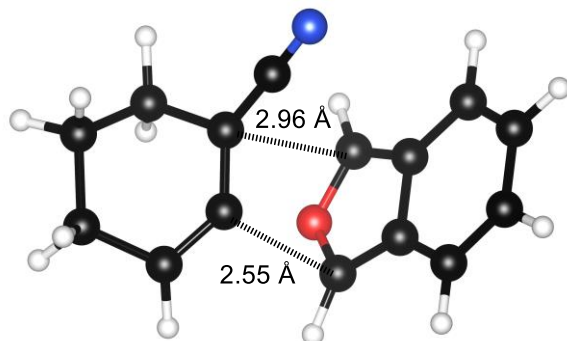
Thermal correction = 0.207807 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.972105	0.475035	0.403169
2	6	0	0.992564	-0.892501	-0.287044
3	6	0	2.071910	-1.373450	-0.896279
4	6	0	2.381571	0.754961	0.949932
5	6	0	3.376504	0.723632	-0.217557
6	1	0	3.134055	1.548365	-0.896604
7	6	0	3.367778	-0.610096	-0.993361
8	1	0	4.145163	-1.275922	-0.597472
9	1	0	2.412674	1.726582	1.452863
10	1	0	2.605926	-0.024153	1.686459
11	1	0	4.385426	0.917679	0.156464
12	1	0	3.635629	-0.435943	-2.041588
13	1	0	2.070788	-2.403699	-1.248164
14	6	0	-0.184369	-1.640887	0.315972
15	6	0	-1.485728	-0.947442	-0.040472
16	6	0	-1.487185	0.229607	0.717352
17	6	0	-0.167993	0.198776	1.464668
18	8	0	-0.006927	-1.205569	1.688937
19	6	0	-2.518033	1.147681	0.622162
20	6	0	-3.576887	0.848507	-0.245852
21	1	0	-4.410610	1.538319	-0.330090
22	6	0	-3.575136	-0.323175	-1.003767

23	1	0	-4.408441	-0.531375	-1.667511
24	6	0	-2.516396	-1.237741	-0.917735
25	1	0	-2.513235	2.068963	1.196724
26	1	0	-2.515752	-2.144169	-1.515444
27	6	0	0.591442	1.564975	-0.510704
28	7	0	0.326057	2.444934	-1.214434
29	1	0	-0.077107	0.764084	2.391376
30	1	0	-0.144390	-2.726011	0.239616

Exo Transition State of trapping Allene 5.45d with Isobenzofuran



HF (M062X/6-31+G(d,p)) = -708.9950869 Hartrees

Imaginary Frequencies: 1 (-99.53 cm⁻¹)

Zero-point correction = 0.240509 (Hartree/Particle)

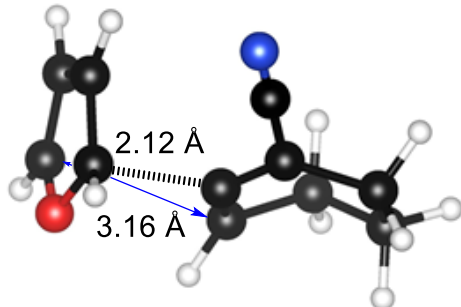
Thermal correction = 0.198520 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.291734	0.681588	0.110565
2	6	0	1.307730	-0.461019	-0.589766
3	6	0	2.292561	-1.258827	-0.953388
4	6	0	2.568983	0.802418	0.938651
5	6	0	3.725559	0.684747	-0.091219
6	1	0	3.698624	1.583655	-0.715355
7	6	0	3.662258	-0.579042	-0.995741
8	1	0	4.371165	-1.334782	-0.638707
9	1	0	2.624574	1.756879	1.468455
10	1	0	2.613091	-0.007059	1.673222
11	1	0	4.684240	0.693085	0.437522
12	1	0	3.966426	-0.326260	-2.016010
13	1	0	2.222983	-2.338294	-1.046675
14	6	0	-0.579746	-1.923585	0.295290
15	6	0	-1.604442	-1.092813	-0.129443
16	6	0	-1.755662	-0.097515	0.897213
17	6	0	-0.826906	-0.415357	1.870333
18	8	0	-0.181750	-1.545307	1.529998
19	6	0	-2.716684	0.948100	0.747417
20	6	0	-3.482990	0.959120	-0.383076
21	1	0	-4.222876	1.740401	-0.524427
22	6	0	-3.332161	-0.038032	-1.407309

23	1	0	-3.966789	0.020585	-2.286023
24	6	0	-2.414692	-1.045323	-1.301614
25	1	0	-2.826703	1.710371	1.511804
26	1	0	-2.300510	-1.790407	-2.082296
27	6	0	0.524852	1.832508	-0.235980
28	7	0	-0.088886	2.787017	-0.485982
29	1	0	-0.577146	0.013168	2.828715
30	1	0	-0.173232	-2.849824	-0.079940

1,3 addition: Endo transition state of Allene 5.45d and furan



HF (M062X/6-31+G(d,p)) = -555.4133096 Hartrees

Imaginary Frequencies: 1 (-287.77 cm⁻¹)

Zero-point correction = 0.193182 (Hartree/Particle)

