THEORETICAL ANALYSIS OF DRUG ANALOGUES AND VOC POLLUTANTS

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While computational chemistry methods have a wide range of applications within the set of traditional physical sciences, very little is being done in terms of expanding their usage into other areas of science where these methods can help clarify research questions. One such promising field is forensic science, where detailed, rapidly acquired sets of chemical data can help in decision-making at a crime scene. As part of an effort to create a database that fits these characteristics, the present work makes use of computational chemistry methods to increase the information readily available for the rapid identification and scheduling of drugs to the forensic scientist. Ab initio geometry optimizations, vibrational spectra calculations and ESI-MS fragmentation prediction of a group of common psychedelics are here presented. In addition, we describe an under development graphical user interface to perform ab initio calculations using the GAMESS software package in a more accessible manner. Results show that the set of theoretical techniques here utilized, closely approximate experimental data. Another aspect covered in this work is the implementation of a boiling point estimation method based on group contributions to generate chemical dispersion areas with the ALOHA software package. Once again, theoretical results showed to be in agreement with experimental boiling point values. A computer program written to facilitate the execution of the boiling point estimation method is also shown.

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CHAPTER 1

INTRODUCTION

Current Trends in the Forensic Community

Forensic Science is the application of the scientific method to the collection, preservation, and analysis of physical evidence found at a crime scene and used within a court of law. Depending on the nature of the object, this evidence can be classified into different categories such as biological, material, fire debris, substance identification, and pattern evidence such as fingerprints, footwear, and others. After analysis and classification, the results are presented to the court during a trial to help establish the innocence or culpability of the defendant.[1]

In general, three distinct areas can be identified within the field of forensic science: forensic DNA analysis, trace evidence, and drugs and poisons.[2] The area of DNA analysis includes everything from collection and characterization of biological material for DNA analysis to the creation of DNA databases for missing persons and disaster victim identification, including all the aspects dealing with short tandem repeat (STR) typing, which is the most utilized method for information recovery from DNA templates. Trace evidence deals with the characterization and discrimination of oil spill samples, the detection and forensic analysis of explosives, and the identification of hairs, fibers, glass, and paint. This area of forensic science also deals with the development and application of new techniques and reagents for latent fingerprint development. Finally, the drugs and poisons branch is concerned with the utilization of spectroscopy and mass spectrometry to characterize, identify, and classify any substance that produces a physiological change (drug) or disturbance in the body (poison). Ethanol and

other volatile materials, cannabinoids, morphine, amphetamines, benzodiazepines, as well as δ-hydroxybutyrate, are among the most commonly examined substances in this area of Forensic Science;[2] for which a wide range of analytical methods are utilized. For instance, gas chromatography/flame ionization detection (GC/FID) has been used to determine the presence of ethanol, acetaldehyde, methanol, and acetone in blood, vitreous humor, and urine.[3] In addition, alcohol concentration in blood has been measured using horizontal attenuated total reflectance-Fourier transform IR spectroscopy (ATR-FT-IR).[4] DELTA-tetrahydrocannabinol and metabolites have been detected in blood, urine, saliva, and oral fluid using techniques such as LC/MS/MS,[5,6] GC/MS,[7] and hollow-fiber liquid-phase microextraction (HF-LPME).[8] Moreover, both quantitative and qualitative determination of major cannabinoids in cannabis plant material has been described using high performance liquid chromatography diode-array detection (HPLC/DAD).[9] Analysis of heroin has been performed by capillary electrophoresis-mass spectrometry (CE-MS),[10] and morphine has been detected in hair using SPE and GC/MS.[11] Simultaneous analysis of cocaine and metabolites in dried blood spots using HPLC coupled to spectrofluorimetric detection has been presented.[12] Additionally, matrix-assisted laser desorption/ionization (MALDI) mass spectrometry has been used to detect cocaine in hair.[13] High throughput chiral analysis of urinary amphetamines by GC/MS using a narrow-bore capillary column has been reported.[14] Furthermore, amphetamines have been detected in urine using *in situ* derivatization and extractive acylation with an ionic liquid-based solid-phase microextraction fiber and ^{1}H NMR spectroscopy.[15] Benzodiazepines have been detected in vitreous humor using SPE and HPLC-DAD.[16] δ-hydroxybutyrate acid (GHB) has been determined in serum and urine by headspace solid-phase dynamic extraction combined with GC-PCIMS[17]

and in urine using GC/MS.[18] Finally, a set of N,N-dialkylated tryptamines has been studied using techniques such as GC, HPLC, and capillary electrophoresis along with spectroscopic methods like FT-IR, UV, and NMR.[19]

Despite the number of analytical tools available to the forensic scientist and law enforcement agencies for the identification and classification of illegal drugs, as more psychotropic substances are designed to bypass controlled substance legislation, new detection and analysis techniques are needed. Current trends in the forensic field show significant effort in the development of techniques that would allow for controlled substance detection and classification in a timely manner, some of them seeking to identify these compounds even before being widely distributed to the public. For example, Feng *et al* reported the design of a portable Raman system for the rapid and convenient identification of counterfeit drugs,[20] Wielbo & Tebbett presented a Micro-FTIR in conjunction with microcrystal tests as a mean for rapid street drug identification,[21] and our very own group designed a vehicle-mounted mobile mass spectrometry unit to detect clandestine methamphetamine laboratories via spatial analysis.[22]

The development of these techniques has also prompted a more active involvement by the chemical community in the forensic field in order to help law enforcement agencies to be better equipped in their battle against drug-facilitated crimes.[23,24] On par with this trend, this project proposes the use of previously established computational chemistry methods to facilitate the rapid detection, characterization, and scheduling of substances of abuse as a complementary source of chemical data to existing and developmental experimental methods. Here, we present the full conformational analysis of a family of psychedelics to demonstrate

how theoretical IR spectra can aid in the characterization of spectral features. Additionally, we set the foundation for a theoretical method to detect point sources of illegal drug manufacture by calculating chemical dispersion areas using theoretical boiling points.

Drug Scheduling in the United Sates[25,26]

In the United States, manufacture, importation, possession, use and distribution of controlled substances is regulated by the Controlled Substances Act (CSA), which encompasses two subchapters. Subchapter I defines Schedules I - V and lists the laws that govern the legal manufacture, distribution, and possession of controlled substances as well as the legal consequences for violations. Subchapter II lists the laws for exportation and importation.

Drugs, substances, and certain chemicals used in drug synthesis are classified (scheduled) into five different classes. The acceptable medical use and the drug's dependency potential are the determining factors when scheduling a drug, with Schedule I drugs considered the most dangerous class and Schedule V representing those drugs with least potential for abuse. A listing of drugs and their schedule can be found in the Controlled Substance Act (CSA) Scheduling by alphabetical order. According to the Drug Enforcement Administration web page, this list is not meant to be comprehensive and a controlled substance does not need to be listed to be treated as a Schedule I substance for criminal prosecution. For legal matters, a controlled substance analogue is defined as a substance intended for legal consumption and is structurally similar to or represented as being similar to a Schedule I or Schedule II substance and is not an approved medication in the United States. Drug schedules are defined as follows:

a) Schedule I. Includes drugs, substances, or chemicals with no current accepted medical use and a high potential for abuse. This is considered the most dangerous class. Examples include: heroin, marijuana, and lysergic acid diethylamide (LSD).

b) Schedule II. This class includes compounds with high potential for abuse and are considered dangerous. Some drugs belonging to this schedule are: cocaine, methamphetamine, and Ritalin.

c) Schedule III. Compounds belonging to this class have a moderate to low potential for physical and psychological dependence. Some examples of Schedule III drugs include: ketamine, anabolic steroids, and testosterone.

d) Schedule IV. Schedule IV drugs are compounds with low potential for abuse and dependence. Some examples are: Xanax, Valium, and Tramadol.

e) Schedule V. These are drugs, substances, or chemicals with the lowest potential for abuse and consist of preparations containing limited quantities of narcotics. This class includes compounds such as Lomotil, Motofen, and Lyrica.

The Problem with Designer Drugs[27]

Although the DEA's list of controlled substances is not comprehensive and drugs with similar physical and psychological effects as Schedule I or II drugs can be treated as such for legal prosecution, criminal organizations have found a way to bypass controlled substance regulation in the form of Synthetic Designer Drugs. According to the 2015 National Drug Threat Assessment Summary published by the Drug Enforcement Administration, synthetic designer drugs refer to 'man-made substances created to mimic the effects of controlled substances, and are often times unscheduled and unregulated.' Synthetic designer drugs include cannabinoids,

cathinones, and phenethylamines, with cannabinoids and cathinones being the two most widely used in the United States.

Synthetic cannabinoids, which are also known as 'Spice' or 'K2', are compounds synthesized with the goal of mimicking the biological effects of THC in the human body. Cathinones or 'bath salts', simulate the effects of cathinone, methcathinone, MDMA, amphetamine, methamphetamine, and cocaine. Phenethylamines are a family of hallucinogens that affect the central nervous system by interacting with neurotransmitters.

Synthetic cannabinoids and cathinones are synthesized in laboratories from countries like China, India, and the Netherlands and then imported into the country as once they are manufactured, little to no processing is needed. Spice is usually processed at homes and warehouses throughout the United States and packaged in individual foil packets with logos and names, which makes them appear as legitimate. Each drug utilizes a different set of precursor chemicals and manufacturing process, and so, while these compounds may have similar effects in the human body, variations in the synthetic process lead to no two packets having the same content. It is this versatility that poses a major challenge to law enforcement agencies, given that 'as certain compounds are scheduled, producers quickly change one or two elements in the banned substance thereby creating a new compound that has similar psychoactive effects but is not yet illegal.' The NDTA Summary adds that 'since 2009, when these drugs were first encountered in the US, more than 250 new synthetic compounds have been encountered.'

Designer drugs are available throughout the United States. They are distributed through convenience stores, head shops, adult stores, hookah and smoke shops, and gas stations. Some

vendors sell these drugs openly, while others will only sell them to trusted customers. While the NDTA 2015 report states that the availability of designer drugs is mostly stable, they still represent a thread primarily among the youth population. 'Due to the changing nature of the chemical formula for synthetic designer drugs, distributors are able to reap significant profits before legislation to control these psychoactive substances is enacted.'

Application of Computational Chemistry Methods Towards the Designer Drug Problem

The purpose of this project is to use previously established methods in the field of Computational Chemistry to increase the amount of chemical information available to the forensic scientist and law enforcement agencies and, in this manner, facilitate the rapid detection, characterization, and scheduling of designer drugs when coupled with experimental data. Quantum chemical calculations have been previously applied to systems of forensic interest. For instance, geometry optimizations have been used to investigate the inhibition of sodium channels in the human body by saxitoxin (paralytic shellfish poison). In another case study, quantum mechanical calculations were utilized to explore possible mechanisms of reaction of ninhydrin and amino acids with the formation of Ruhemann's Purple. This was done with the purpose of finding alternatives to ninhydrin, which is used for fingerprint identification. These examples along with other cases in which computational methods were utilized in the realm of Forensic Science can be found in Chapter 4 of the book titled 'Forensic Science Advances and Their Application in the Judiciary System', edited by D. Sapse and L. Kobilinsky.[28]

In Chapter 2, we describe the full conformational analysis (geometry optimization plus frequency calculations) of a family of amphetamine analogues, and other psychedelics including

phenethylamines, DMCPA, and tryptamines. In addition, we make use of a commercially available fragmentation prediction software with the purpose of evaluating how well the results match to experimental ESI-MS spectra. Finally, we describe a graphical user interface designed to facilitate the creation of input files to perform quantum mechanical calculations. Our goal here is help in the creation of a database where forensic scientists can access a wide range of chemical data (theoretical and experimental) for future reference and comparison.

Chapter 3 describes the implementation of a non-linear group contribution model to predict normal boiling points as part of a graphical user interface. The purpose of this project is to facilitate the calculation of normal boiling points to generate chemical dispersion areas, which in turn will aid in the detection of illegal drug manufacturing sites via spatial analysis.

Finally, Chapter 4, the conclusion chapter, describes the findings of this project and discusses future directions as well as additional physical molecular properties that can be added to our database by making use of theoretical methods. With the creation of a chemical database and a detection method, we seek to better equip law enforcement agencies and forensic scientist in their battle against drug-facilitated crimes and identification, characterization, and scheduling of designer drugs.

Geometry Optimization and Calculation of Vibrational Spectra[29]

This section reviews the underlying principles and assumptions of the *ab initio* mathematical framework as applied to the optimization of molecular structures and the calculation of vibrational spectra. The prediction of molecular properties using *ab initio* methods requires the solution of the time-independent Schrödinger equation:

$$\hat{\mathrm{H}}\Psi(R_1, \dots, R_N, r_1, \dots, r_n) = E\Psi(R_1, \dots, R_N, r_1, \dots, r_n) \qquad (1.1)$$

where $\hat{\mathrm{H}}$ is the Hamiltonian operator, E is the total electron-nuclear energy (kinetic plus potential), and $\Psi(R_1, \dots, R_N, r_1, \dots, r_n)$ is the wave function of the system dependent on both the nuclear (R_i) and electronic (r_i) position coordinates. The explicit form of the non-relativistic Hamiltonian operator, or simply 'the Hamiltonian', is found in equation 1.2. This form of the operator is sufficient because our work only focuses on calculating the structure and spectra of organic molecules, constituted by 2nd row elements in which relativistic effects are unimportant.

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2}\sum_I^N \frac{\nabla_I^2}{m_I} - \frac{\hbar^2}{2m_e}\sum_i^n \nabla_i^2 - \sum_I^N \sum_i^n \frac{Z_I e^2}{4\pi\varepsilon_0 r_{Ii}} + \sum_I^N \sum_{J>I}^N \frac{Z_I Z_J e^2}{4\pi\varepsilon_0 r_{IJ}} + \sum_i^n \sum_{j>i}^n \frac{e^2}{4\pi\varepsilon_0 r_{ij}} \quad (1.2)$$

The first two terms of the Hamiltonian in equation 1.2 constitute the kinetic energy portion of the operator and correspond to both the nuclear and electronic motion of the system, respectively. The potential part is defined by the last three terms, representing, in order of appearance, the nuclear-electron attraction, the repulsion between nuclei, and the electron-electron repulsion.

Because, to a very good approximation, nuclear motion is non-existent in a molecule relative to electronic motion, the wave function of the system can be written as the product of two functions that depend exclusively on a particular set of coordinates—either nuclear or electronic. This is known as the Born-Oppenheimer approximation, named after its proponents. Equation 1.3 shows the Born-Oppenheimer approximation applied to a system made up of N nuclei and n electrons.

$$\Psi(R_1, \dots, R_N, r_1, \dots, r_n) = \Phi(R_1, \dots, R_N)\psi(r_1, \dots, r_n) \quad (1.3)$$

The B.O. approximation allows us to fix the nuclear positions and, in turn, simplify the Hamiltonian by getting rid of the nuclear kinetic energy term. This means that is only necessary to solve the electronic portion of the wave function of the system and equation 1.2 becomes:

$$\hat{\mathrm{H}} = -\frac{\hbar^2}{2m_e}\sum_i^n \nabla_i^2 - \sum_I^N \sum_i^n \frac{Z_I e^2}{4\pi\varepsilon_0 r_{Ii}} + \sum_I^N \sum_{J>I}^N \frac{Z_I Z_J e^2}{4\pi\varepsilon_0 r_{IJ}} + \sum_i^n \sum_{j>i}^n \frac{e^2}{4\pi\varepsilon_0 r_{ij}} \qquad (1.4)$$

By substituting equations 1.3—without the nuclear portion—and 1.4 into equation 1.1, we reduce the complexity of the Schrödinger equation. However, problems still arise from the electron-electron repulsion term. In 1928, Hartree proposed that it is also possible to rewrite the electronic wave function, $\psi(r_1, \dots, r_n)$, as the product of n functions dependent in the position coordinates of one electron each.

$$\psi(r_1, \dots, r_n) = \phi_1(r_1)\phi_2(r_2) \dots \phi_n(r_n) \qquad (1.5)$$

This reinterpretation of the electronic wave function would allow for an exact solution of the Schrödinger equation if the electron-electron repulsion term was negligible. Hartree replaced this term with an effective field (V_i^{eff}) that describes the repulsion felt by an electron from the average position of other electrons. Under these assumptions, the separable functions, ϕ_i, satisfy the Hartree equations.

Because the separable wavefunction employed by Hartree does not satisfy the Pauli exclusion principle, Fock suggested the utilization of a Slater determinant, which satisfies Pauli's principle due to being antisymmetric.

To take into account the electron correlation term, several methods have been employed, one such method being perturbation theory. The basic idea is that the mathematical function to be solved is broken into two—or more—parts, by solving a similar function and adding corrections (perturbations) to it until it matches the desired function. Møller and Plesset

applied perturbation theory to the solution of the Schrödinger equation by dividing the Hamiltonian into two parts, one corresponding to the Hartree-Fock Hamiltonian and the other to the instantaneous electron correlation, the perturbation. Depending on the order of the correction applied, the perturbations can be labeled MP2, MP3, or MP4.

Geometric calculations are performed by quantum mechanical programs by varying the positions of the atoms in the molecule and calculating an energy using the *ab initio* algorithm that was chosen. Once the energy between iterations does not longer changes significantly, it is said that molecular structure has been optimized. This procedure is known as the self-consistent field.

Vibrational spectra are calculated by calculating the matrix of second derivatives of molecular energy with respect to the coordinates of the system, which is known as the Hessian matrix. Because of this, if a molecular structure is not located at an energy minimum, imaginary frequencies appear in the calculated spectrum, as the location of the vibrational bands is the square-root of the second derivatives.

Boiling Point Estimation

Estimation of boiling points of pure substances and mixtures has been the subject of various studies.[30,31,32] The significance of knowing the boiling point of a chemical is due to the fact that knowing this value, chemists are able to determine at which temperature a substance exists as a liquid, get an idea of its volatility and also determine its vapor pressure. Throughout the decades several estimation methods have been developed and a good summary was made by Lyman.[33] In this section, we review the boiling point estimation method developed by Lai *et al* (1987),[34] known as the Nonlinear Group-Contribution Model. Regarded as 'likely the most

accurate boiling point estimation method using a nonlinear group contribution method' by Lyman, the Lai method is also likely one of the most difficult to implement.

Based solely on experimental data—which makes it an empirical method—Lai *et al* developed a method to estimate a temperature range in which the boiling point of a molecule can be found depending on the number of carbon atoms in the molecule (Eq. 1.6).

$$T_b = \left(a + b_c \frac{1-r_c^n}{1-r_c}\right) \quad (1.6)$$

After this value is determined, higher accuracy is achieved by taking into consideration other molecular structural features such as the number and position of functional groups in the molecule, branching, and the presence and number of rings—aromatic or otherwise—and multiple bonds. Lai and coworkers also took into consideration conjugation and whether cis and trans conformations are present.

After determining the presence of any of the features above listed, new terms are added to Equation 1.6 to correct for their presence. Each term is composed by a unique set of characteristic constants, which were determined by fitting experimental data. It is important to note that Lai et al also differentiates between compounds purely composed of carbon and hydrogen atoms and those in which hydrogen-bonding groups are present. So while each correction term has a unique set of characteristic constants, these will also vary depending on what type of groups are present in the molecule.

As an example, we show the calculation of the boiling point of the methamphetamine molecule (Figure 1.1).

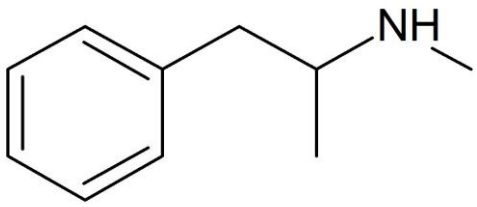


Figure 1.1. Methamphetamine structure.

Inspection of the methamphetamine structure determines that we need the following correction terms in addition to Equation 1.6:

1. NH group correction
2. NH group position correction
3. Three-way branch correction
4. Aromatic ring correction for hydrogen-bonding compound

The equations corresponding to these terms are written as follows:

$$T_b = \left(a + b_c \frac{1-r_c^n}{1-r_c}\right) + \left(b_f + b_{fc} \frac{1-r_c^n}{1-r_c}\right) \qquad (1.7)$$

$$a_{hb,i} = \beta_i \qquad (1.8)$$

$$a_{hf} = \lambda_i \xi'_{ij}; \quad \xi'_{ij} = 1 - \frac{P_{ij}-2}{\frac{(MC+1)}{2}-2} \qquad (1.9)$$

$$a'_{hr,i} = \alpha'_i \qquad (1.10)$$

Where P_{ij} corresponds to the position of the NH functional group and MC to the length of the main chain containing the secondary amine. All other variables are the characteristic constants listed in Lai. After substituting the appropriate values for this molecule, the terms have the following values: $T_b = 474.85$, $a_{hb,i} = -9.50$, $a_{hf} = 7.40$, and $a'_{hr,i} = 5.01$. Adding these values, $T_b = 477.76$ K = 204.63 °C. The experimental value as listed in the CRC Handbook of Chemistry and Physics (96th Edition)[35] is 212.00 °C, yielding an error percent of 3.48%.

CHAPTER 2

IR CALCULATIONS, MASS SPECTRA SIMULATION, AND GUI FOR SIMPLE CALCULATIONS USING PYTHON FOR PREDICTION AND NEW DRUG IDENTIFICATION

Introduction

While there is no shortage in the number of software packages available to calculate molecular properties based on quantum and molecular mechanical (QM/MM) principles, a quick literature search reveals that their application is mostly limited to conducting fundamental physical, chemical and biological research in supercomputing setups. Examples include: studies of force and stress in condensed phase systems[36], mechanistic investigations of organic reactions[37], and conformational and structural research of inorganic biochemical compounds.[38] Indeed, very little effort is being made to expand the number of questions addressed with computational chemistry methods beyond classical chemical problems.

Forensic science represents an area in which theoretical methods can bring clarity to experimental findings. Already, a number of papers have been published in which computational methods aided in the assignment of experimental vibrational spectra and the identification and characterization of synthetic precursors of illegal drugs.[39,40,41,42,43] Other instances in which quantum chemistry has been helpful to forensic research include the investigation of the interaction of saxitoxin with sodium channels, the characterization of fingerprint identification reactions, and the confirmation and differentiation of by-products resulting from MDMA synthesis.[28]

As the amount of chemical information available to the forensic scientist grows thanks to both experiment and theory, so does the need for the creation of a database in which all

these data can be stored for future reference and comparison of known and unknown compounds. The present work encompasses an effort in its early stages to produce such a library. Here, we propose the utilization of computational chemistry methods, coupled to a greater extend with experimental data, to increase the information readily available for the rapid identification and scheduling of drugs and their corresponding derivatives in the form of a database. In addition, because QM/MM programs often have a 'steep learning curve' due to their lack of user-friendly interfaces and require computational knowledge beyond what could be considered common, we include a graphical user interface (GUI) under development to make the creation of input files for the software package GAMESS more accessible to the average computer user. The interface contains preloaded optimized structures of a few controlled substances, some of which can be altered by the user through modification of the functional groups attached to the backbone of the molecule at different positions.

By making theoretical structural information and vibrational spectra available in this manner, we seek to highlight the applicability of computational chemistry to forensic research, and to complement the chemical data obtained from affinity chromatography and PAMPA-BBB.[44] Furthermore, with the inclusion of our GUI, we want to set the stage for the development of new platforms that will bridge the gap between the computational chemical and forensic fields, and meet the needs of an audience beyond that of the traditional physical sciences.

For the purpose of our project, we have performed a complete conformational analysis—structure optimization and vibrational frequency calculation—of the following molecules: eight amphetamines, two phenethylamines, DMCPA, and two tryptamines. In

addition, structure optimizations were completed for other two phenethylamine species and seventeen tryptamine derivatives. Comparison of predicted fragmentation of a small set of tryptamines to ESI-MS experimental data for characterization purposes is also discussed.

Computational Methods

All calculations were performed in the gas phase using the GAMESS[45,46] quantum mechanical software package. Optimization of molecular geometries and calculations of infrared spectra were carried out using the MP2/6-311++G[47] method and basis set, respectively. Optimized ground state structures were verified by the existence of no imaginary frequencies in the calculated vibrational spectra. Both, three-dimensional molecular images and vibrational spectra were generated using Chemcraft[48] with a Lorentzian band width of 10 at half the height. The animation feature of Chemcraft was used for vibrational modes assignment. Molecular structures were built using the Avogadro (v1.0) software package.[49] All structures were pre-optimized using Avogadro's 'Optimize Geometry' built-in molecular mechanical-based feature before performing an optimization under the *ab initio* framework.

In silico characterization of the ESI-MS data was performed using the ACD/MS Fragmenter 2015 Pack 2 (Toronto, ON, Canada).[50] This software package predicts ion fragmentation based on general fragmentation rules. Results were obtained by taking into consideration hydrogen and hydride shifts, double bond cleavage, saturated ring cleavage, resonance reactions, and ring formations only. In addition, all the options found in the Specific Fragmentation tab involving homolytic and heterolytic bond cleavage were checked. ESI was selected as the protonation technique and CID/CAD as the fragmentation activation. Furthermore, charges were removed whenever possible and the option to cleave all bonds was

selected towards the bottom of the Reactions tab. For this analysis, a maximum of one thousand fragments were generated in one fragmentation step. One fragmentation step was sufficient to match the experimental data.

The graphical user-interface for the generation of GAMESS input files was created using the Python 3.4.3 (64-bit) programming language and the JetBrains PyCharm development environment (Community Edition, v5.0.1). The backbone structures included in this interface were created using the Avogadro (v1.0) software package and optimized using GAMESS. Structural images were generated using the Chemcraft software package.

Results and Discussion

The set of compounds studied are listed in Table 2.1. This series of derivatives was designed by placing hydrocarbon chains in place of the hydrogens attached to the amine nitrogen, when applicable. In the case of tryptamine-like species, the hydrocarbons were placed in the nitrogen located in the side chain of tryptamine.

Table 2.1 List of studied compounds

amphetamine
methylamphetamine
N,N-dimethylamphetamine
N-ethyl-N-methylamphetamine
N,N-dimethylamphetamine
N-ethyl-N-propylamphetamine
N,N-dipropylamphetamine
N-isopropyl-N-propylamphetamine
phenethylamine
N-butylphenethylamine
N-hexylphenethylamine
N-octylphenethylamine

(table continues)

Table 2.1 *(continued)*

4-methyl-2,5-methoxyphenylcyclopropylamine
tryptamine
N-methyltryptamine
N,N-dimethyltryptamine
N-ethyl-N-methyltryptamine
N,N-diethyltryptamine
N-ethyl-N-propyltryptamine
N,N-dipropyltryptamine
N-butyltryptamine
N-butyl-N-propyltryptamine
N,N-dibutyltryptamine
N-butyl-N-pentyltryptamine
N-butyl-N-hexyltryptamine
N-butyl-N-octyltryptamine
N,N-dipentyltryptamine
N-hexyl-N-pentyltryptamine
N,N-dihexyltryptamine
N-heptyl-N-hexyltryptamine
N,N-diheptyltryptamine
N-heptyl-N-octyltryptamine

Optimized Structures and Vibrational Spectra

Detailed structural information—optimized coordinates and bonding details—can be found in Tables 2.2-2.29, where harmonic frequencies are also included. Furthermore, a depiction of the optimized compounds and their vibrational spectra can be seen in Figures 2.1-2.5.

Careful consideration of the amphetamine derivatives optimized geometries (Figure 2.1) reveals that they deviate very little from the accepted conformation of amphetamine and amphetamine-like molecules,[51] with side chains pointing away from the ring portion of the

structures. The average carbon-carbon double bond length is 1.41 Å in the aromatic ring and side-chain single carbon-carbon bonds are generally longer, ranging from 1.51 to 1.56 Å. Carbon-nitrogen bond lengths remain constant at about 1.48-1.49 Å, with the amine nitrogen retaining its sp^3 character in the amphetamine series as indicated by its tetrahedral geometry.

Relative bond orders are also in agreement with what is considered acceptable within the chemical community regarding bonding in organic compounds.[52] C—C double bonds have a higher bond order (ca. 1.2 A.U.) relative to the single C—C and C—N bonds present in the molecules. C—H bonds have a similar bond order to that of other single bonds in the structures and possess an average length between 1.09 and 1.10 Å. It is important to note the C—N bonds that connect the amine nitrogen with the hydrocarbon substituents have the lowest bond orders within the amphetamine series, indicative of the weakness of those single bonds. What this implies in terms of the reactivity of these compounds at the active site remains to be considered. The complete data set including optimized geometries and vibrational spectra for all amphetamine species can be found in Tables 2.2 – 2.17.

A much greater wealth of information can be extracted from the systematic analysis of the vibrational spectra of the amphetamine family. In general, there are three key vibrational regions within each spectrum that contain information needed to identify and differentiate between amphetamine species. The first region, located at around 500 cm^{-1}, shows vibrational bands corresponding to twisting and wagging modes of both the amine nitrogen and the C—H ring bonds. Initially, the amine twisting vibration appears at 194.21 cm^{-1} in the amphetamine spectrum (Fig. 2.2a), however, with the addition of the hydrocarbon substituents at this position, this mode is significantly blue-shifted to around 430 cm^{-1} for subsequent

amphetamines. Similarly, the signal corresponding to the ring twisting mode is at first found at 472.56 cm^{-1}, which also shifts to higher frequencies as more methyl groups are added to the molecule and eventually couples with the ring wagging mode for N,N-diethylamphetamine (Fig. 2.2a) and up.

The next mode of interest in this region of the spectrum corresponds to the ring wagging mode, which remains located at around 630 cm^{-1} throughout the series and only shifts to a lower energy from 650.35 cm^{-1} when a methyl group is added to the amine nitrogen of the initial amphetamine molecule. In the same manner, the amine wagging mode is located at 764.81 cm^{-1} in the amphetamine spectrum but it is later found at lower frequencies (ca. 680 cm^{-1}) for other derivatives. It is important to point out that the location of this mode can aid in the discrimination between methamphetamine and disubstituted amphetamine derivatives, as its signal in the methamphetamine spectrum is located at about half-way (711.52 cm^{-1}) between its positions in the amphetamine and the other spectra.

The second region useful for identification purposes is located at around 1700 cm^{-1} and is characterized by a single vibrational mode that corresponds to a primary amine scissoring. This mode can be found at 1739.22 cm^{-1} in the amphetamine spectrum and it owes its significance to the fact that it is absent from the vibrational spectra of the other molecules in the series.

The last region of importance is found at around 3500 cm^{-1}, where the primary and secondary amine stretching modes are located. Visible in Figure 2.2b, these vibrational modes are present at 3460.68 and 3469.12 cm^{-1}, respectively. When compared to vibrational spectra of disubstituted amphetamines, these modes are missing, given that the other amphetamine

species only possess a tertiary amine with less freedom of movement. Because of this, further discrimination between amphetamine species is also possible.

As a final remark regarding the family of amphetamine species, it is important to note that the spectrum corresponding to N-isopropyl-N-propylamphetamine (Fig. 2.2a) is particularly different in the region that corresponds to the twisting and wagging modes. This spectrum is different from the others in that only the amine twisting and ring wagging modes in the spectrum are visible at first glance. The apparent absence of the ring twisting mode is consistent with other amphetamine species in which the energy of this vibration increases enough to match and be overshadowed by the ring wagging mode. The missing amine wagging signal can be explained by considering the bulkiness of the isopropyl group attached to the amine nitrogen and how its presence limits movement in this region of the molecule. Furthermore, it is clear from the spectra shown in Figure 2.2 that data acquired by other means is required in order to differentiate between amphetamine species with hydrocarbon chains longer than two methyl groups, as there is very little variation between the spectra corresponding to the N,N-dimethylamphetamine through the N,N-dipropylamphetamine species.

The following set of molecules is comprised of four phenethylamines (Figures 2.3). Here we present the full analysis—optimization plus frequency calculation—of only two molecules due to time constraints in the completion of this stage of the project. Optimized structures for the set of four are, however, included. For detail structural data see Tables 2.18-2.23

The phenethylamine (PEA) species also show a conformational preference consistent with experimental findings.[53] Compared to the amphetamines, PEAs also possess a

hydrocarbon side chain attached to a benzene ring, albeit with more flexibility. Nevertheless, this section of the molecules remains directed away from the benzene ring, as opposed to bending towards it.

In terms of bond lengths, the PEA family retains the values present in the amphetamine species, with double C—C bonds averaging 1.41 Å and C—C single bonds 1.54 Å. C—N and C—H single bonds also show no difference, as their calculated length is also about 1.48 Å and 1.10 Å, respectively. Bond orders remain consistent: C—C double bonds have the highest bond orders at around 1.2 – 1.3 A.U. and C—N single bonds have the lowest ranging from 0.6 – 0.8 A.U. depending on the species, providing further evidence of structural weakness in the molecules at this position.

Careful consideration of the vibrational spectra of phenethylamine and N-butylphenethylamine (Fig. 2.5a) shows four major areas of differentiation between species. First, in the region below 500 cm^{-1}, the vibration corresponding to an amine twist located at 199.79 cm^{-1} undergoes a shift to 280.07 cm^{-1} when the butyl group is attached to the amine N in PEA. Second, a strong signal grows in the N-butylphenethylamine spectrum just above 1000 cm^{-1} (1166.43 cm^{-1}). This band also corresponds to an amine twisting mode that, though present in the phenethylamine spectrum, is obvious in the N-butylphenethylamine spectrum thanks also to the addition of the hydrocarbon chain.

The third area of interest is the peak located at 1742.89 cm^{-1} in the phenethylamine spectrum. This mode represents the primary amine scissoring and is absent from the N-butylphenethylamine spectrum due to the lack of this structural feature in this molecule. Finally, other amine modes located at around 3500 cm^{-1} can also be considered as comparison

points between the two PEA structures. Two signals corresponding to the symmetric and antisymmetric stretching modes of the amine are present in the phenethylamine spectrum at 3487.44 and 3613.81 cm^{-1}, respectively. Because N-butylphenethylamine only possesses a secondary amine, only one band is found at 3483.47 cm^{-1} (Fig. 2.5b).

From the comparison of the vibrational spectra of the two PEA molecules, it is clear that the major points to be considered in the discrimination between species are those directly related to the presence, or lack thereof, of the primary amine harmonic frequencies. Other modes involving ring and side chain twisting and wagging are present in both spectra, which would make differentiation at these regions (470 – 790 cm^{-1} and 2930 – 3150 $cm^{-}1$) more challenging.

In this study, we also performed a complete conformational analysis of the 4-methyl-2,5-methoxyphenylcyclopropylamine molecule (DMCPA). All the structural and spectral data corresponding to this molecule can be found in Tables 2.24 and 2.25. The optimized DMCPA structure is illustrated in Figure 2.3. The lowest energy conformation of DMCPA is also characterized by bond lengths and orders widely agreed upon.[54] The average double C—C bond length is 1.41 Å in the section of the molecule corresponding to the benzene ring. C—C single bonds average around 1.52 Å and C—O and C—N single bonds range from 1.41 to 1.47 Å. C—H bonds are also consistent with the values of species above described (ca. 1.09 – 1.10 Å). Detailed consideration of the data provided in Table 2.25 shows that the C—C double bonds also have the highest bond order value (1.2 A.U.), with single bonds showing comparable strengths. An exception to this are the O11—C12 and the O14—C15 single bonds, which are longer (1.47 Å) and weaker (B.O. about 0.3) than expected. A possible explanation for this is the

close proximity of the hydrogen atoms attached to these carbons to the lone pairs on the oxygens and the delocalized electron density around the ring, although how exactly this would lead to the elongation of the O—C bonds is not clear and has not been studied.

The vibrational spectra of DMCPA (Fig 2.5) shows five major features in the portion of the spectrum corresponding to 500 – 1750 cm^{-1}. The 620 cm^{-1} to 850 cm^{-1} region corresponds to wagging and twisting modes of various parts of the molecule. The most intense peak at 704.52 cm^{-1} is an amine wagging mode. Next, at 1010.95 cm^{-1}, an aromatic ring twisting mode is located and the strong bands at 1218.39, 1406.09 and 1533.6 cm^{-1} represent combined scissoring vibrations of several structural components. The single peak at 1742.07 cm^{-1} is the primary amine scissoring mode. Above 3400 cm^{-1}, the antisymmetric and symmetric primary amine stretch modes can be seen at 3487.64 and 3613.75 cm^{-1}, respectively.

The last set of molecular species studied in this project belong to the tryptamine family. This series of structures represented a computational challenge because finding an equilibrium geometry for each structure proved to be a difficult task to undertake due to the flexibility of the tryptamine side chain. Here we discuss the geometry and spectra of the near-equilibrium tryptamine and the optimized N,N-dibutyltryptamine structures. The problems faced in the determination of ground state geometries for tryptamine derivatives are addressed in the next section of this chapter.

Continuing the trend seen so far in this study, the bond lengths and orders of the tryptamine derivatives considered in this section (tryptamine and N,N-dibutyltryptamine, see Figure 2.4) also agree with the literature on the subject.[55] Carbon—carbon double bonds in the indole ring have an average length of 1.4 Å and a bond order of about 1.2 A.U. C—C single

bonds and C—N measure about 1.55 Å and 1.48 Å, respectively, with the C—N bond in the indole ring being the shortest of them at 1.40 Å. Bond orders for these bonds also remain constant, taking values ranging from 0.74 to 0.92 in both molecules. The weaker bonds are once again the C—N bonds, however, in the case of tryptamine these correspond to the C—N bonds in the indole ring, whereas for N,N-dibutyltryptamine, they correspond to the C—N bonds at the side-chain amine nitrogen.

A calculation of the vibrational spectrum of tryptamine was attempted after 250 optimization cycles—the equivalent of 5 optimization jobs—were performed in order to determine whether the tryptamine was close to an energy minima or not. While the calculated spectrum of tryptamine here presented is not suitable for inclusion in our database for not meeting our convergence criteria, the data obtained does provide a point of comparison against the spectrum of the optimized N,N-dibutyltryptamine structure, as no imaginary frequencies were found in the set of harmonics of the near-equilibrium tryptamine molecule. Detailed structural information for both molecules can be found in Tables 2.26-2.29.

Once again, there are three regions of importance in both the tryptamine and N,N-dibutyltryptamine spectra (Fig. 2.5). the first region encompasses the set of wagging and twisting modes of the molecule. The first major difference in this portion of the spectra corresponds to the primary side chain amine wagging, this mode is located at about 150.41 cm^{-1}, with a related vibration at 222.39 cm^{-1}. These peaks are clearly absent from the N,N-dibutyltryptamine spectrum, given that N,N-dibutyltryptamine no longer possesses a primary amine. Similarly, the N,N-dibutyltryptamine spectrum features a strong signal at 412.77 cm^{-1} produced by a wagging of the indole nitrogen. This band is not present in the tryptamine

spectrum. It is not why this would be the case, although the rigidity and bulkiness of N,N-dibutyltryptamine could play a role.

The next region of interest for identification purposes corresponds to the primary amine scissoring mode located at 1740.85 cm^{-1} in the tryptamine spectrum. This band is not present in the N,N-dibutyltryptamine vibrational signature because it does not possess a primary amine.

Finally, also concerning amine modes, tryptamine and N,N-dibutyltryptamine can be differentiated in the spectral region around 3400 cm^{-1}. The tryptamine spectrum contains two bands at 3493.56 and 3620.21 cm^{-1}, corresponding to the antisymmetric and symmetric amine stretches, respectively. Because N,N-dibutyltryptamine only has one secondary amine in the indole ring, only one stretching mode signal is seen it its corresponding spectrum. This band is found at 3614 cm^{-1}.

As a final remark for this section, and in order to emphasize the wealth of information that computations can provide, it is important to point out that careful inspection of the C—H bond lengths for each molecule shows an elongation of this bond when located in a periplanar fashion to the lone pairs of the amine nitrogen in the side chains. This is also the case in DMCPA, where the nitrogen is connected to the cyclopropane ring. A possible explanation for this observation is that the arrangement of the atoms in this manner facilitates the flow of electron density from the C—H sigma bond toward the electronegative N atom, leading to the lengthening of the bond.

