

EXPLORING CRITICAL CONFORMATIONS:
STATE SEARCHING AND SAMPLING IN BOTH
GERMANIUM CHAINS AND ICE INTERFACES

By

GENTRY H. SMITH

B.S.

Southern Nazarene University

Bethany, OK, USA

2016

Submitted to the Faculty of the
Graduate College of
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
Master of Science
December 2018

EXPLORING CRITICAL CONFORMATIONS:
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Thesis Approved:

Thesis Advisor

ACKNOWLEDGMENTS

To Oklahoma State University, for providing the environment in which I have been able to study, teach, and research.

To the HPCC and the individuals who manage it for providing a powerful cluster for computations and continuous support for technical issues.

To my advisor, who instructed and assisted me in research.

To my parents, by blood and marriage, who have always encouraged me toward higher goals.

To my wife, Miranda, who has supported me for over five years.

Acknowledgments reflect the views of the author and are not endorsed by committee members or Oklahoma State University.

Name: GENTRY H SMITH

Date of Degree: December 2018

Title of Study: EXPLORING CRITICAL CONFORMATIONS

Major Field: COMPUTATIONAL CHEMISTRY

Abstract: Molecular conformation plays a critical role in the properties of systems in both the condensed or vapor states. The ensemble of conformations dictates structural properties, average energy, heat capacities, and other thermodynamic and dynamic quantities. Here, we explore the role of conformation in proton ordering and orientational defect formation in ice as well as strategies for exhaustive conformer searching for molecules using Group IV element backbones. In the ice systems, we show algorithmic strategies for seeking optimized proton disordered crystals that satisfy the Bernal-Fowler ice rules. In the Group IV molecule investigations, we develop an automated strategy for seeking the optimal low energy conformer and uncover previously unreported deficiencies in common computational software used in investigating Germanium complex energies.

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CHAPTER 1

Introduction

1.1 Computational Chemistry: Chemistry on the Computer

For nearly a century, computational methods have greatly assisted chemists in their efforts of research and discovery and have relatively recently become their own field of focus within chemistry. As a standalone field, computational chemistry uses computer simulations to solve chemical problems. These simulations typically rely on theoretical methods adapted to run highly efficiently on computers. While initial computational methods were designed to solve wave functions and atomic orbitals, the scope quickly expanded into multiple fields of chemistry as more methods were developed to confirm or predict properties of molecules and systems.

With the introduction of *ab initio* and density functional methods, computational methods began to stand as a distinct field within chemistry. This introduction serves to introduce necessary background information generally relevant to the methods developed and utilized in the following chapters.

1.2 Relevant Computational Methods

Modern computational methods take one of several approaches in computing a system. Usually limited by the scale of molecule and scope of system, multiple methods exist to analytically solve or closely approximate a system by way of solving or approximating the quantum mechanical wave function or through a similarly consistent method of generalization by way of statistical solutions. Many other methods exist, but are not directly relevant to this work.

The first hurdle in any computational system is the likely impossibility of analytically solving the problem. In a system with more than two particles, this multi-body problem usually cannot be solved analytically excepting the dihydrogen cation due to the exorbitant amount of information contained in solving the wave function. This is largely due to the complexity introduced into the wave function of multiple interacting species that often lead to prohibitively large or impossible equations to solve.

1.2.1 Quantum Mechanical Methods and Basis Sets

In computational chemistry, quantum mechanical methods generally refer to computational methods that attempt to solve or closely approximate the electronic Schrödinger equation given nuclei and electron position information to determine properties of the system like energies or electron densities. Because the Schrödinger equation is impossible to solve for many-body systems, different methods use different approximations to balance between accuracy of the approximation and efficiency of computation.

1.2.1.1 Basis Sets

While running calculations, both *Ab initio* and DFT methods require basis sets to represent the electronic wave function as a system of algebraic equations that can be efficiently calculated. While basis sets can be designed of atomic orbitals or plane waves, this work focus primarily on basis sets derived by atomic orbitals. The two most often used types of orbitals are Gaussian-type and Slater-type orbitals. Slater-type orbitals (STOs), named after the physicist John Slater who introduced them in 1930,² function as a linear combination of atomic orbitals (LCAO) adopted as a molecular orbital. STOs notably exhibit similar properties to Schrödinger-based orbitals, excepting that STOs have no radial nodes.

Gaussian-type orbitals (GTOs), introduced by S. Francis Boys in 1950,³ also function as orbitals in the LCAO method. GTOs are similar to STOs in premise, but have

further reduced realism when compared to Schrödinger-based orbitals. One example of this is the lack of accuracy of electron density near the nucleus. While exhibiting a lesser accuracy, GTOs excel in computational efficiency compared to STOs by roughly 4-5 orders of magnitude. This allows GTO-based calculations to compute more orbitals. Specifically, Boys designed GTOs as a method of approximating STOs.

Basis sets are often grouped by their sizes. The smallest sets, known as minimal basis sets, use a single basis function for each orbital. The most common minimal basis set, STO-nG where n is an integer usually between 2 and 6, was first proposed by John Pople in 1969.⁴ This method describes that a Slater-type orbital can be approximated using n-Gaussian orbitals. These STO-nG approximations end up fitting electron densities well at all radial distances except those close to the nucleus. The STO-3G basis set used in this work is a popular basis set as the 3 Gaussian-type orbitals works well for atoms in the [H-Xe] range.