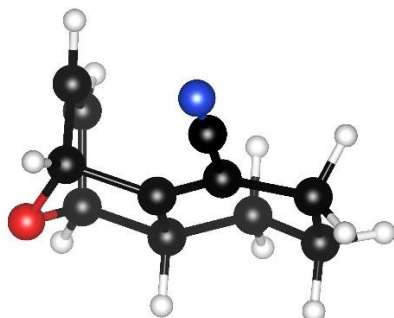
Thermal correction = 0.155138 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.252693	-1.501688	-0.228217
2	6	0	-0.256261	-0.173743	-0.397531
3	6	0	-1.252024	0.713540	-0.228409
4	6	0	-1.397008	-1.922492	0.678749
5	6	0	-2.692139	-1.376411	0.024647
6	1	0	-2.810936	-1.875486	-0.942641
7	6	0	-2.676171	0.156083	-0.186813
8	1	0	-3.176439	0.657238	0.650195
9	1	0	-1.453370	-3.009675	0.777659
10	1	0	-1.277824	-1.497127	1.682041
11	1	0	-3.563826	-1.642480	0.632199
12	1	0	-3.235870	0.421527	-1.089792
13	6	0	2.616775	-1.084692	0.093254
14	6	0	2.515205	-0.167191	1.116572
15	6	0	1.926917	0.978321	0.557557
16	6	0	1.620222	0.646643	-0.766492
17	8	0	2.213878	-0.548085	-1.071782
18	1	0	3.031083	-2.080533	0.044325
19	1	0	2.811150	-0.328337	2.142463
20	1	0	1.662810	1.902157	1.051411
21	1	0	1.400341	1.284546	-1.611143
22	6	0	-1.028096	2.091832	0.064685
23	7	0	-0.868795	3.228213	0.251756

24 1 0 0.235057 -2.205850 -0.892760

1,3 addition: Endo adduct of Allene 5.45d and furan



HF (M062X/6-31+G(d,p)) = -555.4996432 Hartrees

Imaginary Frequencies: none found

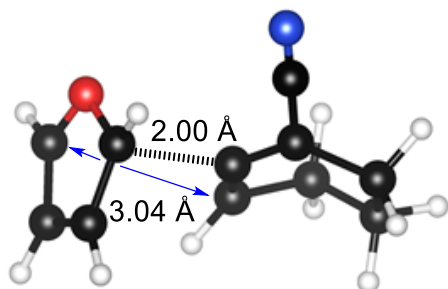
Zero-point correction = 0.198973 (Hartree/Particle)

Thermal correction = 0.163673 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.749709	1.021418	-0.506615
2	6	0	0.101714	-0.223728	-0.433996
3	6	0	1.412129	-0.202219	-0.162566
4	6	0	-0.175717	2.104682	0.394383
5	6	0	1.282789	2.334602	-0.031677
6	1	0	1.288250	2.644839	-1.083194
7	6	0	2.161478	1.084198	0.133541
8	1	0	2.527471	1.015165	1.165929
9	1	0	-0.744923	3.035100	0.306131
10	1	0	-0.219796	1.778234	1.441749
11	1	0	1.725366	3.153707	0.542029
12	1	0	3.049181	1.158308	-0.503061
13	6	0	-2.145427	0.368308	-0.253331
14	6	0	-2.149771	-0.259237	1.133765
15	6	0	-1.378483	-1.345715	1.040100
16	6	0	-0.899929	-1.374415	-0.415729
17	8	0	-2.013438	-0.788877	-1.096709
18	1	0	-3.005974	0.966489	-0.546599
19	1	0	-2.616347	0.162948	2.014531
20	1	0	-1.040226	-2.019788	1.816852
21	1	0	-0.602363	-2.326409	-0.850758
22	6	0	2.124744	-1.442191	-0.016722
23	7	0	2.715580	-2.433104	0.103928
24	1	0	-0.765113	1.379933	-1.544354

1,3 addition: Exo transition state of Allene 5.45d and furan

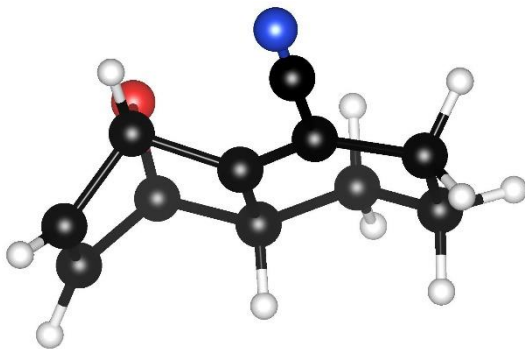


HF (M062X/6-31+G(d,p)) = -555.4138819 Hartrees
 Imaginary Frequencies: 1 (-225.76 cm⁻¹)
 Zero-point correction = 0.193276 (Hartree/Particle)
 Thermal correction = 0.155072 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.114799	-1.409351	0.149848
2	6	0	-0.253793	-0.102731	-0.089655
3	6	0	-1.376340	0.633688	-0.206526
4	6	0	-1.372410	-1.971516	0.785767
5	6	0	-2.521199	-1.647369	-0.206180
6	1	0	-2.313603	-2.180197	-1.139873
7	6	0	-2.671581	-0.135682	-0.494486
8	1	0	-3.436702	0.294987	0.161563
9	1	0	-1.296115	-3.050268	0.942628
10	1	0	-1.570943	-1.497901	1.753256
11	1	0	-3.469199	-2.035839	0.180599
12	1	0	-3.013362	0.019826	-1.523266
13	6	0	1.563178	0.969816	-0.294198
14	6	0	2.111002	0.139138	-1.266670
15	6	0	2.904249	-0.802512	-0.575347
16	6	0	2.845404	-0.449744	0.749581
17	8	0	2.122652	0.672546	0.915729
18	1	0	1.120577	1.953205	-0.370810
19	1	0	1.898541	0.183588	-2.324884
20	1	0	3.435665	-1.648533	-0.985537
21	1	0	3.292042	-0.867001	1.639461
22	6	0	-1.434266	2.014284	0.129983
23	7	0	-1.475997	3.153124	0.365114
24	1	0	0.627191	-2.052225	-0.307464

1,3 addition: Exo adduct of Allene 5.45d and furan



HF (M062X/6-31+G(d,p)) = -555.4969357 Hartrees

Imaginary Frequencies: none found

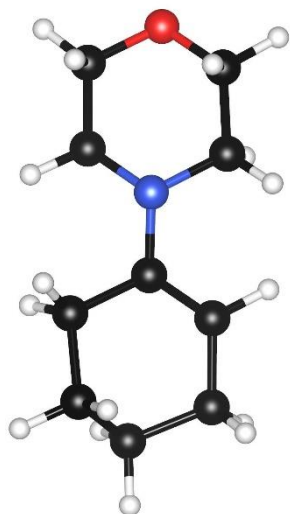
Zero-point correction = 0.199055 (Hartree/Particle)