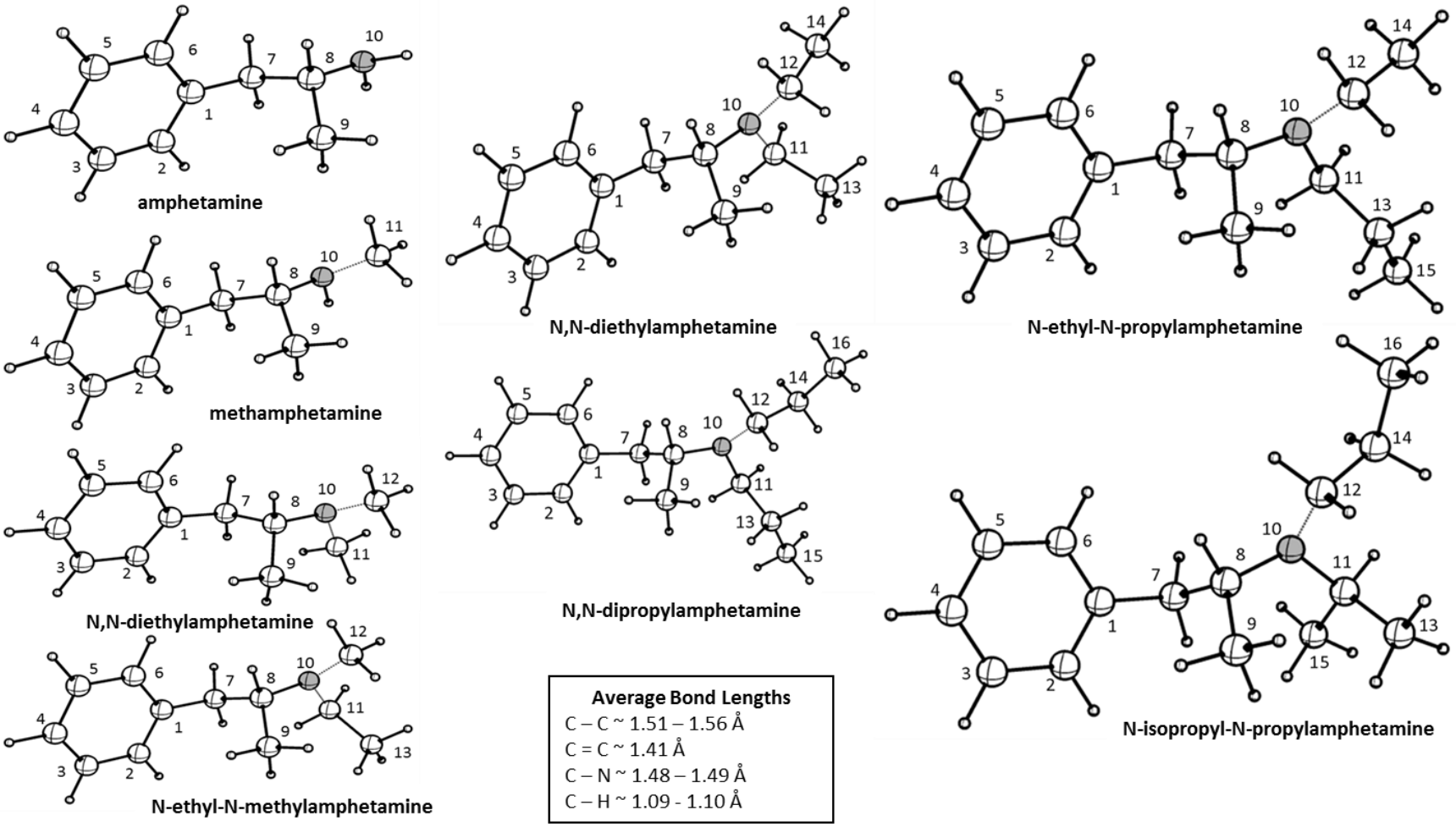


Figure 2.1. Optimized structures of amphetamine derivatives

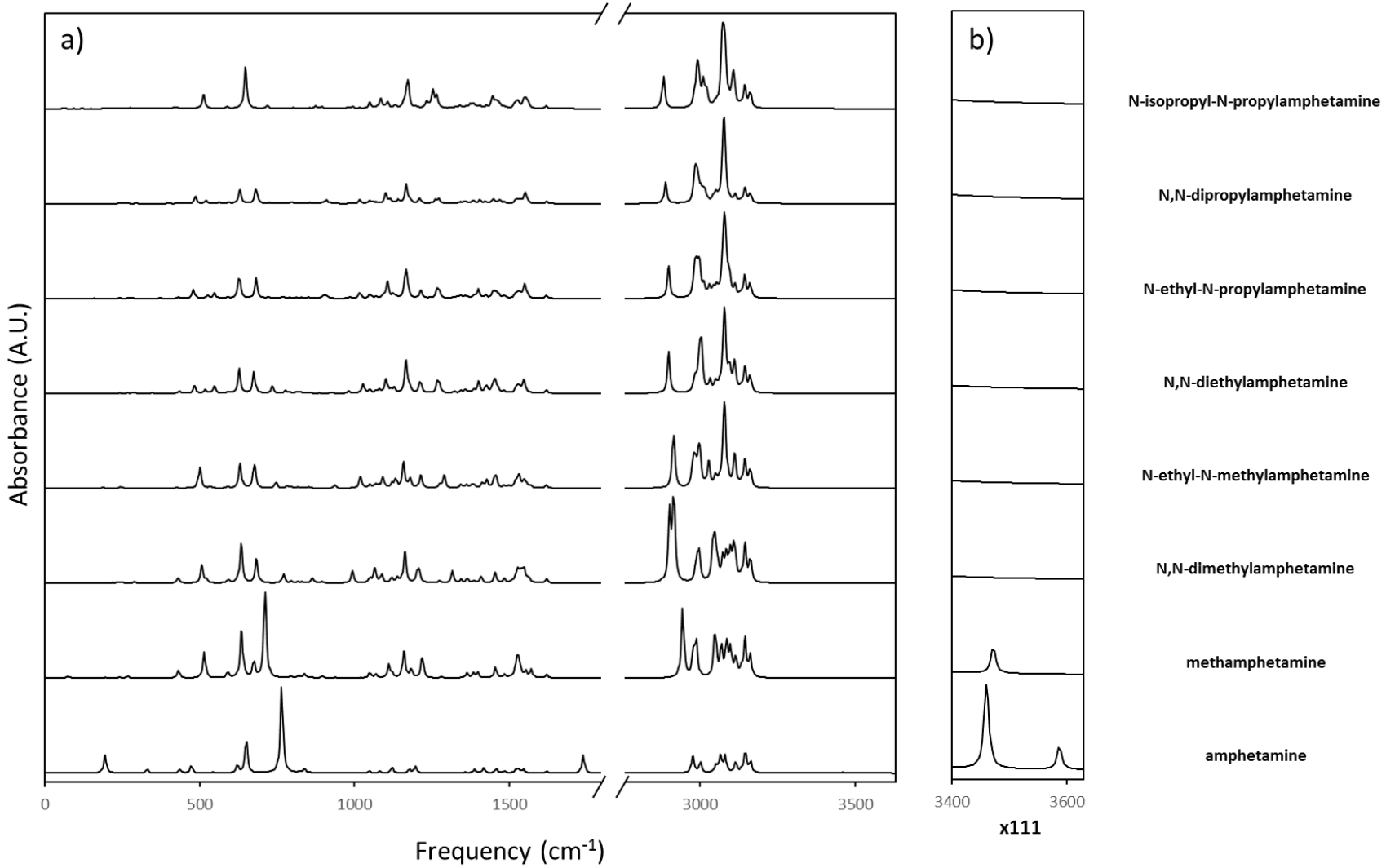
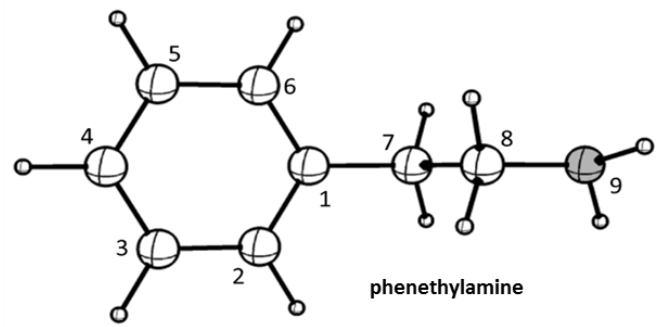
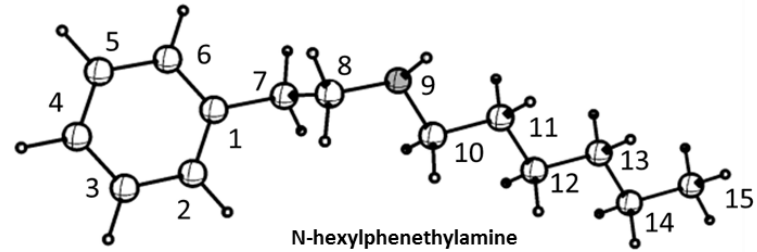
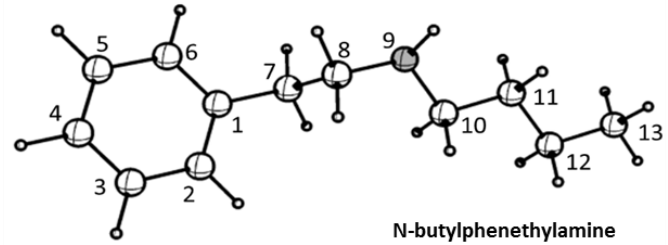
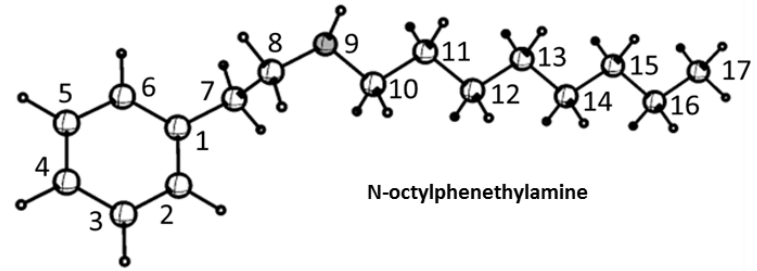


Figure 2.2. a) Vibrational spectra of amphetamine derivatives at the MP2/6-311++G level of theory. b) Zoom into the 3400 - 3630 cm^{-1} region shows side chain amine stretching modes.

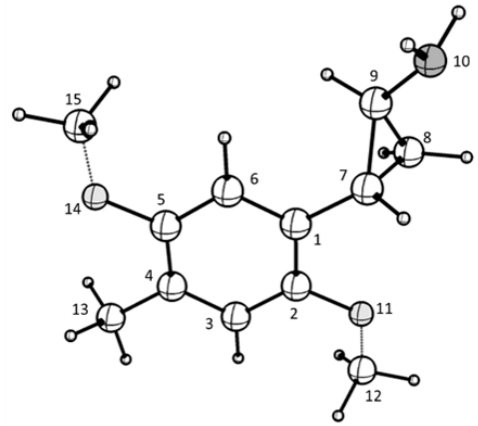






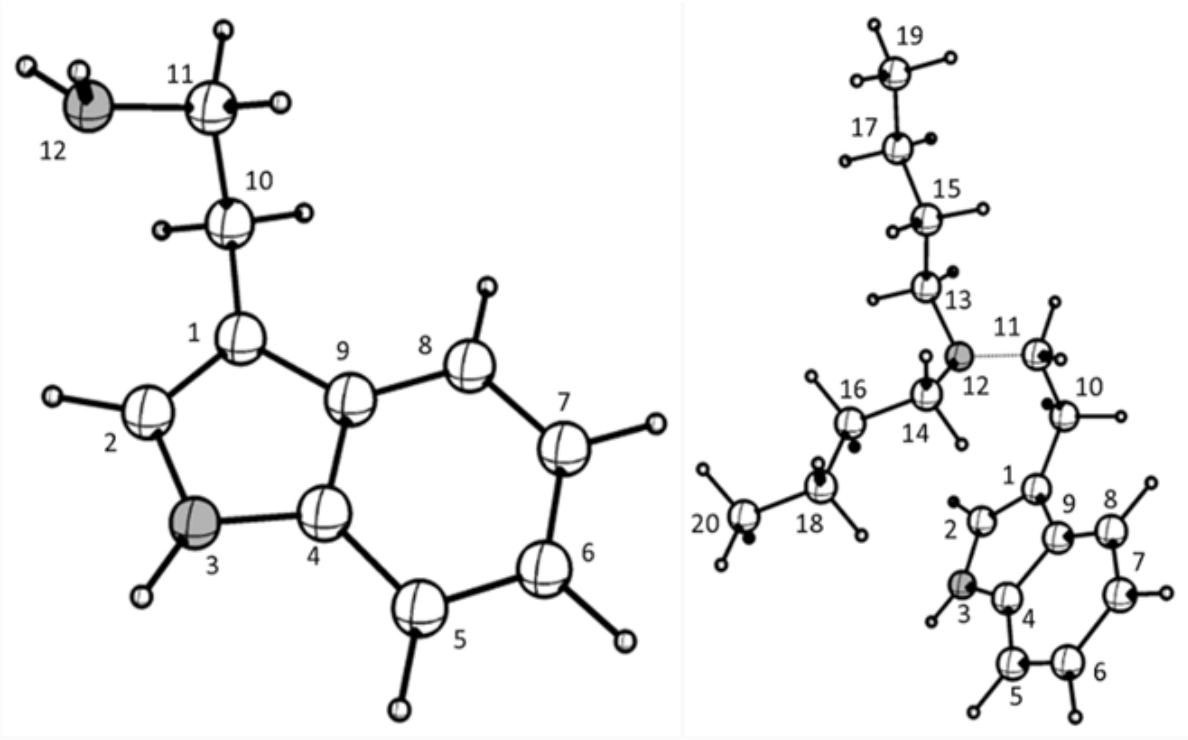


Average Bond Lengths (PEAs)
C – C ~ 1.54 Å
C = C ~ 1.41 Å
C – N ~ 1.48 Å
C – H ~ 1.10 Å



Average Bond Lengths (DMCPA)
C – C ~ 1.52 Å
C = C ~ 1.41 Å
C – N ~ 1.41 – 1.47 Å
C – H ~ 1.09 – 1.10 Å
C – O ~ 1.47 Å

Figure 2.3. Optimized structures of PEA derivatives and DMCPA.



tryptamine **N,N-dibutyltryptamine**

Average Bond Lengths
C – C ~ 1.55 Å
C = C ~ 1.41 Å
C – N ~ 1.48 Å
C – H ~ 1.09 – 1.10 Å

Figure 2.4. Optimized structure of N,N-dibutyltryptamine and near-equilibrium geometry of tryptamine.

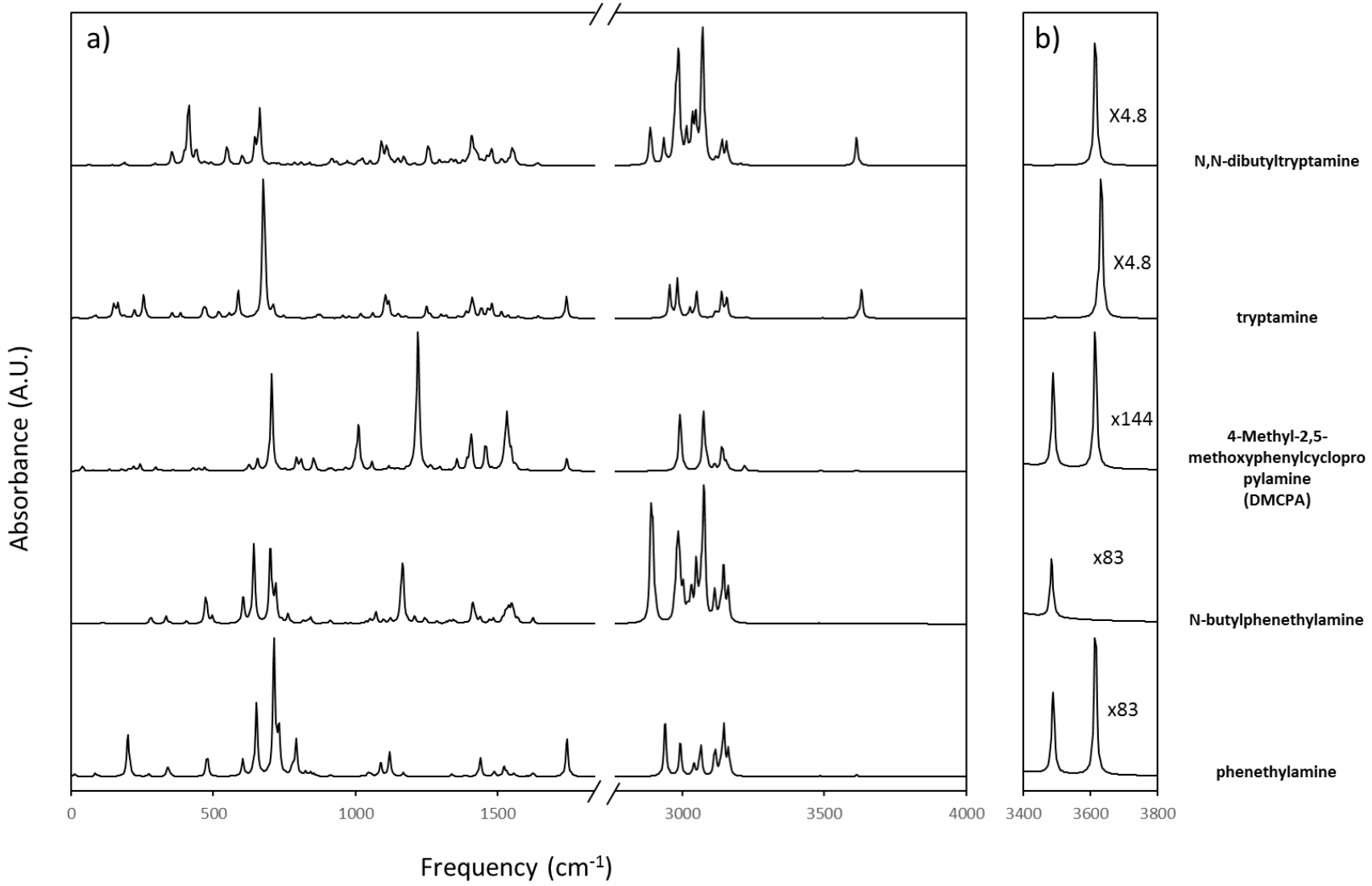


Figure 2.5. a) Calculated vibrational spectrum of a series of organic molecules at the MP2/6-311++G level of theory. b) Zoom into the 3400 - 4000 cm^{-1} region shows side chain amine stretching modes.

Table 2.2 Amphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-0.90818	1.43007	-0.76550
C	6.0	-1.90859	0.45518	-0.95194
C	6.0	-1.94731	-0.68176	-0.12199
C	6.0	-0.92759	-0.88308	0.83046
C	6.0	0.06964	0.09360	1.01120
C	6.0	0.11882	1.24005	0.18455
H	1.0	-2.69819	0.62244	-1.68159
H	1.0	-2.71421	-1.43898	-0.26854
H	1.0	-0.95852	-1.75267	1.48373
H	1.0	0.85066	-0.06215	1.75605
H	1.0	-0.87905	2.30578	-1.41407
C	6.0	1.24663	2.24213	0.33864
C	6.0	2.60309	1.70595	-0.17852
N	7.0	3.63371	2.74624	0.06970
H	1.0	4.58404	2.43149	-0.10920
H	1.0	3.44062	3.61908	-0.41793
H	1.0	1.37214	2.52247	1.39246
H	1.0	0.99490	3.15721	-0.22236
C	6.0	2.51250	1.25040	-1.65036
H	1.0	2.88263	0.84053	0.43962
H	1.0	3.49525	0.90991	-2.00084
H	1.0	2.19148	2.09026	-2.28372
H	1.0	1.79732	0.42791	-1.77120

Table 2.3 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized amphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
7.93	0.01	C1—C2	1.41	1.27
40.13	0.01	C2—C3	1.41	1.24
64.53	0.01	C3—C4	1.41	1.25
89.24	0.01	C4—C5	1.41	1.24
194.21	1.08	C5—C6	1.41	1.26
227.92	0.02	C6—C1	1.41	1.22
254.69	0.03	C1—C7	1.52	0.78
330.49	0.21	C7—C8	1.55	0.88

(table continues)

Table 2.3 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
349.04	0.02	C8—C9	1.54	0.84
370.65	0.01	C8—N10	1.49	0.95
393.75	0.04	C2—H11	1.09	0.85
436.18	0.20	C3—H12	1.09	0.84
472.56	0.42	C4—H13	1.09	0.84
543.27	0.04	C5—H14	1.09	0.85
621.86	0.41	C6—H15	1.09	0.85
643.72	0.06	C7—H16	1.10	0.85
650.35	1.78	C7—H17	1.10	0.89
726.03	0.02	C8—H18	1.10	0.85
764.81	4.92	C9—H19	1.10	0.89
773.33	0.10	C9—H20	1.10	0.89
804.72	0.04	C9—H21	1.10	0.89
821.98	0.06	N10—H22	1.02	0.79
839.04	0.23	N10—H23	1.02	0.82
857.49	0.02			
896.51	0.01			
979.61	0.02			
1019.26	0.03			
1046.15	0.04			
1049.17	0.08			
1081.91	0.14			
1121.89	0.33			
1177.61	0.21			
1197.36	0.38			
1247.86	0.01			
1299.74	0.02			
1359.13	0.05			
1378.49	0.01			
1387.66	0.21			
1417.67	0.30			
1458.99	0.26			
1485.44	0.10			
1520.58	0.15			
1528.17	0.18			
1533.69	0.06			

(table continues)

Table 2.3 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1546.28	0.21			
1600.37	0.01			
1621.97	0.11			
1739.22	1.01			
2974.65	0.59			
2977.82	0.49			
3000.63	0.58			
3050.33	0.40			
3065.22	0.99			
3080.05	0.95			
3113.08	0.28			
3115.00	0.28			
3133.84	0.15			
3145.43	1.11			
3162.44	0.62			
3460.68	0.06			
3587.38	0.02			

Table 2.4 Methylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-0.97279	1.39886	-0.78081
C	6.0	-1.98462	0.42809	-0.92142
C	6.0	-1.94459	-0.74624	-0.14529
C	6.0	-0.94957	-0.89430	0.84243
C	6.0	0.05733	0.07978	0.97686
C	6.0	0.03650	1.25981	0.19698
H	1.0	-2.75235	0.55141	-1.68270
H	1.0	-2.72935	-1.49280	-0.24481
H	1.0	-0.91746	-1.79565	1.45127
H	1.0	0.81450	-0.03181	1.75337
H	1.0	-1.00905	2.30724	-1.38223
C	6.0	1.15245	2.27757	0.33110
C	6.0	2.50959	1.75687	-0.19998
N	7.0	3.53354	2.80483	0.04156

(table continues)

Table 2.4 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	4.94508	2.37373	-0.08029
H	1.0	3.33737	3.63871	-0.51348
H	1.0	1.29133	2.56372	1.38172
H	1.0	0.88241	3.18680	-0.23034
C	6.0	2.40774	1.29939	-1.67206
H	1.0	2.80815	0.89424	0.41631
H	1.0	3.38521	0.97364	-2.04760
H	1.0	2.05367	2.13290	-2.29675
H	1.0	1.70547	0.46450	-1.77922
H	1.0	5.58988	3.22725	0.14908
H	1.0	5.21972	1.98387	-1.07496
H	1.0	5.13367	1.59296	0.66412

Table 2.5 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized methylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
8.23	0.01	C1—C2	1.41	1.26
44.21	0.01	C2—C3	1.41	1.23
72.12	0.05	C3—C4	1.41	1.25
83.37	0.02	C4—C5	1.41	1.24
196.58	0.02	C5—C6	1.41	1.25
212.30	0.01	C6—C1	1.41	1.21
241.74	0.03	C1—C7	1.52	0.80
267.94	0.06	C7—C8	1.55	0.85
317.87	0.01	C8—C9	1.54	0.85
359.24	0.01	C8—N10	1.48	1.02
429.14	0.05	N10—C11	1.48	0.35
432.34	0.18	C2—H12	1.09	0.86
514.34	0.75	C3—H13	1.09	0.84
591.01	0.16	C4—H14	1.09	0.84
635.19	1.45	C5—H15	1.09	0.84
644.41	0.01	C6—H16	1.09	0.85
674.81	0.44	C7—H17	1.10	0.85
711.52	2.49	C7—H18	1.10	0.90

(table continues)

Table 2.5 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
761.25	0.01	C8—H19	1.10	0.84
795.98	0.05	C9—H20	1.10	0.89
816.21	0.04	C9—H21	1.10	0.90
824.74	0.04	C9—H22	1.10	0.89
838.65	0.13	N10—H23	1.02	0.79
861.11	0.03	C11—H24	1.10	0.96
896.64	0.06	C11—H25	1.09	0.91
938.70	0.02	C11—H26	1.10	0.90
1019.93	0.01			
1048.93	0.14			
1055.73	0.02			
1069.43	0.11			
1110.93	0.38			
1121.26	0.11			
1160.08	0.83			
1183.10	0.24			
1218.77	0.60			
1224.87	0.01			
1281.59	0.04			
1342.85	0.01			
1363.46	0.16			
1384.69	0.14			
1398.80	0.16			
1455.53	0.30			
1484.72	0.10			
1500.72	0.03			
1518.96	0.18			
1526.80	0.28			
1527.81	0.30			
1533.82	0.13			
1537.53	0.14			
1554.23	0.20			
1571.11	0.23			
1600.06	0.01			
1621.63	0.11			
2943.26	2.00			

(table continues)

Table 2.5 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
2974.94	0.25			
2979.81	0.53			
2987.91	0.92			
3046.25	0.84			
3050.28	0.56			
3068.11	0.80			
3085.16	0.93			
3097.94	0.78			
3114.03	0.30			
3115.48	0.23			
3133.17	0.19			
3144.67	1.14			
3161.57	0.62			
3469.12	0.02			

Table 2.6 N,N-dimethylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.01177	1.34474	-0.73479
C	6.0	-1.99984	0.35041	-0.87927
C	6.0	-1.92019	-0.83483	-0.12294
C	6.0	-0.90949	-0.97298	0.85016
C	6.0	0.07451	0.02400	0.98770
C	6.0	0.01378	1.21537	0.22753
H	1.0	-2.77982	0.46590	-1.62922
H	1.0	-2.68672	-1.59975	-0.22515
H	1.0	-0.84688	-1.88276	1.44389
H	1.0	0.84385	-0.08030	1.75333
H	1.0	-1.07888	2.26161	-1.32049
C	6.0	1.10587	2.25981	0.36072
C	6.0	2.45727	1.77062	-0.21869
N	7.0	3.52850	2.76488	0.08438
C	6.0	4.88272	2.17068	0.11278
C	6.0	3.49079	3.99319	-0.74088

(table continues)

Table 2.6 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	1.26980	2.51614	1.41596
H	1.0	0.78919	3.17336	-0.16311
C	6.0	2.33833	1.38416	-1.71193
H	1.0	2.74166	0.86836	0.34388
H	1.0	3.32100	1.12720	-2.12763
H	1.0	1.91527	2.21027	-2.29937
H	1.0	1.68068	0.51505	-1.82794
H	1.0	5.58570	2.92270	0.48654
H	1.0	5.23654	1.83116	-0.88080
H	1.0	4.88441	1.31913	0.80013
H	1.0	2.49085	4.43329	-0.70909
H	1.0	3.77278	3.81753	-1.79663
H	1.0	4.19550	4.71403	-0.31306

Table 2.7 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N,N-dimethylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
73.88	0.01	C1—C2	1.41	1.24
88.51	0.01	C2—C3	1.41	1.23
218.75	0.02	C3—C4	1.41	1.24
234.50	0.02	C4—C5	1.41	1.24
243.74	0.01	C5—C6	1.41	1.25
251.53	0.02	C6—C1	1.41	1.22
289.13	0.05	C1—C7	1.52	0.78
354.51	0.01	C7—C8	1.55	0.81
428.03	0.05	C8—C9	1.55	0.78
431.45	0.12	C8—N10	1.49	0.78
507.19	0.57	N10—C11	1.48	0.50
521.03	0.08	N10—C12	1.48	0.44
592.54	0.10	C2—H13	1.09	0.85
633.60	1.22	C3—H14	1.09	0.84
644.36	0.01	C4—H15	1.09	0.84
683.66	0.75	C5—H16	1.09	0.84
770.93	0.26	C6—H17	1.09	0.86

(table continues)

Table 2.7 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
797.34	0.06	C7—H18	1.10	0.84
818.08	0.04	C7—H19	1.10	0.93
831.34	0.03	C8—H20	1.10	0.88
861.46	0.03	C9—H21	1.10	0.89
865.01	0.14	C9—H22	1.10	0.89
896.39	0.05	C9—H23	1.10	0.90
993.57	0.39	C11—H24	1.09	0.92
1019.77	0.01	C11—H25	1.10	0.91
1049.66	0.14	C11—H26	1.11	0.95
1065.35	0.40	C12—H27	1.09	0.95
1068.88	0.08	C12—H28	1.10	0.93
1087.29	0.24	C12—H29	1.11	0.90
1120.21	0.14			
1138.84	0.16			
1162.57	1.00			
1201.99	0.27			
1209.26	0.20			
1209.55	0.15			
1245.68	0.02			
1275.30	0.08			
1316.79	0.37			
1344.94	0.11			
1364.88	0.12			
1387.25	0.06			
1408.62	0.21			
1454.75	0.33			
1483.67	0.13			
1509.04	0.05			
1520.43	0.11			
1527.28	0.15			
1528.02	0.18			
1533.97	0.15			
1540.13	0.23			
1547.56	0.36			
1559.25	0.10			
1566.05	0.09			

(table continues)

Table 2.7 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1599.92	0.01			
1620.88	0.13			
2901.36	2.08			
2914.70	2.39			
2987.22	0.07			
2988.90	0.58			
2996.37	0.81			
3040.10	0.88			
3047.43	1.08			
3054.08	0.44			
3072.88	0.69			
3084.88	0.73			
3096.52	0.81			
3107.51	0.85			
3113.25	0.31			
3115.43	0.26			
3132.98	0.18			
3144.63	1.13			
3161.49	0.64			

Table 2.8 N-ethyl-N-methylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.06085	1.27901	-0.70629
C	6.0	-2.05070	0.28207	-0.81465
C	6.0	-1.96704	-0.88025	-0.02370
C	6.0	-0.94957	-0.99104	0.94579
C	6.0	0.03625	0.00848	1.04722
C	6.0	-0.02841	1.17656	0.25205
H	1.0	-2.83615	0.37643	-1.56189
H	1.0	-2.73485	-1.64707	-0.09823
H	1.0	-0.88429	-1.88271	1.56616
H	1.0	0.81112	-0.07392	1.80999
H	1.0	-1.13066	2.17841	-1.31837

(table continues)

Table 2.8 *(continued)*

Atom	Nuclear charge	X	Y	Z	
C	6.0		1.06564	2.22287	0.34675
C	6.0		2.40591	1.72613	-0.25725
N	7.0		3.49228	2.69584	0.03602
C	6.0		4.83523	2.09460	0.13572
C	6.0		3.46126	4.00861	-0.65410
H	1.0		1.25461	2.48875	1.39550
H	1.0		0.73503	3.13142	-0.17721
C	6.0		2.24644	1.32047	-1.74291
H	1.0		2.68828	0.82155	0.30471
H	1.0		3.21705	1.04929	-2.17644
H	1.0		1.81544	2.14400	-2.32821
H	1.0		1.57719	0.45608	-1.83150
H	1.0		5.53967	2.86809	0.46446
H	1.0		5.21558	1.66138	-0.80840
H	1.0		4.81298	1.30437	0.89433
H	1.0		2.41152	4.31284	-0.73113
C	6.0		4.13259	4.09854	-2.04692
H	1.0		3.95439	4.72874	0.01582
H	1.0		4.06171	5.12985	-2.41800
H	1.0		3.65282	3.43905	-2.77536
H	1.0		5.19588	3.83727	-1.98851

Table 2.9 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N-ethyl-N-methylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
70.67	0.01	C1—C2	1.41	1.24
111.75	0.01	C2—C3	1.41	1.23
186.80	0.05	C3—C4	1.41	1.25
241.18	0.01	C4—C5	1.41	1.24
245.19	0.05	C5—C6	1.41	1.25
260.37	0.01	C6—C1	1.41	1.22
297.98	0.01	C1—C7	1.52	0.77
317.89	0.01	C7—C8	1.55	0.82
354.69	0.01	C8—C9	1.55	0.78

(table continues)

Table 2.9 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
426.01	0.03	C8—N10	1.49	0.74
462.65	0.02	N10—C11	1.48	0.55
500.14	0.85	N10—C12	1.47	0.37
533.95	0.06	C11—C13	1.55	0.94
591.72	0.06	C2—H14	1.09	0.86
630.84	1.02	C3—H15	1.09	0.84
644.27	0.01	C4—H16	1.09	0.84
676.66	0.96	C5—H17	1.09	0.84
746.55	0.22	C6—H18	1.08	0.86
761.93	0.01	C7—H19	1.10	0.84
782.65	0.08	C7—H20	1.10	0.93
795.85	0.05	C8—H21	1.10	0.89
816.61	0.04	C9—H22	1.10	0.88
830.07	0.02	C9—H23	1.10	0.90
850.05	0.04	C9—H24	1.10	0.91
858.82	0.03	C11—H24	1.10	0.89
889.62	0.01	C11—H25	1.10	0.89
936.76	0.12	C12—H26	1.10	0.94
1018.54	0.24	C12—H27	1.10	0.95
1021.16	0.26	C12—H28	1.11	0.91
1049.58	0.14	C13—H29	1.09	0.86
1068.36	0.15	C13—H30	1.10	0.92
1078.69	0.09	C13—H31	1.10	0.89
1092.46	0.44			
1121.26	0.17			
1133.16	0.31			
1158.90	1.06			
1179.32	0.37			
1213.71	0.54			
1224.30	0.01			
1245.30	0.02			
1275.89	0.14			
1289.86	0.55			
1344.73	0.15			
1362.04	0.15			
1380.14	0.13			

(table continues)

Table 2.9 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1387.75	0.09			
1412.80	0.19			
1427.15	0.33			
1450.64	0.17			
1456.38	0.45			
1484.35	0.11			
1499.09	0.09			
1513.50	0.03			
1520.98	0.17			
1527.36	0.10			
1530.03	0.27			
1533.26	0.21			
1547.03	0.20			
1550.05	0.12			
1557.45	0.13			
1569.47	0.08			
1599.64	0.01			
1620.73	0.14			
2914.08	2.09			
2975.49	0.49			
2981.05	0.75			
2985.54	0.42			
2994.23	1.06			
2999.87	0.99			
3026.79	1.03			
3049.50	0.38			
3060.50	0.20			
3073.32	0.43			
3077.20	1.71			
3079.71	0.59			
3081.36	1.32			
3110.30	0.85			
3112.83	0.32			
3114.59	0.26			
3132.72	0.17			

(table continues)

Table 2.9 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
3144.28	1.12			
3161.33	0.66			

Table 2.10 N,N-diethylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.07186	1.42017	-0.52875
C	6.0	-2.15364	0.53330	-0.69778
C	6.0	-2.12051	-0.73866	-0.09399
C	6.0	-1.05073	-1.07680	0.75955
C	6.0	0.02678	-0.18598	0.92238
C	6.0	0.01301	1.09063	0.31337
H	1.0	-2.97876	0.80322	-1.35391
H	1.0	-2.95839	-1.42165	-0.21491
H	1.0	-1.02329	-2.05485	1.23592
H	1.0	0.84385	-0.44543	1.59626
H	1.0	-1.10210	2.40460	-0.99613
C	6.0	1.20254	2.01922	0.46515
C	6.0	2.44678	1.51219	-0.31247
N	7.0	3.63247	2.34859	0.01886
C	6.0	4.92717	1.63275	-0.05559
C	6.0	3.64786	3.73296	-0.52588
H	1.0	1.48917	2.10826	1.52169
H	1.0	0.91976	3.01998	0.10785
C	6.0	2.14682	1.33160	-1.82015
H	1.0	2.68688	0.51862	0.09729
H	1.0	3.05400	1.03150	-2.35932
H	1.0	1.76519	2.26319	-2.25981
H	1.0	1.38752	0.55350	-1.96572
H	1.0	2.60885	4.08060	-0.53971
C	6.0	4.27771	3.93802	-1.92546
H	1.0	4.17850	4.36903	0.19530
H	1.0	4.22152	5.00182	-2.19350
H	1.0	3.75546	3.36430	-2.69627

(table continues)

Table 2.10 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	5.33479	3.64849	-1.93635
C	6.0	6.02958	2.36672	0.72364
H	1.0	5.26128	1.45541	-1.09745
H	1.0	4.75827	0.65006	0.40186
H	1.0	6.31699	3.30748	0.24152
H	1.0	6.92624	1.73780	0.79172
H	1.0	5.67337	2.58577	1.73640

Table 2.11 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N,N-diethylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
68.94	0.01	C1—C2	1.41	1.24
100.26	0.01	C2—C3	1.41	1.23
123.00	0.01	C3—C4	1.41	1.25
174.35	0.02	C4—C5	1.41	1.24
222.03	0.01	C5—C6	1.41	1.25
240.94	0.02	C6—C1	1.41	1.22
266.90	0.02	C1—C7	1.52	0.76
284.78	0.04	C7—C8	1.55	0.82
293.26	0.01	C8—C9	1.55	0.77
345.67	0.02	C8—N10	1.49	0.75
351.60	0.01	N10—C11	1.49	0.47
433.73	0.09	N10—C12	1.48	0.47
482.82	0.34	C11—C13	1.55	0.92
517.31	0.15	C12—C14	1.54	0.98
546.93	0.32	C2—H15	1.09	0.86
591.46	0.06	C3—H16	1.09	0.84
627.43	1.06	C4—H17	1.09	0.84
644.20	0.01	C5—H18	1.09	0.84
675.37	0.91	C6—H19	1.09	0.86
734.96	0.32	C7—H20	1.10	0.84
759.38	0.01	C7—H21	1.10	0.92
777.44	0.12	C8—H22	1.10	0.89

(table continues)

Table 2.11 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
791.69	0.04	C9—H23	1.10	0.88
811.78	0.05	C9—H24	1.10	0.89
821.23	0.04	C9—H25	1.10	0.91
828.41	0.03	C11—H26	1.10	0.89
853.96	0.02	C11—H27	1.10	0.89
854.12	0.02	C12—H28	1.10	0.93
887.74	0.02	C12—H29	1.11	0.88
926.24	0.04	C13—H30	1.09	0.87
982.29	0.10	C13—H31	1.10	0.90
1019.34	0.02	C13—H33	1.10	0.90
1028.66	0.39	C14—H34	1.10	0.88
1049.29	0.14	C14—H35	1.10	0.90
1070.00	0.09	C14—H36	1.10	0.91
1079.83	0.14			
1102.25	0.62			
1117.26	0.12			
1128.78	0.23			
1166.74	1.41			
1176.33	0.23			
1212.65	0.49			
1224.12	0.01			
1245.26	0.02			
1267.53	0.44			
1275.19	0.36			
1322.51	0.06			
1344.21	0.12			
1358.16	0.15			
1368.44	0.05			
1378.78	0.01			
1386.29	0.12			
1400.61	0.52			
1425.85	0.31			
1445.10	0.18			
1451.13	0.19			
1455.76	0.44			
1461.55	0.13			

(table continues)

Table 2.11 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1484.45	0.11			
1518.77	0.05			
1522.12	0.11			
1526.63	0.14			
1531.24	0.21			
1537.00	0.07			
1546.10	0.34			
1548.47	0.22			
1552.43	0.04			
1557.09	0.02			
1564.42	0.03			
1599.71	0.01			
1620.62	0.14			
2898.22	1.80			
2979.28	0.14			
2984.58	0.43			
2993.53	0.45			
2997.40	0.51			
2999.07	0.84			
3004.75	1.71			
3031.37	0.47			
3050.00	0.39			
3061.52	0.24			
3072.75	0.58			
3077.47	1.30			
3079.28	1.82			
3082.23	0.46			
3094.48	0.86			
3109.44	0.84			
3112.58	0.32			
3114.31	0.25			
3132.48	0.17			
3144.08	1.12			
3161.17	0.67			

Table 2.12 N-ethyl-N-propylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.07704	1.38016	-0.55063
C	6.0	-2.16038	0.49232	-0.70424
C	6.0	-2.13903	-0.76056	-0.06103
C	6.0	-1.07935	-1.07654	0.81355
C	6.0	-0.00001	-0.18518	0.96069
C	6.0	-0.00201	1.07214	0.31229
H	1.0	-2.97755	0.74477	-1.37719
H	1.0	-2.97797	-1.44418	-0.17023
H	1.0	-1.06110	-2.03953	1.32029
H	1.0	0.80934	-0.42737	1.65027
H	1.0	-1.09818	2.34991	-1.04848
C	6.0	1.18944	2.00082	0.44884
C	6.0	2.43814	1.46598	-0.30230
N	7.0	3.63026	2.29065	0.03281
C	6.0	4.91754	1.56007	-0.02834
C	6.0	3.66531	3.67288	-0.51089
H	1.0	1.46677	2.12066	1.50500
H	1.0	0.91353	2.99131	0.05854
C	6.0	2.15631	1.26680	-1.81126
H	1.0	2.65998	0.47562	0.12548
H	1.0	3.06786	0.95249	-2.33491
H	1.0	1.78792	2.19556	-2.26822
H	1.0	1.39221	0.49298	-1.95620
H	1.0	2.63098	4.03893	-0.52768
C	6.0	4.29310	3.88412	-1.91072
H	1.0	4.20714	4.30457	0.20872
C	6.0	4.26295	5.37530	-2.30759
H	1.0	3.74998	3.29202	-2.65581
H	1.0	5.33291	3.53008	-1.90757
C	6.0	6.02587	2.29731	0.73938
H	1.0	5.25117	1.36148	-1.06648
H	1.0	4.73759	0.58691	0.44552
H	1.0	6.32686	3.22295	0.23642
H	1.0	6.91413	1.65889	0.82614
H	1.0	5.66805	2.54419	1.74520

(table continues)

Table 2.12 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	4.73005	5.53708	-3.28620
H	1.0	4.80162	5.98277	-1.56846
H	1.0	3.22854	5.73976	-2.36073

Table 2.13 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N-ethyl-N-propylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
62.91	0.01	C1—C2	1.41	1.24
116.65	0.01	C2—C3	1.41	1.23
160.96	0.01	C3—C4	1.41	1.25
206.28	0.01	C4—C5	1.41	1.24
239.89	0.02	C5—C6	1.41	1.25
268.17	0.02	C6—C1	1.41	1.23
279.24	0.04	C1—C7	1.52	0.75
329.26	0.01	C7—C8	1.55	0.81
351.46	0.01	C8—C9	1.55	0.77
371.65	0.02	C8—N10	1.49	0.73
375.19	0.01	N10—C11	1.49	0.62
431.82	0.07	N10—C12	1.48	0.44
479.97	0.45	C11—C13	1.55	0.85
525.88	0.14	C12—C14	1.54	0.95
547.47	0.29	C13—C15	1.54	0.90
590.80	0.05	C2—H16	1.09	0.86
627.51	1.07	C3—H17	1.09	0.84
644.06	0.01	C4—H18	1.09	0.84
682.10	1.06	C5—H19	1.09	0.84
722.76	0.07	C6—H20	1.09	0.86
769.20	0.09	C7—H21	1.10	0.84
790.44	0.05	C7—H22	1.10	0.92
810.62	0.04	C8—H23	1.10	0.89
823.26	0.02	C9—H24	1.10	0.88
829.16	0.04	C9—H25	1.10	0.90
850.88	0.02	C9—H26	1.10	0.90
851.99	0.05	C11—H27	1.10	0.87