The other basis sets used in the work fall under the category of split-valence basis sets. These basis sets represent valence electrons with more than one basis function, which allows for electron density to be more flexible in different molecular systems. The most common form of these basis sets were introduced by John Pople as the X-YZg form and are commonly referred to as Pople basis sets.⁵ These follow the form that each orbital basis function is comprised of X Gaussians. The Y and Z represent the two additional linear combination of Gaussian functions made of Y and Z Gaussians each, respectively, that compose the valence. These basis sets are not limited to two valence functions, referred to as a double-zeta, and can also be triple- or quadruple-zeta. Additional values, typically denoted by one or two stars, one or two plus signs, or explicitly-defined orbital combinations in parentheses can also be used to further complicate the basis set as desired. The star notation defines a polarization function for heavy atoms to account for d and f polarizations. The plus signs denote diffuse functions that more-accurately represent less common valence electrons like

carbanions that may diffuse further out from the nucleus.

1.2.1.2 *Ab Initio* Methods

Ab initio, or "from first principles," methods refer to calculation methods that rely solely on physical constants as external values. By design, *ab initio* methods avoid using any empirically-acquired data and rely on theoretically calculated values. The development of these methods allowed computational chemists to solve a new class of problems and resulted in John Pople and Walter Kohn receiving the Nobel Prize for their work. The *ab initio* method utilized in this work is the Hartree-Fock (HF) method used to determine the energy of a many-body system in a stationary state, which is to say time-independent.⁶ Known initially as the self-consistent field method, the HF method utilizes approximations defined by the basis set to approximate the Schrödinger equation. The consistency of this self-consistent field method arose by the requirement that the final calculated field be self-consistent with the initial field. An additional property of HF is that electron-electron repulsion is not taken into account, requiring that a basis set account for this interaction. As larger basis sets are used, the overall energy of the wavefunction is increased toward a value known as the Hartree-Fock limit. This limit is approached as the larger basis sets approach the exact solution of the non-relativistic Schrödinger equation without spin orbital terms. The calculation of relativistic and spin terms require a further method known as Post-Hartree-Fock, which is not used considered further in this work.

1.2.1.3 Density Functional Theory Methods

Density Function Theory (DFT) Methods function very similarly to *ab initio* methods in how Slater-type orbitals are used to approximate the Schrödinger equation, but differ in that DFT utilizes some empirical data to speed up the calculation process.⁷ These simplifications are stable able to model exchange and correlation

interactions very well, however the reliability of calculated properties, specifically intermolecular interactions, dispersion forces, and other internal properties are greatly reduced. Just as with *ab initio* methods, DFT methods require a basis set definition for the approximation calculations. Many DFT methods exist and even some so-called hybrid functional methods that exchange with HF terms for greater reliability in calculated values. One pure DFT method used in this work is BLYP, which utilizes the Becke exchange with the Lee-Yang-Parr correlation part. Some hybrid functional methods used are the B3LYP, M06L, and PBE methods. The B3LYP utilizes the BLYP but combined Becke's exchange with the exact energy from HF theory. M06L, known as the Minnesota functionals, depend on kinetic energy density values from databases. It specifically was designed to work well with transition metals, inorganics, and organometallics.⁸ The PBE method is another method with similar levels of accuracy to B3LYP that attempts to increase the number of HF-exchanged functionals.⁹

1.2.1.4 Semi-Empirical Methods

Like DFT, Semi-empirical methods also pull somewhat from Hartree-Fock methods, but rely even more on approximations and empirical data to nearly completely substitute out any proper calculation of the Schrödinger equation. These data can produce fairly accurate results to experimental data, but rely heavily on a similarity between the subject molecule and the database molecules. Due to its restrictive scope, semi-empirical methods excel in organic chemistry calculations where relatively few elements are used with moderately sized molecules.¹⁰ Additionally, various semi-empirical methods have been designed to produce results with close accuracies to specific properties of experimental data. Two methods used in this work, AM1¹¹ and PM3,¹² serve particularly well at calculating data to fit heats of formation, dipole moments, ionization potentials, and structural geometries. Unlike the other meth-

ods described so far, basis sets are not used at all in the calculation of energies and properties.

1.2.2 Monte Carlo Molecular Modeling

A major problem in sampling comes with the scale of many molecules of one or more type in a single or mixed phase. A popular method of working around this problem is known as Monte Carlo methods, or MC. While not named until the 1950s, MC methods were first seen in the 18th century thought experiment Buffon's needle.¹³ In his work, Buffon proposed dropping n needles of length l onto a plane with parallel lines spaced t units apart. Buffon worked out that the probability, P , of a needle crossing one of the lines to be $P = \frac{2l}{\pi t}$. Solving for π , the probability can be rearranged as $\pi = \frac{2l}{tP}$ to approximate π . Since P can also be approximated by dividing the number of needles crossing one of the lines, h , by the n needles as $P = \frac{h}{n}$, the approximation can be expressed as $\pi = \frac{2l*n}{t*h}$.