Thermal correction = 0.163698 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.652721	1.073635	-0.253837
2	6	0	0.075687	-0.252939	-0.188583
3	6	0	1.410535	-0.346491	-0.185837
4	6	0	0.194269	2.130471	0.447984
5	6	0	1.541094	2.195124	-0.286602
6	1	0	1.345572	2.466393	-1.330656
7	6	0	2.319545	0.867254	-0.241861
8	1	0	2.948800	0.831552	0.656042
9	1	0	-0.298636	3.107148	0.413569
10	1	0	0.335557	1.857974	1.501304
11	1	0	2.170529	2.985172	0.132285
12	1	0	3.000199	0.794965	-1.096471
13	6	0	-0.970819	-1.260292	0.278820
14	6	0	-2.055197	-1.337941	-0.788647
15	6	0	-2.713625	-0.178873	-0.711033
16	6	0	-2.009503	0.619895	0.378774
17	8	0	-1.591618	-0.425925	1.272096
18	1	0	-0.594516	-2.186554	0.709699
19	1	0	-2.174802	-2.145896	-1.498456
20	1	0	-3.502906	0.194225	-1.351494
21	1	0	-2.573489	1.384933	0.909991
22	6	0	2.031628	-1.627941	0.020130
23	7	0	2.552182	-2.651926	0.178977
24	1	0	-0.814002	1.389559	-1.291260

Enamine 5.58a

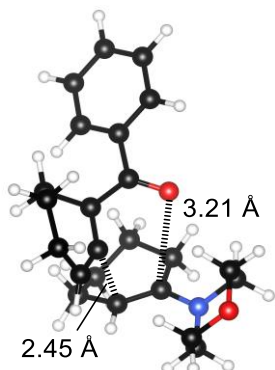


HF (M062X/6-31+G(d,p)) = -521.0482236 Hartrees
 Imaginary Frequencies: none found
 Zero-point correction = 0.264311 (Hartree/Particle)
 Thermal correction = 0.228208 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.373528	1.195389	-0.168792
2	6	0	0.703961	0.052494	0.073064
3	6	0	1.429893	-1.265284	0.261604
4	6	0	2.906014	-1.063046	0.603056
5	6	0	3.542697	-0.082104	-0.378507
6	6	0	2.878026	1.287681	-0.249811
7	1	0	0.927733	-1.832693	1.053842
8	1	0	2.995415	-0.664559	1.622361
9	1	0	3.423334	-2.027713	0.585661
10	1	0	4.620524	0.001920	-0.205241
11	1	0	3.406561	-0.461911	-1.399980
12	1	0	3.262201	1.798787	0.645591
13	1	0	3.155773	1.923590	-1.098593
14	1	0	1.355250	-1.867684	-0.654164
15	1	0	0.831684	2.127886	-0.292270
16	6	0	-1.430088	1.238341	0.122560
17	6	0	-1.357260	-1.066078	-0.549202
18	6	0	-2.887641	1.035026	0.506039
19	1	0	-1.371066	1.642594	-0.904565
20	1	0	-0.987949	1.971871	0.803256
21	6	0	-2.815244	-1.195596	-0.141806
22	1	0	-1.297567	-0.832885	-1.627729
23	1	0	-0.861475	-2.024046	-0.379713
24	1	0	-3.451001	1.957397	0.348516
25	1	0	-2.954414	0.750713	1.567428
26	1	0	-3.324189	-1.922831	-0.778359
27	1	0	-2.877957	-1.528070	0.905955
28	7	0	-0.700549	-0.016775	0.237259
29	8	0	-3.501541	0.035514	-0.290253

Transition state of trapping Allene 5.45a with Enamine 5.58a



HF (M062X/6-31+G(d,p)) = -1098.5687231 Hartrees

Imaginary Frequencies: 1 (-164.98 cm⁻¹)

Zero-point correction = 0.479750 (Hartree/Particle)

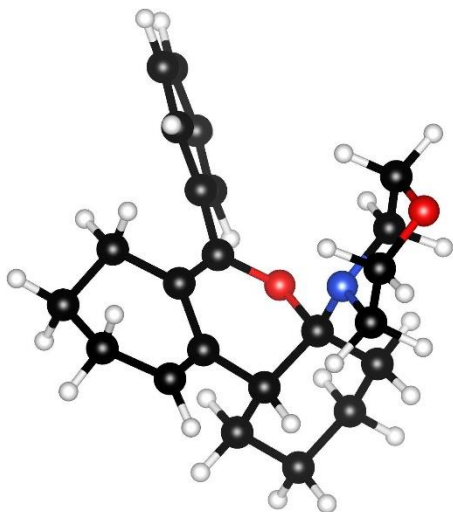
Thermal correction = 0.427048 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.897851	-0.652235	0.327124
2	6	0	-5.462079	-0.769448	-0.943559
3	6	0	-4.679306	-0.549080	-2.078020
4	6	0	-3.334431	-0.215679	-1.940785
5	6	0	-2.768345	-0.074846	-0.669826
6	6	0	-3.557252	-0.297220	0.464197
7	1	0	-5.500715	-0.839497	1.210226
8	1	0	-6.508726	-1.037829	-1.049487
9	1	0	-5.116620	-0.644120	-3.067013
10	1	0	-2.707247	-0.058358	-2.813147
11	1	0	-3.115226	-0.211828	1.454054
12	6	0	-1.303797	0.237227	-0.559508
13	6	0	-0.829323	1.054236	0.550856
14	8	0	-0.527853	-0.240429	-1.393858
15	6	0	0.488582	1.273245	0.745730
16	6	0	1.193787	2.333905	1.086441
17	6	0	-1.615120	2.159332	1.255181
18	6	0	-1.063105	3.493345	0.686618
19	1	0	-1.329633	3.524984	-0.375545
20	6	0	0.470953	3.660793	0.839224
21	1	0	0.695861	4.276855	1.718059
22	1	0	-2.686688	2.095648	1.049153
23	1	0	-1.474687	2.116268	2.341265
24	1	0	-1.564399	4.341440	1.165986
25	1	0	0.878607	4.194116	-0.026104
26	1	0	2.112204	2.326677	1.664007
27	6	0	-0.252485	-2.524496	1.356713
28	6	0	0.826404	-2.463421	0.274493
29	6	0	1.830424	-1.346548	0.490428