(table continues)

Table 2.13 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
885.60	0.03	C11—H28	1.10	0.88
899.87	0.13	C12—H29	1.10	0.94
909.72	0.14	C12—H30	1.11	0.88
984.77	0.06	C13—H31	1.10	0.85
1016.70	0.26	C13—H32	1.10	0.89
1019.55	0.02	C14—H33	1.10	0.89
1048.62	0.10	C14—H34	1.10	0.87
1052.00	0.11	C14—H35	1.10	0.92
1070.14	0.10	C15—H36	1.10	0.90
1095.09	0.11	C15—H37	1.10	0.90
1106.54	0.86	C15—H38	1.10	0.89
1125.10	0.17			
1134.81	0.07			
1166.27	1.44			
1174.41	0.21			
1214.14	0.42			
1224.05	0.01			
1244.91	0.02			
1267.16	0.38			
1272.94	0.31			
1317.88	0.05			
1330.85	0.07			
1343.03	0.13			
1357.81	0.14			
1366.09	0.04			
1372.30	0.02			
1386.47	0.12			
1400.63	0.47			
1423.77	0.15			
1447.28	0.11			
1450.48	0.27			
1459.02	0.22			
1466.94	0.16			
1484.09	0.12			
1517.68	0.02			
1521.38	0.16			

(table continues)

Table 2.13 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1526.88	0.16			
1532.28	0.02			
1534.17	0.23			
1539.81	0.04			
1549.07	0.30			
1550.97	0.18			
1551.86	0.23			
1556.05	0.10			
1562.87	0.01			
1599.17	0.01			
1620.35	0.15			
2898.03	1.72			
2977.44	0.18			
2982.76	0.65			
2986.22	1.17			
2993.14	0.95			
2998.37	1.21			
3012.20	0.57			
3028.90	0.52			
3042.65	0.40			
3053.04	0.45			
3057.56	0.03			
3070.65	0.86			
3076.98	1.52			
3077.25	1.26			
3081.19	1.28			
3084.42	1.02			
3093.30	0.89			
3111.73	0.31			
3113.44	0.27			
3132.08	0.16			
3143.27	1.11			
3160.87	0.68			

Table 2.14 N,N-dipropylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.11785	1.37731	-0.55909
C	6.0	-2.19366	0.48005	-0.71108
C	6.0	-2.16127	-0.77180	-0.06648
C	6.0	-1.09776	-1.07821	0.80682
C	6.0	-0.02560	-0.17784	0.95169
C	6.0	-0.03913	1.07887	0.30245
H	1.0	-3.01398	0.72530	-1.38267
H	1.0	-2.99508	-1.46209	-0.17341
H	1.0	-1.07116	-2.04010	1.31502
H	1.0	0.78649	-0.41251	1.64060
H	1.0	-1.14728	2.34600	-1.05841
C	6.0	1.14376	2.01839	0.43844
C	6.0	2.39938	1.49095	-0.30588
N	7.0	3.58224	2.32978	0.02827
C	6.0	4.87567	1.61252	-0.01769
C	6.0	3.60710	3.70544	-0.53420
H	1.0	1.41664	2.14619	1.49477
H	1.0	0.86067	3.00475	0.04277
C	6.0	2.12593	1.28200	-1.81505
H	1.0	2.62910	0.50499	0.12765
H	1.0	3.04119	0.96571	-2.33098
H	1.0	1.75896	2.20747	-2.27996
H	1.0	1.36378	0.50611	-1.95937
H	1.0	2.56690	4.05195	-0.58232
C	6.0	4.26491	3.90416	-1.92180
H	1.0	4.11996	4.35735	0.18877
C	6.0	4.22337	5.38838	-2.34294
H	1.0	3.74753	3.29266	-2.67005
H	1.0	5.30936	3.56531	-1.88866
C	6.0	5.97458	2.34341	0.77194
H	1.0	5.23094	1.42323	-1.05171
H	1.0	4.70263	0.63407	0.45106
H	1.0	6.21307	3.30035	0.28870
C	6.0	7.25884	1.49719	0.89024
H	1.0	5.57014	2.56676	1.76827

(table continues)

Table 2.14 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	4.70761	5.54070	-3.31480
H	1.0	4.74000	6.01460	-1.60348
H	1.0	3.18564	5.73882	-2.42204
H	1.0	7.65857	1.25263	-0.10257
H	1.0	7.05289	0.55717	1.41813
H	1.0	8.03641	2.03426	1.44604

Table 2.15 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N,N-dipropylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
59.07	0.01	C1—C2	1.41	1.24
207.87	0.01	C2—C3	1.41	1.23
226.19	0.01	C3—C4	1.41	1.25
239.54	0.01	C4—C5	1.41	1.24
245.20	0.03	C5—C6	1.41	1.25
266.20	0.04	C6—C1	1.41	1.22
288.35	0.01	C1—C7	1.52	0.76
297.60	0.02	C7—C8	1.55	0.81
347.37	0.01	C8—C9	1.55	0.78
399.50	0.03	C8—N10	1.49	0.69
430.88	0.05	N10—C11	1.49	0.58
485.88	0.54	N10—C12	1.48	0.50
519.66	0.23	C11—C13	1.55	0.83
562.56	0.11	C12—C14	1.54	0.85
593.57	0.08	C13—C15	1.54	0.88
629.51	1.07	C14—C16	1.54	0.90
644.08	0.02	C2—H17	1.09	0.85
682.04	1.08	C3—H18	1.09	0.84
724.25	0.06	C4—H19	1.09	0.84
754.97	0.01	C5—H20	1.09	0.84
756.70	0.01	C6—H21	1.09	0.86
786.77	0.02	C7—H22	1.10	0.84
796.43	0.10	C7—H23	1.10	0.92
808.02	0.04	C8—H24	1.10	0.90

(table continues)

Table 2.15 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
828.00	0.02	C9—H25	1.10	0.88
848.74	0.03	C9—H26	1.10	0.90
857.51	0.06	C9—H27	1.10	0.89
885.14	0.01	C11—H28	1.10	0.97
898.45	0.08	C11—H29	1.10	0.87
909.39	0.24	C12—H30	1.10	0.97
921.55	0.05	C12—H31	1.11	0.87
939.23	0.01	C13—H32	1.10	0.85
1016.23	0.28	C13—H33	1.10	0.88
1019.62	0.03	C14—H34	1.10	0.87
1047.81	0.01	C14—H35	1.10	0.85
1049.06	0.20	C15—H36	1.10	0.91
1060.75	0.12	C15—H37	1.10	0.90
1070.93	0.07	C15—H38	1.10	0.90
1101.60	0.79	C16—H39	1.10	0.90
1115.48	0.25	C16—H40	1.10	0.89
1128.74	0.04	C16—H41	1.10	0.89
1142.08	0.26			
1167.48	1.38			
1178.73	0.22			
1209.21	0.01			
1211.32	0.39			
1223.80	0.01			
1244.69	0.02			
1260.96	0.25			
1272.76	0.36			
1306.29	0.05			
1323.74	0.02			
1331.47	0.02			
1342.61	0.11			
1356.12	0.14			
1362.87	0.06			
1371.16	0.01			
1378.59	0.01			
1382.86	0.16			
1388.40	0.07			

(table continues)

Table 2.15 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1404.47	0.26			
1423.14	0.14			
1443.67	0.03			
1449.31	0.32			
1466.78	0.17			
1469.64	0.11			
1484.03	0.12			
1517.67	0.02			
1521.35	0.18			
1526.63	0.15			
1528.78	0.02			
1532.33	0.11			
1538.47	0.12			
1544.79	0.04			
1550.46	0.27			
1550.83	0.08			
1551.06	0.29			
1555.45	0.18			
1559.06	0.11			
1599.37	0.01			
1620.37	0.15			
2887.60	1.55			
2977.84	0.16			
2981.72	0.51			
2982.61	0.20			
2985.02	1.10			
2987.85	1.08			
2993.19	0.93			
3001.91	0.73			
3009.98	0.60			
3016.84	0.62			
3041.13	0.31			
3046.98	0.15			
3052.13	0.45			
3056.41	0.05			

(table continues)

Table 2.15 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
3070.09	0.83			
3074.48	1.40			
3076.20	1.45			
3076.86	1.82			
3078.43	1.27			
3082.20	1.11			
3112.10	0.31			
3114.10	0.27			
3132.29	0.17			
3144.15	1.10			
3161.12	0.68			

Table 2.16 N-isopropyl-N-propylamphetamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.19670	1.05711	-0.52427
C	6.0	-2.11889	-0.00596	-0.59871
C	6.0	-1.95235	-1.14018	0.21934
C	6.0	-0.81132	-1.24508	1.04080
C	6.0	0.10767	-0.18083	1.10694
C	6.0	-0.04434	0.96186	0.28704
H	1.0	-3.00397	0.08739	-1.22482
H	1.0	-2.65884	-1.96503	0.15882
H	1.0	-0.68463	-2.11127	1.68710
H	1.0	0.98312	-0.26143	1.75269
H	1.0	-1.33142	1.93555	-1.15596
C	6.0	0.99387	2.06888	0.31763
C	6.0	2.27595	1.65804	-0.46159
N	7.0	3.48689	2.41256	-0.00948
C	6.0	4.69513	1.54194	0.01522
C	6.0	3.76051	3.78984	-0.52972
H	1.0	1.28892	2.29015	1.35204
H	1.0	0.55268	2.97706	-0.10981
C	6.0	2.02091	1.60078	-1.98783

(table continues)

Table 2.16 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	2.48955	0.62524	-0.14640
H	1.0	2.93167	1.30598	-2.52344
H	1.0	1.67879	2.56735	-2.37711
H	1.0	1.24293	0.85535	-2.19943
C	6.0	5.88015	2.14798	0.78513
H	1.0	5.03158	1.24532	-1.00039
H	1.0	4.39396	0.62420	0.53706
H	1.0	6.33513	2.96799	0.21461
C	6.0	6.95666	1.08474	1.08850
H	1.0	5.48807	2.56715	1.72191
H	1.0	7.32302	0.62495	0.16136
H	1.0	6.54436	0.29172	1.72505
H	1.0	7.81361	1.52758	1.60916
C	6.0	2.55595	4.73087	-0.36041
C	6.0	4.33826	3.87736	-1.96843
H	1.0	4.53765	4.17185	0.14539
H	1.0	3.57125	3.70677	-2.72997
H	1.0	5.14754	3.15325	-2.12246
H	1.0	4.75520	4.88201	-2.12646
H	1.0	1.74941	4.50295	-1.06593
H	1.0	2.88053	5.76312	-0.54780
H	1.0	2.16802	4.66908	0.66133

Table 2.17 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N-isopropyl-N-propylamphetamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
119.51	0.01	C1—C2	1.41	1.23
238.28	0.02	C2—C3	1.41	1.22
247.85	0.02	C3—C4	1.41	1.25
277.10	0.05	C4—C5	1.41	1.23
289.85	0.01	C5—C6	1.41	1.24
307.47	0.01	C6—C1	1.41	1.21
330.94	0.02	C1—C7	1.52	0.72
347.89	0.01	C7—C8	1.56	0.82

(table continues)

Table 2.17 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
419.65	0.08	C8—C9	1.55	0.82
430.57	0.03	C8—N10	1.50	0.58
497.13	0.02	N10—C11	1.49	0.54
512.80	0.74	N10—C12	1.50	0.63
575.11	0.01	C11—C13	1.55	0.87
588.39	0.08	C12—C14	1.54	0.85
647.19	2.06	C11—C15	1.54	0.90
654.73	0.06	C14—C16	1.54	0.85
717.72	0.16	C2—H17	1.09	0.85
738.30	0.01	C3—H18	1.09	0.84
760.53	0.01	C4—H19	1.09	0.84
777.72	0.01	C5—H20	1.09	0.84
803.62	0.04	C6—H21	1.09	0.86
833.93	0.02	C7—H22	1.10	0.86
853.86	0.03	C7—H23	1.10	0.90
874.66	0.12	C8—H24	1.10	0.90
894.09	0.11	C9—H25	1.10	0.91
918.22	0.02	C9—H26	1.10	0.88
938.53	0.03	C9—H27	1.10	0.89
977.31	0.06	C11—H28	1.10	0.85
993.44	0.09	C12—H29	1.10	1.01
1018.01	0.03	C12—H30	1.11	0.86
1048.69	0.14	C13—H31	1.10	0.88
1050.56	0.18	C13—H32	1.09	0.87
1072.20	0.07	C13—H33	1.10	0.92
1085.40	0.50	C14—H34	1.10	0.88
1106.35	0.33	C14—H35	1.10	0.88
1130.95	0.15	C15—H36	1.09	0.92
1159.08	0.23	C15—H37	1.10	0.88
1166.23	0.13	C15—H38	1.10	0.85
1172.21	1.35	C16—H39	1.10	0.90
1198.93	0.08	C16—H40	1.10	0.91
1234.09	0.33	C16—H41	1.10	0.89
1244.48	0.06			
1253.10	0.88			
1266.60	0.62			

(table continues)

Table 2.17 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1312.89	0.04			
1326.59	0.07			
1342.09	0.15			
1360.96	0.11			
1375.84	0.22			
1385.05	0.16			
1393.08	0.07			
1405.89	0.12			
1425.99	0.13			
1445.20	0.25			
1448.30	0.36			
1457.39	0.22			
1464.67	0.22			
1471.99	0.10			
1484.50	0.10			
1517.10	0.17			
1525.01	0.20			
1528.05	0.16			
1531.84	0.07			
1532.85	0.01			
1542.73	0.05			
1547.52	0.22			
1549.79	0.11			
1550.62	0.07			
1556.17	0.35			
1559.09	0.03			
1562.94	0.10			
1599.37	0.01			
1620.04	0.14			
2881.47	1.59			
2979.98	0.20			
2988.17	0.28			
2988.69	1.10			
2992.28	0.90			
2996.38	0.56			
2998.55	0.18			

(table continues)

Table 2.17 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
3009.11	0.31			
3010.91	0.92			
3019.99	0.65			
3048.20	0.17			
3066.72	0.24			
3070.05	1.98			
3072.04	0.68			
3075.57	1.54			
3078.77	0.51			
3080.84	1.57			
3084.99	0.47			
3101.49	0.34			
3106.33	1.08			
3108.99	0.40			
3112.48	0.34			
3132.16	0.13			
3143.84	1.09			
3161.23	0.71			

Table 2.18 Phenethylamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-0.74926	1.35609	-0.81066
C	6.0	-1.78455	0.42501	-1.02092
C	6.0	-1.89455	-0.70354	-0.18520
C	6.0	-1.03635	-0.83448	0.92425
C	6.0	-0.00410	0.10120	1.12817
C	6.0	0.12244	1.23654	0.29559
H	1.0	-2.44642	0.53434	-1.87757
H	1.0	-2.70036	-1.41779	-0.33788
H	1.0	-1.11814	-1.70211	1.57569
H	1.0	0.64851	0.00372	1.99585
H	1.0	-0.67679	2.23394	-1.45293
C	6.0	1.26635	2.21300	0.49304

(table continues)

Table 2.18 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	2.53289	1.78313	-0.27932
N	7.0	3.62343	2.76328	-0.07191
H	1.0	4.54511	2.42704	-0.33162
H	1.0	3.43394	3.67628	-0.47509
H	1.0	1.52013	2.28671	1.55778
H	1.0	0.95604	3.21169	0.15121
H	1.0	2.87267	0.81800	0.11511
H	1.0	2.26395	1.63538	-1.33944

Table 2.19 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized phenethylamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
11.97	0.04	C1—C2	1.41	1.21
13.32	0.03	C2—C3	1.41	1.25
84.79	0.08	C3—C4	1.41	1.25
95.84	0.02	C4—C5	1.41	1.25
199.79	1.01	C5—C6	1.41	1.25
272.34	0.06	C6—C1	1.41	1.23
340.21	0.23	C1—C7	1.52	0.82
351.49	0.02	C7—C8	1.54	0.86
477.86	0.45	C8—N9	1.48	0.80
603.47	0.38	C2—H10	1.09	0.86
651.07	1.72	C3—H11	1.09	0.85
713.40	3.17	C4—H12	1.09	0.85
729.91	1.03	C5—H13	1.09	0.85
778.39	0.21	C6—H14	1.09	0.86
790.97	0.84	C7—H15	1.10	0.85
823.93	0.10	C7—H16	1.10	0.90
840.57	0.09	C8—H17	1.10	0.91
853.69	0.06	C8—H18	1.10	0.88
911.56	0.03	N9—H19	1.02	0.84
975.53	0.01	N9—H20	1.01	0.79
1021.96	0.01			
1044.37	0.08			

(table continues)

Table 2.19 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1053.94	0.05			
1088.05	0.34			
1119.56	0.58			
1167.11	0.09			
1295.29	0.01			
1338.22	0.07			
1375.76	0.01			
1381.70	0.01			
1389.47	0.02			
1438.15	0.44			
1486.66	0.11			
1520.83	0.23			
1531.26	0.10			
1556.09	0.08			
1601.48	0.01			
1623.73	0.09			
1742.89	0.91			
2939.97	1.34			
2993.38	0.83			
3040.68	0.30			
3064.87	0.72			
3114.91	0.34			
3116.26	0.26			
3134.44	0.18			
3145.82	1.15			
3162.88	0.60			
3487.44	0.02			
3613.81	0.04			

Table 2.20 N-butylphenethylamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-0.76899	1.26244	-0.54425
C	6.0	-1.80494	0.30997	-0.50243

(table continues)

Table 2.20 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.76553	-0.72967	0.44782
C	6.0	-0.74539	-0.74696	1.41908
C	6.0	0.28732	0.20963	1.37102
C	6.0	0.26537	1.25460	0.41975
H	1.0	-2.59188	0.33087	-1.25372
H	1.0	-2.56990	-1.46050	0.48968
H	1.0	-0.71134	-1.54459	2.15837
H	1.0	1.06937	0.19897	2.13045
H	1.0	-0.81048	2.07205	-1.27341
C	6.0	1.40799	2.24784	0.33374
C	6.0	2.47817	1.79126	-0.68536
N	7.0	3.60253	2.75022	-0.76328
H	1.0	4.46312	2.29736	-1.06922
C	6.0	3.33607	3.96911	-1.56297
H	1.0	1.89245	2.34641	1.31359
H	1.0	1.01617	3.23373	0.04874
H	1.0	2.88016	0.82607	-0.35112
H	1.0	1.99346	1.63360	-1.66981
C	6.0	4.60153	4.82684	-1.69940
H	1.0	2.56305	4.55323	-1.04855
H	1.0	2.95063	3.71438	-2.57140
H	1.0	4.96550	5.06558	-0.69067
C	6.0	4.36430	6.12995	-2.48932
H	1.0	5.38288	4.23780	-2.20646
H	1.0	3.59007	6.71825	-1.97504
H	1.0	3.97301	5.87838	-3.48613
C	6.0	5.64263	6.97946	-2.63684
H	1.0	6.03880	7.25261	-1.65073
H	1.0	5.44455	7.90377	-3.19229
H	1.0	6.41787	6.41829	-3.17386

Table 2.21 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N-butylphenethylamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
9.03	0.01	C1—C2	1.41	1.20
86.12	0.01	C2—C3	1.41	1.24
106.97	0.02	C3—C4	1.41	1.24
117.29	0.01	C4—C5	1.41	1.25
149.85	0.01	C5—C6	1.41	1.23
247.28	0.01	C6—C1	1.41	1.21
280.07	0.13	C1—C7	1.52	0.79
333.29	0.15	C7—C8	1.55	0.70
349.48	0.02	C8—N9	1.48	0.62
403.95	0.05	N9—C10	1.48	0.76
473.69	0.51	C10—C11	1.53	0.98
496.12	0.14	C11—C12	1.54	0.90
604.21	0.54	C12—C13	1.54	0.86
641.58	1.53	C2—H14	1.09	0.86
645.13	0.03	C3—H15	1.09	0.84
701.09	1.56	C4—H16	1.09	0.85
718.41	0.69	C5—H17	1.09	0.85
740.87	0.06	C6—H18	1.09	0.86
761.81	0.18	C7—H19	1.10	0.87
776.99	0.02	C7—H20	1.10	0.91
817.23	0.06	C8—H21	1.10	0.90
831.82	0.05	C8—H22	1.11	0.91
838.78	0.02	N9—H23	1.02	0.78
841.79	0.10	C10—H24	1.10	0.70
885.60	0.03	C10—H25	1.11	0.87
910.31	0.07	C11—H26	1.10	0.90
963.99	0.02	C11—H27	1.10	0.85
981.53	0.01	C12—H28	1.10	0.89
1020.90	0.01	C12—H29	1.10	0.89
1035.72	0.04	C13—H30	1.10	0.90
1048.45	0.02	C13—H31	1.10	0.89
1051.74	0.07	C13—H32	1.10	0.90
1070.38	0.23			
1098.37	0.07			
1122.29	0.11			
1158.87	0.41			

(table continues)

Table 2.21 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1166.43	1.11			
1207.85	0.14			
1242.36	0.10			
1251.15	0.05			
1285.84	0.05			
1318.76	0.03			
1330.36	0.06			
1342.34	0.04			
1342.97	0.03			
1353.17	0.03			
1384.04	0.02			
1412.47	0.42			
1422.08	0.08			
1438.28	0.12			
1470.49	0.07			
1485.26	0.10			
1516.62	0.09			
1527.58	0.06			
1528.34	0.12			
1536.50	0.24			
1540.02	0.02			
1546.06	0.15			
1549.44	0.20			
1555.95	0.15			
1569.33	0.09			
1600.46	0.01			
1622.77	0.13			
2890.08	1.88			
2897.56	1.48			
2973.51	0.28			
2983.87	1.41			
2990.59	0.78			
3003.62	0.62			
3018.61	0.17			
3029.58	0.34			
3033.17	0.33			

(table continues)

Table 2.21 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
3049.98	1.12			
3066.15	0.67			
3075.47	1.73			
3078.39	1.09			
3113.06	0.36			
3115.04	0.26			
3133.38	0.17			
3144.64	1.14			
3162.03	0.66			
3483.47	0.02			

Table 2.22 Phenethylamine derivatives optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
		N-hexylphenethylamine		
C	6.0	-0.80683	1.20483	-0.50376
C	6.0	-1.87152	0.28514	-0.45605
C	6.0	-1.86713	-0.74512	0.50530
C	6.0	-0.85265	-0.78209	1.48162
C	6.0	0.20869	0.14250	1.42796
C	6.0	0.22194	1.17774	0.46607
H	1.0	-2.65409	0.32112	-1.21120
H	1.0	-2.69336	-1.45087	0.55133
H	1.0	-0.84531	-1.57295	2.22895
H	1.0	0.98647	0.11635	2.19119
H	1.0	-0.82145	2.00754	-1.24154
C	6.0	1.39190	2.13833	0.37562
C	6.0	2.43293	1.66563	-0.66638
N	7.0	3.57333	2.60405	-0.75995
H	1.0	4.42482	2.13512	-1.06674
C	6.0	3.32261	3.82203	-1.56619
H	1.0	1.89422	2.20856	1.34884
H	1.0	1.02678	3.14018	0.11144
H	1.0	2.82266	0.69151	-0.34373

(table continues)

Table 2.22 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	1.92825	1.52126	-1.64255
C	6.0	4.58467	4.69159	-1.65856
H	1.0	2.52971	4.39857	-1.07381
H	1.0	2.97096	3.56985	-2.58746
H	1.0	4.90818	4.93758	-0.63806
C	6.0	4.36288	5.98962	-2.46062
H	1.0	5.39037	4.10981	-2.13475
H	1.0	3.56547	6.57586	-1.97756
H	1.0	4.01495	5.73474	-3.47404
C	6.0	5.62979	6.86112	-2.56964
H	1.0	5.98122	7.10720	-1.55532
C	6.0	5.40969	8.16777	-3.35849
H	1.0	6.42510	6.27580	-3.05788
H	1.0	5.04833	7.91473	-4.36637
C	6.0	6.68506	9.02756	-3.46732
H	1.0	4.61520	8.74735	-2.86524
H	1.0	7.48140	8.47134	-3.97811
H	1.0	7.04747	9.30621	-2.46960
H	1.0	6.49846	9.94950	-4.03090
		N-octylphenethylamine		
C	6.0	-0.87686	1.14498	-0.46904
C	6.0	-1.93937	0.22240	-0.42484
C	6.0	-1.92808	-0.81668	0.52691
C	6.0	-0.90813	-0.86112	1.49740
C	6.0	0.15121	0.06581	1.44668
C	6.0	0.15787	1.10979	0.49401
H	1.0	-2.72648	0.26470	-1.17501
H	1.0	-2.75264	-1.52457	0.57048
H	1.0	-0.89570	-1.65860	2.23759
H	1.0	0.93330	0.03400	2.20539
H	1.0	-0.89607	1.95428	-1.19959
C	6.0	1.32793	2.07031	0.40510
C	6.0	2.37815	1.58879	-0.62363
N	7.0	3.52414	2.52125	-0.70867
H	1.0	4.37456	2.04795	-1.01160

(table continues)

Table 2.22 *(continued)*

Atom	Nuclear charge	X	Y	Z	
C	6.0		3.28524	3.74144	-1.51504
H	1.0		1.82197	2.14990	1.38196
H	1.0		0.96361	3.06907	0.12814
H	1.0		2.75960	0.61379	-0.29358
H	1.0		1.88252	1.44350	-1.60455
C	6.0		4.55757	4.59488	-1.61361
H	1.0		2.50140	4.32906	-1.02137
H	1.0		2.92732	3.49176	-2.53488
H	1.0		4.89181	4.83419	-0.59489
C	6.0		4.34639	5.89820	-2.40996
H	1.0		5.35289	4.00514	-2.09766
H	1.0		3.56057	6.49441	-1.91989
H	1.0		3.98859	5.65304	-3.42241
C	6.0		5.62388	6.75382	-2.52452
H	1.0		5.98420	6.99556	-1.51232
C	6.0		5.41348	8.06352	-3.30999
H	1.0		6.40943	6.16078	-3.01910
H	1.0		5.04741	7.81920	-4.31982
C	6.0		6.69039	8.91834	-3.43015
H	1.0		4.62952	8.65568	-2.81190
H	1.0		7.47238	8.32335	-3.92816
H	1.0		7.05628	9.15666	-2.41881
C	6.0		6.48042	10.23063	-4.21238
H	1.0		6.10974	9.98537	-5.21882
C	6.0		7.76485	11.07623	-4.32632
H	1.0		5.69573	10.81726	-3.71193
H	1.0		8.55190	10.51267	-4.84346
H	1.0		8.13654	11.34714	-3.32990
H	1.0		7.58557	12.00198	-4.88611

Table 2.23 Bonding (MP2/6-311++G) for optimized phenethylamine derivatives structures

Bond type	Length/Å	Order
	N-hexylphenethylamine	
C1—C2	1.41	1.19

(table continues)

Table 2.23 *(continued)*

Bond type	Length/Å	Order
C2—C3	1.41	1.25
C3—C4	1.41	1.25
C4—C5	1.41	1.25
C5—C6	1.41	1.24
C6—C1	1.41	1.23
C1—C7	1.52	0.78
C7—C8	1.55	0.80
C8—N9	1.48	0.65
N9—C10	1.48	0.65
C10—C11	1.54	0.99
C11—C12	1.54	0.80
C12—C13	1.54	0.88
C13—C14	1.54	0.86
C14—C15	1.54	0.86
C2—H14	1.09	0.86
C3—H15	1.09	0.85
C4—H16	1.09	0.85
C5—H17	1.09	0.84
C6—H18	1.09	0.86
C7—H19	1.10	0.86
C7—H20	1.10	0.90
C8—H21	1.10	0.91
C8—H22	1.11	0.91
N9—H23	1.02	0.76
C10—H24	1.10	0.87
C10—H25	1.11	0.86
C11—H26	1.10	0.91
C11—H27	1.10	0.85
C12—H28	1.10	0.88
C12—H29	1.10	0.89
C13—H30	1.10	0.89
C13—H31	1.10	0.88
C14—H32	1.10	0.88
C14—H33	1.10	0.88
C15—H34	1.10	0.90
C15—H35	1.10	0.90

(table continues)

Table 2.23 *(continued)*

Bond type	Length/Å	Order
C15—H36	1.10	0.90
	N-octylphenethylamine	
C1—C2	1.41	1.19
C2—C3	1.41	1.25
C3—C4	1.41	1.25
C4—C5	1.41	1.25
C5—C6	1.41	1.24
C6—C1	1.41	1.21
C1—C7	1.52	0.78
C7—C8	1.55	0.75
C8—N9	1.48	0.63
N9—C10	1.48	0.73
C10—C11	1.54	1.02
C11—C12	1.54	0.83
C12—C13	1.54	0.87
C13—C14	1.54	0.83
C14—C15	1.54	0.84
C15—C16	1.54	0.86
C16—C17	1.54	0.86
C2—H14	1.09	0.86
C3—H15	1.09	0.84
C4—H16	1.09	0.85
C5—H17	1.09	0.84
C6—H18	1.09	0.86
C7—H19	1.10	0.87
C7—H20	1.10	0.91
C8—H21	1.10	0.90
C8—H22	1.11	0.91
N9—H23	1.02	0.77
C10—H24	1.10	0.87
C10—H25	1.11	0.86
C11—H26	1.10	0.90
C11—H27	1.10	0.85
C12—H28	1.10	0.88
C12—H29	1.10	0.89

(table continues)

Table 2.23 *(continued)*

Bond type	Length/Å	Order
C13—H30	1.10	0.88
C13—H31	1.10	0.89
C14—H32	1.10	0.89
C14—H33	1.10	0.88
C15—H34	1.10	0.89
C15—H35	1.10	0.88
C16—H36	1.10	0.88
C16—H37	1.10	0.88
C17—H38	1.10	0.90
C17—H39	1.10	0.90
C17—H40	1.10	0.90

Table 2.24 4-methyl-2,5-methoxyphenylcyclopropylamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-4.11012	3.11518	-0.11692
C	6.0	-5.10759	2.12948	0.01257
C	6.0	-4.76645	0.77139	0.18080
C	6.0	-3.40901	0.41397	0.04931
C	6.0	-2.40955	1.39463	-0.08511
C	6.0	-2.74841	2.75838	-0.22538
C	6.0	-5.82360	-0.30182	0.32942
H	1.0	-5.65643	-0.89605	1.23563
H	1.0	-5.80103	-0.99580	-0.51925
H	1.0	-6.81939	0.15385	0.38408
O	8.0	-3.14229	-0.96928	0.19398
O	8.0	-4.38424	4.49177	-0.28209
C	6.0	-5.77958	4.92893	-0.15116
H	1.0	-6.40586	4.48312	-0.93241
H	1.0	-5.73244	6.00972	-0.28003
H	1.0	-6.17424	4.68287	0.84156
C	6.0	-1.75169	-1.41372	0.03975
H	1.0	-1.36790	-1.15733	-0.95451
H	1.0	-1.80247	-2.49572	0.15648
H	1.0	-1.11407	-0.97966	0.81848

(table continues)

Table 2.24 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-6.15364	2.40767	0.11563
H	1.0	-1.36464	1.11738	-0.19464
C	6.0	-1.71097	3.81692	-0.41590
C	6.0	-0.33181	3.68378	0.21412
C	6.0	-1.30595	4.72480	0.74460
H	1.0	-1.71506	4.31084	-1.38440
H	1.0	-1.77374	4.53655	1.70573
H	1.0	-1.09868	5.76357	0.51216
N	7.0	0.80508	4.16267	-0.55518
H	1.0	-0.18599	2.81661	0.85963
H	1.0	1.14576	3.51573	-1.25924
H	1.0	1.55573	4.55353	0.00520

Table 2.25 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized 4-methyl-2,5-methoxyphenylcyclopropylamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
32.92	0.01	C1—C2	1.41	1.24
39.96	0.22	C2—C3	1.41	1.18
77.09	0.06	C3—C4	1.41	1.23
94.84	0.01	C4—C5	1.41	1.29
134.04	0.10	C5—C6	1.41	1.19
177.51	0.09	C6—C1	1.41	1.16
187.82	0.01	C1—C7	1.49	0.97
202.67	0.09	C7—C8	1.53	0.75
219.74	0.24	C7—C9	1.52	0.82
230.96	0.01	C8—C9	1.52	0.76
241.74	0.37	C9—N10	1.45	0.91
296.98	0.21	C2—O11	1.41	0.79
309.26	0.01	O11—C12	1.47	0.27
315.48	0.06	C4—C13	1.51	0.88
358.21	0.07	C5—O14	1.42	0.73
374.87	0.02	O14—C15	1.47	0.31
428.13	0.16	C3—H16	1.09	0.81
447.96	0.13	C6—H17	1.09	0.84

(table continues)

Table 2.25 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
469.15	0.19	C7—H18	1.09	0.78
483.51	0.02	C8—H19	1.09	0.90
538.23	0.01	C8—H20	1.08	0.90
622.38	0.18	C9—H21	1.09	0.82
627.29	0.19	N10—H22	1.02	0.80
655.37	0.62	N10—H23	1.02	0.79
704.52	4.77	C12—H24	1.10	0.90
719.07	0.02	C12—H25	1.10	0.90
751.07	0.07	C12—H26	1.09	0.92
792.20	0.66	C13—H27	1.10	0.84
807.76	0.53	C13—H28	1.10	0.84
852.74	0.67	C13—H29	1.10	0.90
903.60	0.10	C15—H30	1.09	0.92
915.71	0.13	C15—H31	1.10	0.89
944.24	0.05	C15—H32	1.10	0.90
966.17	0.15			
1000.44	0.72			
1010.95	2.28			
1056.81	0.42			
1098.83	0.06			
1116.43	0.23			
1130.53	0.08			
1141.92	0.06			
1150.38	0.04			
1151.36	0.04			
1178.47	0.10			
1194.14	0.06			
1197.51	0.09			
1205.27	0.12			
1218.39	6.80			
1224.96	0.72			
1263.72	0.20			
1287.75	0.03			
1295.60	0.17			
1327.74	0.05			
1355.61	0.57			

(table continues)

Table 2.25 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1391.92	0.46			
1406.09	1.77			
1457.11	1.30			
1479.81	0.12			
1499.26	0.01			
1501.01	0.04			
1515.27	0.20			
1524.46	0.93			
1531.38	0.57			
1532.00	0.06			
1533.60	2.05			
1546.17	0.79			
1560.84	0.06			
1562.88	0.18			
1603.95	0.07			
1626.43	0.02			
1742.07	0.63			
2991.03	2.33			
2991.40	0.04			
2996.93	0.97			
3073.17	0.90			
3073.64	0.28			
3075.64	0.65			
3075.84	1.22			
3085.12	0.50			
3114.32	0.26			
3140.14	0.58			
3140.65	0.50			
3141.54	0.09			
3153.89	0.38			
3162.46	0.15			
3220.67	0.27			
3487.64	0.03			
3613.75	0.05			

Table 2.26 Tryptamine unoptimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-3.90145	3.17825	-0.04000
C	6.0	-5.00493	2.42048	-0.45265
C	6.0	-4.89311	1.01476	-0.66157
C	6.0	-3.69998	0.33501	-0.37884
C	6.0	-2.58045	1.11143	-0.01298
C	6.0	-2.69143	2.51083	0.28286
N	7.0	-1.28595	0.72349	0.33993
C	6.0	-1.38362	2.97316	0.70694
H	1.0	-5.77421	0.44785	-0.95493
H	1.0	-3.61595	-0.73728	-0.55144
H	1.0	-4.00950	4.24735	0.14074
H	1.0	-5.94103	2.91910	-0.69626
C	6.0	-0.55908	1.85557	0.74528
H	1.0	0.49636	1.79325	0.97266
H	1.0	-0.89125	-0.19476	0.19990
C	6.0	-0.99290	4.39748	0.99364
C	6.0	-0.31659	5.07780	-0.22145
H	1.0	-0.30569	4.44634	1.85092
H	1.0	-1.89500	4.96695	1.26803
N	7.0	1.01700	4.48380	-0.48119
H	1.0	-0.25412	6.16456	-0.04888
H	1.0	-0.94288	4.91335	-1.10701
H	1.0	1.78525	4.94837	-0.00714
H	1.0	1.22786	4.30236	-1.45730

Table 2.27 Calculated (MP2/6-311++G) IR spectrum and bonding for unoptimized tryptamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
12.15	0.01	C1—C2	1.39	1.46
10.43	0.01	C2—N3	1.41	0.66
20.28	0.02	N3—C4	1.40	0.68
79.39	0.08	C4—C5	1.41	1.14
87.59	0.10	C5—C6	1.40	1.31
150.41	0.56	C6—C7	1.43	1.18

(table continues)

Table 2.27 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
164.09	0.57	C7—C8	1.40	1.31
186.95	0.09	C8—C9	1.42	1.10
222.39	0.35	C9—C1	1.45	1.18
255.58	1.00	C4—C9	1.43	1.25
354.59	0.24	C1—C10	1.50	0.78
385.10	0.22	C10—C11	1.55	0.85
464.50	0.27	C11—N12	1.48	0.74
471.70	0.39	C2—H13	1.08	0.76
519.15	0.28	N3—H14	1.01	0.74
554.52	0.18	C5—H15	1.09	0.85
567.18	0.05	C6—H16	1.09	0.84
586.82	1.12	C7—H17	1.09	0.84
589.00	0.04	C8—H18	1.09	0.83
674.41	1.72	C10—H19	1.10	0.90
677.26	4.44	C10—H20	1.10	0.89
709.89	0.44	C11—H21	1.10	0.90
746.40	0.08	C11—H22	1.10	0.92
852.45	0.03	N12—H23	1.01	0.79
866.54	0.12	N12—H24	1.02	0.83
876.12	0.14			
909.94	0.02			
954.03	0.12			
976.83	0.07			
994.31	0.01			
1018.38	0.20			
1060.11	0.21			
1104.29	0.90			
1117.33	0.61			
1149.48	0.17			
1176.22	0.10			
1249.94	0.49			
1261.43	0.12			
1300.37	0.16			
1316.67	0.13			
1362.47	0.08			

(table continues)

Table 2.27 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1389.41	0.22			
1403.83	0.24			
1411.24	0.79			
1442.02	0.39			
1465.53	0.35			
1478.83	0.57			
1512.33	0.23			
1516.70	0.05			
1536.44	0.11			
1571.04	0.08			
1641.57	0.10			
1740.85	0.92			
2956.03	1.35			
2983.51	1.62			
3026.76	0.40			
3049.94	1.11			
3117.05	0.21			
3123.66	0.07			
3139.31	1.04			
3156.90	0.83			
3225.95	0.05			
3493.56	0.02			
3620.21	0.10			
3631.53	1.21			

Table 2.28 N,N-dibutyltryptamine optimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
C	6.0	-3.28838	2.32387	-0.27585
C	6.0	-3.80397	1.10210	-0.72908
C	6.0	-3.05609	-0.10396	-0.59790
C	6.0	-1.81191	-0.11914	0.04994
C	6.0	-1.28347	1.12106	0.46275
C	6.0	-2.05408	2.33035	0.42289
N	7.0	-0.05942	1.43158	1.06470

(table continues)

Table 2.28 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	-1.22376	3.39447	0.95424
H	1.0	-3.48901	-1.04019	-0.94417
H	1.0	-1.23074	-1.03828	0.11801
H	1.0	-3.88315	3.23299	-0.35813
H	1.0	-4.75530	1.07996	-1.25721
C	6.0	-0.04302	2.80259	1.38282
H	1.0	0.84658	3.27012	1.78676
H	1.0	0.58689	0.74989	1.43688
C	6.0	-1.51002	4.86962	0.90905
C	6.0	-1.28762	5.45394	-0.51204
H	1.0	-0.82404	5.38734	1.59454
H	1.0	-2.54029	5.07830	1.23995
N	7.0	0.07396	5.11900	-0.99508
H	1.0	-1.40540	6.54716	-0.47649
H	1.0	-2.05543	5.06427	-1.20452
C	6.0	0.09764	3.94711	-1.90546
C	6.0	0.87762	6.28174	-1.44285
C	6.0	1.47687	3.27585	-1.96701
H	1.0	-0.24646	4.21092	-2.92748
H	1.0	-0.62043	3.22440	-1.50428
H	1.0	0.80451	7.03606	-0.64598
C	6.0	0.46777	6.92153	-2.78937
H	1.0	1.92954	5.96815	-1.49270
H	1.0	2.17869	3.88122	-2.56197
C	6.0	1.40242	1.85231	-2.55679
H	1.0	1.86166	3.23058	-0.93754
H	1.0	-0.60789	7.15783	-2.76274
H	1.0	0.62609	6.20212	-3.60635
C	6.0	1.26400	8.20721	-3.09281
H	1.0	0.96659	1.90081	-3.56659
H	1.0	0.71342	1.26225	-1.93433
C	6.0	2.77693	1.15711	-2.61901
H	1.0	1.08060	8.93412	-2.28706
C	6.0	0.89563	8.83799	-4.45069
H	1.0	2.33886	7.97055	-3.07557
H	1.0	3.47296	1.72965	-3.24592

(table continues)

Table 2.28 *(continued)*

Atom	Nuclear charge	X	Y	Z	
H	1.0		2.69659	0.14551	-3.03566
H	1.0		3.20981	1.07840	-1.61274
H	1.0		-0.17096	9.09520	-4.47721
H	1.0		1.09901	8.13504	-5.26850
H	1.0		1.47107	9.75302	-4.63631

Table 2.29 Calculated (MP2/6-311++G) IR spectrum and bonding for optimized N,N-dibutyltryptamine structure

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
18.90	0.01	C1—C2	1.39	1.58
21.12	0.01	C2—N3	1.41	0.80
60.87	0.03	N3—C4	1.40	0.82
69.69	0.01	C4—C5	1.41	1.12
119.26	0.01	C5—C6	1.40	1.28
143.38	0.03	C6—C7	1.43	1.19
177.97	0.03	C7—C8	1.40	1.32
187.91	0.11	C8—C9	1.42	1.11
244.94	0.01	C9—C1	1.45	1.13
295.64	0.09	C4—C9	1.43	1.17
317.30	0.01	C1—C10	1.50	0.76
327.30	0.01	C10—C11	1.55	0.80
354.85	0.53	C11—N12	1.48	0.46
397.13	0.34	N12—C13	1.48	0.63
412.77	2.22	N12—C14	1.48	0.63
439.45	0.55	C13—C15	1.55	0.83
466.18	0.09	C14—C16	1.54	0.87
475.79	0.06	C15—C17	1.54	0.84
492.11	0.09	C16—C18	1.54	0.88
530.79	0.01	C17—C19	1.54	0.87
546.56	0.33	C18—C20	1.54	0.84
549.06	0.39	C2—H21	1.08	0.79
563.13	0.04	N3—H22	1.01	0.68
601.71	0.36	C5—H23	1.09	0.84
646.09	0.92	C6—H24	1.09	0.83

(table continues)

Table 2.29 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
662.26	2.03	C7—H25	1.09	0.84
704.63	0.01	C8—H26	1.09	0.83
707.67	0.06	C10—H27	1.10	0.90
717.66	0.05	C10—H28	1.10	0.90
729.74	0.08	C11—H29	1.10	0.89
762.85	0.05	C11—H30	1.10	0.95
785.56	0.10	C13—H31	1.10	0.87
807.36	0.07	C13—H32	1.10	0.88
809.97	0.07	C14—H33	1.11	0.83
828.20	0.03	C14—H34	1.09	0.87
838.80	0.10	C15—H35	1.10	0.89
902.55	0.04	C15—H36	1.10	0.91
912.01	0.14	C16—H37	1.10	0.86
918.18	0.16	C16—H38	1.10	0.90
921.29	0.05	C17—H39	1.10	0.89
932.69	0.12	C17—H40	1.10	0.89
957.98	0.04	C18—H41	1.10	0.79
969.81	0.15	C18—H42	1.10	0.88
981.72	0.06	C19—H43	1.10	0.90
1007.69	0.10	C19—H44	1.10	0.89
1015.27	0.11	C19—H45	1.10	0.90
1024.00	0.24	C20—H46	1.10	0.89
1050.90	0.16	C20—H47	1.10	0.90
1083.28	0.02	C20—H48	1.10	0.91
1089.82	0.24			
1091.48	0.62			
1107.74	0.55			
1114.90	0.34			
1128.85	0.12			
1147.53	0.20			
1151.32	0.04			
1169.59	0.33			
1206.07	0.09			
1237.95	0.01			
1253.61	0.50			
1258.51	0.35			

(table continues)

Table 2.29 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1288.80	0.02			
1292.31	0.06			
1294.75	0.15			
1310.68	0.08			
1318.03	0.06			
1326.92	0.01			
1334.56	0.18			
1339.23	0.06			
1346.15	0.01			
1351.47	0.18			
1373.00	0.06			
1378.11	0.11			
1395.09	0.16			
1406.40	0.75			
1411.55	0.55			
1420.36	0.11			
1420.87	0.18			
1428.77	0.27			
1444.08	0.14			
1460.57	0.19			
1463.90	0.10			
1468.06	0.08			
1477.74	0.57			
1508.92	0.13			
1513.17	0.03			
1514.99	0.07			
1518.97	0.06			
1526.48	0.01			
1532.21	0.01			
1537.09	0.16			
1543.71	0.01			
1545.10	0.04			
1549.65	0.15			
1549.88	0.24			
1553.27	0.19			
1556.77	0.19			

(table continues)

Table 2.29 *(continued)*

Frequency/cm^{-1}	Intensities	Bond type	Length/Å	Order
1569.38	0.05			
1639.36	0.10			
2888.16	1.39			
2935.73	0.93			
2972.77	0.09			
2973.09	0.02			
2974.95	1.11			
2978.03	0.90			
2979.79	0.35			
2983.83	0.84			
2987.99	2.52			
2988.66	0.93			
3009.23	0.10			
3012.18	0.01			
3015.38	1.08			
3025.91	0.06			
3035.35	0.98			
3035.86	0.56			
3048.32	1.62			
3065.48	0.46			
3069.08	1.51			
3072.32	1.28			
3073.69	1.70			
3075.39	1.20			
3117.52	0.17			
3123.12	0.07			
3139.44	0.86			
3156.72	0.80			
3207.24	0.07			
3614.39	1.09			

Unoptimized Tryptamine Derivatives

As mentioned in the previous section, optimization of tryptamine-like molecules represented a challenge due to the degrees of freedom that characterize the tryptamine side-

chain and the nature of indolealkylamines.[32] While the structural values are consistent with those calculated for other organic molecules in this study at the MP2/6-311++G level (see Tables 2.31-2.32), tryptamine and derivatives did not meet the convergence criteria set for the other species studied in this work, with the exception of N,N-dibutyltryptamine. Further investigation of the issue revealed that the problem has been previously addressed in the literature[56,57] and our results where compared to those found in Inoue et al.[26] Table 2.30 lists two dihedral angles (χ and θ) for the tryptamine molecules as defined by Inoue (see Figure 2.9). Determination of these angles for each one of the nineteen tryptamine species here studied was followed by the creation of a plot of χ vs θ. This plot is similar to one found in the literature[26] and represents the potential energy surface of the tryptamine family as function of χ and θ. Comparison of the plot in Figure 2.10(a) to Inoue *et al* (Fig. 2.10(b)), shows an agreement between both data sets. In their study of the conformation of tryptamine and similar molecules, Inoue concluded that their preferred structure is due to fact that the region—'Region II'—in the potential energy surface in which they are found is larger than that of the alternative global minimum. Overlaying our plot with that found in Inoue shows that our calculated structures fall within the region considered as region II in their work, which means that instead of falling into a local minimum, as we previously thought, our structures indeed found the favorable global minimum. Furthermore, comparison of both studies shows that our structures are found near equilibrium and that in order to reach the ground state more optimization cycles are needed.