This method of randomness was improved upon by Stanislaw Ulam while working at Los Alamos National Laboratory in the late 1940s by introducing markov chains to favor the probability of events occurring. Ulam shared this work with John von Neumann and together they created a program to run on the ENIAC computer capable of computing this favored version of random sampling. As the project was secretive due to being used as a part of the Manhattan Project, a collaborator named Nikolas Metropolis suggested the name Monte Carlo due to Ulam's uncle's propensity to gambling at a casino in Monaco of the same name.¹⁴ Later dubbed Markov Chain Monte Carlo (MCMC) sampling, this allowed for random sampling to instead become a virtual statistically-appropriate sampling method. Eventually published in 1949 by Metropolis and Ulam, this laid the groundwork for modern MC methods used in modern chemical simulation packages.

1.3 Hardware

Since computation methods were developed slightly before and during the rise of modern computers, early calculations were performed by hand with minimal assistance by machines. Over time, these methods were increasingly assisted by early computers and further development eventually led to the first computational programs. These first computers, like the ENIAC and EDSAC offered computation power in the order of a few dozen to a few thousand operations per second.

For this work, the majority of calculations were computed on the Oklahoma State University Cowboy Cluster. Available since 2014, this cluster collectively offers the computing power of 3048 cores and 8576 GB of RAM, totalling 48.8 trillion FLoating Point Operations Per Second (Tera FLOPS or TFLOPS).

1.4 Software

If hardware denotes the realm of study of a computational chemist, software denotes the tools. By utilizing preexisting packages of and developing new and more advanced tools, computational chemists are able to simulate a wide variety of chemical systems.

1.4.1 Programs

While computational programs have existed for nearly 50 years, additional programs have relatively recently developed to aid in the visualization and depiction of chemical systems. Gaussian, developed by John Pople and his team is one of the earliest *ab initio* computation programs developed. Released as Gaussian 70 in 1970, it has received regular updates and capability expansions is still in use today and is one of the most widely-used computational chemistry tools available in its latest iteration, Gaussian 16. Gaussian tends to carry a lot of clout in the computational community as founder John Pople won a Nobel Prize in 1998 with Walter Kohn for

his work in *ab initio* quantum mechanical systems and for being one of the oldest packages around.

In addition to Gaussian, many other packages exist with a large set of available tools for investigators. Two additional packages used in this work are GAMESS,¹⁵ a package also in active development since the 1970s led by Mark Gordon, and NWChem,¹⁶ a popular open source package developed by Pacific Northwest National Laboratory since the late 2000s.

Once the rounds computation has completed, investigators often report the calculated system graphically through visualization tools. These tools are also popular among any investigator wishing to represent a compound or system as more than its molecular formula. Two visualization tools used in this work are Avogadro and UCSF Chimera. Avogadro, in development since 2008, is a relatively simple molecular visualization tool designed to work across multiple operating systems across multiple languages and with many extensions.¹⁷ UCSF Chimera, developed by the Resource for Biocomputing, Visualization, and Informatics (RBVI) at the University of California, San Francisco, focuses on more advanced representations of compounds and systems. It allows for multi-structure files to generate videos of simulations and also provides a powerful Application Program Interface for programmatically creating or altering molecules and systems.

1.4.2 Programming Languages

A final note should be made about programming languages and their usage in general and in this work. Programming languages have existed for as long as computers. From original punch cards and bitwise commands to modern interpreted languages, programming languages allows investigators to control computers to enact explicit commands. In a way, the job command files in computational tools like those in Gaussian and GAMESS are programmatically used as a programming language to

tell a system to enact a calculation of type X on system Y with Z parameters. Even these tools utilize code to enact their commands, usually in older and highly efficient languages like C and Fortran. Because these tools directly interact with hardware to calculate an immense number of calculations, efficiency is key.

One language almost exclusively used in this work is Python.¹⁸ The Python programming language has recently become one of the most used programming languages for scientific analysis. This is possibly due to Python's initial development focus of data analysis, support for extensions by the development team, and ease of use. As a scripted type languages, Python does not directly interface with hardware in assembly like the more efficient C and Fortran languages, but certain packages and extensions can take advantage of those efficiency boosts to improve Python's effectiveness. Math and science packages like NumPy¹⁹ and SciPy²⁰ interface with C code to rapidly speed up complex mathematic evaluations like matrix manipulations while retaining the usability expected in Python. Additional packages like Cython²¹ will take a completed Python script and compile much of it in C code to greatly improve efficiency and reduce the computational strain on the system.

As will be seen in this work, code can be used to generate and run these sets of code, effectively creating a train of code that can operate as a tool within a tool. One aspect of this is abstracting out method and basis sets to that of a computational requirement and level of accuracy. Effectively, an investigator could remove any necessary knowledge of which basis set or method is necessary for a specific system, although a tool with sufficient awareness to automatically enact this has not been published.

CHAPTER 2

On Algorithms for Building and Sampling Disordered Crystal States

2.1 States and Properties of Ice

Ice has many forms, each with unique environments and structures that give rise to similar and distinct properties.