30	6	0	1.808029	-0.595127	1.636011
31	6	0	0.959808	-0.937574	2.839843
32	6	0	0.358215	-2.339045	2.742053
33	1	0	-0.992783	-1.732590	1.186176
34	1	0	1.399282	-3.401902	0.264708
35	1	0	1.567570	-0.844194	3.747612
36	1	0	-0.394882	-2.482251	3.523840
37	1	0	2.584935	0.147027	1.788183
38	1	0	0.139804	-0.209962	2.937850
39	1	0	1.140687	-3.093445	2.899523
40	1	0	-0.781991	-3.479579	1.279157
41	1	0	0.348989	-2.370032	-0.701221
42	6	0	4.083185	-0.556540	-0.202480
43	6	0	2.537684	-1.280925	-1.892454
44	6	0	4.084033	0.843166	-0.805402
45	1	0	4.881598	-1.135080	-0.687232
46	1	0	4.287115	-0.532603	0.869408
47	6	0	2.557880	0.143127	-2.443158
48	1	0	3.303899	-1.882819	-2.398476
49	1	0	1.560430	-1.723153	-2.077429
50	1	0	5.066451	1.310600	-0.699149
51	1	0	3.326055	1.470876	-0.315119
52	1	0	2.417886	0.138298	-3.527436
53	1	0	1.748739	0.717294	-1.970769
54	8	0	3.812946	0.769878	-2.198722
55	7	0	2.831057	-1.256225	-0.458394

Product 5.59a



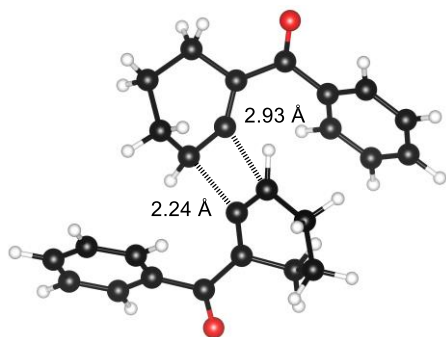
HF (M062X/6-31+G(d,p)) = -1098.689286 Hartrees
Imaginary Frequencies: none found
Zero-point correction = 0.485730 (Hartree/Particle)
Thermal correction = 0.435890 Hartrees

Coordinates from last standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.469847	-0.388207	3.459037
2	6	0	1.729244	-1.147253	2.156119
3	6	0	1.167251	-0.429996	0.925926
4	6	0	1.631782	1.032852	0.847076
5	6	0	1.323576	1.760478	2.169319
6	6	0	1.964921	1.053959	3.362469
7	6	0	0.929355	1.704347	-0.306577
8	6	0	-0.479757	1.332235	-0.508605
9	6	0	-0.997477	0.310868	0.209995
10	6	0	-1.256689	2.108557	-1.551514
11	1	0	-2.319332	2.142540	-1.293536
12	6	0	-0.703970	3.524944	-1.723915
13	6	0	0.786460	3.483127	-2.062740
14	6	0	1.526608	2.655079	-1.046456
15	1	0	0.392599	-0.388347	3.665547
16	1	0	2.810657	-1.265824	2.003463
17	1	0	1.686338	2.790207	2.082594
18	1	0	1.742150	1.597358	4.286878
19	1	0	-1.262519	4.047857	-2.506385
20	1	0	0.928821	3.070045	-3.072241
21	1	0	2.580290	2.871224	-0.870611
22	6	0	-2.397597	-0.176191	0.188518
23	6	0	-3.106221	-0.359670	-1.004920
24	6	0	-3.020526	-0.505554	1.401639
25	6	0	-4.416362	-0.836884	-0.984193
26	1	0	-2.624434	-0.153002	-1.955081
27	6	0	-4.330098	-0.975605	1.421532
28	1	0	-2.468339	-0.386404	2.329079
29	6	0	-5.034651	-1.140325	0.227604
30	1	0	-4.949654	-0.979500	-1.919051
31	1	0	-4.802165	-1.214976	2.369582
32	1	0	-6.055462	-1.509214	0.242602
33	8	0	-0.254744	-0.417362	1.113164
34	1	0	-1.181113	1.594010	-2.521084
35	1	0	-0.841174	4.084165	-0.789879
36	1	0	1.203079	4.495939	-2.086138
37	1	0	2.717782	1.072357	0.705085
38	1	0	0.235736	1.810647	2.308752
39	1	0	3.057702	1.059084	3.242709
40	1	0	1.957632	-0.910115	4.289064
41	1	0	1.294744	-2.150448	2.210029
42	6	0	2.770836	-1.063568	-0.878127
43	6	0	0.927398	-2.501301	-0.387981
44	6	0	2.759807	-1.593755	-2.305929
45	1	0	3.485934	-1.656084	-0.277604
46	1	0	3.120910	-0.029963	-0.914636
47	6	0	0.941686	-2.979198	-1.830804
48	1	0	1.554506	-3.185760	0.211238
49	1	0	-0.094174	-2.533865	0.001374
50	1	0	3.773540	-1.624915	-2.712021
51	1	0	2.139500	-0.930930	-2.929342
52	1	0	0.624469	-4.022518	-1.896902
53	1	0	0.263671	-2.355045	-2.433255
54	8	0	2.253589	-2.916691	-2.370680
55	7	0	1.417858	-1.125674	-0.339277