By looking at the values of χ and θ in Table 2.30, the reader can see that their absolute values decrease as the size of the substituents increases, reaching a minimum at N,N-

dibutyltryptamine, and then increasing again toward the end of the series. This observation clarifies why N,N-dibutyltryptamine was the only tryptamine species to actually 'officially' converge, however, what makes this particular structure more likely to fall into the global minimum quickly is not obvious.

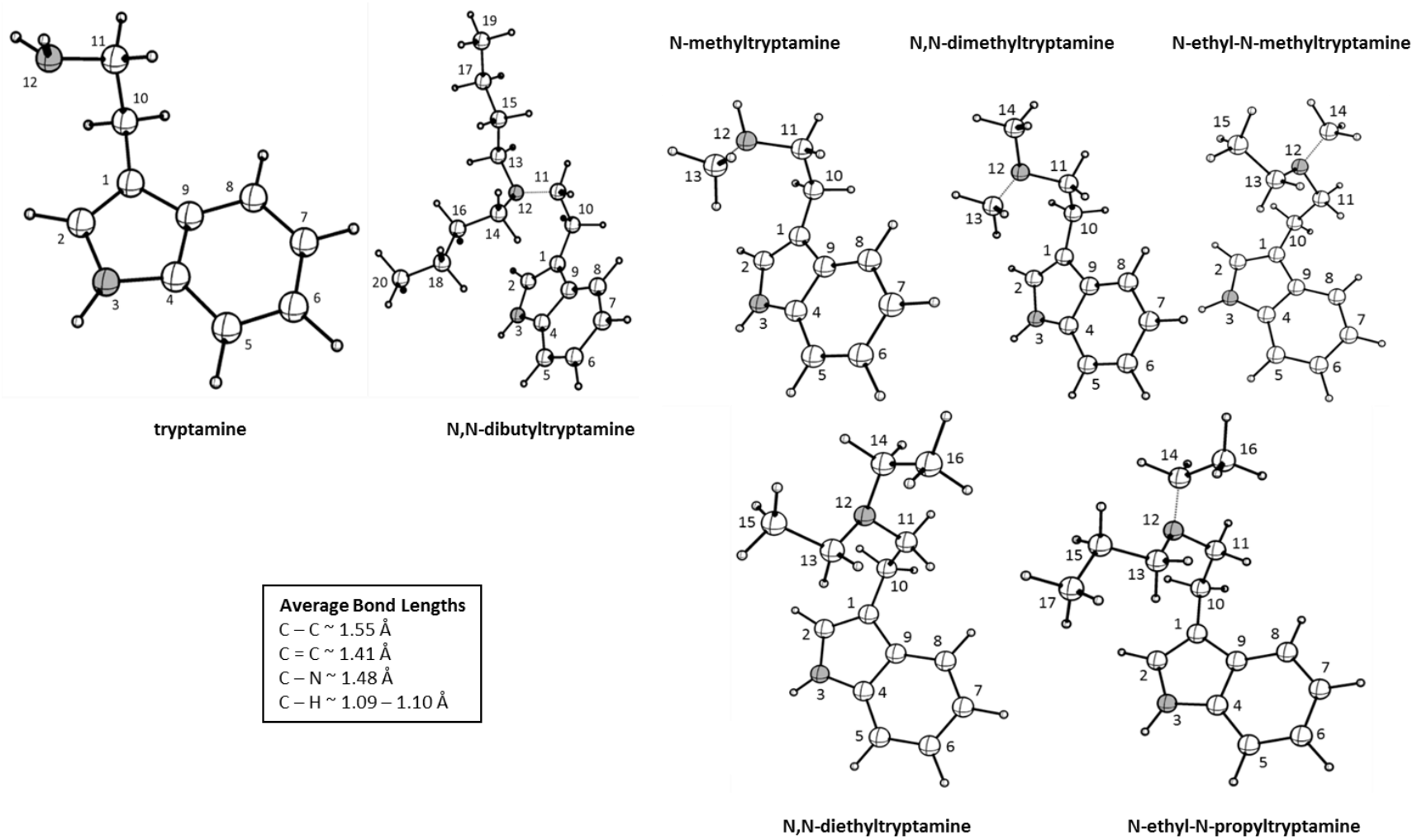


Figure 2.6. Near-equilibrium structures of tryptamine derivatives and optimized structure of N,N-dibutyltryptamine.

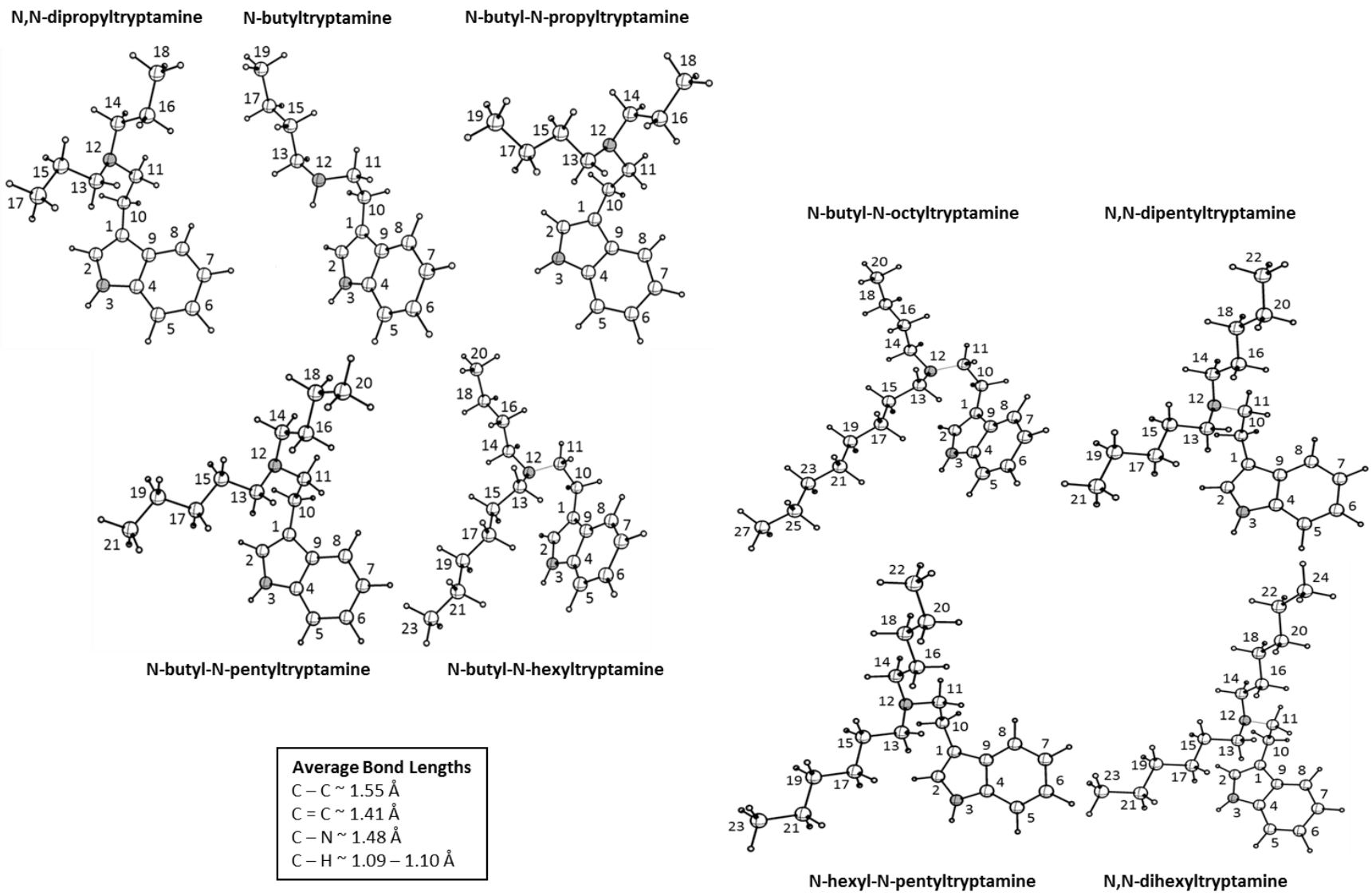


Figure 2.7. Near-equilibrium structures of tryptamine derivatives.

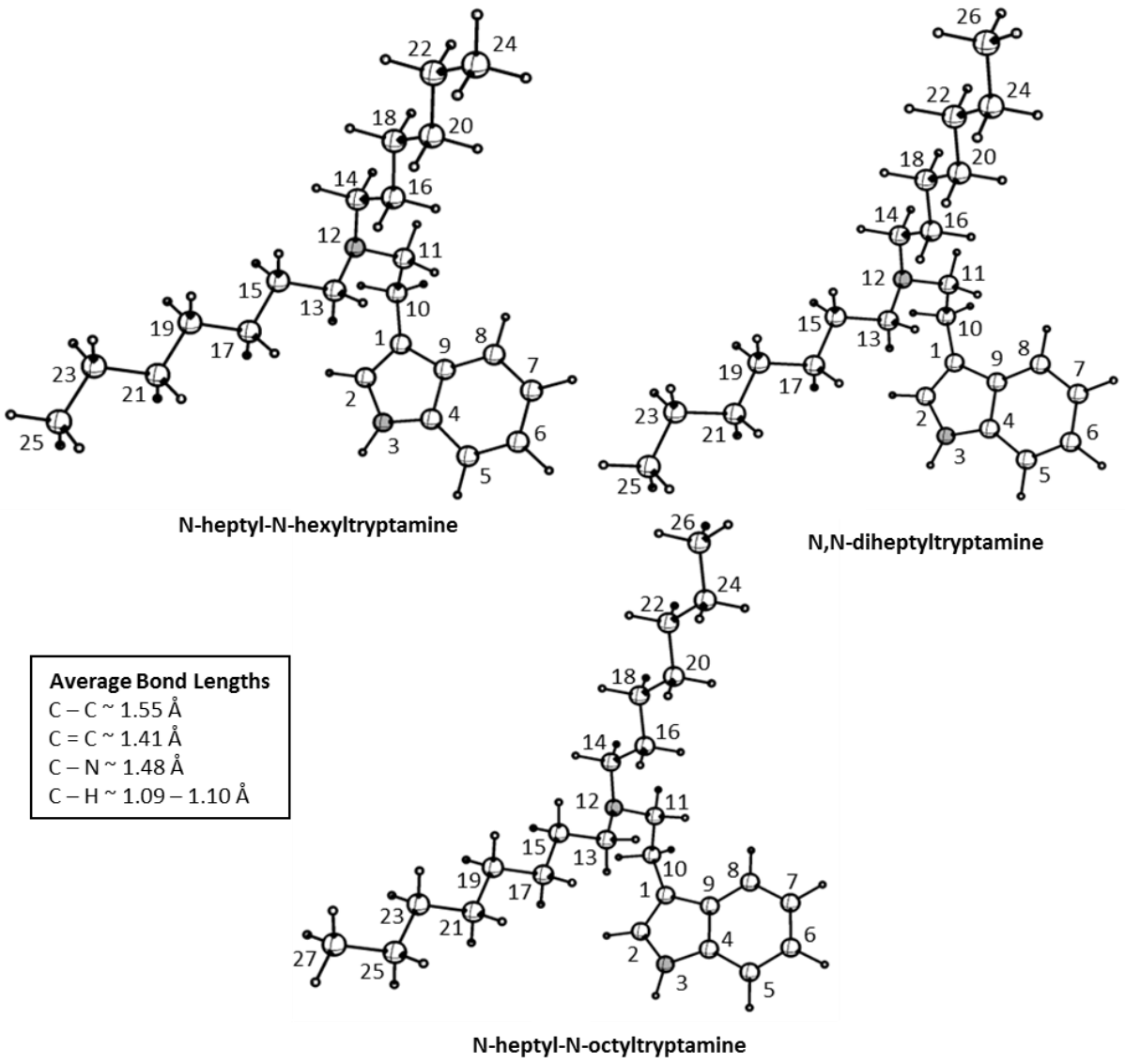


Figure 2.8. Near-equilibrium structures of tryptamine derivatives.

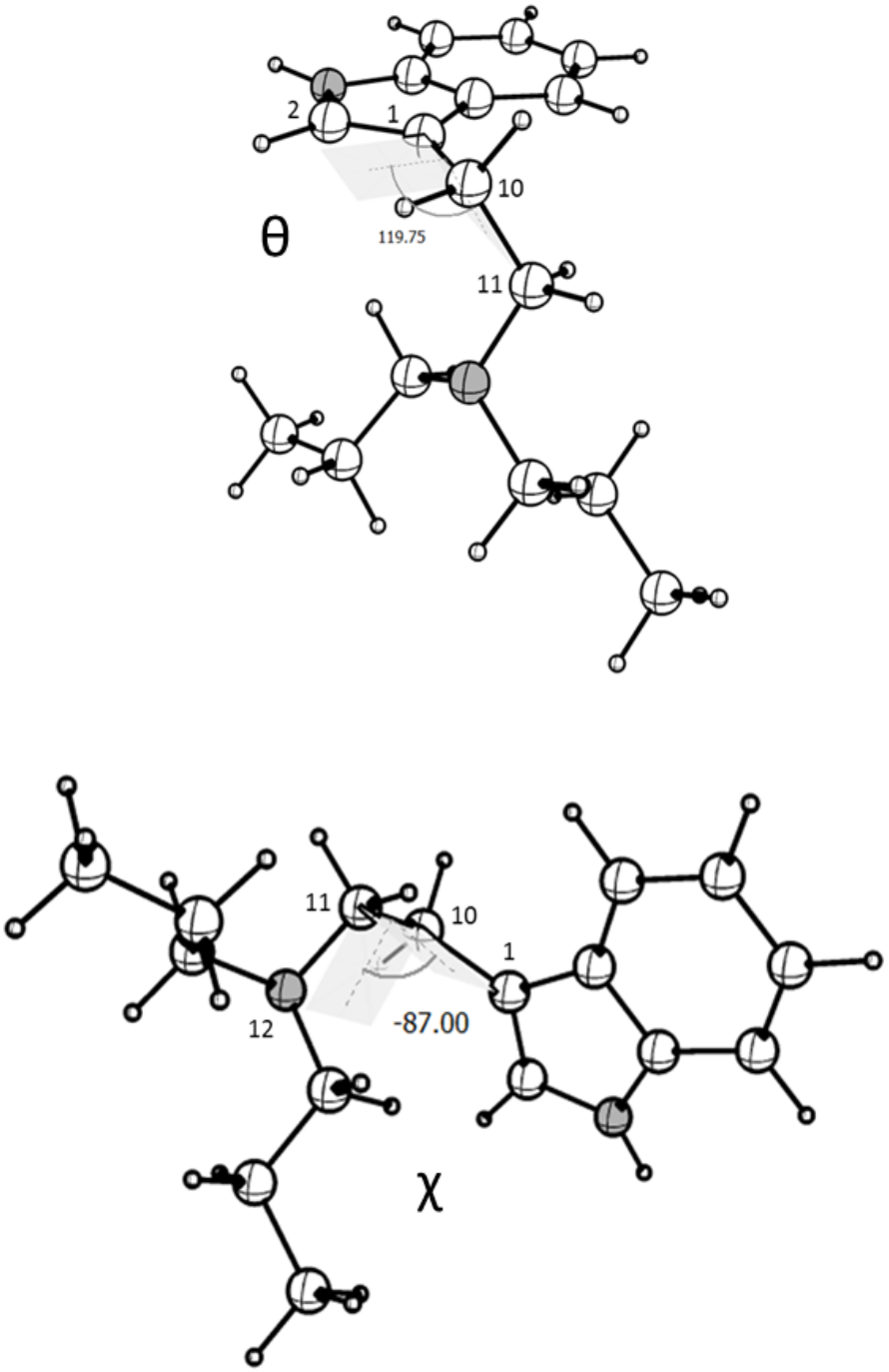


Figure 2.9. Definition of χ (C2-C1-C10-C11) and ϑ (C1-C10-C11-C12) dihedral angles.

Table 2.30 Conformations of tryptamine derivatives

Molecule	χ/°	θ/°
tryptamine	81.21	-68.74
N-methyltryptamine	108.87	-68.30
N,N-dimethyltryptamine	119.40	-79.59
N-ethyl-N-methyltryptamine	121.46	-86.05
N,N-diethyltryptamine	117.39	-83.16
N-ethyl-N-propyltryptamine	118.26	-81.94
N,N-dipropyltryptamine	119.75	-87.00
N-butyltryptamine	110.86	-62.63
N-butyl-N-propyltryptamine	119.97	-87.36
N,N-dibutyltryptamine	97.91	-53.90
N-butyl-N-pentyltryptamine	120.32	-86.26
N-butyl-N-hexyltryptamine	96.90	-52.83
N-butyl-N-octyltryptamine	95.97	-54.58
N,N-dipentyltryptamine	120.82	-86.11
N-hexyl-N-pentyltryptamine	120.86	-85.89
N,N-dihexyltryptamine	106.31	-66.00
N-heptyl-N-hexyltryptamine	122.53	-88.01
N,N-diheptyltryptamine	121.92	-87.35
N-heptyl-N-octyltryptamine	122.04	-87.70

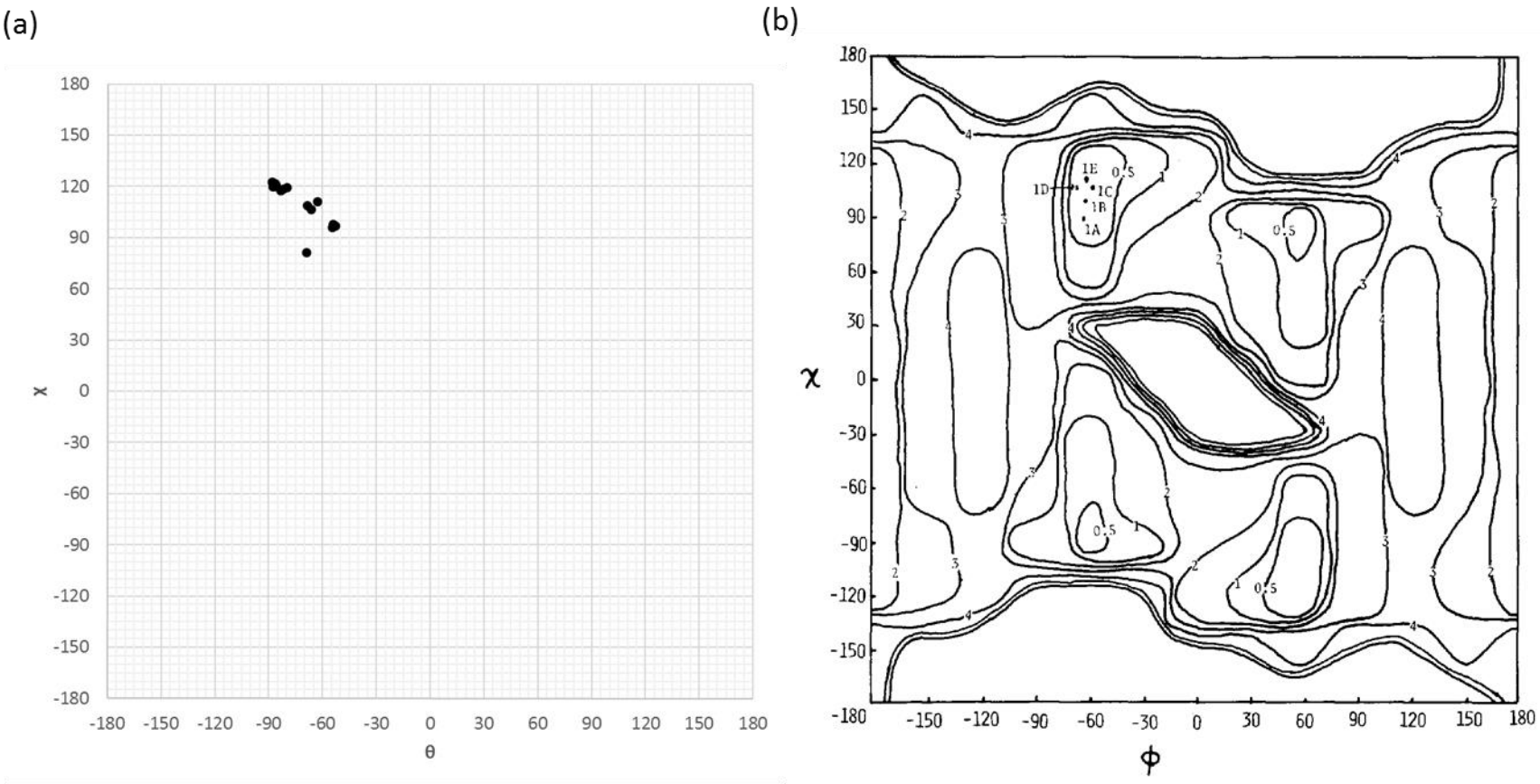


Figure 2.10. (a) Plot of χ vs ϑ shows location of near-equilibrium tryptamine derivatives structures on their corresponding potential energy surface. (b) From Inoue: "CNDO/2 conformational energy map for the present neutral tryptamine. Isoenergy in kcal per mol with respect to the global energy taken as energy zero. Five conformers found in the crystal structures are represented by the letters, 1A-1E, which are in accordance with the numbers in Table VII.[i]"

[i] Reprinted from Biochimica et Biophysica Acta (BBA) - General Subjects, Vol 543, Masatoshi Inoue, Toshimasa Sakaki, Akio Wakahara, Ken-Ichi Tomita, X-ray crystallographic and molecular orbital studies on the conformation of tryptamine, Page 131, Copyright (1978), with permission from Elsevier.

Table 2.31 Tryptamine derivatives unoptimized (MP2/6-311++G) coordinates

Atom	Nuclear charge	X	Y	Z
		N-methyltryptamine		
C	6.0	-3.48725	3.28557	-0.37398
C	6.0	-4.54904	2.56209	-0.93030
C	6.0	-4.49401	1.14153	-1.02733
C	6.0	-3.41403	0.42122	-0.49808
C	6.0	-2.32914	1.16091	0.01815
C	6.0	-2.40144	2.58056	0.20346
N	7.0	-1.13358	0.73345	0.60958
C	6.0	-1.17339	3.00344	0.84801
H	1.0	-5.34407	0.60340	-1.44100
H	1.0	-3.37059	-0.66360	-0.59128
H	1.0	-3.55924	4.36907	-0.27565
H	1.0	-5.39353	3.09065	-1.36960
C	6.0	-0.45822	1.84824	1.13625
H	1.0	0.52328	1.74216	1.58323
H	1.0	-0.90028	-0.22586	0.79334
C	6.0	-0.78406	4.42006	1.17664
C	6.0	-0.37423	5.26044	-0.05597
H	1.0	0.07290	4.41092	1.86543
H	1.0	-1.62322	4.91838	1.68755
N	7.0	0.90425	4.79017	-0.64657
H	1.0	-0.24396	6.30299	0.26025
H	1.0	-1.18463	5.23345	-0.81030
C	6.0	0.78811	3.79762	-1.73926
H	1.0	1.49879	5.57392	-0.91259
H	1.0	1.78294	3.65906	-2.17712
H	1.0	0.08145	4.11670	-2.52975
H	1.0	0.45566	2.84034	-1.33373
		N,N-dimethyltryptamine		
C	6.0	-3.49449	3.23469	-0.39421
C	6.0	-4.58415	2.53014	-0.92023
C	6.0	-4.57194	1.10309	-0.94934
C	6.0	-3.50963	0.35620	-0.42132
C	6.0	-2.39547	1.08319	0.05336
C	6.0	-2.41704	2.50909	0.18524

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
N	7.0	-1.23677	0.62785	0.69258
C	6.0	-1.17124	2.91366	0.80691
H	1.0	-5.45744	0.57494	-1.30455
H	1.0	-3.50992	-0.73365	-0.45624
H	1.0	-3.53096	4.32725	-0.36662
H	1.0	-5.41402	3.08237	-1.37430
C	6.0	-0.49392	1.74196	1.12138
H	1.0	0.47491	1.61538	1.59422
H	1.0	-0.87190	-0.31410	0.65078
C	6.0	-0.73828	4.31861	1.14103
C	6.0	-0.51464	5.22624	-0.09843
H	1.0	0.20737	4.29704	1.70534
H	1.0	-1.50765	4.79881	1.76764
N	7.0	0.79109	4.99729	-0.76225
H	1.0	-0.50104	6.26555	0.24485
H	1.0	-1.32499	5.11479	-0.84089
C	6.0	0.83233	3.79987	-1.60122
C	6.0	1.22927	6.17277	-1.53959
H	1.0	1.84032	3.69077	-1.99600
H	1.0	0.13004	3.83936	-2.42702
H	1.0	0.57363	2.94381	-0.98757
H	1.0	1.21428	7.03504	-0.91495
H	1.0	0.58046	6.37631	-2.39278
H	1.0	2.23287	6.01583	-1.91992
		N-ethyl-N-methyltryptamine		
C	6.0	-3.52988	3.21811	-0.35732
C	6.0	-4.62409	2.50477	-0.86285
C	6.0	-4.60455	1.08199	-0.93177
C	6.0	-3.53480	0.34704	-0.40217
C	6.0	-2.41819	1.07087	0.06590
C	6.0	-2.43802	2.49852	0.19542
N	7.0	-1.24917	0.62271	0.68868
C	6.0	-1.17650	2.90375	0.78650
H	1.0	-5.47734	0.55547	-1.31116
H	1.0	-3.52605	-0.74059	-0.45342

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-3.57347	4.30332	-0.28441
H	1.0	-5.47022	3.04378	-1.28440
C	6.0	-0.49745	1.73302	1.10616
H	1.0	0.47972	1.60596	1.55818
H	1.0	-0.91519	-0.33104	0.69002
C	6.0	-0.74552	4.31407	1.10154
C	6.0	-0.57258	5.25231	-0.12178
H	1.0	0.21959	4.29363	1.62983
H	1.0	-1.48630	4.77020	1.77891
N	7.0	0.77506	5.16303	-0.74859
H	1.0	-0.67543	6.28815	0.22777
H	1.0	-1.37169	5.06797	-0.86958
C	6.0	0.93968	3.93098	-1.57369
C	6.0	1.07846	6.39333	-1.52343
C	6.0	2.41537	3.63748	-1.89820
H	1.0	0.34109	4.01725	-2.51094
H	1.0	0.52357	3.10203	-0.99352
H	1.0	0.97516	7.26657	-0.86866
H	1.0	0.39913	6.51618	-2.39558
H	1.0	2.11226	6.35688	-1.87978
H	1.0	2.83746	4.37089	-2.60334
H	1.0	2.50712	2.63702	-2.35263
H	1.0	3.00816	3.66223	-0.96896
		N,N-diethyltryptamine		
C	6.0	-3.56089	3.14029	-0.32373
C	6.0	-4.61916	2.38646	-0.84720
C	6.0	-4.54971	0.96549	-0.90349
C	6.0	-3.46282	0.27254	-0.35109
C	6.0	-2.38313	1.03871	0.13618
C	6.0	-2.45860	2.46464	0.26149
N	7.0	-1.18507	0.63804	0.73648
C	6.0	-1.22184	2.91835	0.87173
H	1.0	-5.39292	0.40759	-1.30370
H	1.0	-3.40580	-0.81261	-0.41868
H	1.0	-3.64226	4.22398	-0.26192

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-5.47367	2.89253	-1.29253
C	6.0	-0.51071	1.77551	1.21745
H	1.0	0.47574	1.68732	1.65844
H	1.0	-0.95620	-0.31191	0.98749
C	6.0	-0.82805	4.35181	1.12369
C	6.0	-0.61596	5.20377	-0.15809
H	1.0	0.11436	4.37825	1.69241
H	1.0	-1.60861	4.83679	1.73545
N	7.0	0.73840	5.04036	-0.75560
H	1.0	-0.70045	6.26390	0.12255
H	1.0	-1.41605	4.98137	-0.89141
C	6.0	0.86977	3.79385	-1.56773
C	6.0	1.20498	6.27377	-1.45214
C	6.0	2.32927	3.50593	-1.95827
H	1.0	0.22753	3.83208	-2.47342
H	1.0	0.49031	2.97831	-0.94760
H	1.0	1.12092	7.09202	-0.72332
C	6.0	0.44206	6.65479	-2.74811
H	1.0	2.27340	6.14751	-1.66965
H	1.0	2.69807	4.19413	-2.72887
H	1.0	2.42016	2.48213	-2.34907
H	1.0	2.96965	3.59992	-1.07090
H	1.0	-0.63575	6.77541	-2.55776
H	1.0	0.57113	5.89194	-3.52923
H	1.0	0.82489	7.60715	-3.14193
		N-ethyl-N-propyltryptamine		
C	6.0	-3.49842	3.12377	-0.38763
C	6.0	-4.52222	2.32589	-0.91385
C	6.0	-4.40767	0.90665	-0.94819
C	6.0	-3.30110	0.25717	-0.39136
C	6.0	-2.25348	1.06622	0.09718
C	6.0	-2.38711	2.48687	0.21603
N	7.0	-1.05460	0.71337	0.71898
C	6.0	-1.19264	2.98721	0.86859
H	1.0	-5.23413	0.31477	-1.33264

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-3.21276	-0.82747	-0.42725
H	1.0	-3.62224	4.20359	-0.33248
H	1.0	-5.38607	2.80131	-1.37040
C	6.0	-0.44646	1.87395	1.23495
H	1.0	0.52613	1.82040	1.70728
H	1.0	-0.80647	-0.22928	1.00041
C	6.0	-0.86863	4.43066	1.14869
C	6.0	-0.66421	5.29411	-0.12450
H	1.0	0.05337	4.49519	1.74356
H	1.0	-1.68762	4.87806	1.74037
N	7.0	0.70129	5.16125	-0.69676
H	1.0	-0.78003	6.34850	0.15637
H	1.0	-1.44353	5.04997	-0.87147
C	6.0	0.89304	3.91669	-1.48156
C	6.0	1.14530	6.39406	-1.40331
C	6.0	2.36497	3.64405	-1.81808
H	1.0	0.29173	3.91951	-2.40936
H	1.0	0.49961	3.09675	-0.87015
H	1.0	1.02328	7.21471	-0.69281
C	6.0	0.40588	6.73039	-2.71499
H	1.0	2.21660	6.29283	-1.60885
H	1.0	2.71124	4.34348	-2.58590
C	6.0	2.59145	2.20101	-2.31719
H	1.0	2.94406	3.82538	-0.89824
H	1.0	-0.67672	6.85309	-2.53815
H	1.0	0.55170	5.95027	-3.47379
H	1.0	0.79121	7.67557	-3.12685
H	1.0	1.95769	1.96992	-3.17724
H	1.0	2.36226	1.48871	-1.52103
H	1.0	3.63309	2.04360	-2.61117
		N,N-dipropyltryptamine		
C	6.0	-3.55304	3.09854	-0.31110
C	6.0	-4.60856	2.33394	-0.82262
C	6.0	-4.53198	0.91133	-0.86622
C	6.0	-3.43691	0.22974	-0.31775

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	-2.35790	1.00668	0.15404
C	6.0	-2.44258	2.43320	0.27198
N	7.0	-1.15909	0.61692	0.75841
C	6.0	-1.20951	2.89725	0.87875
H	1.0	-5.37754	0.34363	-1.24817
H	1.0	-3.37537	-0.85631	-0.36944
H	1.0	-3.64154	4.18235	-0.25848
H	1.0	-5.47028	2.83111	-1.26341
C	6.0	-0.48857	1.76003	1.22557
H	1.0	0.49908	1.68167	1.66533
H	1.0	-0.90937	-0.33364	0.98920
C	6.0	-0.82359	4.33098	1.13912
C	6.0	-0.66582	5.20518	-0.13454
H	1.0	0.13416	4.36419	1.67807
H	1.0	-1.58497	4.79646	1.78606
N	7.0	0.69807	5.13215	-0.72241
H	1.0	-0.81610	6.25566	0.14876
H	1.0	-1.44730	4.93414	-0.87113
C	6.0	0.96111	3.84634	-1.42253
C	6.0	1.03518	6.34026	-1.52543
C	6.0	2.43490	3.68014	-1.82501
H	1.0	0.30701	3.72354	-2.31265
H	1.0	0.69355	3.05099	-0.72221
H	1.0	0.83568	7.20544	-0.87759
C	6.0	0.27357	6.51642	-2.86086
H	1.0	2.11527	6.32712	-1.71838
H	1.0	2.67681	4.33173	-2.67666
C	6.0	2.76121	2.21735	-2.19301
H	1.0	3.05147	4.00365	-0.97463
H	1.0	-0.80818	6.46916	-2.66933
H	1.0	0.52010	5.68784	-3.53877
C	6.0	0.61887	7.85620	-3.54402
H	1.0	2.10835	1.86416	-3.00194
H	1.0	2.61270	1.56340	-1.32342
H	1.0	3.80175	2.11275	-2.52358
H	1.0	0.34354	8.70147	-2.89961

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	0.08610	7.96550	-4.49617
H	1.0	1.69630	7.92012	-3.74788
		N-butyltryptamine		
C	6.0	-3.26772	2.23268	-0.23916
C	6.0	-3.82095	0.96705	-0.47618
C	6.0	-3.09421	-0.22209	-0.17679
C	6.0	-1.84464	-0.16332	0.45674
C	6.0	-1.27277	1.11354	0.65243
C	6.0	-2.00617	2.32159	0.40844
N	7.0	-0.06979	1.48255	1.26784
C	6.0	-1.15018	3.43773	0.78021
H	1.0	-3.55903	-1.19178	-0.35337
H	1.0	-1.29215	-1.07553	0.68011
H	1.0	-3.84943	3.12928	-0.44800
H	1.0	-4.78555	0.88501	-0.97350
C	6.0	0.01755	2.88601	1.29912
H	1.0	0.88958	3.38383	1.71018
H	1.0	0.69726	0.85621	1.46700
C	6.0	-1.44478	4.90025	0.56953
C	6.0	-1.49794	5.23390	-0.95104
H	1.0	-0.64487	5.49850	1.03506
H	1.0	-2.39458	5.18331	1.05156
N	7.0	-0.21404	5.00142	-1.64391
H	1.0	-1.75976	6.29109	-1.09747
H	1.0	-2.27597	4.62754	-1.43234
C	6.0	0.73682	6.14096	-1.62488
H	1.0	0.68385	6.71009	-0.67191
C	6.0	0.46801	7.08951	-2.81282
H	1.0	1.75467	5.73639	-1.70860
H	1.0	-0.57745	7.42898	-2.75914
H	1.0	0.57022	6.49462	-3.73238
C	6.0	1.39841	8.32103	-2.87453
H	1.0	1.27812	8.91406	-1.95416
C	6.0	1.11510	9.21267	-4.10645
H	1.0	2.44368	7.97976	-2.90298

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	0.08095	9.57805	-4.08420
H	1.0	1.25634	8.63930	-5.03202
H	1.0	1.78357	10.08310	-4.14039
H	1.0	0.20220	4.10995	-1.37348
		N-butyl-N-propyltryptamine		
C	6.0	-3.57449	3.09296	-0.30144
C	6.0	-4.62689	2.32443	-0.81458
C	6.0	-4.53876	0.90313	-0.87371
C	6.0	-3.43614	0.22399	-0.33698
C	6.0	-2.36089	1.00546	0.13729
C	6.0	-2.45566	2.43076	0.26897
N	7.0	-1.15706	0.61876	0.73470
C	6.0	-1.22347	2.89805	0.87714
H	1.0	-5.38128	0.33193	-1.25845
H	1.0	-3.36766	-0.86115	-0.39859
H	1.0	-3.67099	4.17564	-0.23784
H	1.0	-5.49562	2.81899	-1.24465
C	6.0	-0.49372	1.76270	1.21201
H	1.0	0.49419	1.68596	1.65200
H	1.0	-0.90089	-0.33253	0.95765
C	6.0	-0.84786	4.33284	1.15097
C	6.0	-0.70367	5.22118	-0.11505
H	1.0	0.11421	4.36627	1.68342
H	1.0	-1.60848	4.78624	1.80784
N	7.0	0.66043	5.17086	-0.70396
H	1.0	-0.86822	6.26734	0.17714
H	1.0	-1.48202	4.94625	-0.85374
C	6.0	0.94000	3.89429	-1.41531
C	6.0	0.98068	6.38744	-1.50115
C	6.0	2.41214	3.76862	-1.83802
H	1.0	0.27430	3.76371	-2.29644
H	1.0	0.70225	3.08787	-0.71553
H	1.0	0.76868	7.24763	-0.85007
C	6.0	0.22042	6.55725	-2.83820
H	1.0	2.06183	6.38996	-1.69227