2.1.1 Bernal-Fowler Ice Rules

Based on their paper published in 1933, the Bernal-Fowler Ice Rules are the foundational observations of how water molecules interact in an ice structure and have remained the standard for ice bonding rules for nearly a century. Although a bent, divalent molecule, water possesses an electronic tetrahedral structure that allows for four interactions on each molecule. The two protons allow for a hydrogen bond with a lone pair from a neighboring oxygen atom. Similarly, the oxygen atom's two lone pairs allow for a hydrogen bond with a neighboring proton. These rules are fairly rigid in the sense that every water molecule can interact with two oxygen atoms and two protons from four surrounding water molecules. These are also relatively relaxed in the sense that each of the four attached water molecules can occupy one of three rotational positions, allowing for 81 possible microstates when including rotational duplicates.

2.1.2 Forms of Ice

While ubiquitous in the ' I_h ' form, ice water has many known forms. As of the writing of this work, there are 17 established forms of ice. These forms usually occur

in cubic, hexagonal, and orthorhombic crystal structures. The relationship between external pressure and temperature are the primary defining characteristics of which form will form in a given system, although doping may be required to produce some structures. The subject of this work will be on the proton-ordered orthorhombic ice XI and its proton-disordered isomer, ice I_h.

2.1.3 Ice I_h

Ice I_h naturally forms in pure solution at temperatures in the 72 K to 273.15 K range at pressures in the 1 Pa to 100 MPa range, with some temperature curving off into the vapour and liquid phases at very high and very low pressures. As the most commonly found form on earth, ice I_h is a highly desired form for computational studies involving ice systems for investigators investigating ice simulations in normal earth conditions.

As famously discussed by Linus Pauling, hexagonal ice water contains a residual entropy at very low temperatures.²² This residual entropy goes according to Boltzmann's entropy equation $K = \ln(W)$ where $W = (\frac{3}{2})^N$ for N molecules in the crystal. He additionally predicted that an ice structure may exist at sufficiently low temperatures with zero residual entropy.

2.1.4 Efforts to Generate Ice I_h

A commonly referenced effort to create an ice I_h crystal comes from Victoria Buch's 1998 paper.²³ Her work involved a monte carlo effort to generate ice I_h by initializing a deprotonated oxygen structure, randomly placing the appropriate number of protons, and then using MC methods to adjust the structure until every oxygen atom was bonded to exactly two hydrogen bonds.

2.1.5 Comparison between Ice XI and Ice I_h

While ice I_h is known as the most common form of ice found on the planet, it is much more difficult to computationally generate than an ice XI crystal. The ease of generation of an ice XI structure stems from the repetition of a unit cell with consistent layering and orientation throughout the crystal lattice.

With ice I_h crystals, the proton-disordered form introduces entropy by way of rotational disorder. The disordered protons allow for a greater number of microstates in the organization of the crystal, increasing the multiplicity and, by its very definition, entropy. As the protons and lone pairs are no longer consistently ordered, hydrogen bonds may no longer form properly at all interaction sites. The interaction of proton with proton or lone pair with lone pair are not hydrogen bonds and are considered defects in the lattice. An ice structure of randomly oriented molecules without consideration of hydrogen bonds will likely produce defects at many interaction sites across the lattice and weaken the integrity of the system, leading to stability problems while running simulations. In generating the crystal, the cause of these defects must be considered and countered effectively. While other stable hydrogen bonding structures may exist, they would either break the Bernal-Fowler ice rules or alter the structure away from the specified form.

2.2 Method Design

2.2.1 Overview

The big idea is to convert an easy-to-make ice XI crystal into an ice I_h crystal. Because the key difference in structure is the proton-orderedness, it might be possible to rearrange the water molecule orientations in a pseudorandom way to create an ice I_h crystal. This section walks through the method developed to convert ice XI into ice I_h, the results of initial testing, and imperfections discovered in the design.

2.2.2 Selection of Software Tools

Python was chosen as the language of the tool due to the versatility of the language and the ease of development due to the "pseudocode" written style of the language and the availability of scientific packages including SciPy and NumPy. Python version 2.7 was specifically chosen due to familiarity with the language. Crystal files were defined and saved as Protein Data Bank (.pdb) files as this format allows for defining multiple molecules within a larger structure with a simple X, Y, Z grid position format.

2.2.3 Generation of Source Ice XI

This is Dr. Fennell's method to create an ice XI .pdb file. Basically, the ice XI unit cell of eight water molecules is repeated as desired to create a sufficiently large crystal. The primarily used crystal consists of a 3 x 3 x 6 unit cell repetition totaling 432 water molecules.

2.2.4 Source Ingestion

It is important that the crystal be read and stored in an efficient method to keep relevant information about each molecule easily accessible. As the file is read in, each molecule is stored as an entry in a multidimensional array where the first index is the molecule number. Further, the second index defines the molecule number where 0 is oxygen and 1 and 2 are the protons. The third, fourth, and fifth indices define the X, Y, and Z position coordinates.

2.2.5 Identifying Neighboring Molecules

Identifying the neighboring molecules proved computationally difficult. The most effective method is to find the closest four molecules by computing a distance calculation between every two oxygen atoms. This ensures every molecule is considered, but

also presents significant hurdles. First, a distance calculation utilizes an extremely computationally-inefficient square root calculation. The inefficiency lies in the binary-based command for calculating a square root that often utilizes either a logarithmic solution or a Newtonian approximation that requires 16-64 processor cycles. This square root computation can be entirely bypassed by instead comparing the squared-distance between molecules and finding the lowest values. These squared-distances scale identically to the square root value for all distances greater than one, which is true for the ice XI structures sampled in this work.