Transition state of Allene 5.45a [2+2] dimerization



HF (M062X/6-31+G(d,p)) = -1155.0522239 Hartrees

Imaginary Frequencies: 1 (-171.76 cm⁻¹)

Zero-point correction = 0.429073 (Hartree/Particle)

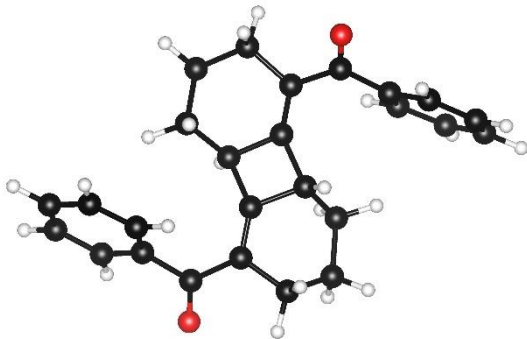
Thermal correction = 0.373502 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.395960	-1.660030	-1.571462
2	6	0	4.296028	-2.185334	-0.645148
3	6	0	4.794946	-1.378091	0.379390
4	6	0	4.390702	-0.050691	0.476337
5	6	0	3.463642	0.473396	-0.433949
6	6	0	2.970267	-0.336782	-1.462750
7	1	0	3.021904	-2.281007	-2.379388
8	1	0	4.615391	-3.219846	-0.725530
9	1	0	5.498426	-1.783981	1.099329
10	1	0	4.773062	0.591577	1.263759
11	1	0	2.274086	0.065955	-2.190778
12	6	0	3.034760	1.893473	-0.233514
13	6	0	1.630403	2.263509	-0.533379
14	8	0	3.807596	2.719836	0.233256
15	6	0	0.630537	1.414817	-0.700599
16	6	0	-0.658648	1.345044	-0.369832
17	6	0	1.135684	3.692335	-0.271210
18	6	0	-0.348177	3.721193	0.179462
19	1	0	-0.471550	4.502029	0.936899
20	6	0	-0.880173	2.378069	0.746189
21	1	0	-1.940281	2.456604	1.000168
22	1	0	1.793281	4.066475	0.521822
23	1	0	1.284396	4.342238	-1.138379
24	1	0	-0.983191	3.998918	-0.668128
25	1	0	-0.327579	2.088470	1.645453
26	1	0	-1.461042	1.098888	-1.058658
27	6	0	-4.410695	0.992655	1.149636
28	6	0	-5.361700	1.253238	0.163357
29	6	0	-5.364146	0.506517	-1.016192
30	6	0	-4.419864	-0.499030	-1.203016
31	6	0	-3.449399	-0.749854	-0.226464
32	6	0	-3.449152	0.001471	0.953089

33	1	0	-4.415964	1.562091	2.074184
34	1	0	-6.103258	2.031277	0.315773
35	1	0	-6.105360	0.703196	-1.784415
36	1	0	-4.420798	-1.100695	-2.106659
37	1	0	-2.711122	-0.196637	1.725050
38	6	0	-2.478130	-1.868627	-0.477475
39	6	0	-1.081608	-1.729342	-0.082695
40	8	0	-2.874857	-2.876761	-1.066503
41	6	0	-0.494018	-0.692371	0.554867
42	6	0	0.553183	-0.663300	1.374233
43	6	0	-0.124099	-2.908765	-0.151105
44	6	0	0.293975	-3.203693	1.309478
45	1	0	-0.597494	-3.548683	1.844197
46	6	0	0.898511	-1.979961	2.046586
47	1	0	1.995645	-2.023292	2.014750
48	1	0	-0.619721	-3.776735	-0.592101
49	1	0	0.755327	-2.662889	-0.756557
50	1	0	1.018911	-4.024547	1.332480
51	1	0	0.622211	-1.994596	3.106353
52	1	0	1.230088	0.181535	1.463351

Dimerization of Allene 5.45a [2+2] cycloadduct



HF (M062X/6-31+G(d,p)) = -1155.1972599 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.435416 (Hartree/Particle)

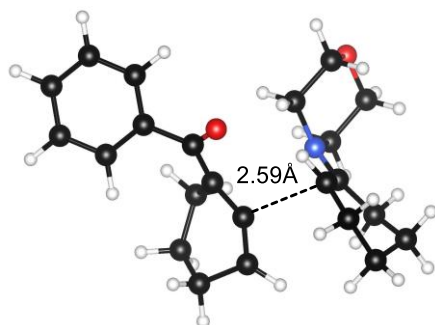
Thermal correction = 0.380774 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.793701	-0.978148	1.316908
2	6	0	-5.639195	-1.370019	0.280524
3	6	0	-5.552292	-0.748819	-0.968292
4	6	0	-4.630983	0.273084	-1.172251
5	6	0	-3.763067	0.652616	-0.141620
6	6	0	-3.843417	0.020032	1.102665
7	1	0	-4.866812	-1.454387	2.289612
8	1	0	-6.369518	-2.156395	0.444138
9	1	0	-6.209874	-1.055502	-1.775455