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	2.61800	4.40124	-2.71531
C	6.0	2.79992	2.31319	-2.17146
H	1.0	3.03429	4.13508	-1.00715
H	1.0	-0.86159	6.51083	-2.64729
H	1.0	0.46948	5.72627	-3.51255
C	6.0	0.56699	7.89529	-3.52414
H	1.0	2.10955	1.92411	-2.93549
H	1.0	2.66146	1.70156	-1.26728
C	6.0	4.25285	2.18160	-2.66945
H	1.0	0.29646	8.74300	-2.88063
H	1.0	0.03357	8.00514	-4.47637
H	1.0	1.64433	7.95558	-3.72960
H	1.0	4.39866	2.75960	-3.59084
H	1.0	4.51348	1.13684	-2.87686
H	1.0	4.95289	2.56328	-1.91436
		N-butyl-N-pentyltryptamine		
C	6.0	-3.53256	3.03159	-0.30622
C	6.0	-4.55682	2.23746	-0.83667
C	6.0	-4.43364	0.81931	-0.89243
C	6.0	-3.32691	0.16624	-0.33359
C	6.0	-2.27958	0.97443	0.15892
C	6.0	-2.40976	2.39695	0.28653
N	7.0	-1.07896	0.61506	0.77750
C	6.0	-1.19922	2.89214	0.91451
H	1.0	-5.25177	0.22615	-1.29686
H	1.0	-3.23100	-0.91703	-0.38913
H	1.0	-3.65554	4.11164	-0.24750
H	1.0	-5.42692	2.71067	-1.28875
C	6.0	-0.44850	1.77446	1.25954
H	1.0	0.53123	1.71783	1.71722
H	1.0	-0.80533	-0.32806	1.00091
C	6.0	-0.86245	4.33536	1.19503
C	6.0	-0.72791	5.23197	-0.06538
H	1.0	0.09391	4.38867	1.73641
H	1.0	-1.64027	4.76878	1.84473

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
N	7.0	0.63578	5.19857	-0.65656
H	1.0	-0.90340	6.27450	0.23413
H	1.0	-1.50457	4.95768	-0.80627
C	6.0	0.92481	3.92788	-1.37617
C	6.0	0.93903	6.41995	-1.45609
C	6.0	2.39476	3.82795	-1.81328
H	1.0	0.25190	3.79287	-2.25035
H	1.0	0.70516	3.11338	-0.67998
H	1.0	0.70354	7.27785	-0.81024
C	6.0	0.18620	6.56515	-2.79913
H	1.0	2.02111	6.44371	-1.63747
H	1.0	2.58275	4.47384	-2.68470
C	6.0	2.80377	2.38388	-2.16754
H	1.0	3.01729	4.19218	-0.98154
H	1.0	-0.89812	6.50029	-2.62044
H	1.0	0.45780	5.73523	-3.46809
C	6.0	0.50387	7.89747	-3.50908
H	1.0	2.11919	1.98684	-2.93460
H	1.0	2.68551	1.75434	-1.27143
C	6.0	4.25575	2.27628	-2.67388
H	1.0	0.19916	8.72895	-2.85576
C	6.0	-0.20153	8.02749	-4.87408
H	1.0	1.59306	7.97542	-3.64764
H	1.0	4.35942	2.89040	-3.57942
C	6.0	4.68311	0.82830	-2.97871
H	1.0	4.92565	2.70203	-1.91173
H	1.0	-1.29035	7.96309	-4.75280
H	1.0	0.11343	7.21948	-5.54637
H	1.0	0.03374	8.98414	-5.35553
H	1.0	4.03465	0.39155	-3.74909
H	1.0	4.60677	0.20788	-2.07821
H	1.0	5.71669	0.78557	-3.34042
		N-butyl-N-hexyltryptamine		
C	6.0	-3.21484	2.27304	-0.24403
C	6.0	-3.63818	1.06053	-0.80505

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	-2.81675	-0.10317	-0.74751
C	6.0	-1.52975	-0.05341	-0.19209
C	6.0	-1.12594	1.15885	0.40532
C	6.0	-1.90469	2.35738	0.29204
N	7.0	0.10488	1.52242	0.96578
C	6.0	-1.15645	3.43007	0.92069
H	1.0	-3.16549	-1.02554	-1.20777
H	1.0	-0.91162	-0.94905	-0.13773
H	1.0	-3.84390	3.16053	-0.31225
H	1.0	-4.63661	0.98319	-1.23126
C	6.0	0.06260	2.88704	1.30531
H	1.0	0.91040	3.37188	1.77398
H	1.0	0.78690	0.86942	1.32604
C	6.0	-1.49627	4.89474	0.90734
C	6.0	-1.31888	5.52272	-0.50310
H	1.0	-0.81692	5.42143	1.59297
H	1.0	-2.52782	5.06338	1.25716
N	7.0	0.03425	5.23420	-1.03255
H	1.0	-1.45908	6.61141	-0.42914
H	1.0	-2.09865	5.13812	-1.18510
C	6.0	0.07043	4.08601	-1.97183
C	6.0	0.81233	6.42269	-1.45428
C	6.0	1.43305	3.37494	-1.98816
H	1.0	-0.22133	4.38120	-3.00096
H	1.0	-0.67955	3.37018	-1.62056
H	1.0	0.76215	7.14206	-0.62374
C	6.0	0.35390	7.11708	-2.75792
H	1.0	1.86370	6.11797	-1.55345
H	1.0	2.17255	3.95132	-2.56613
C	6.0	1.32386	1.94740	-2.56180
H	1.0	1.78275	3.32571	-0.94722
H	1.0	-0.71903	7.35425	-2.67987
H	1.0	0.47747	6.43014	-3.60805
C	6.0	1.14320	8.41142	-3.04136
H	1.0	0.97687	1.99472	-3.60710
H	1.0	0.55613	1.40603	-1.98697

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	2.64464	1.15819	-2.49845
H	1.0	0.99732	9.10609	-2.20016
C	6.0	0.72282	9.09725	-4.35670
H	1.0	2.21657	8.17024	-3.07882
H	1.0	3.41589	1.68872	-3.08013
C	6.0	2.51734	-0.28710	-3.02012
H	1.0	2.98810	1.13304	-1.45082
H	1.0	-0.34231	9.36047	-4.32888
H	1.0	0.88828	8.42640	-5.20941
H	1.0	1.29582	10.01631	-4.52981
H	1.0	2.17408	-0.25683	-4.06497
H	1.0	1.73617	-0.80047	-2.43875
C	6.0	3.83720	-1.07922	-2.93031
H	1.0	4.62195	-0.58679	-3.51854
H	1.0	3.71832	-2.10146	-3.30942
H	1.0	4.17863	-1.13948	-1.88873
		N-butyl-N-octyltryptamine		
C	6.0	-3.44516	2.49619	-0.13739
C	6.0	-3.97473	1.27858	-0.58755
C	6.0	-3.21922	0.07332	-0.50291
C	6.0	-1.95169	0.05332	0.09818
C	6.0	-1.41215	1.28921	0.51103
C	6.0	-2.18597	2.49695	0.51576
N	7.0	-0.16662	1.59424	1.07218
C	6.0	-1.34161	3.55510	1.03897
H	1.0	-3.66284	-0.85954	-0.84507
H	1.0	-1.36434	-0.86481	0.12865
H	1.0	-4.04445	3.40475	-0.18562
H	1.0	-4.94533	1.26013	-1.07958
C	6.0	-0.14499	2.96004	1.41567
H	1.0	0.75715	3.42430	1.79508
H	1.0	0.48541	0.90697	1.42346
C	6.0	-1.62573	5.03157	1.00996
C	6.0	-1.41470	5.62732	-0.40917
H	1.0	-0.93274	5.54294	1.69315

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-2.65351	5.23799	1.35101
N	7.0	-0.05197	5.30735	-0.89986
H	1.0	-1.54026	6.71947	-0.36570
H	1.0	-2.18289	5.23588	-1.10068
C	6.0	-0.01991	4.12941	-1.80250
C	6.0	0.73271	6.47679	-1.36560
C	6.0	1.37235	3.48833	-1.88092
H	1.0	-0.38391	4.37827	-2.82148
H	1.0	-0.71649	3.39378	-1.38732
H	1.0	0.63735	7.24517	-0.58504
C	6.0	0.32352	7.07822	-2.72918
H	1.0	1.79121	6.18426	-1.40053
H	1.0	2.05609	4.10877	-2.48125
C	6.0	1.32215	2.06613	-2.47419
H	1.0	1.77084	3.44514	-0.85645
H	1.0	-0.75515	7.30166	-2.71578
H	1.0	0.49649	6.34120	-3.52738
C	6.0	1.10585	8.36533	-3.06092
H	1.0	0.89887	2.10522	-3.49151
H	1.0	0.64134	1.45646	-1.85877
C	6.0	2.70454	1.38690	-2.52804
H	1.0	0.89648	9.11725	-2.28502
C	6.0	0.75328	8.94034	-4.44662
H	1.0	2.18326	8.14568	-3.01589
H	1.0	3.39299	2.01585	-3.11565
C	6.0	2.67268	-0.02813	-3.13932
H	1.0	3.11065	1.32838	-1.50469
H	1.0	-0.31709	9.17458	-4.50356
H	1.0	0.98735	8.21244	-5.23384
H	1.0	1.31472	9.85956	-4.65376
H	1.0	2.24572	0.03134	-4.15281
H	1.0	2.00081	-0.66188	-2.53844
C	6.0	4.06149	-0.69160	-3.21786
H	1.0	4.73280	-0.04202	-3.80257
C	6.0	4.03899	-2.09591	-3.85623
H	1.0	4.48186	-0.76395	-2.20175

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	3.59597	-2.01710	-4.86006
H	1.0	3.37936	-2.74491	-3.26104
C	6.0	5.43905	-2.73194	-3.95795
H	1.0	6.10130	-2.10549	-4.56930
H	1.0	5.39392	-3.72813	-4.41535
H	1.0	5.88860	-2.83387	-2.96198
		N,N-dipentyltryptamine		
C	6.0	-3.51866	3.00348	-0.29087
C	6.0	-4.53932	2.20619	-0.82374
C	6.0	-4.41884	0.78698	-0.86340
C	6.0	-3.31528	0.13908	-0.29260
C	6.0	-2.27041	0.94961	0.20018
C	6.0	-2.40156	2.37264	0.31627
N	7.0	-1.07588	0.59657	0.83384
C	6.0	-1.19846	2.87345	0.95496
H	1.0	-5.23971	0.19399	-1.26069
H	1.0	-3.22140	-0.94466	-0.33888
H	1.0	-3.64448	4.08320	-0.23948
H	1.0	-5.40533	2.67874	-1.28107
C	6.0	-0.45167	1.75796	1.31724
H	1.0	0.52603	1.70834	1.78247
H	1.0	-0.80439	-0.34488	1.06558
C	6.0	-0.86222	4.31842	1.22821
C	6.0	-0.72554	5.20576	-0.03955
H	1.0	0.09112	4.37886	1.77368
H	1.0	-1.64267	4.75872	1.87237
N	7.0	0.63699	5.16843	-0.63404
H	1.0	-0.90148	6.25062	0.24954
H	1.0	-1.49910	4.91872	-0.77860
C	6.0	0.93374	3.88192	-1.32109
C	6.0	0.91990	6.36973	-1.47166
C	6.0	2.39430	3.79090	-1.78804
H	1.0	0.24623	3.70999	-2.17647
H	1.0	0.74413	3.08727	-0.59613
H	1.0	0.68304	7.24483	-0.85032

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	0.14904	6.46747	-2.80899
H	1.0	1.99856	6.39829	-1.66863
H	1.0	2.55662	4.42061	-2.67586
C	6.0	2.81223	2.34565	-2.12362
H	1.0	3.03177	4.18204	-0.98108
H	1.0	-0.93302	6.41121	-2.61420
H	1.0	0.41206	5.61509	-3.45247
C	6.0	0.45505	7.77118	-3.57239
H	1.0	2.11405	1.92462	-2.86476
H	1.0	2.72494	1.73454	-1.21143
C	6.0	4.25238	2.24241	-2.66195
H	1.0	0.15183	8.63125	-2.95383
C	6.0	-0.25876	7.85508	-4.93683
H	1.0	1.54331	7.84968	-3.72900
H	1.0	4.32539	2.83665	-3.58326
C	6.0	4.68624	0.79401	-2.94600
H	1.0	4.93622	2.69514	-1.92924
H	1.0	-1.34214	7.75868	-4.77292
H	1.0	0.05436	6.99547	-5.54746
C	6.0	0.03523	9.16253	-5.69636
H	1.0	4.02472	0.33150	-3.68901
H	1.0	4.64089	0.19444	-2.03015
H	1.0	5.71199	0.75223	-3.32984
H	1.0	-0.29231	10.03032	-5.11036
H	1.0	-0.48286	9.18932	-6.66210
H	1.0	1.11171	9.26388	-5.88421
		N-hexyl-N-pentyltryptamine		
C	6.0	-3.53627	2.98874	-0.27539
C	6.0	-4.54569	2.18158	-0.81163
C	6.0	-4.40862	0.76460	-0.85817
C	6.0	-3.29918	0.12930	-0.28633
C	6.0	-2.26459	0.94927	0.21010
C	6.0	-2.41187	2.37002	0.32739
N	7.0	-1.06537	0.60775	0.84236
C	6.0	-1.21619	2.88284	0.96858

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-5.22001	0.16251	-1.25990
H	1.0	-3.19199	-0.95285	-0.33698
H	1.0	-3.67143	4.06667	-0.22041
H	1.0	-5.41738	2.64339	-1.26792
C	6.0	-0.45754	1.77612	1.33207
H	1.0	0.52054	1.73806	1.79693
H	1.0	-0.79353	-0.33106	1.09091
C	6.0	-0.89411	4.33002	1.23992
C	6.0	-0.76768	5.21754	-0.02752
H	1.0	0.05571	4.40072	1.78807
H	1.0	-1.68063	4.75741	1.88277
N	7.0	0.59508	5.18543	-0.62234
H	1.0	-0.94412	6.26109	0.26748
H	1.0	-1.54471	4.93136	-0.76228
C	6.0	0.89394	3.90494	-1.31988
C	6.0	0.87367	6.39311	-1.45309
C	6.0	2.35233	3.82741	-1.79535
H	1.0	0.20348	3.73677	-2.17445
H	1.0	0.70901	3.10120	-0.60190
H	1.0	0.63169	7.26250	-0.82645
C	6.0	0.10976	6.49309	-2.79370
H	1.0	1.95311	6.42889	-1.64593
H	1.0	2.50660	4.46857	-2.67634
C	6.0	2.78097	2.38920	-2.15033
H	1.0	2.99108	4.21022	-0.98506
H	1.0	-0.97381	6.44584	-2.60470
H	1.0	0.36890	5.63851	-3.43494
C	6.0	0.42955	7.79483	-3.55494
H	1.0	2.08632	1.97337	-2.89842
H	1.0	2.70140	1.76306	-1.24760
C	6.0	4.21914	2.31011	-2.69733
H	1.0	0.13262	8.65784	-2.93773
C	6.0	-0.27591	7.88447	-4.92339
H	1.0	1.51952	7.86304	-3.70658
H	1.0	4.28559	2.92168	-3.61065
C	6.0	4.68108	0.87560	-3.01474

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	4.90443	2.75259	-1.95625
H	1.0	-1.36138	7.80135	-4.76497
H	1.0	0.02975	7.02018	-5.53091
C	6.0	0.04090	9.18677	-5.68296
H	1.0	3.98718	0.43451	-3.74606
H	1.0	4.61119	0.27473	-2.09615
C	6.0	6.12108	0.81291	-3.56235
H	1.0	-0.28016	10.05920	-5.09906
H	1.0	-0.47699	9.22179	-6.64902
H	1.0	1.11902	9.27554	-5.86614
H	1.0	6.20174	1.38853	-4.49297
H	1.0	6.42483	-0.21792	-3.77524
H	1.0	6.82843	1.23643	-2.83630
		N,N-dihexyltryptamine		
C	6.0	-3.23157	2.36202	-0.29676
C	6.0	-3.83450	1.21098	-0.82248
C	6.0	-3.20736	-0.06393	-0.70662
C	6.0	-2.00798	-0.22082	0.00579
C	6.0	-1.38565	0.94888	0.49185
C	6.0	-2.03751	2.22534	0.45747
N	7.0	-0.18535	1.11754	1.19409
C	6.0	-1.15587	3.18489	1.09733
H	1.0	-3.71065	-0.94226	-1.10568
H	1.0	-1.52246	-1.19495	0.06721
H	1.0	-3.73776	3.32481	-0.36666
H	1.0	-4.75589	1.29947	-1.39570
C	6.0	-0.07132	2.46641	1.58629
H	1.0	0.82452	2.82846	2.07880
H	1.0	0.36775	0.36099	1.57502
C	6.0	-1.33117	4.67890	1.09993
C	6.0	-1.15591	5.30567	-0.30576
H	1.0	-0.57806	5.13167	1.76078
H	1.0	-2.32980	4.94319	1.48498
N	7.0	0.23921	5.16367	-0.80340
H	1.0	-1.37790	6.38007	-0.23638

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-1.88048	4.85763	-1.01226
C	6.0	0.45532	3.90547	-1.57293
C	6.0	0.72111	6.38332	-1.51504
C	6.0	1.94412	3.64721	-1.84968
H	1.0	-0.11852	3.90502	-2.52386
H	1.0	0.06534	3.08743	-0.96128
H	1.0	0.53986	7.23038	-0.83884
C	6.0	0.05881	6.66547	-2.88416
H	1.0	1.80809	6.29975	-1.64149
H	1.0	2.31168	4.30852	-2.64971
C	6.0	2.22344	2.18272	-2.24403
H	1.0	2.49989	3.89203	-0.93175
H	1.0	-1.03476	6.70498	-2.75694
H	1.0	0.27820	5.84227	-3.58007
C	6.0	0.53580	7.98587	-3.52268
H	1.0	1.58588	1.90595	-3.09944
H	1.0	1.93738	1.53323	-1.40104
C	6.0	3.70034	1.93353	-2.60866
H	1.0	0.29936	8.82132	-2.84449
C	6.0	-0.10888	8.25065	-4.89810
H	1.0	1.63145	7.95604	-3.63684
H	1.0	3.96938	2.57557	-3.46306
C	6.0	4.01582	0.46666	-2.96232
H	1.0	4.33119	2.24251	-1.75950
H	1.0	-1.20387	8.27436	-4.77772
H	1.0	0.12662	7.40796	-5.56738
C	6.0	0.35222	9.56387	-5.56204
H	1.0	3.36695	0.15674	-3.79498
H	1.0	3.76014	-0.16609	-2.09913
C	6.0	5.49304	0.24777	-3.34735
H	1.0	0.11586	10.40193	-4.88975
C	6.0	-0.30511	9.80076	-6.93697
H	1.0	1.44629	9.53633	-5.67545
H	1.0	5.75474	0.85468	-4.22360
H	1.0	5.69362	-0.80325	-3.58832
H	1.0	6.15302	0.53950	-2.51996

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
H	1.0	-1.39700	9.84951	-6.83702
H	1.0	-0.06081	8.98210	-7.62586
H	1.0	0.03750	10.73948	-7.38870
		N-heptyl-N-hexyltryptamine		
C	6.0	-3.55302	3.01241	-0.24499
C	6.0	-4.57532	2.23657	-0.80777
C	6.0	-4.46463	0.81708	-0.88291
C	6.0	-3.37577	0.14645	-0.30679
C	6.0	-2.32780	0.93467	0.21622
C	6.0	-2.44090	2.35918	0.35236
N	7.0	-1.16094	0.55296	0.88655
C	6.0	-1.22884	2.83502	0.99558
H	1.0	-5.28543	0.24034	-1.30548
H	1.0	-3.29549	-0.93851	-0.36773
H	1.0	-3.66927	4.09286	-0.16785
H	1.0	-5.43482	2.72576	-1.26353
C	6.0	-0.49545	1.70380	1.34045
H	1.0	0.47024	1.63134	1.82997
H	1.0	-0.77918	-0.38216	0.91277
C	6.0	-0.87795	4.27029	1.30628
C	6.0	-0.75917	5.19579	0.06601
H	1.0	0.08599	4.30750	1.83628
H	1.0	-1.64140	4.69382	1.97982
N	7.0	0.60473	5.20285	-0.52723
H	1.0	-0.95256	6.22889	0.38511
H	1.0	-1.52855	4.91716	-0.68009
C	6.0	0.94103	3.92372	-1.21041
C	6.0	0.84107	6.40853	-1.37240
C	6.0	2.39265	3.88680	-1.71018
H	1.0	0.24414	3.71440	-2.05012
H	1.0	0.79935	3.12529	-0.47727
H	1.0	0.56470	7.27743	-0.75812
C	6.0	0.07603	6.46502	-2.71539
H	1.0	1.91909	6.48134	-1.56464
H	1.0	2.51842	4.54271	-2.58454

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	2.84269	2.46289	-2.09629
H	1.0	3.03848	4.27156	-0.90664
H	1.0	-1.00712	6.40746	-2.52681
H	1.0	0.34805	5.59748	-3.33518
C	6.0	0.38212	7.75044	-3.51006
H	1.0	2.14157	2.04776	-2.83836
H	1.0	2.79431	1.81774	-1.20425
C	6.0	4.27235	2.42371	-2.67238
H	1.0	0.06817	8.62503	-2.91798
C	6.0	-0.31314	7.79329	-4.88507
H	1.0	1.47171	7.82850	-3.65586
H	1.0	4.31558	3.07423	-3.56071
C	6.0	4.74669	1.00988	-3.06186
H	1.0	4.96580	2.84323	-1.92615
H	1.0	-1.40232	7.72062	-4.73738
H	1.0	-0.00288	6.90950	-5.46531
C	6.0	0.00311	9.06525	-5.69690
H	1.0	4.04799	0.59113	-3.80342
H	1.0	4.70672	0.36160	-2.17163
C	6.0	6.17554	0.98301	-3.64309
H	1.0	-0.31227	9.94337	-5.11411
C	6.0	-0.68483	9.08446	-7.07606
H	1.0	1.09305	9.13639	-5.82710
H	1.0	6.20958	1.64394	-4.52248
C	6.0	6.64117	-0.43249	-4.04130
H	1.0	6.86657	1.40196	-2.89634
H	1.0	-1.77518	9.03385	-6.96300
H	1.0	-0.36272	8.22487	-7.67781
H	1.0	-0.44246	9.99848	-7.63118
H	1.0	5.97496	-0.85523	-4.80442
H	1.0	6.63271	-1.10057	-3.17018
H	1.0	7.65893	-0.41795	-4.44979
		N,N-diheptyltryptamine		
C	6.0	-3.53590	2.97536	-0.21369
C	6.0	-4.55111	2.19241	-0.77308

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	-4.43139	0.77516	-0.84430
C	6.0	-3.33902	0.11451	-0.27119
C	6.0	-2.29861	0.91062	0.25084
C	6.0	-2.42363	2.33168	0.38835
N	7.0	-1.12733	0.54047	0.91129
C	6.0	-1.21745	2.81753	1.02924
H	1.0	-5.24754	0.19368	-1.26462
H	1.0	-3.25221	-0.96779	-0.33274
H	1.0	-3.65879	4.05396	-0.14338
H	1.0	-5.41115	2.67495	-1.23043
C	6.0	-0.47455	1.69478	1.36919
H	1.0	0.49374	1.63131	1.84926
H	1.0	-0.74564	-0.39153	0.95072
C	6.0	-0.88130	4.25454	1.34005
C	6.0	-0.76206	5.17499	0.09595
H	1.0	0.07800	4.30009	1.87635
H	1.0	-1.65656	4.67125	2.00506
N	7.0	0.60041	5.18113	-0.49960
H	1.0	-0.95569	6.20948	0.41095
H	1.0	-1.53148	4.89439	-0.64888
C	6.0	0.93871	3.89903	-1.17645
C	6.0	0.83318	6.38418	-1.35187
C	6.0	2.38714	3.86802	-1.68471
H	1.0	0.23849	3.68354	-2.01160
H	1.0	0.80304	3.10502	-0.43847
H	1.0	0.55473	7.25525	-0.74252
C	6.0	0.06712	6.42743	-2.69417
H	1.0	1.91050	6.45830	-1.54387
H	1.0	2.50529	4.52310	-2.55974
C	6.0	2.84230	2.44568	-2.06912
H	1.0	3.03589	4.25671	-0.88468
H	1.0	-1.01600	6.37287	-2.50501
H	1.0	0.33727	5.55357	-3.30488
C	6.0	0.36938	7.70253	-3.50647
H	1.0	2.13791	2.02763	-2.80630
H	1.0	2.80364	1.80237	-1.17667

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
C	6.0	4.26690	2.41155	-2.65545
H	1.0	0.06067	8.58671	-2.92618
C	6.0	-0.33911	7.71974	-4.87547
H	1.0	1.45778	7.77764	-3.66476
H	1.0	4.30218	3.06283	-3.54254
C	6.0	4.73474	0.99865	-3.04961
H	1.0	4.96675	2.82878	-1.91440
H	1.0	-1.42653	7.65002	-4.71399
H	1.0	-0.03380	6.82561	-5.44189
C	6.0	-0.03462	8.97371	-5.71596
H	1.0	4.03213	0.58460	-3.78998
H	1.0	4.69251	0.34923	-2.16175
C	6.0	6.16278	0.96396	-3.63104
H	1.0	-0.34829	9.86800	-5.15470
C	6.0	-0.72996	8.97025	-7.09141
H	1.0	1.05453	9.04842	-5.86353
H	1.0	6.19953	1.61530	-4.51697
C	6.0	6.62078	-0.45576	-4.01959
H	1.0	6.85554	1.38651	-2.88851
H	1.0	-1.81603	8.89224	-6.93612
H	1.0	-0.41466	8.07099	-7.64144
C	6.0	-0.41499	10.22381	-7.92996
H	1.0	5.95164	-0.88491	-4.77517
H	1.0	6.61389	-1.11387	-3.14137
H	1.0	7.64103	-0.45085	-4.42238
H	1.0	-0.74439	11.12972	-7.40526
H	1.0	-0.92146	10.19319	-8.90176
H	1.0	0.66422	10.30563	-8.10981
		N-heptyl-N-octyltryptamine		
C	6.0	-3.58017	3.02446	-0.19692
C	6.0	-4.60656	2.25620	-0.76200
C	6.0	-4.50072	0.83706	-0.84683
C	6.0	-3.40903	0.15883	-0.28629
C	6.0	-2.35728	0.94122	0.23816
C	6.0	-2.47101	2.36327	0.39487

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z
N	7.0	-1.17238	0.55404	0.87116
C	6.0	-1.26255	2.83036	1.04975
H	1.0	-5.32447	0.26602	-1.27081
H	1.0	-3.32748	-0.92477	-0.36531
H	1.0	-3.69269	4.10457	-0.11275
H	1.0	-5.46504	2.75180	-1.21141
C	6.0	-0.53341	1.69450	1.38780
H	1.0	0.44128	1.61774	1.85697
H	1.0	-0.90108	-0.39904	1.06721
C	6.0	-0.90932	4.26288	1.36672
C	6.0	-0.77848	5.18716	0.12685
H	1.0	0.04849	4.29735	1.90787
H	1.0	-1.67973	4.68767	2.03204
N	7.0	0.58708	5.18572	-0.46308
H	1.0	-0.96677	6.22169	0.44350
H	1.0	-1.54640	4.91242	-0.62218
C	6.0	0.92364	3.90094	-1.13627
C	6.0	0.81968	6.38361	-1.32160
C	6.0	2.36953	3.86962	-1.65233
H	1.0	0.21820	3.68082	-1.96591
H	1.0	0.79400	3.10787	-0.39542
H	1.0	0.54618	7.25891	-0.71571
C	6.0	0.04677	6.42055	-2.66035
H	1.0	1.89638	6.45448	-1.51972
H	1.0	2.48284	4.52865	-2.52591
C	6.0	2.82282	2.45036	-2.05187
H	1.0	3.02442	4.25531	-0.85646
H	1.0	-1.03526	6.37066	-2.46345
H	1.0	0.31092	5.54152	-3.26682
C	6.0	0.34908	7.68923	-3.48308
H	1.0	2.11707	2.03561	-2.78970
H	1.0	2.79017	1.79827	-1.16434
C	6.0	4.24559	2.42843	-2.64558
H	1.0	0.03869	8.57842	-2.91156
C	6.0	-0.35375	7.69461	-4.85549
H	1.0	1.43778	7.76396	-3.63916

(table continues)

Table 2.31 *(continued)*

Atom	Nuclear charge	X	Y	Z	
H	1.0	4.27462	3.09096	-3.52514	
C	6.0	4.72567	1.02407	-3.06110	
H	1.0	4.94657	2.84151	-1.90271	
H	1.0	-1.44235	7.63108	-4.69781	
H	1.0	-0.05083	6.79307	-5.41132	
C	6.0	-0.03967	8.93974	-5.70702	
H	1.0	4.01808	0.60905	-3.79623	
H	1.0	4.70935	0.36335	-2.18002	
C	6.0	6.14204	1.02265	-3.66997	
H	1.0	-0.35381	9.84062	-5.15653	
C	6.0	-0.72655	8.92560	-7.08742	
H	1.0	1.05073	9.00676	-5.84851	
H	1.0	6.15515	1.69729	-4.54082	
C	6.0	6.62702	-0.37412	-4.10819	
H	1.0	6.84755	1.43223	-2.92945	
H	1.0	-1.81443	8.85612	-6.93970	
H	1.0	-0.41461	8.01773	-7.62517	
C	6.0	-0.39763	10.16779	-7.93838	
H	1.0	5.91360	-0.78031	-4.84076	
H	1.0	6.61214	-1.04421	-3.23570	
C	6.0	8.04106	-0.35490	-4.72170	
H	1.0	-0.72201	11.08209	-7.42505	
H	1.0	-0.89839	10.12975	-8.91299	
H	1.0	0.68342	10.23904	-8.11252	
H	1.0	8.06706	0.29260	-5.60758	
H	1.0	8.36111	-1.35918	-5.02428	
H	1.0	8.76891	0.03055	-3.99612	

Table 2.32 Bonding (MP2/6-311++G) for unoptimized tryptamine derivatives structures

Bond type	Length/Å	Order
	N-methyltryptamine	
C1—C2	1.39	1.48
C2—N3	1.41	0.69
N3—C4	1.40	0.77

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.42	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.09
C4—C9	1.43	1.23
C1—C10	1.51	0.80
C10—C11	1.55	0.76
C11—N12	1.48	0.67
N12—C13	1.48	0.47
C2—H14	1.08	0.77
N3—H15	1.00	0.71
C5—H16	1.09	0.84
C6—H17	1.09	0.84
C7—H18	1.09	0.83
C8—H19	1.09	0.84
C10—H20	1.10	0.90
C10—H21	1.10	0.89
C11—H22	1.11	0.91
C11—H23	1.10	0.90
N12—H24	1.02	0.75
C13—H25	1.11	0.93
C13—H26	1.10	0.94
C13—H27	1.09	0.81
	N,N-dimethyltryptamine	
C1—C2	1.39	1.49
C2—N3	1.41	0.67
N3—C4	1.40	0.75
C4—C5	1.41	1.14
C5—C6	1.40	1.31
C6—C7	1.43	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.12

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C4—C9	1.43	1.24
C1—C10	1.51	0.71
C10—C11	1.55	0.80
C11—N12	1.48	0.70
N12—C13	1.46	0.48
N12—C14	1.48	0.56
C2—H15	1.09	0.77
N3—H16	1.01	0.73
C5—H17	1.09	0.85
C6—H18	1.09	0.84
C7—H19	1.10	0.83
C8—H20	1.09	0.83
C10—H21	1.10	0.91
C10—H22	1.10	0.88
C11—H23	1.10	0.89
C11—H24	1.09	0.88
C13—H25	1.08	0.80
C13—H26	1.09	0.93
C13—H27	1.08	0.93
C14—H28	1.06	0.93
C14—H29	1.08	0.92
C14—H30	1.09	0.92
	N-ethyl-N-methyltryptamine	
C1—C2	1.39	1.46
C2—N3	1.40	0.70
N3—C4	1.40	0.77
C4—C5	1.41	1.14
C5—C6	1.40	1.31
C6—C7	1.42	1.18
C7—C8	1.40	1.31
C8—C9	1.42	1.09
C9—C1	1.45	1.14
C4—C9	1.43	1.24
C1—C10	1.51	0.73
C10—C11	1.55	0.75

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C11—N12	1.49	0.67
N12—C13	1.49	0.63
N12—C14	1.49	0.48
C13—C15	1.54	1.00
C2—H16	1.08	0.77
N3—H17	1.01	0.73
C5—H18	1.09	0.84
C6—H19	1.09	0.84
C7—H20	1.09	0.83
C8—H21	1.09	0.83
C10—H22	1.10	0.89
C10—H23	1.10	0.89
C11—H24	1.11	0.88
C11—H25	1.10	0.89
C13—H26	1.09	0.95
C13—H27	1.12	0.87
C14—H28	1.10	0.92
C14—H29	1.11	0.93
C14—H30	1.09	0.94
C15—H31	1.10	0.89
C15—H32	1.10	0.88
C15—H33	1.10	0.90
	N,N-diethyltryptamine	
C1—C2	1.39	1.46
C2—N3	1.41	0.70
N3—C4	1.40	1.14
C4—C5	1.41	1.30
C5—C6	1.40	1.19
C6—C7	1.42	1.29
C7—C8	1.40	1.11
C8—C9	1.42	1.09
C9—C1	1.45	1.23
C4—C9	1.43	1.23
C1—C10	1.51	0.72
C10—C11	1.55	0.76

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C11—N12	1.49	0.62
N12—C13	1.49	0.56
N12—C14	1.49	0.58
C13—C15	1.54	0.98
C14—C16	1.55	0.83
C2—H17	1.08	0.78
N3—H18	1.01	0.71
C5—H19	1.09	0.85
C6—H20	1.09	0.83
C7—H21	1.09	0.83
C8—H22	1.09	0.83
C10—H23	1.10	0.90
C10—H24	1.10	0.89
C11—H25	1.11	0.91
C11—H26	1.10	0.88
C13—H27	1.09	0.97
C13—H28	1.11	0.86
C14—H29	1.10	0.90
C14—H30	1.10	0.91
C15—H31	1.10	0.89
C15—H32	1.10	0.87
C15—H33	1.10	0.90
C16—H34	1.10	0.91
C16—H35	1.10	0.90
C16—H36	1.10	0.89
	N-ethyl-N-propyltryptamine	
C1—C2	1.39	1.53
C2—N3	1.41	0.71
N3—C4	1.40	0.77
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.42	1.19
C7—C8	1.40	1.30
C8—C9	1.42	1.14
C9—C1	1.45	1.08

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C4—C9	1.43	1.24
C1—C10	1.51	0.70
C10—C11	1.55	0.79
C11—N12	1.49	0.61
N12—C13	1.48	0.73
N12—C14	1.49	0.55
C13—C15	1.53	0.81
C14—C16	1.54	0.84
C15—C17	1.54	0.82
C2—H18	1.08	0.78
N3—H19	1.01	0.71
C5—H20	1.09	0.84
C6—H21	1.09	0.83
C7—H22	1.09	0.84
C8—H23	1.09	0.83
C10—H24	1.10	0.90
C10—H25	1.10	0.88
C11—H26	1.11	0.94
C11—H27	1.10	0.89
C13—H28	1.10	0.90
C13—H29	1.11	0.86
C14—H30	1.09	0.90
C14—H31	1.10	0.91
C15—H32	1.10	0.88
C15—H33	1.09	0.90
C16—H34	1.10	0.89
C16—H35	1.10	0.89
C16—H36	1.10	0.91
C17—H37	1.09	0.89
C17—H38	1.09	0.90
C17—H39	1.09	0.91
	N,N-dipropyltryptamine	
C1—C2	1.39	1.47
C2—N3	1.41	0.72
N3—C4	1.40	0.75

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.43	1.18
C7—C8	1.40	1.31
C8—C9	1.42	1.11
C9—C1	1.45	1.09
C4—C9	1.43	1.26
C1—C10	1.51	0.71
C10—C11	1.55	0.80
C11—N12	1.49	0.58
N12—C13	1.49	0.68
N12—C14	1.49	0.69
C13—C15	1.54	0.82
C14—C16	1.55	0.75
C15—C17	1.54	0.81
C16—C18	1.54	0.90
C2—H19	1.08	0.78
N3—H20	1.01	0.71
C5—H21	1.09	0.85
C6—H22	1.09	0.83
C7—H23	1.09	0.84
C8—H24	1.09	0.83
C10—H25	1.10	0.89
C10—H26	1.10	0.88
C11—H27	1.11	1.00
C11—H28	1.10	0.89
C13—H29	1.09	0.90
C13—H30	1.11	0.85
C14—H31	1.10	0.89
C14—H32	1.10	0.89
C15—H33	1.10	0.88
C15—H34	1.10	0.88
C16—H35	1.10	0.88
C16—H36	1.10	0.89
C17—H37	1.10	0.91
C17—H38	1.10	0.89

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C17—H39	1.10	0.89
C18—H40	1.10	0.90
C18—H41	1.10	0.89
C18—H42	1.10	0.90
	N-butyltryptamine	
C1—C2	1.39	1.50
C2—N3	1.41	0.69
N3—C4	1.40	0.70
C4—C5	1.41	1.14
C5—C6	1.40	1.31
C6—C7	1.43	1.18
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.12
C4—C9	1.43	0.72
C1—C10	1.56	0.86
C10—C11	1.48	0.75
C11—N12	1.48	0.60
N12—C13	1.54	0.93
C13—C15	1.54	0.88
C15—C17	1.55	0.84
C2—H18	1.09	0.76
N3—H19	1.01	0.74
C5—H20	1.09	0.84
C6—H21	1.09	0.84
C7—H22	1.09	0.83
C8—H23	1.09	0.84
C10—H24	1.10	0.89
C10—H25	1.10	0.89
C11—H26	1.10	0.82
C11—H27	1.10	0.92
N12—H28	1.02	0.74
C13—H29	1.11	0.90
C13—H30	1.10	0.91
C15—H31	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C15—H32	1.10	0.86
C17—H33	1.10	0.88
C17—H34	1.10	0.89
C19—H35	1.10	0.89
C19—H36	1.10	0.90
C19—H37	1.10	0.90
	N-butyl-N-propyltryptamine	
C1—C2	1.39	1.54
C2—N3	1.41	0.70
N3—C4	1.40	0.76
C4—C5	1.41	1.15
C5—C6	1.40	1.31
C6—C7	1.43	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.13
C9—C1	1.45	1.09
C4—C9	1.43	1.24
C1—C10	1.51	0.79
C10—C11	1.55	0.78
C11—N12	1.49	0.56
N12—C13	1.49	0.65
N12—C14	1.49	0.69
C13—C15	1.54	0.85
C14—C16	1.55	0.75
C15—C17	1.54	0.81
C16—C18	1.54	0.89
C17—C19	1.54	0.86
C2—H20	1.08	0.80
N3—H21	1.01	0.72
C5—H22	1.09	0.84
C6—H23	1.09	0.84
C7—H24	1.09	0.85
C8—H25	1.09	0.84
C10—H26	1.10	0.87
C10—H27	1.10	0.91

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C11—H28	1.10	0.90
C11—H29	1.10	0.98
C13—H30	1.09	0.91
C13—H31	1.11	0.84
C14—H32	1.10	0.87
C14—H33	1.10	0.90
C15—H34	1.10	0.87
C15—H35	1.10	0.89
C16—H36	1.10	0.89
C16—H37	1.10	0.88
C17—H38	1.10	0.89
C17—H39	1.10	0.88
C18—H40	1.10	0.90
C18—H41	1.10	0.90
C18—H42	1.10	0.90
C19—H43	1.10	0.88
C19—H44	1.10	0.90
C19—H45	1.10	0.90
	N-butyl-N-pentyltryptamine	
C1—C2	1.39	1.48
C2—N3	1.41	0.71
N3—C4	1.40	0.78
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.42	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.09
C4—C9	1.43	1.24
C1—C10	1.51	0.73
C10—C11	1.55	0.81
C11—N12	1.49	0.55
N12—C13	1.49	0.66
N12—C14	1.49	0.65
C13—C15	1.54	0.81