Second, molecules on the walls and edges of the molecule will not have four neighbors in the non-periodic crystal. This is accounted for by shifting all six sides to make a pseudo-periodicity for these edge cases. Those periodically-neighboring molecules are flagged with a shifting value in the neighboring atom array by specifying a translation in the x, y, or z axis values. Unfortunately, the necessary code to implement the periodically-neighboring molecule detections requires a major rewrite of the entire tool and has not yet been implemented.

Once these closest neighboring oxygen atoms have been discovered, the appropriate interacting tetrahedral position is identified by finding the closest of the four tetrahedral positions using the same squared-distance calculation with the four defined tetrahedral positions detailed in the next subsection.

2.2.6 Defining Tetrahedral Positions

An important aspect of pseudorandom selection is the existence of a bank of options. Utilizing the ingestion portion of the tool to calculate and store all tetrahedral possibilities proves effective for tracking position options. For each water molecule, the first two tetrahedral positions are known by the positions of the two hydrogen atoms. The other two positions are found by rotating one hydrogen atom 120° twice about the vector from the oxygen atom through the other hydrogen atom and storing

the resulting positions as tetrahedral positions three and four.

This does not produce an exactly correct tetrahedral position of potential hydrogen atoms due to the slight acuteness of the H-O-H bond created by the variance in repulsive forces between the two lone pairs of electrons and two hydrogen atoms. Fortunately, this difference is sufficiently small for visualization programs like Avogadro to still recognize hydrogen bonds between a rotated hydrogen atom and corresponding neighboring lone pair. Currently, the method does not correct for these minor angle variations and relies on the user to anneal the crystal by way of simulation to fully adjust the angles. Future versions of this method may account for the variations.

2.2.7 Pseudorandom Rearrangement of Water Molecules

Once the tetrahedral positions have been defined, each water molecule is ready to rotate. What may seem the most crucial step in this methods ends up being the most simple. As designed, the rotation of water molecules is as simple as using a stepwise iterator to pseudorandomly select two tetrahedral positions for the hydrogen bonds and store the new positions in a new crystal array. These new positions are determined sequentially and immediately, so to speak, in the time-independent manipulation of the crystal. An extremely important note is that this rearrangement does not consider the orientations of neighboring molecules and likely introduces defects of hydrogen - hydrogen and lone pair - lone pair interactions. The likelihood of a defect-free interaction lattice forming is nearly zero and is assumed to have a great deal of defects within the lattice.

2.2.8 Detecting Hydrogen Bond Defects

After all water molecules have been rearranged, defects between incorrectly-interacting hydrogen bonds must be found and corrected. Discovering the defects relies on the detection of neighboring molecules and the appropriate interacting hydrogen atom or

electron lone pair. As previously discussed, the initial data ingest records and detects the nearest water molecules and determines the tetrahedral position containing the interacting space, be it electron lone pair or hydrogen atom. From that data, the detection of a valid hydrogen bond is as simple as checking both all interacting tetrahedral positions and confirming that they both do not contain or lack a hydrogen atom. Additionally, each water molecule keeps a count of how many defects are present among the four positions. This allows for contextual changes during the correction step.

2.2.9 Correcting Hydrogen Bond Defects

Once the hydrogen bond defects have been discovered and marked, each needs to be corrected. The most direct approach to this is to sequentially walk through each defect and repeat the pseudorandom rotation until the number of defective regions is zero or a user-specified value. The current implementation sorts the defect list by the number of defects and attempts to fix the most defective molecules first because of the highest-density entropy introduced into the system. These most defective molecules may include defects impossible to solve by simple rotation, specifically when neighboring molecules have collectively directed three or four hydrogen atoms or electron lone pairs at the target water. These can only be solved by adjusting one or more of the neighboring molecules until the number of hydrogen atoms and electron lone pairs have balanced. Unfortunately, this high-defect problem can quickly escalate if the neighboring molecules contain the same problem of unbalanced hydrogen atoms and electron lone pairs. The current solution is to recursively check for and fix these impossible interactions first, but has not yet yielded a defect-free crystal in testing.

The current design of the method allows for the user to specify a threshold of defects as an average per molecule. For example, a threshold of 2.5 will allow a maximum of 3 defects on any given molecule and will continue to correct defects until