10	1	0	-4.568010	0.783907	-2.128384
11	1	0	-3.174521	0.317592	1.904942
12	6	0	-2.831228	1.800656	-0.373856
13	6	0	-1.481710	1.795772	0.249547
14	8	0	-3.187283	2.743638	-1.070334
15	6	0	-0.762071	0.671563	0.368608
16	6	0	0.735409	0.622845	0.634563
17	6	0	-0.835499	3.142959	0.495670
18	6	0	0.615963	3.046650	0.986026
19	1	0	1.103764	4.015901	0.846123
20	6	0	1.407205	1.943642	0.269510
21	1	0	2.458334	1.955232	0.571705
22	1	0	-0.876973	3.691271	-0.453660
23	1	0	-1.437285	3.726137	1.202558
24	1	0	0.628933	2.838974	2.063615
25	1	0	1.369809	2.093507	-0.817300
26	1	0	0.965975	0.378513	1.682472
27	6	0	4.567847	1.289143	-1.337119
28	6	0	5.529628	1.505256	-0.350979
29	6	0	5.623954	0.636469	0.739193
30	6	0	4.764841	-0.453649	0.834346
31	6	0	3.781328	-0.658431	-0.140128
32	6	0	3.682412	0.218438	-1.224555
33	1	0	4.499558	1.959754	-2.187884
34	1	0	6.208683	2.348484	-0.431435
35	1	0	6.372529	0.805741	1.506554
36	1	0	4.840320	-1.150932	1.663272
37	1	0	2.921566	0.056828	-1.982663
38	6	0	2.903522	-1.864968	-0.035164
39	6	0	1.476781	-1.755834	-0.419404
40	8	0	3.356881	-2.924072	0.381166
41	6	0	0.726236	-0.672751	-0.175405
42	6	0	-0.789636	-0.727839	-0.241149
43	6	0	0.703859	-2.973951	-0.867190
44	6	0	-0.533143	-3.239992	0.035666
45	1	0	-1.248179	-3.837129	-0.538016
46	6	0	-1.226738	-1.962863	0.571933
47	1	0	-0.947219	-1.790666	1.618151
48	1	0	0.362739	-2.810606	-1.896536
49	1	0	1.354277	-3.851149	-0.876648
50	1	0	-0.219183	-3.854169	0.884526
51	1	0	-2.312985	-2.073690	0.541844
52	1	0	-1.230535	-0.764922	-1.246476

Transition state: Nucleophilic attack of Enamine 5.58a on Allene 5.45a



HF (M062X/6-31+G(d,p)) = -1098.5691451 Hartrees

Imaginary Frequencies: 1 (-125.20 cm^{-1})

Zero-point correction = 0.479276 (Hartree/Particle)

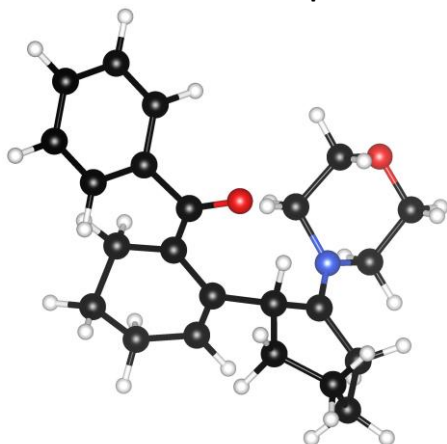
Thermal correction = 0.425119 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.358757	0.412520	-0.420967
2	6	0	5.918507	-0.744193	0.122561
3	6	0	5.134417	-1.605488	0.891853
4	6	0	3.793732	-1.306953	1.120827
5	6	0	3.222445	-0.160474	0.560480
6	6	0	4.011434	0.699050	-0.210636
7	1	0	5.971200	1.090243	-1.007189
8	1	0	6.966034	-0.971322	-0.049626
9	1	0	5.569971	-2.504016	1.317391
10	1	0	3.175673	-1.955700	1.734246
11	1	0	3.577910	1.606380	-0.624385
12	6	0	1.791735	0.163619	0.876867
13	6	0	0.945058	0.775928	-0.144432
14	8	0	1.352004	-0.097564	1.998585
15	6	0	-0.064934	1.610395	0.148073
16	6	0	-0.490076	2.716387	-0.426826
17	6	0	1.173862	0.781516	-1.657176
18	6	0	1.244381	2.246437	-2.200290
19	1	0	2.287583	2.513188	-2.400705
20	6	0	0.635320	3.334294	-1.256497
21	1	0	0.260775	4.176845	-1.844052
22	1	0	2.078410	0.227521	-1.922194
23	1	0	0.332316	0.263080	-2.126865
24	1	0	0.723374	2.284547	-3.161308
25	1	0	1.415948	3.720117	-0.594553
26	1	0	-1.516332	3.058328	-0.489891
27	6	0	-4.608994	1.249075	0.517696
28	6	0	-3.705385	0.495497	-0.459674
29	6	0	-2.444753	-0.034766	0.199749
30	6	0	-2.031868	0.467708	1.396086
31	6	0	-2.754856	1.549868	2.159034
32	6	0	-3.813942	2.267444	1.324695
33	1	0	-5.420142	1.730527	-0.037928
34	1	0	-4.275789	-0.335074	-0.887138
35	1	0	-3.230740	1.115764	3.051192

36	1	0	-3.336617	2.975645	0.636138
37	1	0	-1.170661	0.044317	1.901395
38	1	0	-2.018147	2.271676	2.533982
39	1	0	-4.474361	2.853342	1.972282
40	1	0	-5.071498	0.528477	1.205083
41	1	0	-3.432060	1.148445	-1.301561
42	6	0	-2.218956	-1.605534	-1.730014
43	6	0	-0.827186	-1.917847	0.180016
44	6	0	-2.943505	-2.910577	-1.408972
45	1	0	-1.354717	-1.834824	-2.367826
46	1	0	-2.860789	-0.924155	-2.288159
47	6	0	-1.580953	-3.208194	0.485895
48	1	0	0.020336	-2.141255	-0.482782
49	1	0	-0.421014	-1.479112	1.089559
50	1	0	-3.250791	-3.428246	-2.321261
51	1	0	-3.836104	-2.702496	-0.796423
52	1	0	-0.923636	-3.950590	0.945114
53	1	0	-2.415970	-2.993999	1.171861
54	8	0	-2.083997	-3.797261	-0.708092
55	7	0	-1.711381	-0.983331	-0.512632