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C14—C16	1.55	0.81
C15—C17	1.54	0.82
C16—C18	1.54	0.88
C17—C19	1.54	0.86
C18—C20	1.54	0.84
C19—C21	1.54	0.85
C2—H22	1.08	0.77
N3—H23	1.01	0.71
C5—H24	1.09	0.84
C6—H25	1.09	0.84
C7—H26	1.09	0.84
C8—H27	1.09	0.82
C10—H28	1.10	0.88
C10—H29	1.10	0.88
C11—H30	1.11	0.93
C11—H31	1.10	0.91
C13—H32	1.09	0.90
C13—H33	1.11	0.85
C14—H34	1.10	0.89
C14—H35	1.10	0.86
C15—H36	1.10	0.88
C15—H37	1.10	0.88
C16—H38	1.10	0.88
C16—H39	1.10	0.90
C17—H40	1.10	0.90
C17—H41	1.10	0.87
C18—H42	1.10	0.89
C18—H43	1.10	0.89
C19—H44	1.10	0.88
C19—H45	1.10	0.88
C20—H46	1.10	0.90
C20—H47	1.10	0.89
C20—H48	1.10	0.90
C21—H49	1.10	0.89
C21—H50	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C21—H51	1.10	0.90
	N-butyl-N-hexyltryptamine	
C1—C2	1.39	1.60
C2—N3	1.41	0.77
N3—C4	1.40	0.79
C4—C5	1.41	1.14
C5—C6	1.40	1.28
C6—C7	1.43	1.20
C7—C8	1.40	1.31
C8—C9	1.42	1.10
C9—C1	1.45	1.07
C4—C9	1.43	1.20
C1—C10	1.50	0.79
C10—C11	1.55	0.84
C11—N12	1.48	0.41
N12—C13	1.48	0.61
N12—C14	1.48	0.61
C13—C15	1.54	0.83
C14—C16	1.55	0.87
C15—C17	1.54	0.82
C16—C18	1.54	0.86
C17—C19	1.54	0.88
C18—C20	1.54	0.84
C19—C21	1.54	0.83
C21—C23	1.54	0.86
C2—H24	1.08	0.78
N3—H25	1.01	0.68
C5—H26	1.09	0.83
C6—H27	1.09	0.84
C7—H28	1.09	0.83
C8—H29	1.09	0.83
C10—H30	1.10	0.90
C10—H31	1.10	0.90
C11—H32	1.11	0.93
C11—H33	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C13—H34	1.10	0.91
C13—H35	1.11	0.82
C14—H36	1.10	0.88
C14—H37	1.10	0.87
C15—H38	1.10	0.89
C15—H39	1.10	0.87
C16—H40	1.10	0.89
C16—H41	1.10	0.92
C17—H42	1.10	0.84
C17—H43	1.10	0.85
C18—H44	1.10	0.89
C18—H45	1.10	0.89
C19—H46	1.10	0.89
C19—H47	1.10	0.90
C20—H48	1.10	0.90
C20—H49	1.10	0.89
C20—H50	1.10	0.90
C21—H51	1.10	0.87
C21—H52	1.10	0.88
C23—H53	1.10	0.89
C23—H54	1.10	0.90
C23—H55	1.10	0.90
	N-butyl-N-octyltryptamine	
C1—C2	1.39	1.59
C2—N3	1.41	0.79
N3—C4	1.40	0.81
C4—C5	1.41	1.12
C5—C6	1.40	1.28
C6—C7	1.43	1.19
C7—C8	1.40	1.32
C8—C9	1.42	1.11
C9—C1	1.45	1.12
C4—C9	1.43	1.18
C1—C10	1.50	0.75
C10—C11	1.55	0.81

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C11—N12	1.48	0.47
N12—C13	1.48	0.62
N12—C14	1.48	0.60
C13—C15	1.53	0.83
C14—C16	1.55	0.88
C15—C17	1.54	0.82
C16—C18	1.54	0.87
C17—C19	1.54	0.87
C18—C20	1.54	0.84
C19—C21	1.54	0.81
C21—C23	1.54	0.86
C23—C25	1.54	0.85
C25—C27	1.54	0.85
C2—H28	1.08	0.78
N3—H29	1.01	0.68
C5—H30	1.09	0.84
C6—H31	1.09	0.83
C7—H32	1.09	0.84
C8—H33	1.09	0.83
C10—H34	1.10	0.90
C10—H35	1.10	0.90
C11—H36	1.11	0.96
C11—H37	1.10	0.89
C13—H38	1.09	0.89
C13—H39	1.11	0.84
C14—H40	1.10	0.88
C14—H41	1.10	0.87
C15—H42	1.10	0.88
C15—H43	1.10	0.87
C16—H44	1.10	0.88
C16—H45	1.10	0.92
C17—H46	1.10	0.88
C17—H47	1.10	0.84
C18—H48	1.10	0.89
C18—H49	1.10	0.89
C19—H50	1.10	0.88

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C19—H51	1.10	0.90
C20—H52	1.10	0.90
C20—H53	1.10	0.89
C20—H54	1.10	0.90
C21—H55	1.10	0.90
C21—H56	1.10	0.88
C23—H57	1.10	0.88
C23—H58	1.10	0.89
C25—H59	1.10	0.88
C25—H60	1.10	0.88
C27—H61	1.10	0.90
C27—H62	1.10	0.90
C27—H63	1.10	0.90
	N,N-dipentyltryptamine	
C1—C2	1.39	1.56
C2—N3	1.40	0.69
N3—C4	1.40	0.76
C4—C5	1.41	1.14
C5—C6	1.40	1.31
C6—C7	1.42	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.15
C9—C1	1.45	1.10
C4—C9	1.43	1.21
C1—C10	1.51	0.75
C10—C11	1.55	0.76
C11—N12	1.49	0.52
N12—C13	1.49	0.63
N12—C14	1.49	0.68
C13—C15	1.54	0.80
C14—C16	1.55	0.81
C15—C17	1.54	0.83
C16—C18	1.54	0.81
C17—C19	1.54	0.86
C18—C20	1.54	0.89

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C19—C21	1.59	0.85
C20—C22	1.54	0.85
C2—H23	1.08	0.80
N3—H24	1.01	0.71
C5—H25	1.09	0.84
C6—H26	1.09	0.84
C7—H27	1.09	0.84
C8—H28	1.09	0.84
C10—H29	1.10	0.88
C10—H30	1.10	0.89
C11—H31	1.11	0.93
C11—H32	1.10	0.91
C13—H33	1.09	0.90
C13—H34	1.11	0.84
C14—H35	1.10	0.87
C14—H36	1.10	0.87
C15—H37	1.10	0.88
C15—H38	1.10	0.87
C16—H39	1.10	0.89
C16—H40	1.10	0.87
C17—H41	1.10	0.91
C17—H42	1.10	0.88
C18—H43	1.10	0.89
C18—H44	1.10	0.88
C19—H45	1.10	0.88
C19—H46	1.10	0.88
C20—H47	1.10	0.89
C20—H48	1.10	0.88
C21—H49	1.10	0.90
C21—H50	1.10	0.90
C21—H51	1.10	0.90
C22—H52	1.10	0.90
C22—H53	1.10	0.89
C22—H54	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
	N-hexyl-N-pentyltryptamine	
C1—C2	1.39	1.55
C2—N3	1.41	0.69
N3—C4	1.40	0.77
C4—C5	1.41	1.14
C5—C6	1.40	1.30
C6—C7	1.42	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.14
C9—C1	1.45	1.10
C4—C9	1.43	1.24
C1—C10	1.51	0.75
C10—C11	1.55	0.78
C11—N12	1.49	0.56
N12—C13	1.49	0.62
N12—C14	1.49	0.67
C13—C15	1.54	0.82
C14—C16	1.55	0.84
C15—C17	1.54	0.79
C16—C18	1.54	0.88
C17—C19	1.54	0.87
C18—C20	1.54	0.86
C19—C21	1.54	0.85
C20—C22	1.54	0.85
C21—C23	1.54	0.85
C2—H24	1.08	0.79
N3—H25	1.01	0.71
C5—H26	1.09	0.84
C6—H27	1.09	0.84
C7—H28	1.09	0.84
C8—H29	1.09	0.84
C10—H30	1.10	0.89
C10—H31	1.10	0.89
C11—H32	1.11	0.92
C11—H33	1.10	0.91
C13—H34	1.09	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C13—H35	1.11	0.87
C14—H36	1.10	0.88
C14—H37	1.10	0.85
C15—H38	1.10	0.87
C15—H39	1.10	0.86
C16—H40	1.10	0.89
C16—H41	1.10	0.88
C17—H42	1.10	0.91
C17—H43	1.10	0.87
C18—H44	1.10	0.89
C18—H45	1.10	0.88
C19—H46	1.10	0.91
C19—H47	1.10	0.87
C20—H48	1.10	0.89
C20—H49	1.10	0.88
C21—H50	1.10	0.89
C21—H51	1.10	0.88
C22—H52	1.10	0.90
C22—H53	1.10	0.89
C22—H54	1.10	0.90
C23—H55	1.10	0.90
C23—H56	1.10	0.90
C23—H57	1.10	0.90
	N,N-dihexyltryptamine	
C1—C2	1.39	1.54
C2—N3	1.41	0.74
N3—C4	1.40	0.79
C4—C5	1.41	1.12
C5—C6	1.40	1.30
C6—C7	1.43	1.20
C7—C8	1.40	1.29
C8—C9	1.42	1.13
C9—C1	1.45	1.07
C4—C9	1.43	1.18
C1—C10	1.50	0.77

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C10—C11	1.55	0.83
C11—N12	1.49	0.46
N12—C13	1.49	0.63
N12—C14	1.49	0.66
C13—C15	1.54	0.86
C14—C16	1.55	0.84
C15—C17	1.54	0.82
C16—C18	1.54	0.87
C17—C19	1.54	0.87
C18—C20	1.54	0.86
C19—C21	1.54	0.85
C20—C22	1.54	0.84
C21—C23	1.54	0.84
C22—C24	1.54	0.86
C2—H25	1.08	0.77
N3—H26	1.01	0.67
C5—H27	1.09	0.84
C6—H28	1.09	0.84
C7—H29	1.09	0.84
C8—H30	1.09	0.83
C10—H31	1.10	0.89
C10—H32	1.10	0.89
C11—H33	1.11	0.94
C11—H34	1.10	0.90
C13—H35	1.09	0.86
C13—H36	1.11	0.85
C14—H37	1.10	0.87
C14—H38	1.10	0.86
C15—H39	1.10	0.85
C15—H40	1.10	0.90
C16—H41	1.10	0.89
C16—H42	1.10	0.88
C17—H43	1.10	0.86
C17—H44	1.10	0.86
C18—H45	1.10	0.89
C18—H46	1.10	0.89

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C19—H47	1.10	0.87
C19—H48	1.10	0.89
C20—H49	1.10	0.89
C20—H50	1.10	0.88
C21—H51	1.10	0.89
C21—H52	1.10	0.88
C22—H53	1.10	0.88
C22—H54	1.10	0.88
C23—H55	1.10	0.89
C23—H56	1.10	0.90
C23—H57	1.10	0.90
C24—H58	1.10	0.90
C24—H59	1.10	0.90
C24—H60	1.10	0.90
	N-heptyl-N-hexyltryptamine	
C1—C2	1.39	1.53
C2—N3	1.40	0.68
N3—C4	1.40	0.75
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.43	1.18
C7—C8	1.40	1.31
C8—C9	1.42	1.13
C9—C1	1.45	1.14
C4—C9	1.44	1.24
C1—C10	1.51	0.73
C10—C11	1.55	0.77
C11—N12	1.49	0.55
N12—C13	1.49	0.61
N12—C14	1.49	0.67
C13—C15	1.54	0.84
C14—C16	1.55	0.86
C15—C17	1.54	0.80
C16—C18	1.54	0.86
C17—C19	1.54	0.85

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C18—C20	1.54	0.85
C19—C21	1.54	0.85
C20—C22	1.54	0.85
C21—C23	1.54	0.85
C22—C24	1.54	0.86
C23—C25	1.54	0.86
C2—H26	1.09	0.78
N3—H27	1.01	0.72
C5—H28	1.09	0.84
C6—H29	1.09	0.84
C7—H30	1.09	0.84
C8—H31	1.09	0.84
C10—H32	1.10	0.88
C10—H33	1.10	0.89
C11—H34	1.11	0.93
C11—H35	1.10	0.90
C13—H36	1.09	0.92
C13—H37	1.11	0.86
C14—H38	1.10	0.87
C14—H39	1.10	0.85
C15—H40	1.10	0.85
C15—H41	1.10	0.87
C16—H42	1.10	0.87
C16—H43	1.10	0.86
C17—H44	1.10	0.91
C17—H45	1.10	0.87
C18—H46	1.10	0.89
C18—H47	1.10	0.89
C19—H48	1.10	0.88
C19—H49	1.10	0.89
C20—H50	1.10	0.89
C20—H51	1.10	0.88
C21—H52	1.10	0.88
C21—H53	1.10	0.88
C22—H54	1.10	0.88
C22—H55	1.10	0.88

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C23—H56	1.10	0.88
C23—H57	1.10	0.88
C24—H58	1.10	0.90
C24—H59	1.10	0.89
C24—H60	1.10	0.90
C25—H61	1.10	0.90
C25—H62	1.10	0.90
C25—H63	1.10	0.90
	N,N-diheptyltryptamine	
C1—C2	1.39	1.49
C2—N3	1.40	0.70
N3—C4	1.39	0.75
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.42	1.18
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.13
C4—C9	1.43	1.25
C1—C10	1.51	0.71
C10—C11	1.55	0.77
C11—N12	1.49	0.56
N12—C13	1.49	0.61
N12—C14	1.49	0.81
C13—C15	1.54	0.85
C14—C16	1.55	0.81
C15—C17	1.54	0.80
C16—C18	1.54	0.88
C17—C19	1.54	0.85
C18—C20	1.54	0.82
C19—C21	1.54	0.85
C20—C22	1.54	0.86
C21—C23	1.54	0.85
C22—C24	1.54	0.86
C23—C25	1.54	0.86

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C24—C26	1.54	0.85
C2—H27	1.08	0.77
N3—H28	1.01	0.71
C5—H29	1.09	0.84
C6—H30	1.09	0.84
C7—H31	1.09	0.83
C8—H32	1.09	0.83
C10—H33	1.10	0.89
C10—H34	1.10	0.88
C11—H35	1.11	0.94
C11—H36	1.10	0.90
C13—H37	1.09	0.90
C13—H38	1.11	0.89
C14—H39	1.10	0.86
C14—H40	1.10	0.86
C15—H41	1.10	0.85
C15—H42	1.10	0.86
C16—H43	1.10	0.88
C16—H44	1.10	0.85
C17—H45	1.10	0.91
C17—H46	1.10	0.87
C18—H47	1.10	0.89
C18—H48	1.10	0.89
C19—H49	1.10	0.88
C19—H50	1.10	0.89
C20—H51	1.10	0.89
C20—H52	1.10	0.90
C21—H53	1.10	0.89
C21—H54	1.10	0.88
C22—H55	1.10	0.88
C22—H56	1.10	0.88
C23—H57	1.10	0.88
C23—H58	1.10	0.88
C24—H59	1.10	0.88
C24—H60	1.10	0.88
C25—H61	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C25—H62	1.10	0.90
C25—H63	1.10	0.90
C26—H64	1.10	0.90
C26—H65	1.10	0.90
C26—H66	1.10	0.90
	N-heptyl-N-octyltryptamine	
C1—C2	1.39	1.47
C2—N3	1.41	0.71
N3—C4	1.40	0.76
C4—C5	1.41	1.13
C5—C6	1.40	1.30
C6—C7	1.43	1.19
C7—C8	1.40	1.31
C8—C9	1.42	1.12
C9—C1	1.45	1.12
C4—C9	1.44	1.23
C1—C10	1.51	0.72
C10—C11	1.55	0.77
C11—N12	1.49	0.55
N12—C13	1.49	0.61
N12—C14	1.49	0.68
C13—C15	1.54	0.85
C14—C16	1.55	0.81
C15—C17	1.54	0.80
C16—C18	1.54	0.88
C17—C19	1.54	0.86
C18—C20	1.54	0.81
C19—C21	1.54	0.83
C20—C22	1.54	0.86
C21—C23	1.54	0.85
C22—C24	1.54	0.86
C23—C25	1.54	0.86
C24—C26	1.54	0.85
C25—C27	1.54	0.85
C2—H28	1.08	0.78

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
N3—H29	1.01	0.71
C5—H30	1.09	0.84
C6—H31	1.09	0.84
C7—H32	1.09	0.83
C8—H33	1.09	0.83
C10—H34	1.10	0.89
C10—H35	1.10	0.88
C11—H36	1.11	0.94
C11—H37	1.10	0.90
C13—H38	1.09	0.90
C13—H39	1.11	0.88
C14—H40	1.10	0.86
C14—H41	1.10	0.86
C15—H42	1.10	0.85
C15—H43	1.10	0.85
C16—H44	1.10	0.87
C16—H45	1.10	0.85
C17—H46	1.10	0.91
C17—H47	1.10	0.87
C18—H48	1.10	0.89
C18—H49	1.10	0.89
C19—H50	1.10	0.87
C19—H51	1.10	0.89
C20—H52	1.10	0.89
C20—H53	1.10	0.88
C21—H54	1.10	0.89
C21—H55	1.10	0.88
C22—H56	1.10	0.88
C22—H57	1.10	0.88
C23—H58	1.10	0.88
C23—H59	1.10	0.89
C24—H60	1.10	0.88
C24—H61	1.10	0.88
C25—H62	1.10	0.88
C25—H63	1.10	0.88
C26—H64	1.10	0.90

(table continues)

Table 2.32 *(continued)*

Bond type	Length/Å	Order
C26—H65	1.10	0.90
C26—H66	1.10	0.90
C27—H67	1.10	0.90
C27—H68	1.10	0.90
C27—H69	1.10	0.90

Fragmentation Predictions

As a collaboration effort and in order to further emphasize the application of theoretical methods to forensic research, a comparison of predicted fragmentation against ESI-MS experimental spectra was carried out. The molecules considered were three tryptamines species. Analysis of these compounds using PAMPA-BBB has been described elsewhere.[14] The experimental data set was provided by former Verbeck lab member Dr. Kristina Clemons.

The comparison (Table 2.33) shows that the predicted fragmentation obtained using ACD labs software is in very good agreement with the portion of experimental ESI-MS data available for structure identification purposes. For both tryptamine and N-methyltryptamine, ACD's Fragmenter predicted each one of the peaks seen in the experimental data, albeit with slight variations in the decimal place. For N,N,N-trimethyltryptamine, however, only two experimental peaks are present in the predicted set, 203.4 and 144.1. The rest of the peaks shown for this molecule cannot be compared between both sets of data, as it is obvious that they do not match at plain sight. One possible explanation is that the structure of the ionic tryptamine species might fall into the realm of 'unusual' for the ACD program, given that it determines fragmentation based on the fragmentation rules for common organic molecules. This hypothesis, however, remains to be tested. Nevertheless, close approximation in the case

of the neutral species means that the software can be confidently used in the study and identification of unknown compounds.

Table 2.33 Predicted fragmentation and ESI-MS data comparison

tryptamine		N-methyltryptamine		N,N,N-trimethyltryptamine	
Predicted (m/z)	Experimental (m/z)	Predicted (m/z)	Experimental (m/z)	Predicted (m/z)	Experimental (m/z)
130.1	—	58.1	—	—	59.6
—	143.6	130.1	—	—	59.8
144.1	144.1	—	131.7	—	60.2
159.1	—	—	131.7	73.1	—
160.1	160.6	—	131.9	—	83.2
161.1	161.0	—	132.2	—	100.3
		144.1	144.0	—	101.2
		173.1	—	130.1	—
		174.1	174.8	—	143.4
		175.1	175.0	—	143.7
		—	175.3	144.1	144.1
				202.1	—
				203.2	203.4

User interface written in Python

In the last section of this chapter we discuss the development of a graphical user interface to facilitate the creation of input files for the quantum mechanical software GAMESS. Figure 2.11 shows the GUI designed as part of this project. The GUI here included was developed with an audience not familiar with computational chemistry programs in mind. With this program we wanted to make the process of calculating optimized molecular geometries and vibrational spectra more automated and minimize the number of steps required to create input files for GAMESS. The structures included in this interface were incorporated as follows: after a back bone optimized structured was found in GAMESS, the new Cartesian coordinates were imported into Avogadro and modified to accommodate new functional groups at the sites of interest (i.e. amine nitrogen for amphetamine and tryptamine). Once the modification was performed, a quick molecular mechanics optimization was carried out using the Avogadro built-in optimization tool. This was done in order to improve the quality of the initial guess fed into GAMESS for the *ab initio* optimization. The Python script was designed so when the user wants to modify one of the backbones with a fragment, the program will search for the Cartesian coordinates corresponding to that specific fragment and overwrite the necessary lines in the backbone input file. In this manner, the user interface makes quantum mechanical calculations more accessible for everyday use, as the process of input file generation and execution can now be performed within a few clicks.

The interface is still in its initial stages of development and we hope for continued work in order to eventually bring it to members in the forensic science community. The full code can

be found in Appendix A. Python 3.4 and up (64-bit) and the pyqt4 library are necessary to run this program.

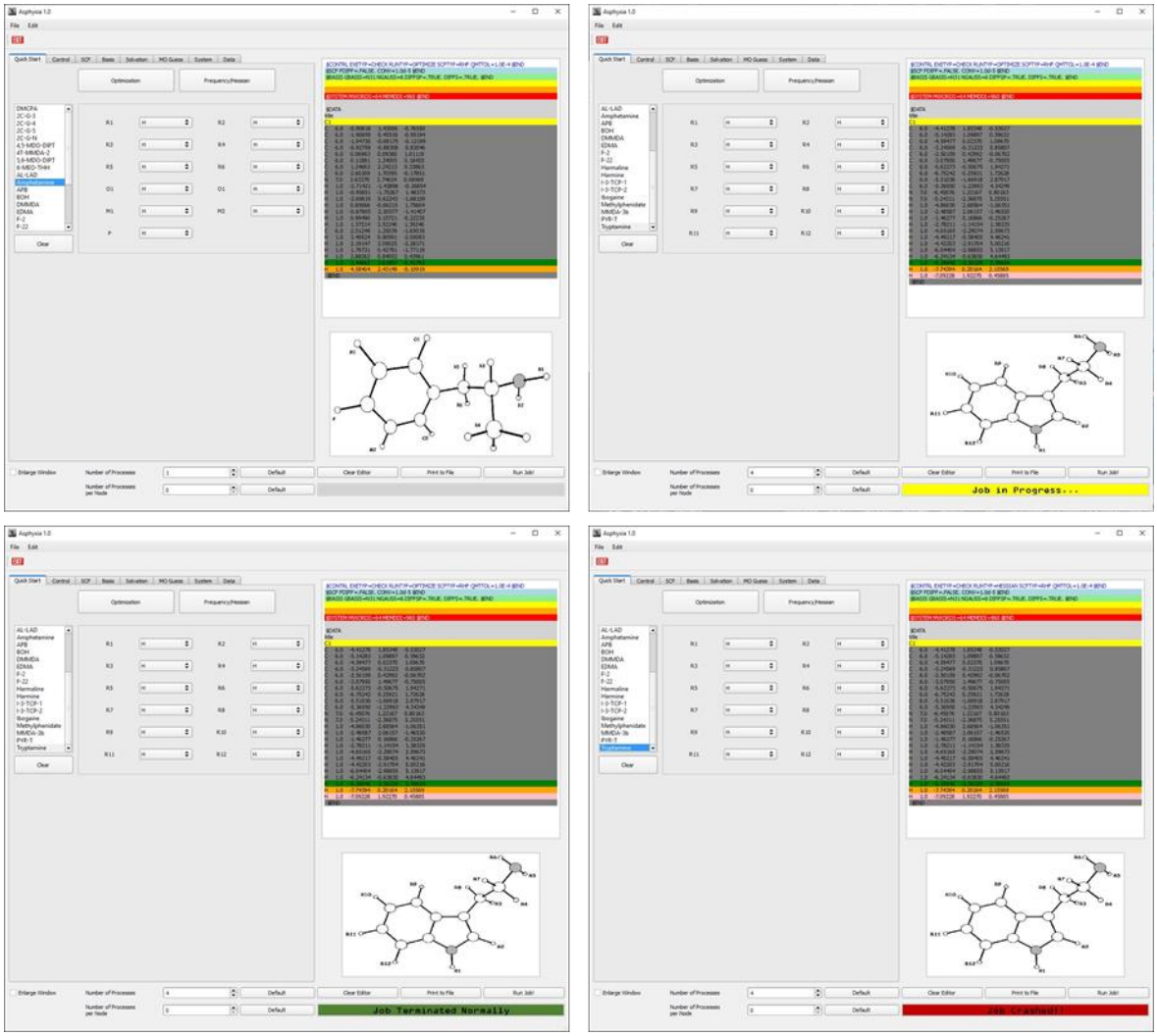


Figure 2.11. Graphical user interface for the creation of GAMESS input files.

Conclusions

In this chapter we hoped to highlight the applicability of computational chemistry methods in the field of forensic science through the systematic analysis of structural and vibrational data of different controlled substances and to set initial efforts towards the creation

of a database that will be helpful to the forensic science community. A full conformational analysis—geometry optimization plus frequency calculation—was performed for eight amphetamine species, two phenethylamine derivatives, DMCPA and two tryptamines. In addition, geometry optimizations for two other members of the phenethylamine series and for seventeen tryptamine-like molecules were also carried out.

In general, calculated bond lengths and orders for all molecules were determined to be in agreement with widely accepted values within the chemical community. Calculated vibrational spectra was also found to be detailed enough to allow for differentiation between molecules belonging to the same family, though limitations are also clear. Data obtained by other means—experimental techniques—is necessary to further discriminate between molecules with similar structures.

While the geometry optimizations of tryptamine-like molecules did not converge, by comparison to previous literature on the subject we determined that the structures where located near the correct global minimum on their corresponding potential energy surface. This provides further evidence of the wealth of information that can be obtained from computational methods.

Comparison of predicted fragmentation to experimental ESI-MS data also shows the benefit of considering the utilization of fragmentation prediction software to help in the identification of novel molecules with structures that resemble common organic compounds.

The predicted fragmentation showed very good agreement with experimental data and variations from it are possibly due to the ‘unusual’ structure of one of the molecules under study. Finally, we included a graphical user interface created in Python language that facilitates

the creation of GAMESS input files and the execution of geometry and spectra calculations by making available preloaded optimized back bone structures of common controlled substances. These structures can be modified by the user by incorporating functional groups at different backbone positions, which are also included in the interface.

CHAPTER 3

BOILING POINT ESTIMATION FOR PREDICTION IN REVERSE GAS STACK MODELING

Introduction

Each year an increasing number of illicit drugs and synthetic routes are identified by forensic analysis of clandestine manufacturing sites.[58] At this places, synthesis of illicit drugs often emits trace chemicals that can be detected in the atmosphere of the areas surrounding the 'cooking' site. In a previous article published by Mach *et al*,[22] a novel vehicle-based mass spectrometer was introduced in order to aid in the characterization of such trace chemicals and, in this manner, facilitate the detection of precursors and synthetic by-products. In addition, they sought to supplement current law enforcement identification techniques with a 'powerful, mobile system.' To demonstrate the advantages of possessing such a system, they performed a mock covert methamphetamine synthesis that was followed by the detection of precursors and by-products using the mobile mass spectrometer unit.

The present work encompasses the initial stages of a follow-up project; in which we seek to enhance the detection capabilities of the mobile unit through the creation of a signal-strength-detection-based navigation system. This new addition would allow not only for the characterization of uncovered manufacturing sites of illicit drugs, but also provides a mean for uncovering such places by guiding the operator of the mobile unit in the direction of greater target chemical concentration.

Because new synthetic routes can lead to novel pharmacologically active by-products, we see the need for our navigation algorithm to rapidly incorporate such compounds. In this chapter we present a method for the calculation of boiling points of organic molecules and its

application in the generation of 'thread chemical zones.' By having the model unit compare the signal detected with the intensity gradient of the modeled thread zones, one can create directions that will lead the operator to the point source of the molecule of interest. While in this chapter we used a program already available to generate dispersion areas, in the future we hope to make heavier use of the concepts of gas stack modeling.

Computational Methods

Considered by Lyman[33] 'likely the most accurate boiling point estimation method using non-linear group contributions', the Lai *et al* (1987) boiling point estimation method was used to theoretically determine the boiling point of volatile organic compounds. In order to facilitate the implementation of the Lai method, a graphical user-interface was created using the Python 3.4.3 (64-bit) programming language. The code was written in the JetBrains PyCharm development environment (Community Edition, v5.0.1).

Once a boiling point for a particular molecule was calculated, the value was entered—in Kelvin—in the ALOHA 5.4.5 (Areal Locations of Hazardous Atmospheres) software package along with the molecular weight of the compound—in grams per mole. ALOHA is the hazard modeling program for the CAMEO software suite and it is made available to the public through the Environmental Protection Agency (EPA) web page. The software is used widely to plan for and respond to chemical emergencies.

To generate 'Thread Zones' in ALOHA, the following parameters were used:

1. Under SetUp/Atmospheric/User Input: Wind Speed is 8 mph and Direction is S, Ground Roughness is 'Open Country', and Cloud Cover is between 'Partly Cloudy' and 'Clear.' Temperature is 80°F. Other options were left with the default values.

2. Under SetUp/Source/Direct: Source Strength Unit is grams, Amount of Pollutant is 1 for either grams/min or grams/hr, Source height is 0 meters (ground source). Everything else was left unchanged.
3. Under SetUp/Calculation Options: Check 'Let ALOHA decide.'
4. Under Display/Thread Zone: User specified values were given as follows:
    a. For a pollutant rate of 1 grams/min: Red = 0.0001 ppm, Orange = 0.00001 ppm, Yellow = 0.000001 ppm.
    b. For a pollutant rate of 1 grams/hr: Red = 0.01 ppm, Orange = 0.001 ppm, Yellow = 0.0001 ppm.

Confidence lines are shown for each thread zone.

Because ALOHA adjusts the dispersion areas according to the time and location, one must use the same settings to replicate the data. Here we used the following coordinates: 33°12'27.23"N (latitude), 97°10'23.26"W (longitude). The data was generated on February 15, 2016 at 5:18 AM.

Results and Discussion

Table 3.1 shows the estimated and experimental boiling points—both °C and K—for twenty-five organic molecules, along with their molecular masses and percent errors. Our results were compared to the boiling points listed in the CRC Handbook of Chemistry and Physics (96th Edition). The average percent error was found to be 6.86% in °C and 2.82% in K, which is consistent with the value claimed by Lai et al. Percent errors ranged from 0.18% for 1-phenyl-1,2-propanedione to 15.65% for benzene in degrees Celsius.

Figure 3.1 shows a correlation plot of estimated boiling points vs experimental boiling points. Using Microsoft Excel, the data points shown in Fig. 3.1 were fitted to a line (R^2 = 0.9468). This shows that our results very closely approximate experimental values.

Theoretical and experimental agreement was further confirmed by comparing the appropriate (experimental or theoretical) boiling point vs molecular weight trends (see Fig. 3.2). This plot also shows that the calculated boiling points closely resembling the experimental data, as both sets follow a hyperbolic pattern which was fitted to a logarithmic function using the built-in features of Microsoft Excel.

In order to determine whether or not the percent error is specific to certain compounds, a plot of percent error vs molecular weight was also generated (Fig. 3.3). This plot shows that the percent error is distributed in a parabolic pattern, with its minimum located at about 150 g/mol. This means that better boiling point predictions can be expected for molecules whose molecular weight is closer to this value. The data points in Fig. 3.3 were fitted to a fourth degree polynomial to make the pattern clearer to the reader.

'Thread zones' for all compounds are shown in Figures 3.4 – 3.8 and Figures 3.9 – 3.13, each set of figures corresponding to the two pollutant rates mentioned in the Computational Methods section of this document, 1 gr/hr and 1 gr/min, respectively.

Careful consideration of the 'Thread Zone' areas found in Figures 3.4 – 3.13 and the maximum dispersion distances listed in Table 3.2, show that the maximum distance traveled by an organic compound is inversely proportional to its molecular weight and boiling point. From these plots, it is clear that benzene, the lightest molecule of the set and also the one with the lowest boiling point, covered a greater distance relative to the other compounds in this study.

This is clearer by looking at the first set of figures (Fig. 3.4 — 3.13). The plots also show that 1,3-diphenyl-2-propanone is the compound that traveled the least amount, being also the heaviest and with the highest boiling point. In the case of molecules like 4-ethyltoluene and 1,2,3-trimethylbenzene, who possess the same molecular mass and similar boiling points, no difference in terms of the distance traveled is observed, implying that structure plays a small role, if any, in the amount of distance traveled by a molecule in the atmosphere.

As a final point, Figure 3.14 contains an image of the boiling point estimation program created in Python. The program was designed with the intention of facilitating boiling point calculations. Even though this GUI can keep the user from making mathematical mistakes, it is still important to be familiar with the calculation criteria as outlined by Lai et al. To insure that the boiling point is calculated correctly, one must press the 'Set' button besides the entry box for each desired variable, it is also recommended to draw the molecule of interest to make sure the correct variables and variable values are being utilized and enter, respectively, in the interface.

The program does not possess a clear all button at this point, which means that before each calculation one must insure that all fields are blank or set to zero. In addition, values of double bonds under the category of 'Others' as listed in Lai, have not been yet implemented, which means that these values must be added manually when applicable. The complete Python code for this application is found in Appendix B. Python 3.4 and up (64-bit) and the Pyqt4 library are necessary to run this program.

Table 3.1 Estimated boiling points for various organic compounds

Name	T_b (Calc.)/°C	T_b (Expt.)/°C	% Error	M.W./g*mol^{-1}	T_b (Calc.)/K	T_b (Expt.)/K	% Error
benzene	67.55	80.08	15.65	78.11	340.70	353.23	3.55
toluene	98.14	110.6	11.27	92.14	371.29	383.75	3.25
benzaldehyde	165.33	178.70	7.48	106.12	438.48	451.85	2.96
o-xylene	132.03	144.40	8.57	106.17	405.18	417.55	2.96
ethylbenzene	126.89	136.20	6.84	106.17	400.04	409.35	2.27
acetophenone	172.35	202.10	14.72	120.15	445.50	475.25	6.26
4-ethyltoluene	157.60	162.00	2.72	120.19	430.75	435.15	1.01
1,2,3-trimethylbenzene	165.11	176.00	6.19	120.19	438.26	449.15	2.43
1,2,4-trimethylbenzene	163.65	169.40	3.40	120.19	436.80	442.55	1.30
benzoic acid	234.06	250.20	6.45	122.12	507.21	523.35	3.08
benzyl chloride	162.62	174.00	6.54	126.58	435.77	447.15	2.54
(2-methyl-1-propenyl)benzene	175.76	189.00	7.00	132.20	448.91	462.15	2.86
amphetamine	218.61	198.00	10.41	135.21	491.76	471.15	4.37
methyl benzoate	186.30	199.00	6.38	136.15	459.45	472.15	2.69
benzeneacetic acid	252.02	268.00	5.96	136.15	525.17	541.15	2.95
phthalic anhydride	292.74	285.30	2.61	148.12	565.89	558.45	1.33
1-phenyl-1,2-propanedione	221.60	222.00	0.18	148.16	494.75	495.15	0.08
methamphetamine	204.61	212.00	3.49	149.23	477.76	485.15	1.52
benzyl acetate	206.99	215.00	3.72	150.17	480.14	488.15	1.64
3,5-dimethylbenzoic acid	268.90	275.00	2.22	150.17	542.05	548.15	1.11
1,4-dimethylnaphthalene	282.19	264.00	6.89	156.22	555.34	537.15	3.39
diphenylmethane	254.68	264.20	3.60	168.23	527.83	537.35	1.77
trans-stilbene	289.70	307.00	5.63	180.25	562.85	580.15	2.98
2,2'-dimethylbiphenyl	284.79	258.00	10.39	182.26	557.94	531.15	5.04
1,3-diphenyl-2-propanone	285.54	329.00	13.21	210.27	558.69	602.15	7.22

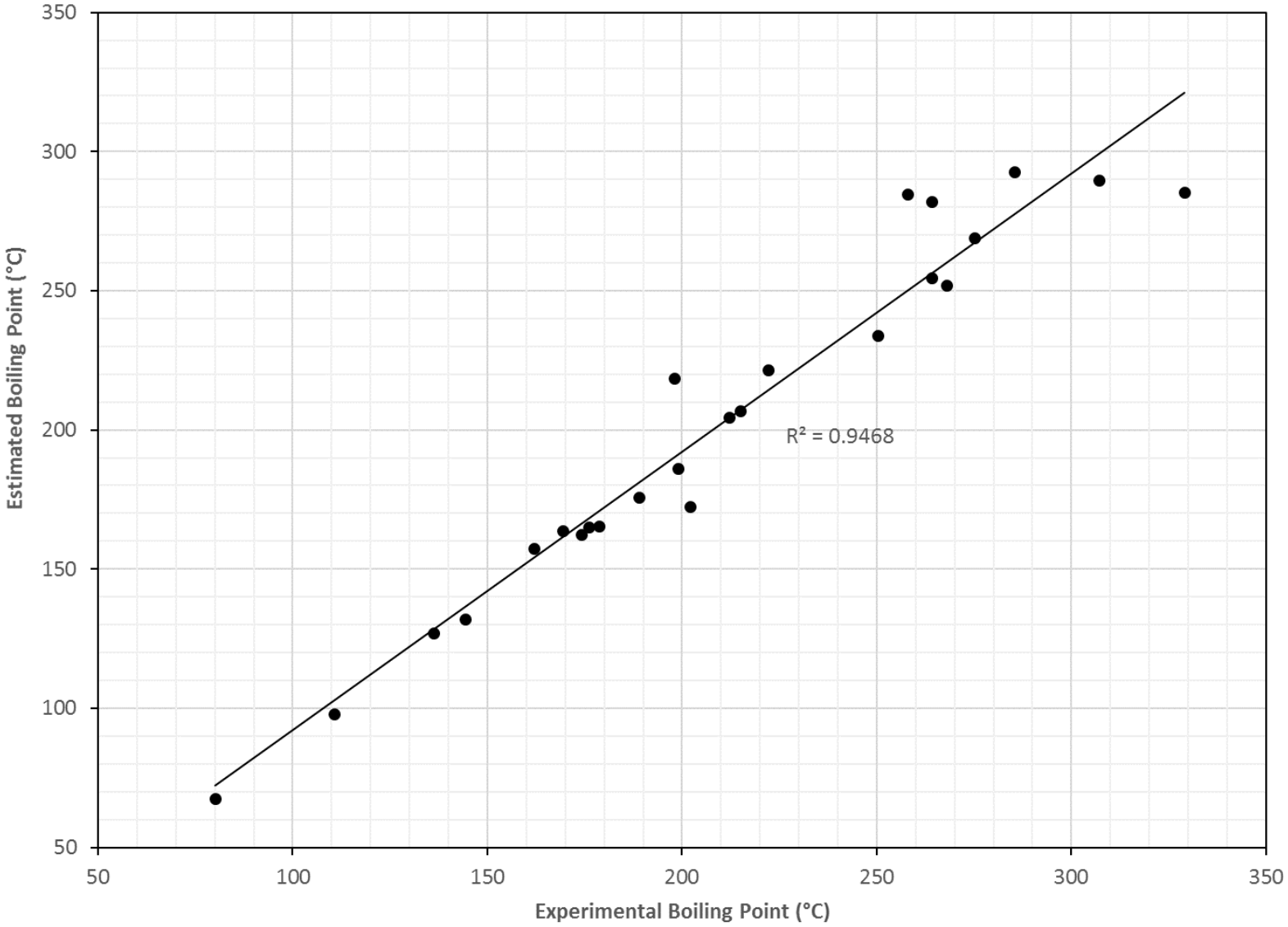


Figure 3.1. Correlation plot of estimated boiling points vs experimental boiling points. Data shows very good agreement between both data sets.

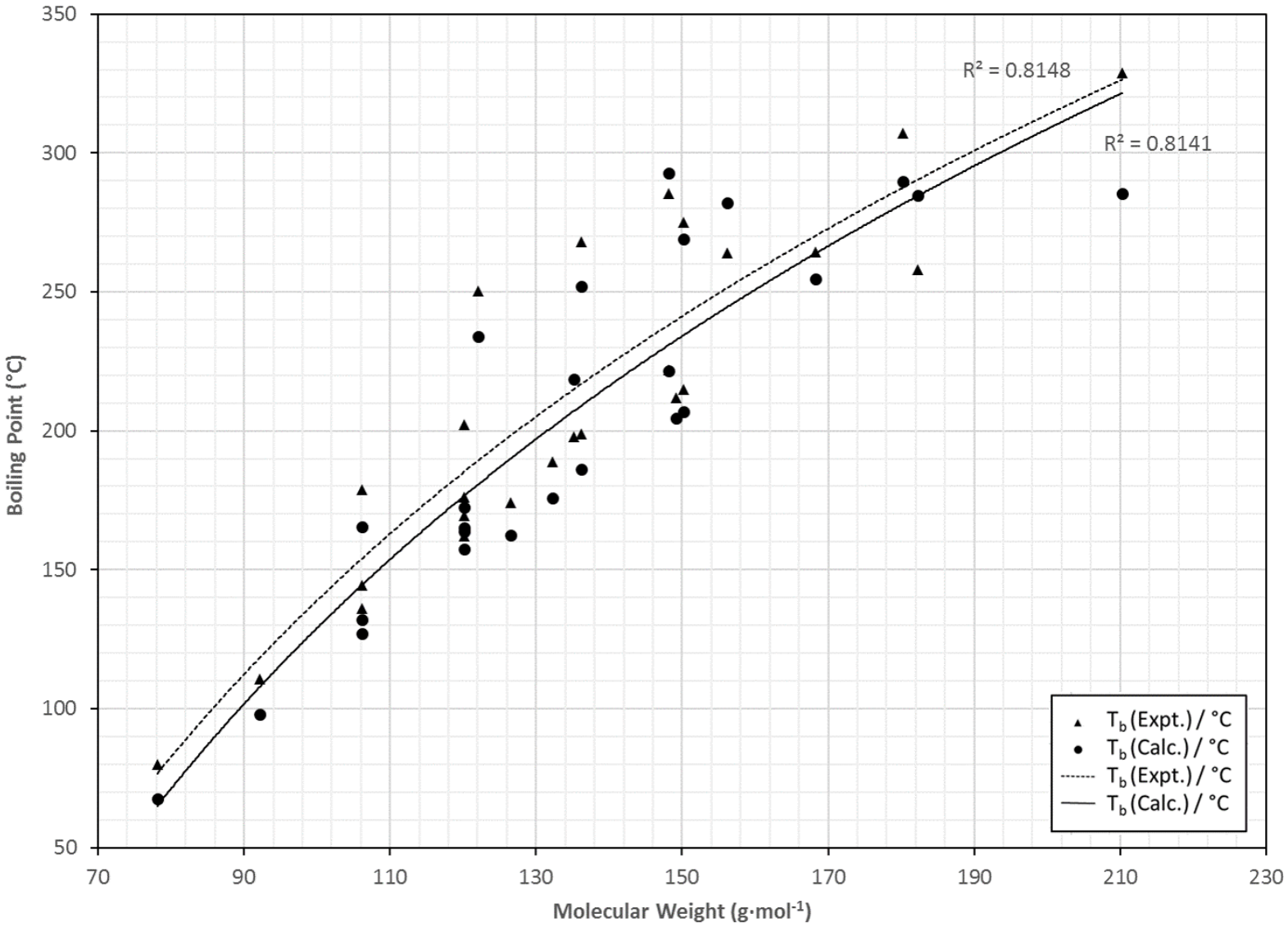


Figure 3.2. Boiling point vs molecular weight plots. Both have a hyperbolic pattern.