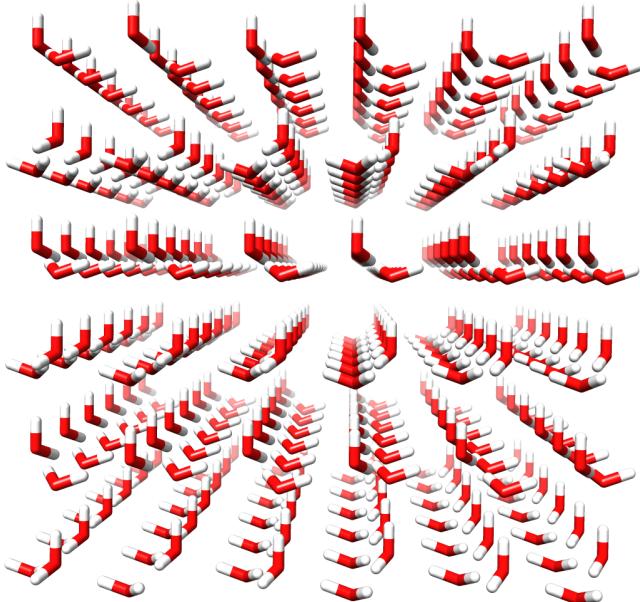


Figure 2.1: "Before" image of Ice XI

the average number of defects per molecule is equal to or below 2.5. Because each of these defects will be counted twice, once for each molecule, the total number of defects in a crystal can be determined by multiplying the average defect value by the number of molecules and dividing by two. As of the current implementation, the method cannot reliably produce a crystal with a threshold below 2 as it will continue to recursively search until the system runs out of available memory and crashes without finalizing the structure.

2.3 Results of Method

When supplied with an input ice XI crystal, an output structure with rotated water molecule orientations strictly consistent with ice I_h describes a success at the most basic level. An example before and after of the method is given in figures 2.1 and 2.2. As can be seen, the "after" image has experienced rotation and can no longer be classified as ice XI. However, as ice I_h also has a standard shape, the generated crystal can not be considered ice I_h . Instead, it can be considered a proton-disordered orthorhombic ice crystal similar to ice I_h .

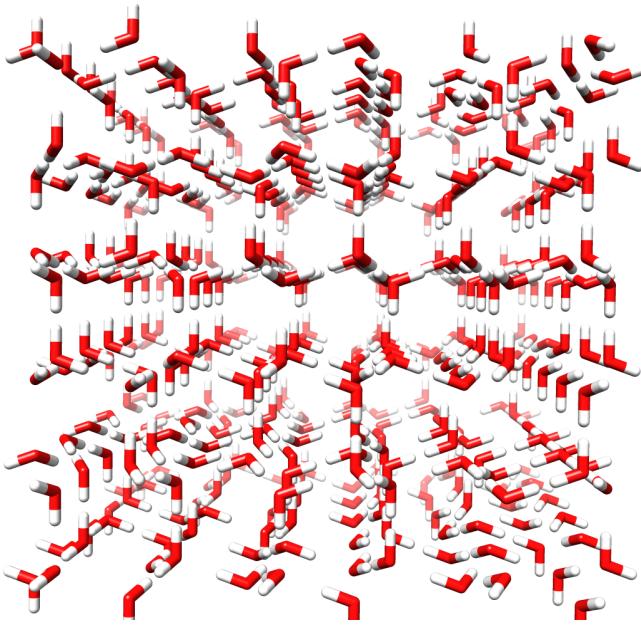


Figure 2.2: "After" image of generated ice I_h

Unfortunately, the result is not without defect. When following the subsequent layers in the crystal, patterns emerge. Inconsistently, some rows of waters remain consistent. Some of these are a uniform rotation of both hydrogen atoms, while others are just one consistently placed hydrogen atom. Multiple trials yield internally unique results, yet all contain these strange consistencies. This may be due to some accidental pattern in the method's implementation.

2.4 Comparison to Buch's Method

Currently in progress, this section will primarily compare the results of this method with²³.

2.4.1 benefits of own method over others

2.4.2 benefits of other methods over this

2.5 Comments on Limitations and Proposed Improvements

During the hydrogen bond defect correction step, a weakness in the design is that any clustering or regions of high defect density will not be treated uniquely. This allows the existence of a highly-defective region within the larger structure that could potentially cause problems when the crystal is used in simulations. The prevalence and occurrence of these defects have not been studied in this work, but seem a natural inevitability of statistics. A potential solution with partial development will score regions based on the number of defects as a weighted function expanding out from a central molecule for N connections. For example, consider a specific water defined as level 1. The neighboring four molecules are defined as level 2, and continued onward excepting already-defined molecules out to an N^{th} level. The number of defects in each level can be counted and averaged. Then a depressive factor along the lines of $\frac{1}{level}$ can be used to diminish the value of defects further away from the first-level molecule. This would create a value for each molecule that shows the relative density of defects centered about that specific molecule and could even be plotted as a gradient change within the crystal. The general approach to a scoring mechanism may take a form similar to equation 2.1.

$$Value = \sum_{l=1}^{N_{levels}} \left[\frac{1}{l} * \frac{1}{N_{molecules}} * \sum_{m=1}^{N_{molecules}} [N_{defects,m}] \right] \quad (2.1)$$

CHAPTER 3

Germanium Compounds and QM Concerns

3.1 Modeling Germanium Compounds

While primarily used in optical applications including fiber optic cables and solar cell systems, germanium-based compounds are also used as polymerization catalysts. Relative to many other elements on the periodic table, computational reports on germanium are not common. Recent works have shown germanium's potential to polarize light.