Intermediate: Nucleophilic attack of Enamine 5.58a on Allene 5.45a



HF (M062X/6-31+G(d,p)) = -1098.630231 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.483149 (Hartree/Particle)

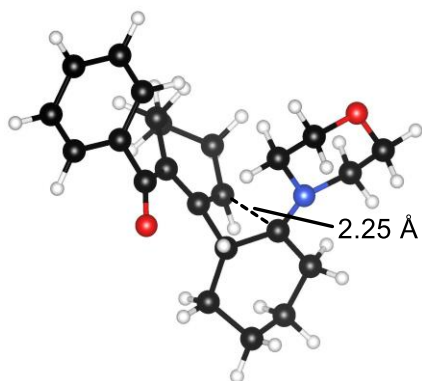
Thermal correction = 0.428032 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.517758	0.294225	0.605198
2	6	0	5.905596	-1.043915	0.533057
3	6	0	4.931264	-2.040201	0.451926
4	6	0	3.580373	-1.696682	0.445834
5	6	0	3.180328	-0.357322	0.495337
6	6	0	4.164506	0.633053	0.581820
7	1	0	6.269255	1.074763	0.682430

8	1	0	6.958565	-1.308982	0.546414
9	1	0	5.225341	-3.084665	0.399878
10	1	0	2.817469	-2.469992	0.405777
11	1	0	3.862382	1.676782	0.633489
12	6	0	1.702594	-0.033677	0.562210
13	6	0	1.135321	0.777140	-0.423636
14	8	0	1.098496	-0.593290	1.549995
15	6	0	-0.256469	1.207600	-0.423369
16	6	0	-0.793160	1.972115	-1.409584
17	6	0	1.874510	1.123094	-1.704952
18	6	0	1.498996	2.512744	-2.226450
19	1	0	1.729574	3.257759	-1.453591
20	6	0	0.004515	2.559904	-2.544869
21	1	0	-0.189636	2.018588	-3.482996
22	1	0	2.955250	1.048027	-1.575908
23	1	0	1.607995	0.393686	-2.490837
24	1	0	2.086889	2.766569	-3.115334
25	1	0	-0.316459	3.594112	-2.723413
26	1	0	-1.843958	2.260570	-1.339932
27	6	0	-3.742172	2.198269	1.409674
28	6	0	-3.814209	0.922853	0.566985
29	6	0	-2.479174	0.282749	0.266401
30	6	0	-1.179490	0.857749	0.757162
31	6	0	-1.305983	2.050395	1.728888
32	6	0	-2.642401	2.088630	2.459933
33	1	0	-3.532559	3.061184	0.766758
34	1	0	-4.411305	0.174971	1.104417
35	1	0	-0.463738	1.990878	2.425471
36	1	0	-2.673576	2.944614	3.140127
37	1	0	-0.687481	0.051377	1.318394
38	1	0	-1.195132	2.985447	1.168687
39	1	0	-2.785664	1.184431	3.067830
40	1	0	-4.724549	2.363766	1.859718
41	1	0	-4.332919	1.113846	-0.379851
42	6	0	-3.660005	-1.503456	-0.953201
43	6	0	-1.247712	-1.631120	-0.677214
44	6	0	-3.754747	-2.926640	-0.410500
45	1	0	-3.527493	-1.525947	-2.039663
46	1	0	-4.563307	-0.948071	-0.719685
47	6	0	-1.445791	-3.051428	-0.160599
48	1	0	-1.107391	-1.623636	-1.763488
49	1	0	-0.375089	-1.192892	-0.198737
50	1	0	-4.599901	-3.436358	-0.875656
51	1	0	-3.906911	-2.898871	0.679041
52	1	0	-0.582820	-3.657416	-0.440475
53	1	0	-1.527468	-3.033932	0.936282
54	8	0	-2.591868	-3.663407	-0.722488
55	7	0	-2.466441	-0.843356	-0.390788

Transition state: Formation of [2+2] adduct with Enamine 5.58a and Allene 5.45a



HF (M062X/6-31+G(d,p)) = -1098.6150561 Hartrees

Imaginary Frequencies: 1 (-353.13 cm^{-1})

Zero-point correction = 0.482486 (Hartree/Particle)

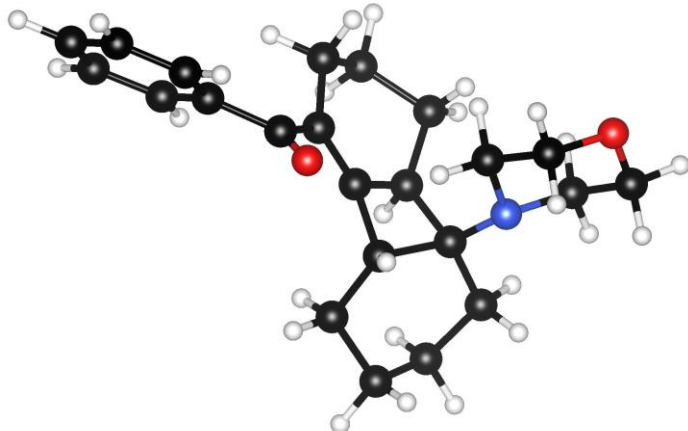
Thermal correction = 0.431290 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.507076	0.539199	-0.969695
2	6	0	-5.732996	-0.722098	-0.415551
3	6	0	-4.669169	-1.439406	0.131259
4	6	0	-3.388032	-0.888788	0.140597
5	6	0	-3.153725	0.374378	-0.411893
6	6	0	-4.222001	1.076606	-0.979340
7	1	0	-6.332013	1.098945	-1.400257
8	1	0	-6.732790	-1.145595	-0.414684
9	1	0	-4.835840	-2.427046	0.550605
10	1	0	-2.561602	-1.453334	0.564671
11	1	0	-4.032526	2.047165	-1.428593
12	6	0	-1.764297	0.957671	-0.502341
13	6	0	-0.908741	0.923530	0.646875
14	8	0	-1.433787	1.444312	-1.608350
15	6	0	0.451569	1.200265	0.506383
16	6	0	1.390253	1.156925	1.552333
17	6	0	-1.397553	0.563718	2.037306
18	6	0	-0.541291	1.225587	3.123837
19	1	0	-0.643953	2.315396	3.048852
20	6	0	0.938472	0.850386	2.962686
21	1	0	1.060658	-0.218367	3.187468
22	1	0	-2.446658	0.850341	2.165439
23	1	0	-1.357092	-0.526906	2.199950
24	1	0	-0.901244	0.928619	4.114625
25	1	0	1.552295	1.391176	3.690663
26	1	0	2.291635	1.752437	1.438228
27	6	0	4.059234	2.030151	-0.575140
28	6	0	3.755199	0.568557	-0.239056
29	6	0	2.280350	0.188137	-0.268859
30	6	0	1.235447	1.164424	-0.793543
31	6	0	1.740681	2.538571	-1.274991
32	6	0	3.193668	2.508480	-1.736224
33	1	0	3.881448	2.676433	0.293689