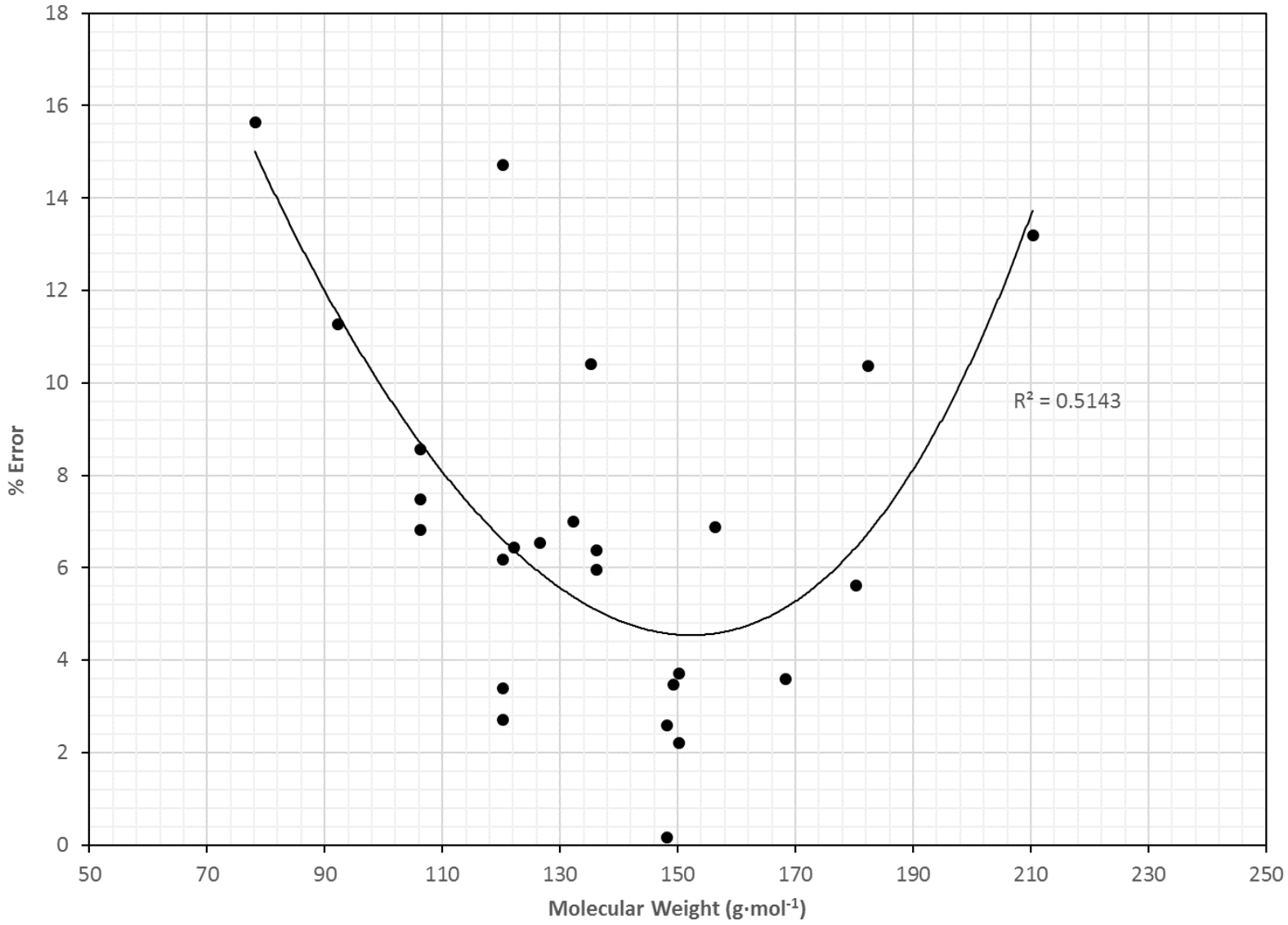


Figure 3.3. Plot of error percent vs molecular weight. Data shows that more accurate predictions can be expected for molecules with a M.W. near 150 g/mol

Table 3.2 Maximum dispersion distance of various organic compounds

		Dispersion Distance/m					
		Dispersion Rate 1 gr/hr			Dispersion Rate (1 gr/min)		
Name	M.W./g *mol^{-1}	Red (0.01 ppm)	Orange (0.001 ppm)	Yellow (0.0001 ppm)	Red (0.0001 ppm)	Orange (0.00001 ppm)	Yellow (0.000001 ppm)
benzene	78.11	21.03	66.75	215.80	2253.08	>9656.06	>9656.06
toluene	92.14	19.20	61.26	198.43	1931.21	>9656.06	>9656.06
benzaldehyde	106.12	18.29	56.69	183.79	1770.28	>9656.06	>9656.06
o-xylene	106.17	18.29	56.69	183.79	1770.28	>9656.06	>9656.06
ethylbenzene	106.17	18.29	56.69	183.79	1770.28	>9656.06	>9656.06
acetophenone	120.15	16.46	53.04	172.82	1609.34	9495.13	>9656.06
4-ethyltoluene	120.19	16.46	53.04	172.82	1609.34	9495.13	>9656.06
1,2,3-trimethylbenzene	120.19	16.46	53.04	172.82	1609.34	9495.13	>9656.06
1,2,4-trimethylbenzene	120.19	16.46	53.04	172.82	1609.34	9495.13	>9656.06
benzoic acid	122.12	16.46	53.04	170.99	1609.34	9334.20	>9656.06
benzyl chloride	126.58	16.46	52.12	168.25	1597.46	9012.33	>9656.06
(2-methyl-1-propenyl)benzene	132.20	16.46	51.21	164.59	1554.48	8690.46	>9656.06
amphetamine	135.21	15.54	50.29	162.76	1533.45	8529.52	>9656.06
methyl benzoate	136.15	15.54	50.29	161.85	1529.05	8529.52	>9656.06
benzeneacetic acid	136.15	15.54	50.29	161.85	1529.05	8529.52	>9656.06
phthalic anhydride	148.12	14.63	47.55	155.44	1450.24	7885.79	>9656.06
1-phenyl-1,2-propanedione	148.16	14.63	47.55	155.44	1449.32	7885.79	>9656.06
methamphetamine	149.23	14.63	47.55	154.53	1442.92	7724.85	>9656.06
benzyl acetate	150.17	14.63	47.55	154.53	1437.44	7724.85	>9656.06
3,5-dimethylbenzoic acid	150.17	14.63	47.55	154.53	1437.44	7724.85	>9656.06

(table continues)

Table 3.2 *(continued)*

		Dispersion Distance/m					
		Dispersion Rate 1 gr/hr			Dispersion Rate (1 gr/min)		
Name	M.W./g *mol^{-1}	Red (0.01 ppm)	Orange (0.001 ppm)	Yellow (0.0001 ppm)	Red (0.0001 ppm)	Orange (0.00001 ppm)	Yellow (0.000001 ppm)
1,4-dimethylnaphthalene	156.22	14.63	46.63	150.88	1403.60	7402.98	>9656.06
diphenylmethane	168.23	14.63	45.72	145.39	1341.43	6920.18	>9656.06
trans-stilbene	180.25	13.72	43.89	139.90	1286.56	6598.31	>9656.06
2,2'-dimethylbiphenyl	182.26	13.72	43.89	139.90	1278.33	6437.38	>9656.06
1,3-diphenyl-2-propanone	210.27	12.80	40.23	129.85	1174.09	5793.64	>9656.06

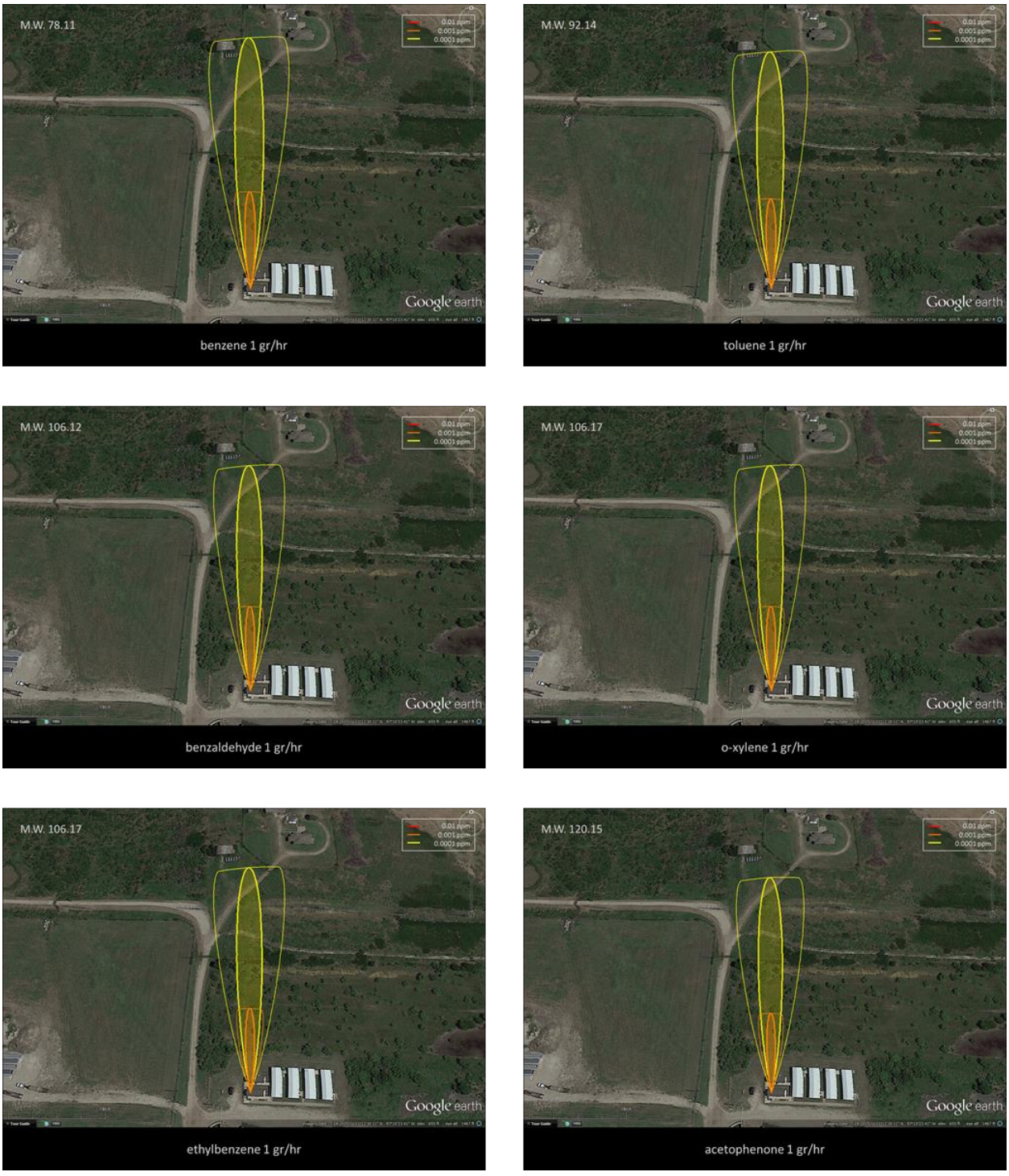


Figure 3.4. Thread zones of organic compounds at a pollutant rate of 1 gr/hr.

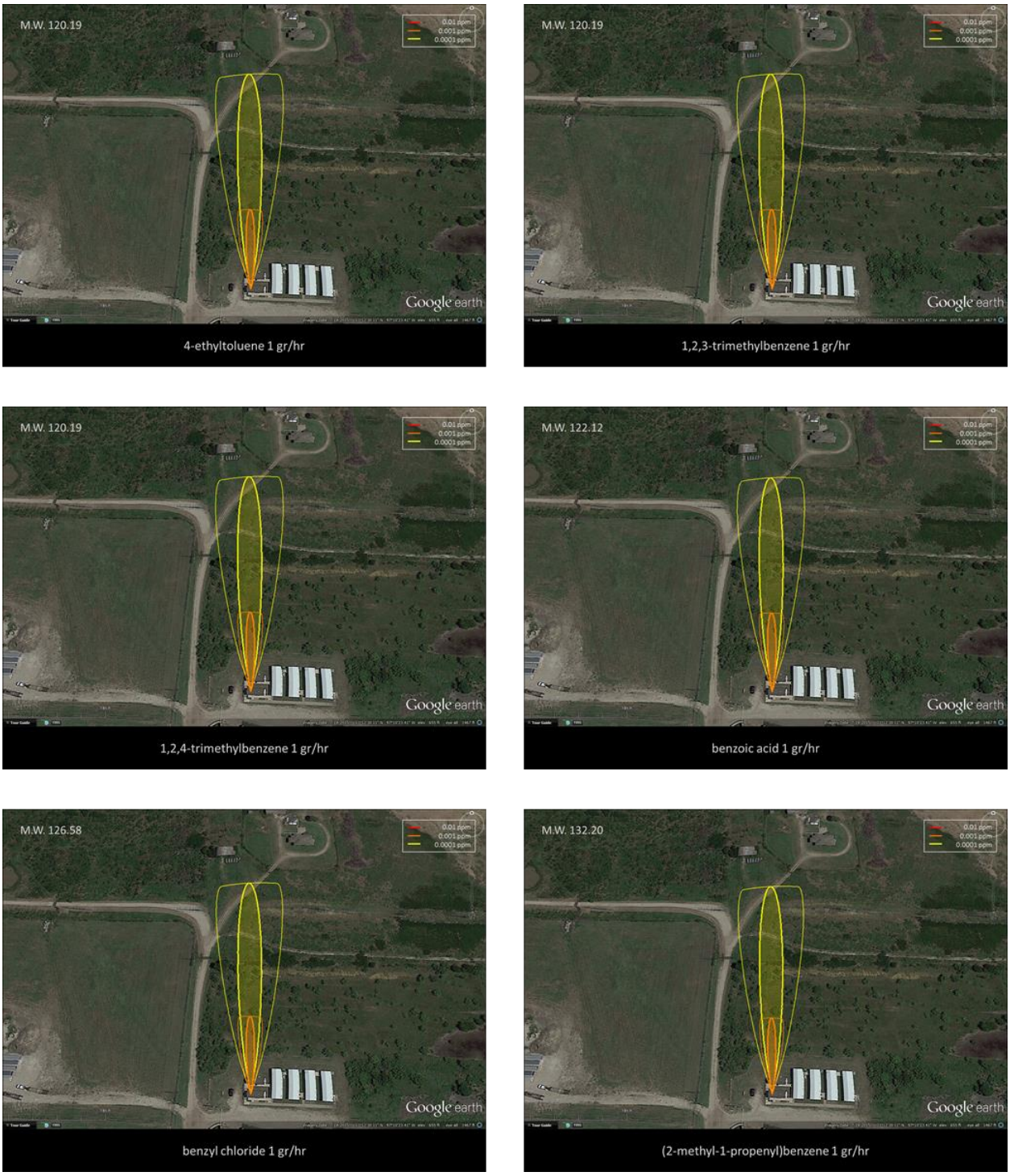


Figure 3.5. Thread zones of organic compounds at a pollutant rate of 1 gr/hr.

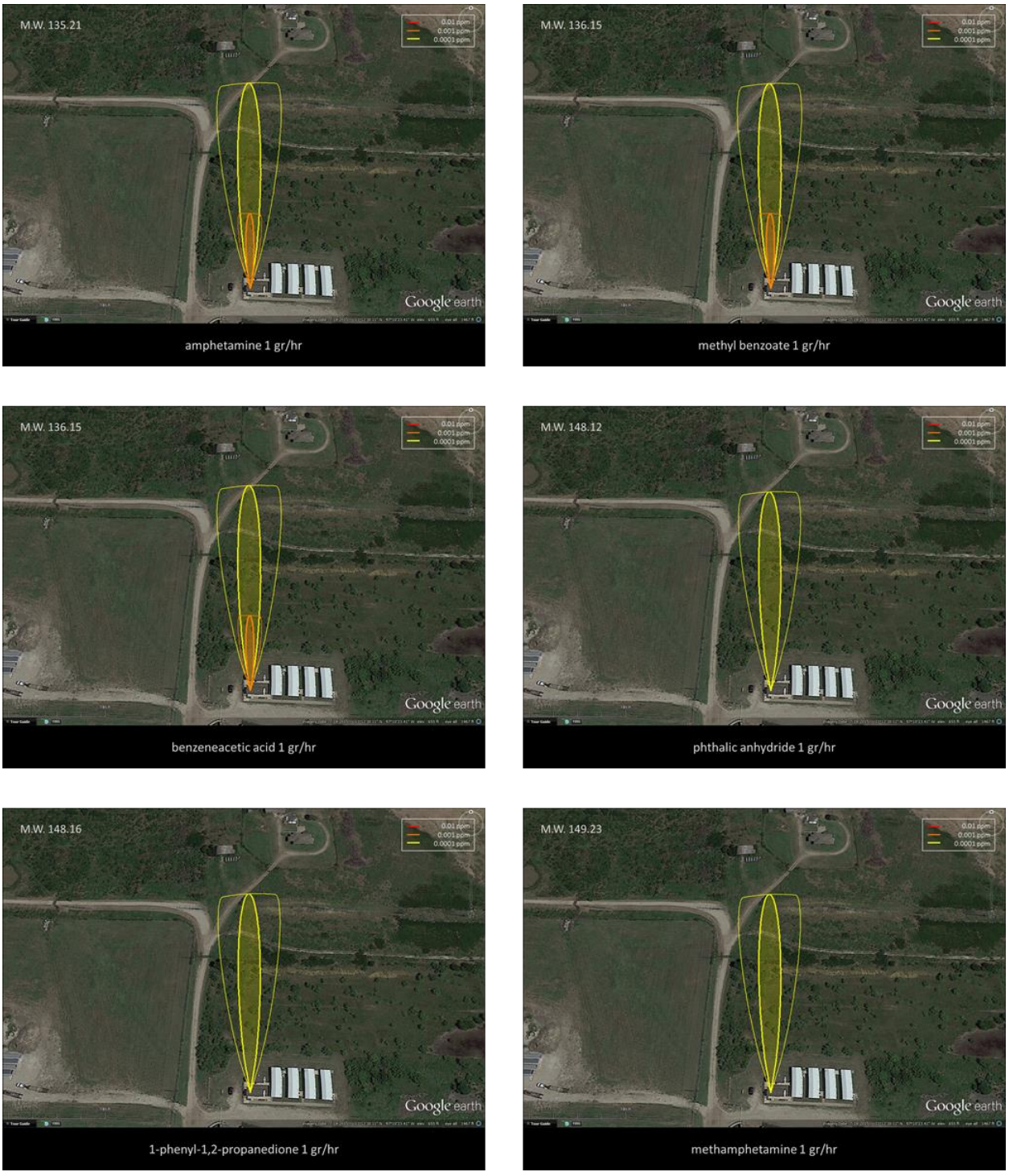


Figure 3.6. Thread zones of organic compounds at a pollutant rate of 1 gr/hr.

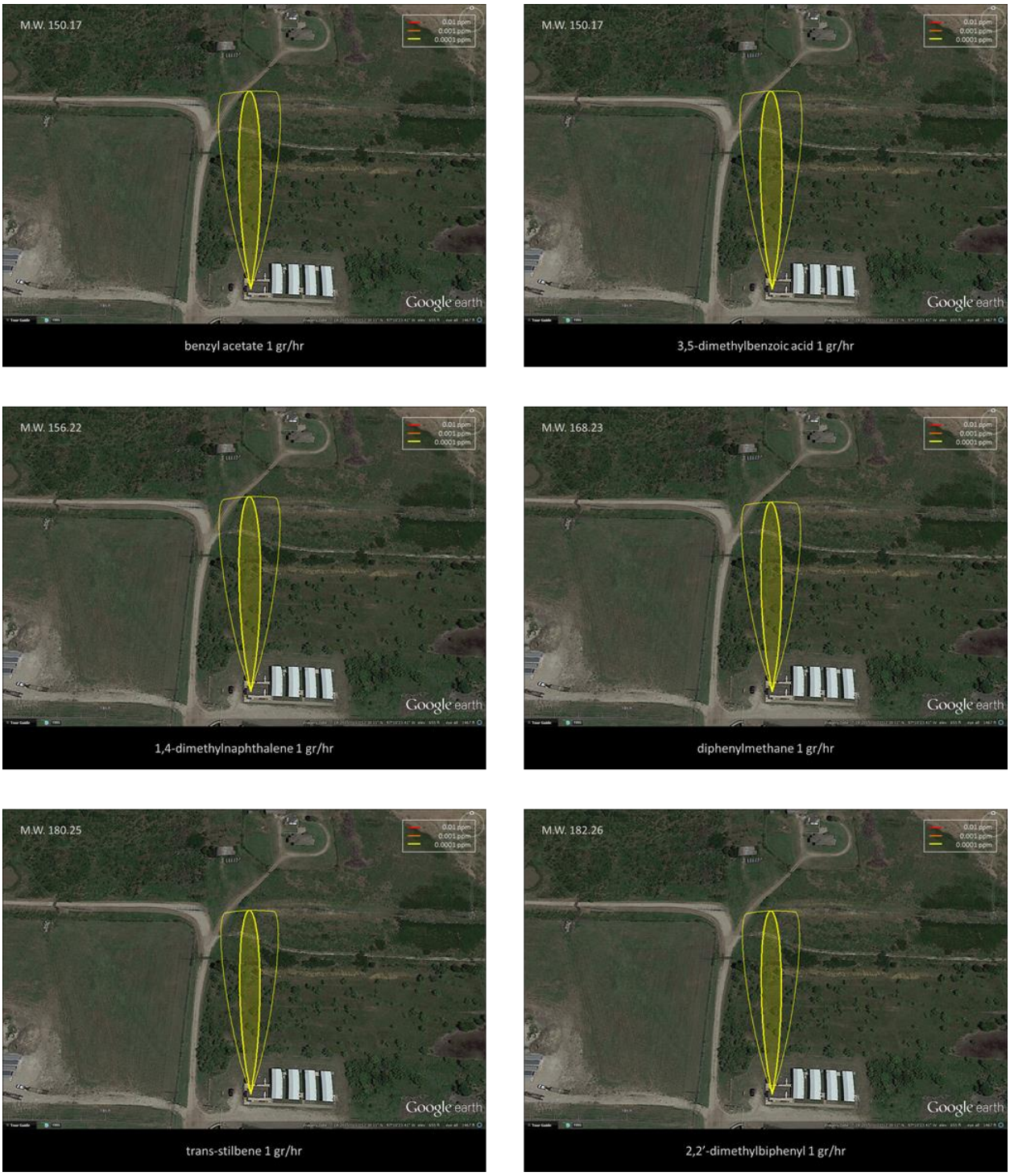


Figure 3.7. Thread zones of organic compounds at a pollutant rate of 1 gr/hr.

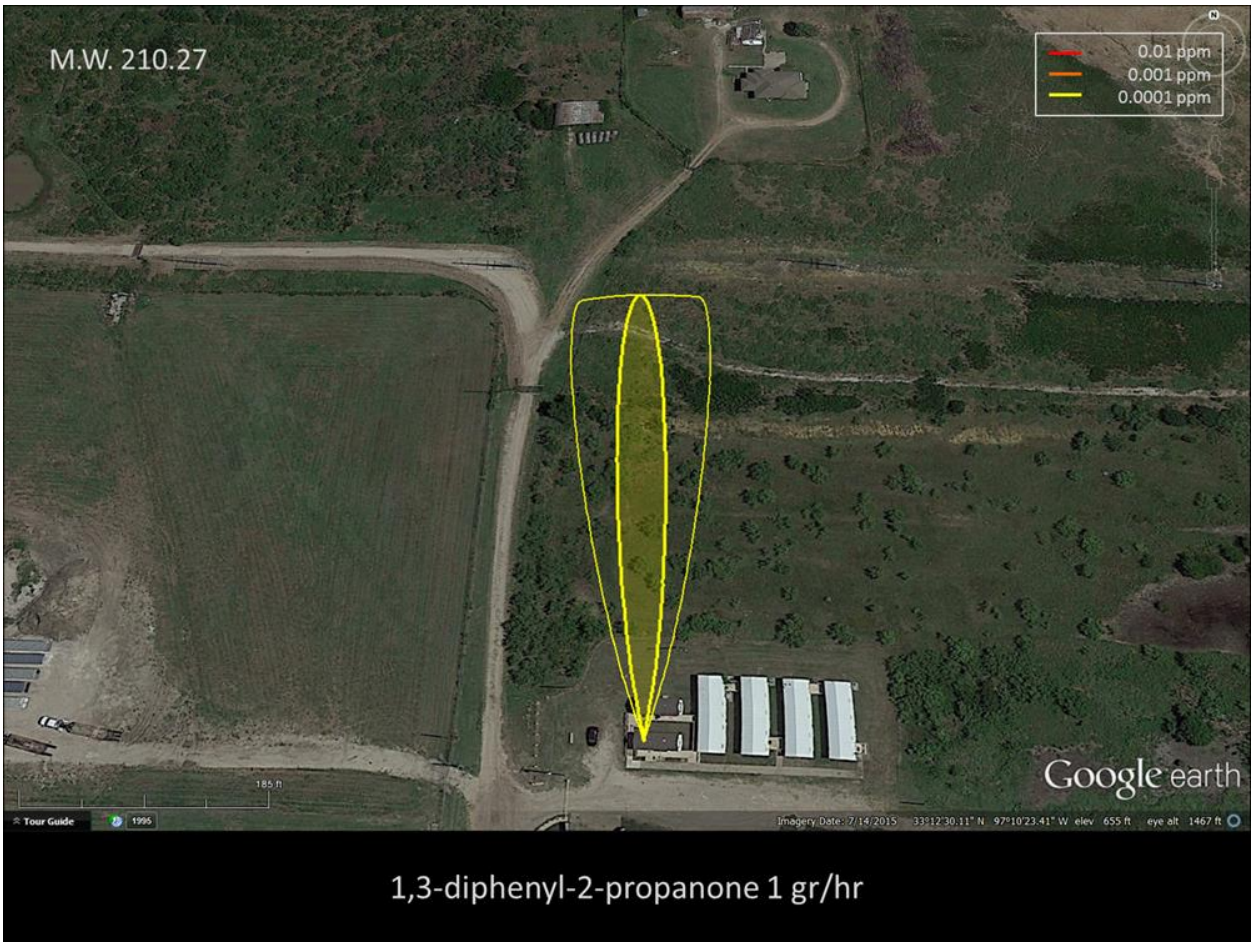


Figure 3.8. Thread zones of 1,3-diphenyl-2-propanone at a pollutant rate of 1 gr/hr.

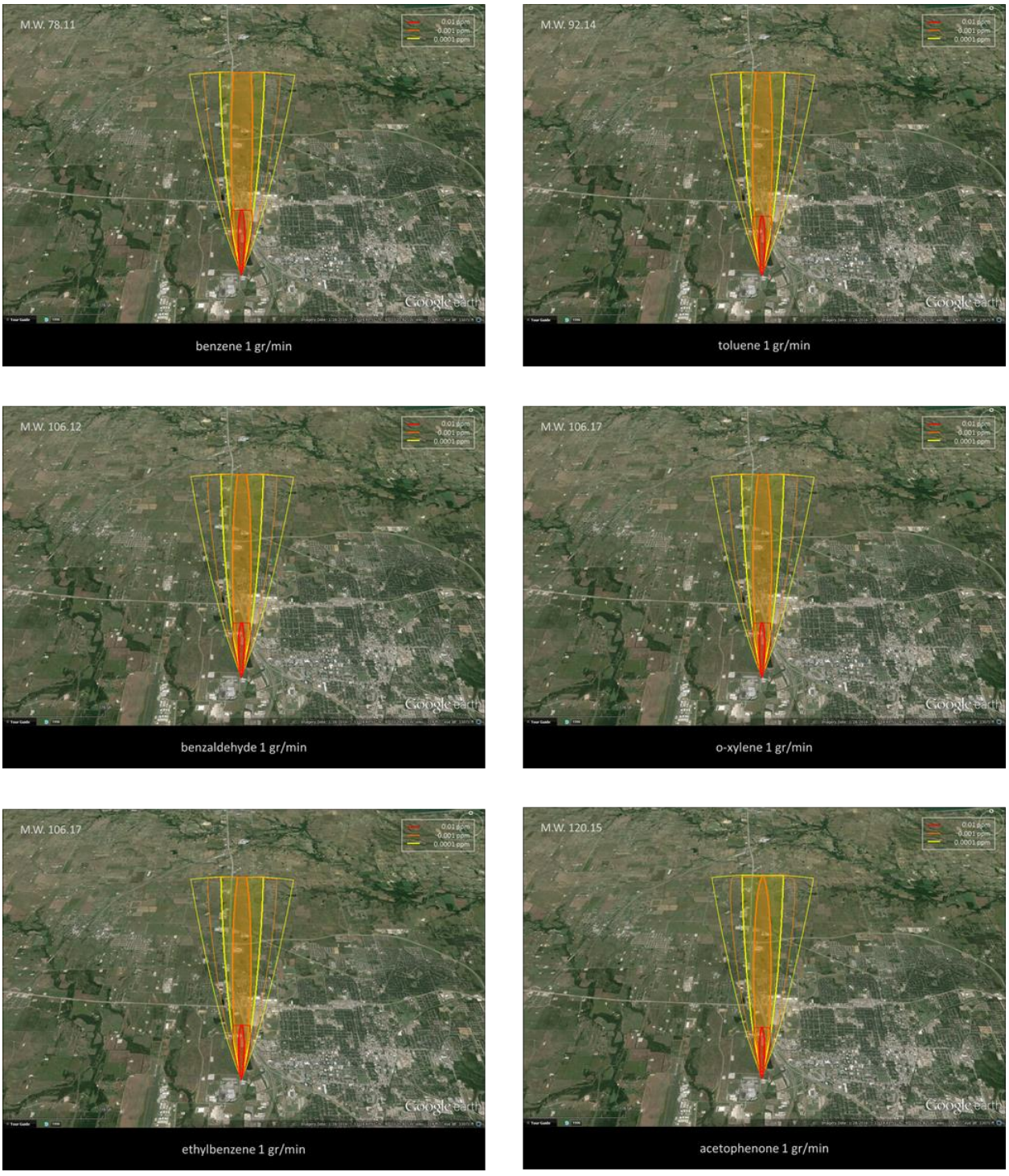
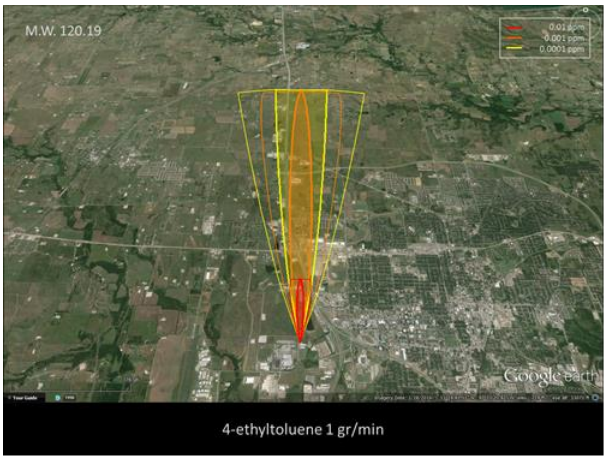
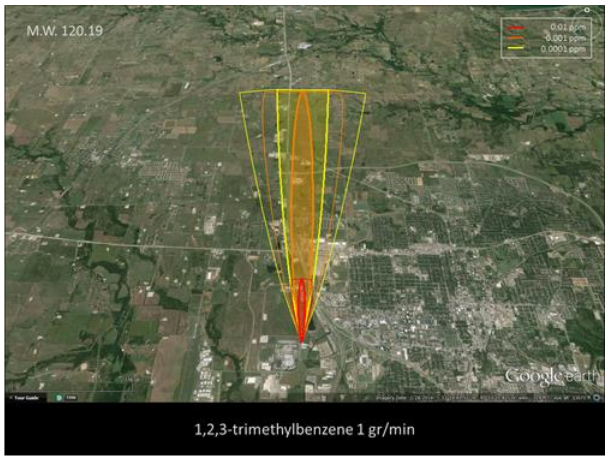
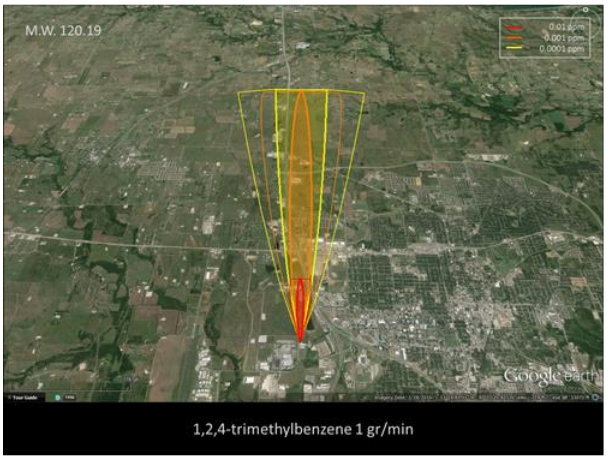
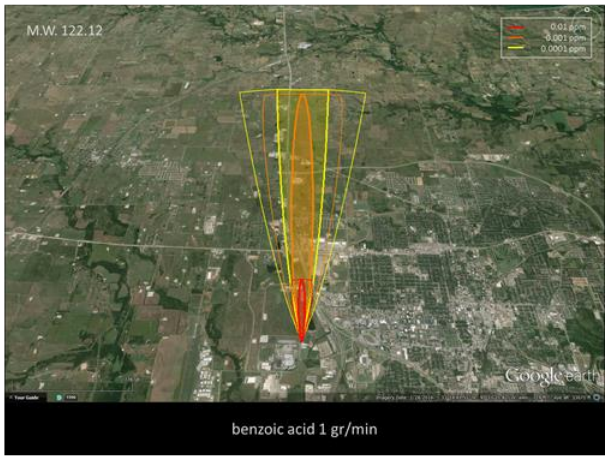


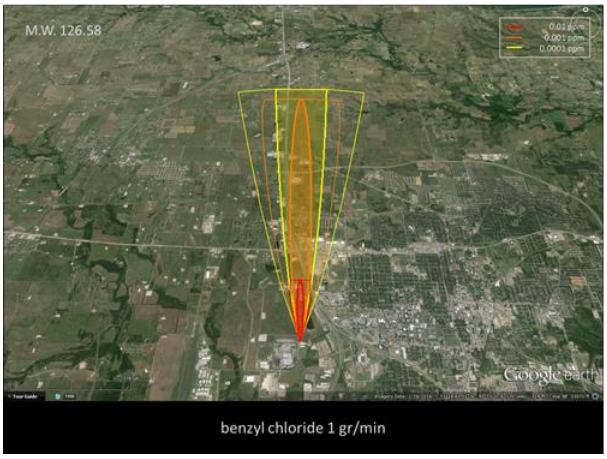
Figure 3.9. Thread zones of organic compounds at a pollutant rate of 1 gr/min.











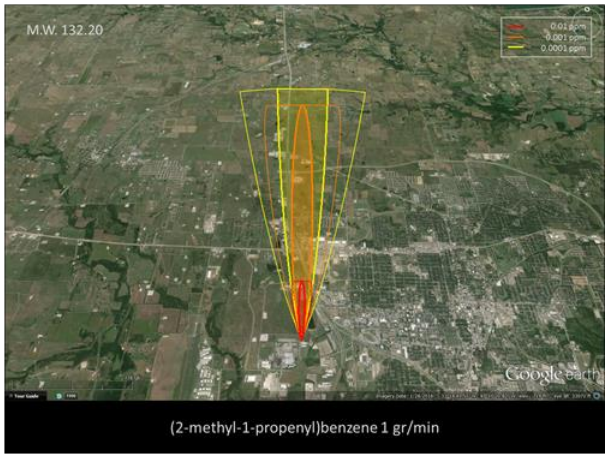
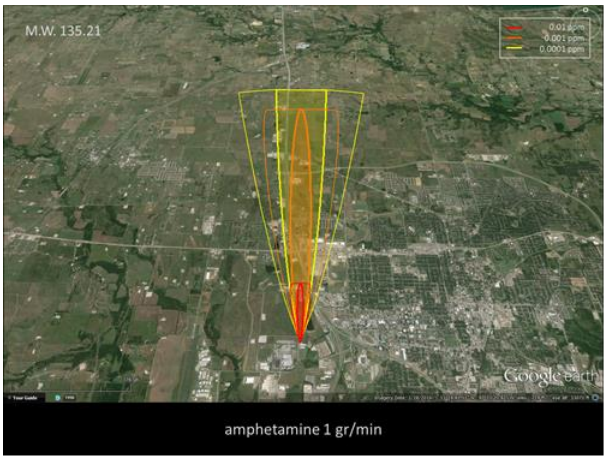
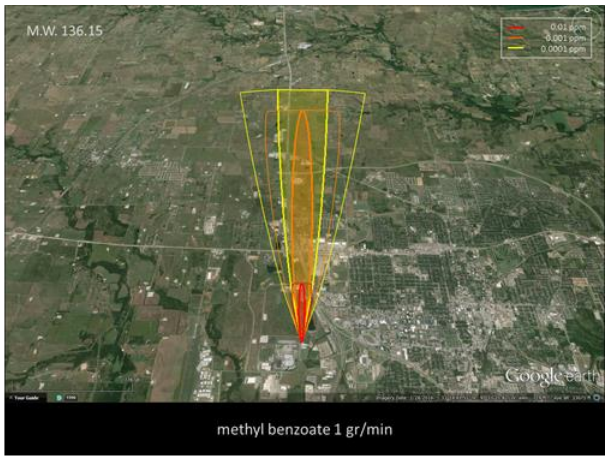
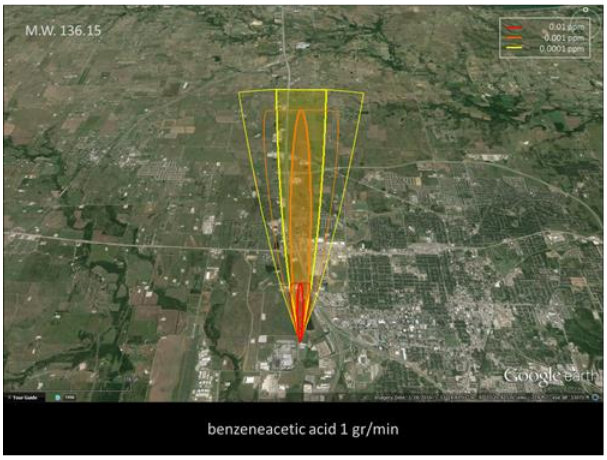
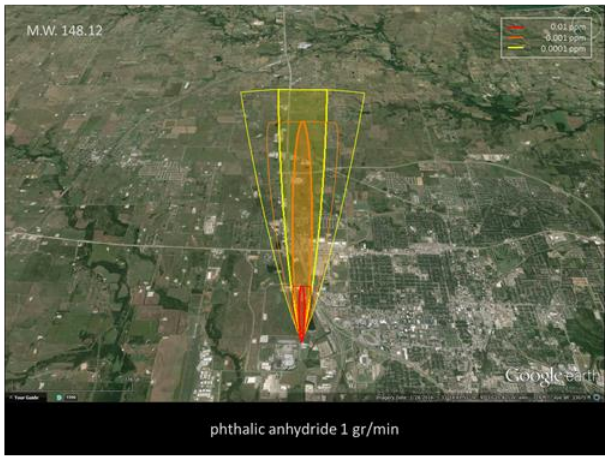


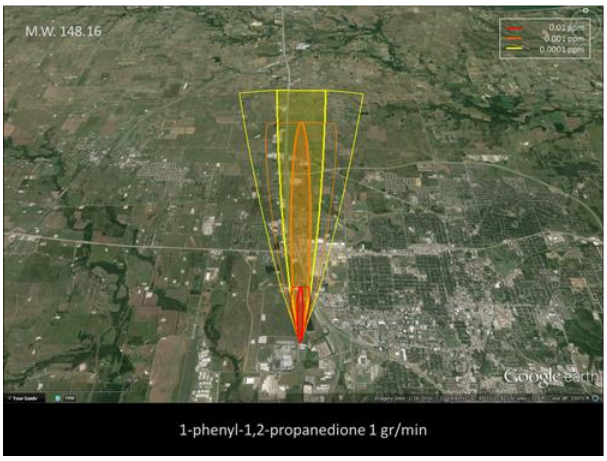
Figure 3.10. Thread zones of organic compounds at a pollutant rate of 1 gr/min.