3.1.1 Computational Complexity of Germanium Compounds

Publications on germanium computational efforts are not as common as many other main group elements. Of those extant publications, the majority of final published data involve a Density Functional Theory (DFT) with either the 6-31G(d), 6-31G(d,p), or 6-311G(2d) basis set.²⁴ As with most other lighter elements calculated with Pople basis sets, the 6-31G(d,p) basis set is most commonly used for the final energy calculation.^{25;26}

3.2 The Initial Problem: Germanium Study

During Fall 2017, Dr. Christopher Fennell was approached by Dr. Charles Weinert of OSU to continue a collaborative effort in sampling conformation energies of two germanium-based compounds of interest to Dr. Weinert's work. Seen as an opportunity to train a new graduate student in conformational calculations, this project was delegated to me. The initial focus was to create the two compounds in a 3D

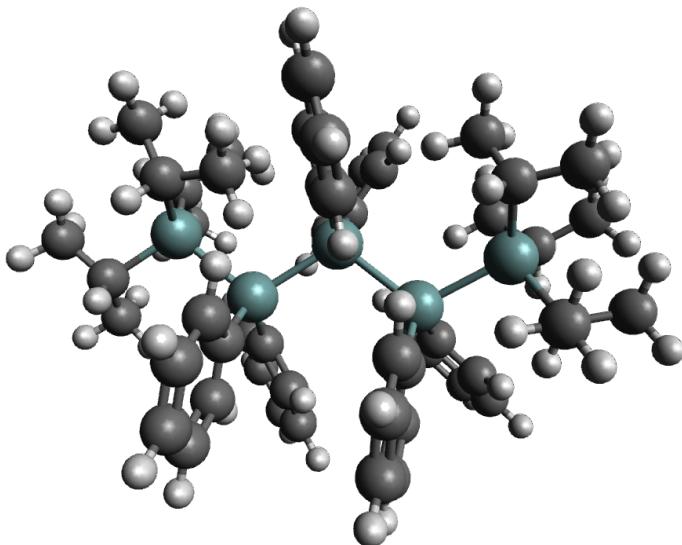


Figure 3.1: Fully trans configuration of pentagermanium-based compound.

modeling program, save a file of each, run a conformation optimization program on a supercomputer, and read the output to report the findings. As detailed below, this work led to impossibilities, curiosities, and inconsistencies that resulted in a general solution and a discovery of a flaw in a popular computational program.

3.2.1 Parameters of Work and Previous Collaborator's Results

The two subject germanium-based compounds are very similar: a germanium backbone with terminal isopropyl groups and internal phenyl rings. One compound constituted a pentagermanium chain while the other a hexagermanium backbone. The molecular formula for both is $\text{Pr}_3^i\text{Ge}(\text{GePh}_2)_n\text{GePr}_3^i$ where n equals 3 for the pentagermanium or 4 for the hexagermanium compounds, respectively. An example image of both compounds in their fully-trans configurations are provided in figures 3.1 and 3.2.

Dr. Weinert had worked previously with a collaborator who provided conformation data supplied in table 3.1. While the basis set was not explicitly provided, it is likely that the most common 6-31G(d,p) basis set was used. Unfortunately, the collaborator is no longer active in research and was inaccessible for clarification.

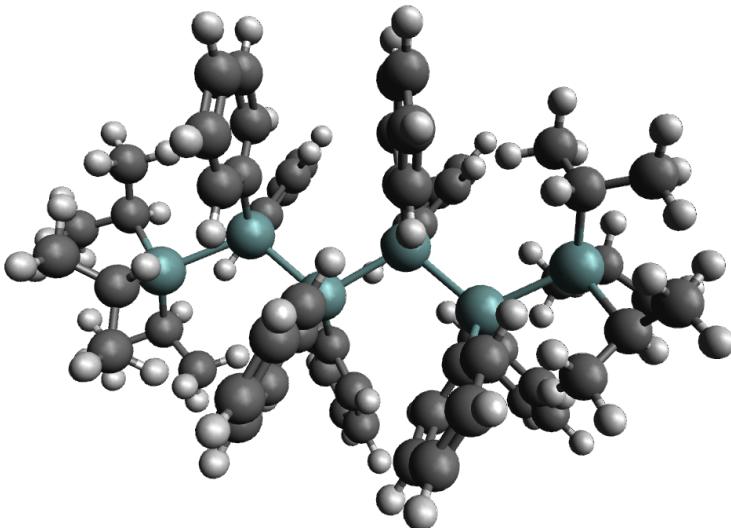


Figure 3.2: Fully trans configuration of hexagermanium-based compound.

Conformation	Energy (E_h)	Δ Energy (E_h)	Δ Energy ($\frac{kJ}{mol}$)
Trans-coplanar	-15014.8403143	0.0066255	17.39525025
Cis-Trans-Cis	-15014.7983311	0.0486087	127.6221418
Trans-Cis-Trans	-15014.8469398	0.0000000	0.0000000
Cis-Trans-Trans	-15014.8246918	0.0222480	58.412124

Table 3.1: Collaborator's Hexagermanium Energies by Conformation
(density functional theory, unknown basis set, energy in Hartrees and kJ/mol)