34	1	0	4.234939	-0.054465	-1.007396
35	1	0	1.067433	2.881623	-2.064801
36	1	0	3.502313	3.506414	-2.062064
37	1	0	0.657000	0.712835	-1.602031
38	1	0	1.660640	3.260445	-0.453437
39	1	0	3.314775	1.834530	-2.595752
40	1	0	5.125231	2.106736	-0.809185
41	1	0	4.204339	0.292146	0.718768
42	6	0	2.930270	-2.078827	0.352815
43	6	0	0.661683	-1.668228	-0.357427
44	6	0	2.804494	-3.481831	-0.221387
45	1	0	2.669309	-2.080701	1.423190
46	1	0	3.966002	-1.761784	0.250854
47	6	0	0.629671	-3.085339	-0.907766
48	1	0	0.273053	-1.657199	0.673789
49	1	0	0.017809	-1.037512	-0.970112
50	1	0	3.414465	-4.172949	0.363504
51	1	0	3.157966	-3.486355	-1.263631
52	1	0	-0.384962	-3.481575	-0.833481
53	1	0	0.935676	-3.083099	-1.964666
54	8	0	1.471464	-3.950269	-0.168146
55	7	0	2.031946	-1.147588	-0.343932

Intermediate: Formation of [2+2] adduct with Enamine 5.58a and Allene 5.45a



HF (M062X/6-31+G(d,p)) = -1098.6531182 Hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.484799 (Hartree/Particle)

Thermal correction = 0.434081 Hartrees

Coordinates from last standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.439982	0.729523	0.570168
2	6	0	-6.269718	-0.143471	-0.133698
3	6	0	-5.717019	-1.114512	-0.971328
4	6	0	-4.335256	-1.208472	-1.108764
5	6	0	-3.498858	-0.348009	-0.390350

6	6	0	-4.056226	0.620831	0.451038
7	1	0	-5.869996	1.491319	1.212497
8	1	0	-7.347831	-0.065707	-0.032000
9	1	0	-6.364006	-1.791855	-1.519720
10	1	0	-3.889221	-1.946738	-1.768182
11	1	0	-3.406331	1.302628	0.993865
12	6	0	-2.015859	-0.437998	-0.584710
13	6	0	-1.119171	-0.048456	0.541051
14	8	0	-1.562670	-0.818432	-1.657298
15	6	0	-0.007832	0.651549	0.294088
16	6	0	1.117061	0.904449	1.258409
17	6	0	-1.371283	-0.564137	1.949252
18	6	0	-0.384648	0.005134	2.981817
19	1	0	-0.665942	1.040597	3.214948
20	6	0	1.068657	-0.009037	2.476214
21	1	0	1.342401	-1.033655	2.207955
22	1	0	-2.397516	-0.358456	2.270095
23	1	0	-1.281536	-1.660586	1.924384
24	1	0	-0.472349	-0.566465	3.910892
25	1	0	1.757001	0.319752	3.261531
26	1	0	1.106563	1.954060	1.588922
27	6	0	2.772141	3.288331	-0.329390
28	6	0	3.210810	1.850109	-0.047516
29	6	0	2.073045	0.817441	-0.000910
30	6	0	0.803335	1.120076	-0.890914
31	6	0	0.555280	2.608031	-1.210021
32	6	0	1.843887	3.354191	-1.538498
33	1	0	2.254086	3.714014	0.541153
34	1	0	3.899751	1.538971	-0.843458
35	1	0	-0.167761	2.666260	-2.029831
36	1	0	1.618059	4.393961	-1.797036
37	1	0	0.739913	0.531150	-1.808182
38	1	0	0.087027	3.099527	-0.346884
39	1	0	2.335620	2.900374	-2.410118
40	1	0	3.667326	3.898985	-0.487224
41	1	0	3.768765	1.823734	0.895876
42	6	0	3.737680	-0.939709	0.526911
43	6	0	1.723462	-1.639100	-0.537700
44	6	0	4.456765	-2.115201	-0.119781
45	1	0	3.394218	-1.239341	1.532182
46	1	0	4.462205	-0.132750	0.648051
47	6	0	2.495004	-2.784118	-1.177450
48	1	0	1.283546	-2.009024	0.404779
49	1	0	0.896609	-1.362988	-1.194960
50	1	0	5.247722	-2.487422	0.535933
51	1	0	4.901794	-1.788285	-1.072618
52	1	0	1.846424	-3.653829	-1.307821
53	1	0	2.878583	-2.467999	-2.159876
54	8	0	3.576010	-3.199959	-0.357105
55	7	0	2.631501	-0.506825	-0.328206