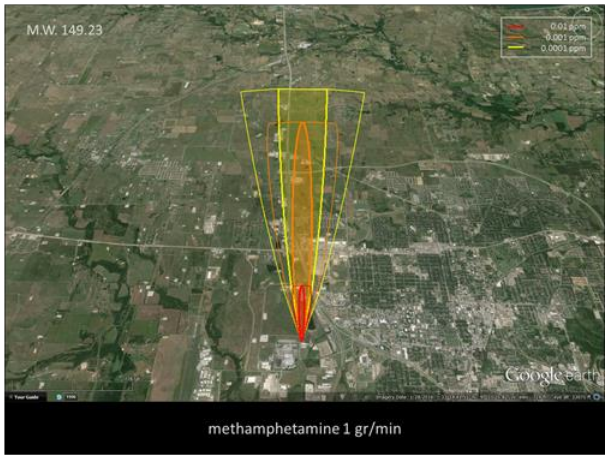
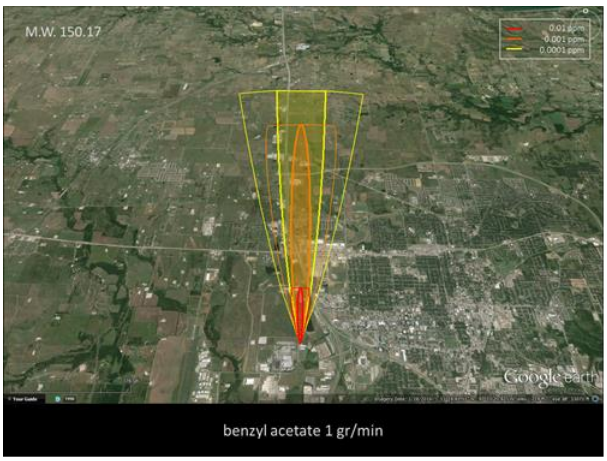
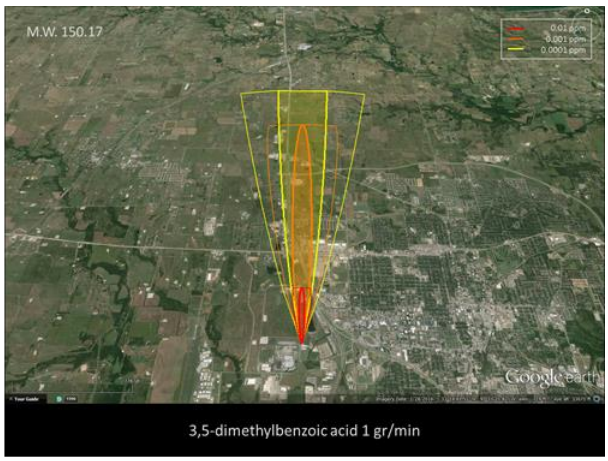
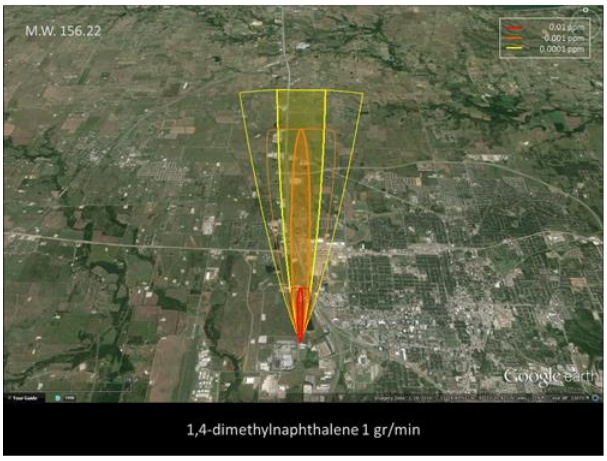
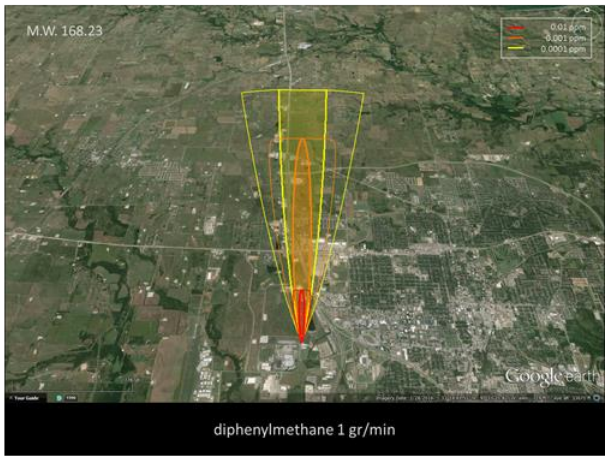


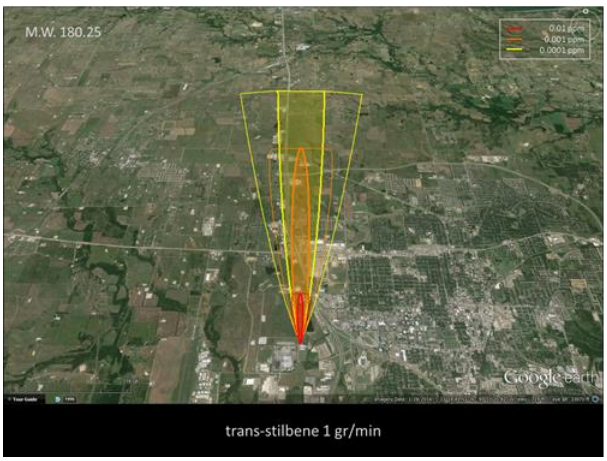
Figure 3.11. Thread zones of organic compounds at a pollutant rate of 1 gr/min.











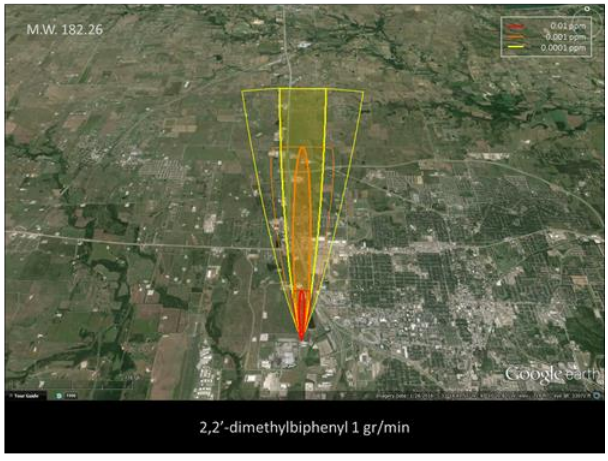


Figure 3.12. Thread zones of organic compounds at a pollutant rate of 1 gr/min.

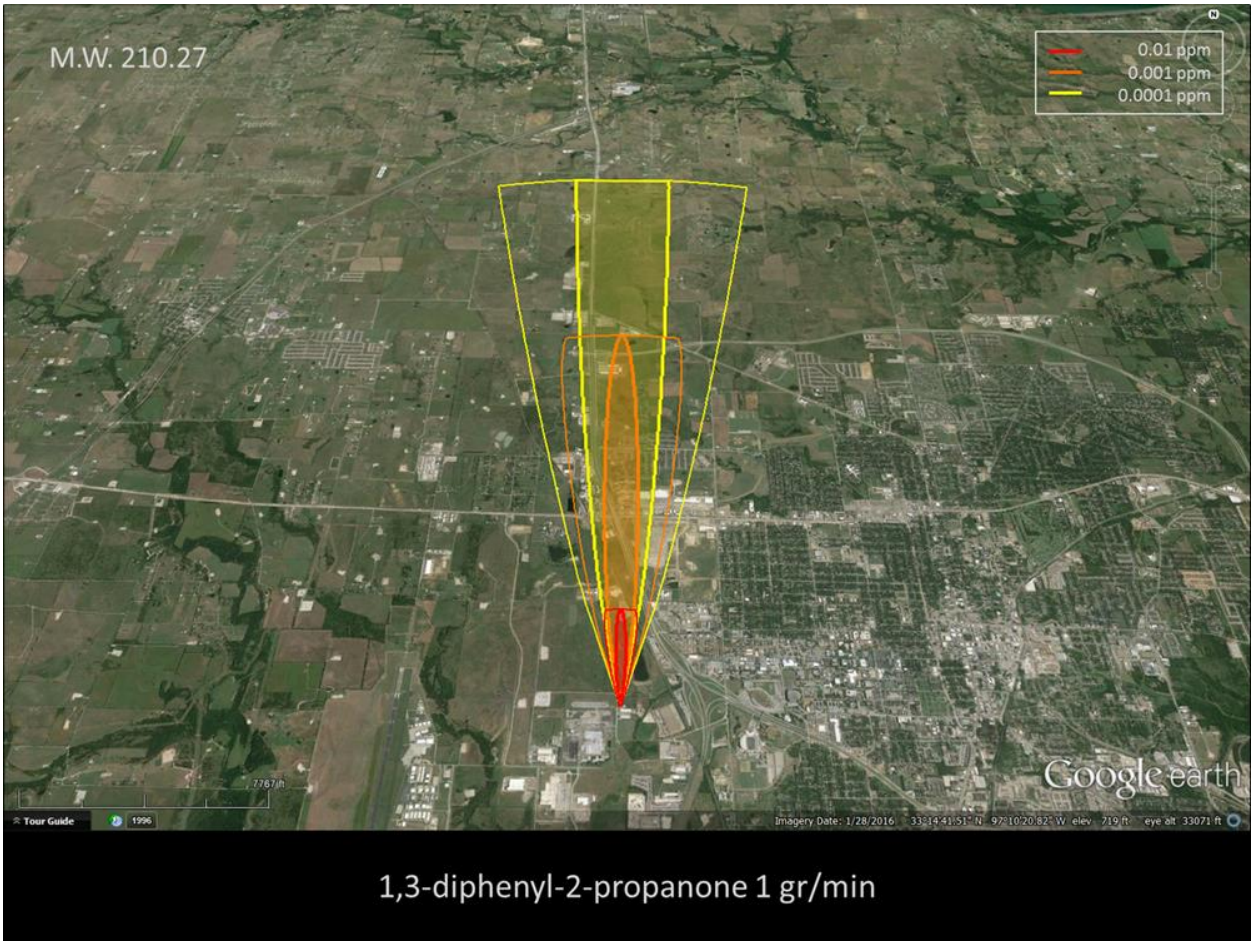


Figure 3.13. Thread zones of 1,3-diphenyl-2-propanone at a pollutant rate of 1 gr/min.

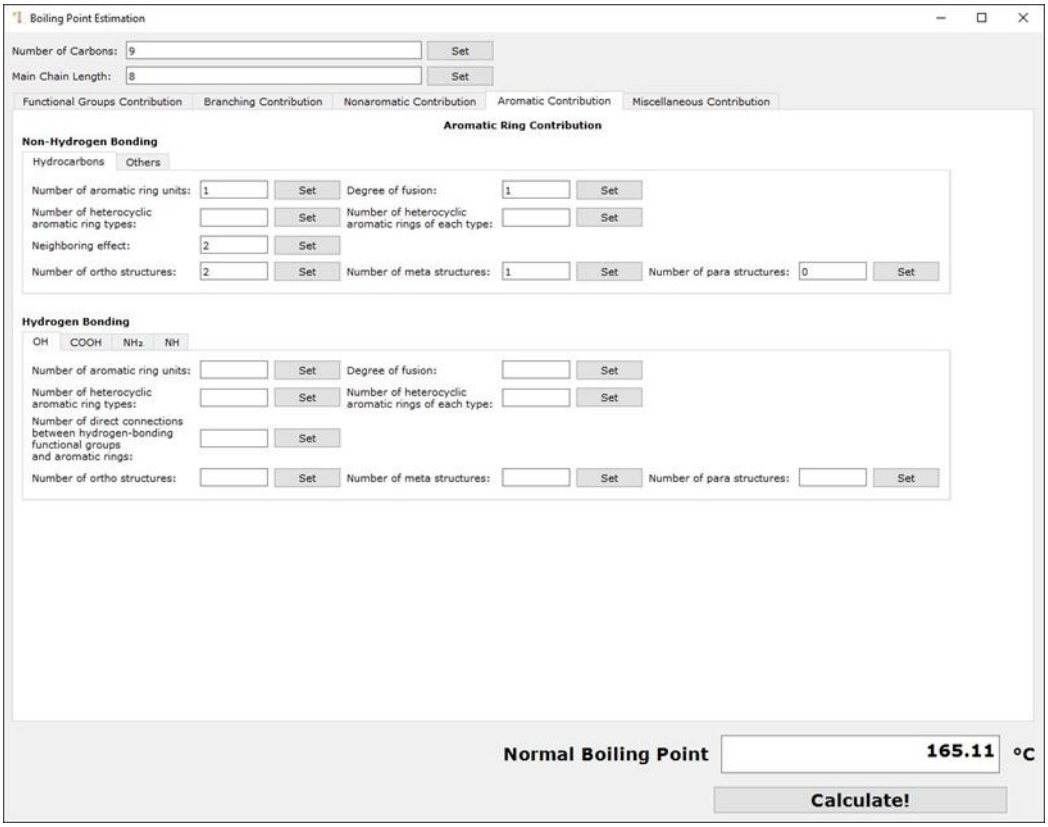


Figure 3.14. Boling point estimation program. Image shows the calculation of the normal boiling point of 1,2,3-trimethylbenzene.

Conclusions

Here, boiling points of a set of twenty-five organic compounds were calculated using the Lai method. Data comparison between the estimated and experimental values further supports the claim that the Lai method is very accurate and closely follows experiment.

Using the software package ALOHA and the calculated boiling points, we generated 'Thread Zones' for each compound in this study at different pollutant rates. In general, these 'Thread Zones' follow a pattern that one would expect when considering only boiling point and molecular weight values of a molecule, with larger areas and distances being covered by lighter, low-boiling point molecules. The data shows that the Lai method is sufficiently accurate to allow us to make predictions regarding the area a compound would cover under specified

weather conditions. In turn, it will be possible to implement this method to direct the signal-strength-based-navigation of the vehicle-mounted portable mass spectrometer system to detect source points of known and unknown chemical organic species.

Finally, we include a graphical user interface to facilitate the calculation of boiling points. Though the interface facilitates the mathematics involved in the problem, it is still important for the user to be familiar with the calculation rules set by Lai et al.

CHAPTER 4

CONCLUSIONS AND FUTURE WORK

As part of this project, different computational techniques have been applied to solve problems in the fields of forensic science and atmospheric chemistry. First, *ab initio* methods were employed in the full conformational analysis of several organic molecules as part of an early effort to create a database for the forensic science community. The purpose of this database is to make chemical information readily available to facilitate the identification and scheduling of known and unknown drugs. Here we showed that the amount of structural information provided by computational chemistry methods is detailed enough to help in the differentiation between drug analogues and that, coupled with experimental data, these tools can be used to provide a more complete picture of common and novel organic compounds, which could be of interest to the forensic scientist.

In addition, we performed a comparison of theoretical fragmentation of tryptamine species to experimental ESI-MS data, to further show the applicability of theoretical tools in the interpretation of experimental data. In general, we demonstrated that theoretical results closely resemble experiment. A graphical user interface was also designed as an attempt to bring computational chemistry methods to a wider audience by facilitating the creating of GAMES input files.

As part of this work, we also implemented an empirical model for the prediction of boiling points though the creation of a graphical user interface and the calculation of 'Thread Zones' for different organic compounds using the program ALOHA. This was done with the purpose of creating a source point detection algorithm based on MS signal intensity and

'Thread Zone' areas for the mobile mass spectrum system designed by the Verbeck lab. Estimated boiling points also were proven to be in very good agreement with experimental values.

As part of the future work, we want to increase the wealth of information available in our database by incorporating the parameters considered in Lipinski's rule of five.[59] Lipinski's paper describes experimental and computational methods to aid in the search for leads of potential drugs using 'high throughput screening.' They tested 2,287 compounds that entered Phase II efficacy studies and 'are likely to have superior physical-chemical properties.' Their goal was to set up an 'absorption-permeability alert procedure to guide medicinal chemists' in the search for leads (asses drug-likeness).

'The rule of 5' predicts that poor absorption or permeation is more likely when:

1. There are more than 5 H-bond donors (defined as the number of OH and NH bonds in the molecule).
2. There are more than 10 H-bond acceptors (defined as the number of Os and Ns in the molecule).
3. The molecular weight is greater than 500.
4. The calculated log P (ClogP) is greater than 5 (or MlogP > 4.15); where log P is the lipophilicity of the molecule expressed as the ratio of octanol solubility to aqueous solubility. ClogP refers to the value of log P calculated using the Pomona College Medicinal Chemistry program and MlogP to the value of log P calculated using the rule-based Moriguchi algorithm.

Furthermore, we would like the accuracy of our boiling point estimation method to generate 'Thread zones' in ALOHA by comparing our predictions to experimental data collected using the mobile mass spectrum system. Should our predictions match the experimental results, the next step would be to implement the boiling point estimation method in the development of a navigation algorithm that would help the mobile unit in the detection of point sources.

Finally, we hope to keep expanding our library with data generated using ab initio computational methods and finalize our software platform for the automated calculation of structures and vibrational spectra.

APPENDIX A

GRAPHICAL USER INTERFACE FOR THE GENERATION OF GAMESS INPUT FILES

As described in the main text, this program is a user-graphical interface designed to facilitate the generation of GAMESS input files. The foundation of this interface is the text editor available through Python and the PyQt4 library. The program puts together portions of precreated input files to form the skeleton of a GAMESS input file and then overwrites the appropriate keywords and/or coordinates at their corresponding positions within the file depending on what the user is trying to achieve. This appendix shows how the program edits the RUNTYP portion of the GAMESS file, how the backbone coordinates of amphetamine are loaded onto the text editor and, finally, how substituents are added to this backbone. Regardless of the GAMESS keyword that the user tries to modify (i.e. regardless of the parameter that the user wants to change), the text editing/input file overwriting algorithm is always the same. The same can be said about the process through which backbone coordinates are loaded and modified with substituents.

Below is the portion of the code that shows how the user can choose between types of GAMESS jobs (i.e. edit the value of the RUNTYP keyword). Specifically, when the user requests a certain calculation type, the function below gets executed and moves the cursor in the GUI's text editor to the position where the RUNTYP keyword is found, then proceeds to select the text at that position and replaces it with the corresponding RUNTYP keyword. The program knows where to place the cursor by looking at what has been previously written in the text editor and counting the number of characters accordingly. For this to work, GAMESS keywords and blocks must preserve their relative position within the text editor (input file).

```
def run_typ(self, text):
        if self.a1 == 0:
```

```
            pass
        else:
            if text == "Energy":
                x = " RUNTYP=ENERGY"
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            elif text == "Gradient":
                x = " RUNTYP=GRADIENT"
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            elif text == "Hessian":
                x = " RUNTYP=HESSIAN"
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            elif text == "FMOHess":
                x = " RUNTYP=FMOHess"
```

```
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            elif text == "Gamma":
                x = " RUNTYP=GAMMA"
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            elif text == "Optimization":
                x = " RUNTYP=OPTIMIZE"
                self.cursor.setPosition(self.a1 + self.b1 +
self.c1, self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a1 + self.b1,
self.cursor.KeepAnchor)
                self.cursor.insertText(x)
                self.c1 = len(x)
                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.PreviousCharacter,
self.cursor.KeepAnchor, 5)
                self.cursor.insertText(" $END")
            else:
                pass
```

This section shows how the amphetamine backbone is inserted into the text editor (i.e. the amphetamine coordinates are loaded onto the program). In this example, the program

moves the text editor cursor to the section corresponding to the molecular Cartesian coordinates as previously described and then proceeds to write (or overwrite) the contents in this section. Molecular backbones are loaded onto the text editor as a collection of different fragments, which correspond to the different positions where the user may want to place a substituent. For instance, if the user wants to enter the coordinates for methamphetamine, the program will load the entire amphetamine backbone as a collection of fragments and then, after the user selects a methyl group to be placed at the amine nitrogen, procceds to replace the coordinates corresponding to one of the amine hydrogens with the coordinates corresponding to a methyl group. The code also shows from where these coordinates will be loaded onto the text file.

```
def amphetamine_frag(self):

.
.
.

self.cursor.setPosition(self.a7, self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

            data = "amphetamine_gamess"

            from itertools import islice
            with open(data, 'r') as file:
                lines_gen = islice(file, 0, 9)
                for line in lines_gen:
                    self.cursor.insertText(line)
```

```
            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            coordinates = self.cursor.selectedText()
            self.d7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub1 =
"Substituents/Amphetamine/P/amphetamine_hydrogen_p"

            from itertools import islice
            with open(sub1, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            coordinates = self.cursor.selectedText()
            self.e7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub2 =
"Substituents/Amphetamine/MI/amphetamine_hydrogen_m1"

            from itertools import islice
            with open(sub2, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.f7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub3 =
"Substituents/Amphetamine/MII/amphetamine_hydrogen_m2"
```

```
            from itertools import islice
            with open(sub3, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.g7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub4 =
"Substituents/Amphetamine/OI/amphetamine_hydrogen_o1"

            from itertools import islice
            with open(sub4, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.h7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub5 =
"Substituents/Amphetamine/OII/amphetamine_hydrogen_o2"

            from itertools import islice
            with open(sub5, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.i7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub6 =
"Substituents/Amphetamine/RVI/amphetamine_hydrogen_r6"

            from itertools import islice
            with open(sub6, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.j7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub7 =
"Substituents/Amphetamine/RV/amphetamine_hydrogen_r5"

            from itertools import islice
            with open(sub7, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.k7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub8 =
"Substituents/Amphetamine/RIV/amphetamine_methyl_r4"

            from itertools import islice
            with open(sub8, 'r') as file:
                lines_gen = islice(file, 0, 4)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.l7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub9 =
"Substituents/Amphetamine/RIII/amphetamine_hydrogen_r3"

            from itertools import islice
            with open(sub9, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.m7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.n7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub10 =
"Substituents/Amphetamine/RII/amphetamine_hydrogen_r2"

            from itertools import islice
            with open(sub10, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.n7 = len(coordinates)

            self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.n7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.o7)
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

            sub11 =
"Substituents/Amphetamine/RI/amphetamine_hydrogen_r1"

            from itertools import islice
            with open(sub11, 'r') as file:
                lines_gen = islice(file, 0, 1)
                for line in lines_gen:
                    self.cursor.insertText(line)

            self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
```

```
            self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
```

```
            self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
            coordinates = self.cursor.selectedText()
            self.o7 = len(coordinates)
.
.
.
```

The following portion of the code shows how a substituent is added to the amine Nitrogen of amphetamine (position R1 of amphetamine in the program which corresponds to one of the amine hydrogens). Essentially, this section shows the algorithm the program follows to replace the coordinates of a specific substituent (i.e. a fragment that makes up the entire backbone). As before, the program moves the cursor to the position of the backbone fragment's coordinates, selects the text at that position, and finally replaces it with the new coordinates. As mentioned above, the code also shows from where these coordinates will be loaded onto the text file.

```
def amp_sub1_typ(self, text):
        if self.d7 < 10:
            pass
        else:
            if text == "H":
                self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.o7)
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

                sub11 =
"Substituents/Amphetamine/RI/amphetamine_hydrogen_r1"

                from itertools import islice
                with open(sub11, 'r') as file:
                    lines_gen = islice(file, 0, 1)
                    for line in lines_gen:
                        self.cursor.insertText(line)

                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
                coordinates = self.cursor.selectedText()
                self.o7 = len(coordinates)
            elif text == "CH\u2083":
                self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.o7)
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

                sub11 =
"Substituents/Amphetamine/RI/amphetamine_methyl_r1"

                from itertools import islice
                with open(sub11, 'r') as file:
                    lines_gen = islice(file, 0, 4)
                    for line in lines_gen:
                        self.cursor.insertText(line)

                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
                coordinates = self.cursor.selectedText()
                self.o7 = len(coordinates)
            elif text == "CH\u2082CH\u2083":
                self.cursor.setPosition(self.a7,
self.cursor.MoveAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.MoveAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.MoveAnchor, self.o7)
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
```

```
self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

                sub11 =
"Substituents/Amphetamine/RI/amphetamine_ethyl_r1"

                from itertools import islice
                with open(sub11, 'r') as file:
                    lines_gen = islice(file, 0, 7)
                    for line in lines_gen:
                        self.cursor.insertText(line)

                self.cursor.movePosition(self.cursor.EndOfBlock,
self.cursor.MoveAnchor)
```

```
                self.cursor.setPosition(self.a7,
self.cursor.KeepAnchor)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor, 3)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.d7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.e7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.f7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.g7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.h7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.i7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.j7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.k7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.l7)
```

```
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.m7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)

self.cursor.movePosition(self.cursor.NextCharacter,
self.cursor.KeepAnchor, self.n7)
                self.cursor.movePosition(self.cursor.NextBlock,
self.cursor.KeepAnchor)
                coordinates = self.cursor.selectedText()
                self.o7 = len(coordinates)
            else:
                pass
```

APPENDIX B

GRAPHICAL USER INTERFACE FOR THE ESTIMATION OF NORMAL BOILING POINTS OF ORGANIC MOLECULE

This graphical-user interface was designed to facilitate the calculation of normal boiling points using the group contribution Lai method. The interface allows the user to enter the values corresponding to each parameter mentioned in Lai's, with the characteristic constants already written within the code for the appropriate correction. The values entered by the user are determined by visual inspection based on the structural features of the molecule in question.

Here we show the Python implementation of the Lai method that corresponds to the main equation, the aromatic ring contribution correction, and the final portion of the code where all the corrections are added to give the normal boiling point. The code is broken into sections corresponding to the main equation and each of the corrections mentioned in Lai's work. The algorithm used to translate the equations into the Python programming language is essentially the same for each major portion of this work, and only the portions corresponding to Lai's equations vary within each section.

Below are the Python instructions that correspond to the main Lai equation, including the functional group portion. For instance, the first block corresponds to the main term of the Lai model, which yields a value for the boling point of the molecule based solely on the number of carbons that the compound possesses. This block is followed by a section that indicates the length of the main chain of the molecule. Both of these values are entered by the user and then stored for further calculations as above stated.

The next portion of code deals with functional group presence and location in the molecule's main chain. All possible functional groups are specified in the code, and depending on which ones the user selects, a value of 0 (zero) or 1 is assign to it in order to tell the program

to take into consideration the corresponding terms for the calculation of the boling point. Finally, the code calculates the contribution of the functional group based on its position in the main chain and adds up all the terms to yield a value for the boiling point. If no other structural corrections are needed, this value is final, otherwise, the value is stored and then added to contribution values from other corractions located in different tabs of the program.

```
def ncarbons_term(self):
        if self.ncarbons_box.text() != "":
            self.n = float(self.ncarbons_box.text())
            self.n_term = 103.59 + 44.34 * ((1 - math.pow(0.94,
self.n))/(1 - 0.94))
            print(self.n_term)

    def nmain_chain_term(self):
        if self.mc_box.text() != "":
            self.MC_val = float(self.mc_box.text())
        else:
            self.MC_val = 0

    def fg_term(self):
.
.
.
self.fg_1 = ((l_oh * (179.75 - 15.35 * ((1 - math.pow(0.94,
self.n))/(1 - 0.94))) * r_oh) +
                          (l_o * (72.83 - 6.98 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_o) +
                          (l_co * (126.16 - 10.17 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_co) +
                          (l_cooh * (235.91 - 16.64 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_cooh) +
                          (l_coh * (119.29 - 9.32 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_coh) +
                          (l_coo * (124.51 - 10.39 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_coo) +
                          (l_nh2 * (109.52 - 6.81 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_nh2) +
                          (l_nh * (86.20 - 7.27 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_nh) +
```

```
                          (l_n * (60.94 - 4.51 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_n) +
                          (l_conh2 * (361.4 - 35.80 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_conh2) +
                          (l_conhr * (325.41 - 30.32 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_conhr) +
                          (l_conrr * (276.30 - 28.91 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_conrr) +
                          (l_cn * (171.31 - 12.57 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_cn) +
                          (l_no2 * (222.34 - 16.08 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_no2) +
                          (l_sh * (139.04 - 8.73 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_sh) +
                          (l_s * (133.38 - 7.47 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_s) +
                          (l_f * (49.05 - 3.42 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_f) +
                          (l_cl * (108.14 - 6.76 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_cl) +
                          (l_br * (135.23 - 8.61 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_br) +
                          (l_i * (178.36 - 9.79 * ((1 -
math.pow(0.94, self.n))/(1 - 0.94))) * r_i))

            self.fg_2 = (l_oh * l_cooh * (-28.53) * r_oh *
r_cooh +
                         l_oh * l_o * (-14.88) * r_oh * r_o +
                         l_oh * l_nh2 * 4.18 * r_oh * r_nh2 +
                         l_oh * l_nh * (-4.26) * r_oh * r_nh +
                         l_oh * l_cn * (-21.98) * r_oh * r_cn +
                         l_oh * l_no2 * (-40.27) * r_oh * r_no2
+
                         l_oh * l_cl * (-30.97) * r_oh * r_cl +
                         l_oh * l_br * (-39.75) * r_oh * r_br +
                         l_cooh * l_o * (-14.08) * r_cooh * r_o
+
                         l_cooh * l_nh2 * (-15.84) * r_cooh *
r_nh2 +
                         l_cooh * l_nh * (-13.97) * r_cooh *
r_nh +
                         l_cooh * l_cn * (-40.83) * r_cooh *
r_cn +
                         l_cooh * l_no2 * (-53.17) * r_cooh *
r_no2 +
                         l_cooh * l_cl * (-27.26) * r_cooh *
r_cl +
```

```
                        l_cooh * l_br * (-31.71) * r_cooh *
r_br +
                        l_o * l_nh2 * (-6.02) * r_o * r_nh2 +
                        l_o * l_nh * (-5.20) * r_o * r_nh +
                        l_o * l_cn * (-14.37) * r_o * r_cn +
                        l_o * l_no2 * (-18.70) * r_o * r_no2 +
                        l_o * l_cl * (-13.16) * r_o * r_cl +
                        l_o * l_br * (-16.26) * r_o * r_br +
                        l_nh2 * l_nh * (-5.87) * r_nh2 * r_nh +
                        l_nh2 * l_cn * (-17.73) * r_nh2 * r_cn
+
                        l_nh2 * l_no2 * (-23.10) * r_nh2 *
r_no2 +
                        l_nh2 * l_cl * (-16.93) * r_nh2 * r_cl
+
                        l_nh2 * l_br * (-13.37) * r_nh2 * r_br
+
                        l_nh * l_cn * (-15.05) * r_nh * r_cn +
                        l_nh * l_no2 * (-19.60) * r_nh * r_no2
+
                        l_nh * l_cl * (-14.02) * r_nh * r_cl +
                        l_nh * l_br * (-11.38) * r_nh * r_br +
                        l_cn * l_no2 * (-51.26) * r_cn * r_no2
+
                        l_cn * l_cl * (-9.88) * r_cn * r_cl +
                        l_cn * l_br * (-27.61) * r_cn * r_br +
                        l_no2 * l_cl * (-36.00) * r_no2 * r_cl
+
                        l_no2 * l_br * (-32.58) * r_no2 * r_br
+
                        l_cl * l_br * (-23.66) * r_cl * r_br)

            l_total = int(l_oh + l_o + l_co + l_cooh + l_coh +
l_coo + l_nh2 + l_nh + l_n + l_conh2 + l_conhr +
                          l_conrr + l_cn + l_no2 + l_sh + l_s +
l_f + l_cl + l_br + l_i)

            d = [int(self.m_o), int(self.m_co),
int(self.m_cooh), int(self.m_coh), int(self.m_coo),
int(self.m_n),
                 int(self.m_conh2), int(self.m_conhr),
int(self.m_conrr), int(self.m_cn), int(self.m_no2),
                 int(self.m_sh), int(self.m_s), int(self.m_f),
int(self.m_cl), int(self.m_br), int(self.m_i)]
            m = ([d for d in d if d] + ([0] * l_total))
            g = [int(self.m_oh), int(self.m_nh2)]
            m1 = ([g for g in g if g] + ([0] * l_total))
```

```
            x = [int(self.m_nh)]
            m2 = ([x for x in x if x] + ([0] * l_total))

            e = [l_o * -3.13, l_co * -14.70, l_cooh * 0, l_coh *
0, l_coo * -9.01, l_n * 0, l_conh2 * 0, l_conhr * 0,
                 l_conrr * 3.51, l_cn * 0, l_no2 * -11.32, l_sh
* 0, l_s * -10.60, l_f * -9.01, l_cl * 2.85,
                 l_br * -3.90, l_i * -7]
            lam = ([e for e in e if e] + ([0] * l_total))
            h = [l_oh * -0.39, l_nh2 * -3.91]
            lam1 = ([h for h in h if h] + ([0] * l_total))
            y = [l_nh * 7.40]
            lam2 = ([y for y in y if y] + ([0] * l_total))

            f = [int(l_o) * self.po_o, int(l_co) * self.po_co,
                 int(l_cooh) * self.po_cooh, int(l_coh) *
self.po_coh, int(l_coo) * self.po_coo, int(l_n) * self.po_n,
                 int(l_conh2) * self.po_conh2, int(l_conhr) *
self.po_conhr, int(l_conrr) * self.po_conrr,
                 int(l_cn) * self.po_cn, int(l_no2) *
self.po_no2, int(l_sh) * self.po_sh, int(l_s) * self.po_s,
                 int(l_f) * self.po_f, int(l_cl) * self.po_cl,
int(l_br) * self.po_br, int(l_i) * self.po_i]

            if l_total == 1:
                p = ([f for f in f if f] + ([[0] * 100] * 100))
            else:
                p = ([f for f in f if f] + ([[0] * l_total] *
l_total))

            k = [int(l_oh) * self.po_oh, int(l_nh2) *
self.po_nh2]

            if l_total == 1:
                p1 = ([k for k in k if k] + ([[0] * 100] * 100))
            else:
                p1 = ([k for k in k if k] + ([[0] * l_total] *
l_total))

            l = [l_oh * -19.90, l_nh2 * -14.75]

            sig = ([l for l in l if l] + ([0] * l_total))

            z = [int(l_nh) * self.po_nh]

            if l_total == 1:
                p2 = ([z for z in z if z] + ([[0] * 100] * 100))
```

```
            else:
                p2 = ([z for z in z if z] + ([[0] * l_total] *
l_total))

            w = [int(self.m_k)]
            m3 = ([w for w in w if w] + ([0] * l_total))
            q = [self.po_k]

            if l_total == 1:
                p3 = ([q for q in q if q] + ([[0] * 100] * 100))
            else:
                p3 = ([q for q in q if q] + ([[0] * l_total] *
l_total))

            if self.MC_val != 0 and p != [0]:
                for i in range(1, (l_total + 1)):
                    for j in range(1, (m[i - 1]) + 1):
                        if 0 < p[i - 1][j - 1] <= ((self.MC_val
+ 1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p1 = lam[i - 1] * (p[i - 1][j -
1] - 2)/(((self.MC_val + 1)/2) - 2)
                            self.fg_3 += fg_p1
                        if p[i - 1][j - 1] > ((self.MC_val +
1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p2 = lam[i - 1] * (self.MC_val -
p[i - 1][j - 1] - 1)/(((self.MC_val + 1)/2) - 2)
                            self.fg_4 += fg_p2

            if self.MC_val != 0 and p1 != [0]:
                for i in range(1, (l_total + 1)):
                    for j in range(1, (m1[i - 1]) + 1):
                        if 0 < p1[i - 1][j - 1] <= ((self.MC_val
+ 1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p1 = (lam1[i - 1] * (p1[i - 1][j
- 1] - 2)/(((self.MC_val + 1)/2) - 2)) + sig[i - 1]
                            self.fg_3 += fg_p1
                        if p1[i - 1][j - 1] > ((self.MC_val +
1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p2 = ((lam1[i - 1] * (self.MC_val
- p1[i - 1][j - 1] - 1)/(((self.MC_val +

1)/2) - 2)) + sig[i - 1])
                            self.fg_4 += fg_p2

            if self.MC_val != 0 and p2 != [0]:
                for i in range(1, (l_total + 1)):
                    for j in range(1, (m2[i - 1]) + 1):
```

```
                        if 0 < p2[i - 1][j - 1] <= ((self.MC_val
+ 1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p1 = lam2[i - 1] * (1 - (p2[i -
1][j - 1] - 2)/(((self.MC_val + 1)/2) - 2))
                            self.fg_3 += fg_p1
                        if p2[i - 1][j - 1] > ((self.MC_val +
1)/2) and (self.MC_val + 1)/2 != 2:
                            fg_p2 = lam2[i - 1] * (1 -
(self.MC_val - p2[i - 1][j - 1] - 1)/(((self.MC_val + 1)/2) -
2))
                            self.fg_4 += fg_p2

            if self.MC_val != 0 and p3 != [0]:
                for i in range(1, (l_total + 1)):
                    for j in range(1, (m3[i - 1]) + 1):
                        cof_0 = -11.03 * (math.factorial(p3[i -
1][j - 1])/(math.factorial(p3[i - 1][j - 1] - 2) *

math.factorial(2)))
                        self.cof += cof_0
        print(self.fg_1)
        print(self.fg_2)
        print(self.fg_3)
        print(self.fg_4)
        print(self.cof)

        self.fugr_term = self.fg_1 + self.fg_2 + self.fg_3 +
self.fg_4 + self.cof
```

This portion of the code shows how the aromatic ring contribution is implemented in Python. The different block in this portion of the code correspond to different structural corrections depending on whether the molecule is made up of carbons only or oother elements. Whether the molecule is hydrogen bonding or not is also taken into consideration. Corrections go further by taking into consideration what type of functional group is responsible for the hydrogen bonding.

The code also shows how corrections corresponding to neighboring effects between functional groups attached to the aromatic ring are implemented as well as ortho, meta, and

para interactions. Finally, an aromatic contribution term is calculated based on the values entered by the user, which is later added to the main term to yield a boling point value.

```
def arom_term(self):
.
.
.
            alpha = [-9.29, 41.76, 66.17] + [0] * (self.a_nh)
            alpha1 = [-9.29, 41.76, 66.17] + [0] * (self.a_nh1)
            alpha2 = [-9.29, 41.76, 66.17] + [0] * (self.ha_nh)
            alpha3 = [-9.29, 41.76, 66.17] + [0] * (self.ha_nh1)
            alpha4 = [-9.29, 41.76, 66.17] + [0] * (self.ha_nh2)
            alpha5 = [-9.29, 41.76, 66.17] + [0] * (self.ha_nh3)

            for j in range(1, (self.a_nb + 1)):
                at1 = 7.92 * (math.pow((self.a_fb[j - 1]),
1.94))
                self.ar1 += at1
            for k in range(1, (self.a_nh + 1)):
                at2 = (alpha[k - 1]) * (self.a_hk[k - 1])
                self.ar2 += at2
            self.ar3 = (15.80 * self.a_ne - 10.66 * self.a_ortho
+ 0.91 * self.a_meta +
                        3.68 * self.a_para)

            for j in range(1, (self.a_nb1 + 1)):
                at1 = 5.01 * (math.pow((self.a_fb1[j - 1]),
2.50))
                self.ar4 += at1
            for k in range(1, (self.a_nh1 + 1)):
                at2 = (alpha1[k - 1]) * (self.a_hk1[k - 1])
                self.ar5 += at2
            self.ar6 = (2.45 * self.a_ne1 - 6.51 * self.a_ortho1
- 6.24 * self.a_meta1 -
                        7.69 * self.a_para1)

            for j in range(1, (self.ha_nb + 1)):
                at1 = 24.00 * (math.pow((self.ha_fb[j - 1]), 0))
                self.ar7 += at1
            for k in range(1, (self.ha_nh + 1)):
                at2 = (alpha2[k - 1]) * (self.ha_hk[k - 1])
                self.ar8 += at2
            self.ar9 = (0 * self.ha_c - 14.00 * self.ha_ortho -
3.00 * self.ha_meta -
```

```
                        3.00 * self.ha_para)

            for j in range(1, (self.ha_nb1 + 1)):
                at1 = 0 * (math.pow((self.ha_fb1[j - 1]), 0))
                self.ar10 += at1
            for k in range(1, (self.ha_nh1 + 1)):
                at2 = (alpha3[k - 1]) * (self.ha_hk1[k - 1])
                self.ar11 += at2
            self.ar12 = (0 * self.ha_c1 + 0 * self.ha_ortho1 + 0
* self.ha_meta1 +
                        0 * self.ha_para1)

            for j in range(1, (self.ha_nb2 + 1)):
                at1 = 25.00 * (math.pow((self.ha_fb2[j - 1]),
0))
                self.ar13 += at1
            for k in range(1, (self.ha_nh2 + 1)):
                at2 = (alpha4[k - 1]) * (self.ha_hk2[k - 1])
                self.ar14 += at2
            self.ar15 = (25.00 * self.ha_c2 - 10.28 *
self.ha_ortho2 - 7.28 * self.ha_meta2 -
                        10.28 * self.ha_para2)

            for j in range(1, (self.ha_nb3 + 1)):
                at1 = 5.01 * (math.pow((self.ha_fb3[j - 1]), 0))
                self.ar16 += at1
            for k in range(1, (self.ha_nh3 + 1)):
                at2 = (alpha5[k - 1]) * (self.ha_hk3[k - 1])
                self.ar17 += at2
            self.ar18 = (15.00 * self.ha_c3 - 10.00 *
self.ha_ortho3 - 7.00 * self.ha_meta3 -
                        10.00 * self.ha_para3)

            m_total = self.m_oh + self.m_cooh + self.m_nh2 +
self.m_nh

            if m_total != 0:
                self.ar_hb = (self.ar7 + self.ar8 + self.ar9 +
self.ar10 + self.ar11 + self.ar12 + self.ar13 +
                              self.ar14 + self.ar15 + self.ar16 +
self.ar17 + self.ar18)/m_total
            else:
                self.ar_hb = 0

            self.ar_term += self.ar1 + self.ar2 + self.ar3 +
self.ar4 + self.ar5 + self.ar6 + self.ar_hb
```

```
            print(self.ar_term)
```

Finally, this section shows how all the terms corresponding to each main correction mentioned in Lai's work is added to the main equation to determine the normal boiling point.

```
def calculate(self):
            point = (self.n_term + self.fugr_term + self.br_term
+
                     self.nonar_term + self.ar_term +
self.mic_term - 273.15)
            print(point + 273.15)
            print(point)
            t_b = "{:.2f}".format(point)
            frm = QtGui.QTextCharFormat()
            font = QtGui.QFont('Verdana')
            font.setBold(1)
            font.setPointSize(14)
            frm.setFont(font)
            self.cursor.setPosition(0, self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.End,
self.cursor.MoveAnchor)
            self.cursor.movePosition(self.cursor.Start,
self.cursor.KeepAnchor)
            x = str(t_b)
            self.cursor.insertText(x, frm)
```

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