The approach of labeling the conformation shape of each compound, given the many points of torsion, focuses on the backbone structure. As the raw data from the collaborator was not available, the general dihedral angles of cis and trans proved a vexing focus for initial efforts at conformer design. Using Newman projections like in figure 3.3 as a visual guide, each Ge-Ge bond was defined as cis or trans based on the relative angle produced by the two adjacent bonded Ge atoms to each subject Ge. Specifically, the bonds are marked cis if the most acute angle is 90° or fewer, and likewise trans if greater than 90° up to the maximum 180° . Effectively the cis and trans angles coincide with gauche and anti-periplanar in organic structure nomenclature. These cis and trans terms are preferred over gauche and anti as the dihedral angles are not necessarily restricted to eclipsed or staggered angles. Terminal germanium atoms are not considered as a part of the conformation state. This is partly due to the definition in labeling where the terminal germanium does not have an adjacent germanium for the measured relative angle, in addition to the assumed C_3 symmetry of the terminal Ge with three isopropyl groups reducing the relative effects of terminal germanium rotation. Effectively, only dihedrals formed by four consecutive Ge are given a cis or trans label.

3.2.2 Design and Approach to Solution

The initial approach involved an attempt at basic replication of the collaborative results. As detailed below, the design gradually grew in complexity as a learning process. Eventually, curiosities in results and a desire to automate an objective search algorithm developed into two unique investigations.

3.2.2.1 Design 1: Occam's Smallest Razor

With each non-terminal Ge-Ge dihedral initially labeled cis or trans for 0° or 180° , about 3 unique pentagermanium and 6 unique hexagermanium structures were

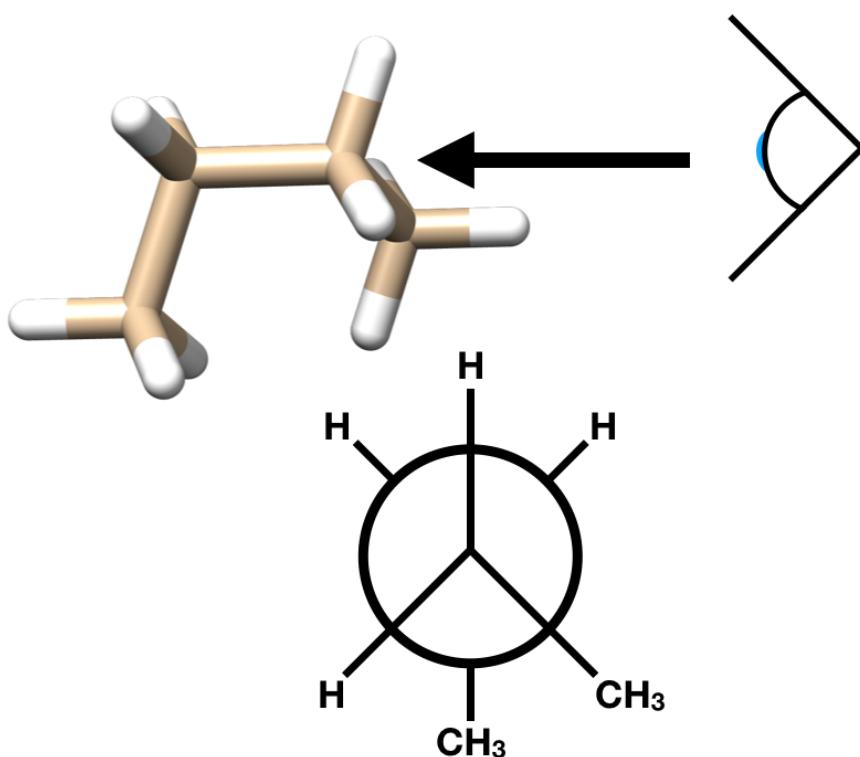


Figure 3.3: Sample Newman projection of cis-butane.

built visually on a 3D visualization program (Avogadro). These were rotated without consideration for the phenyl rings populating the non-terminal Ge atoms. Each molecule was subjected to an energy minimization in Gaussian 09 with the B3LYP hybrid function and STO-3G basis set as a single particle in a vacuum at otherwise default settings.

Unsurprisingly, only the fully trans conformers successfully converged (a 22% success rate) into a stable form. These troubles were likely caused by the poor design of the initial conformers. With initial results, the conformer design was altered into a more systematic approach with some consideration for the phenyl rings.

3.2.2.2 Design 2: A Blunt Effort

In the second iteration of the conformer design process, a greater number of backbone conformers were generated. Instead of the simple 180° opposition between the cis and trans conformers, more intentional initial angles seen in Newman projections

were selected. Specifically, the anti and both gauche angles were chosen for the natural local minima in a non-bulky molecule, with both gauche angles (60 and 300) labeled as cis and the anti angle (180) as trans. For initial conformer design, these backbone angles were limited to three positions: 60°, 180°, or 300°. For the hexagermanium compound, these structures were sequentially labeled trans-trans-trans, trans-trans-cis, trans-cis-trans, et cetera until all major unique conformers were produced. For clarity, each conformer was identified by the dihedral angles (60-60-60, 60-60-180) in increasing order (Ge 1-2-3-4, Ge 2-3-4-5, Ge 3-4-5-6 dihedral). The phenyl rings on the non-terminal Ge atoms were left untouched from an initial steepest-descent minimization available from Avogadro ran in the fully trans conformer.

To prevent potentially strong interactions between adjacent phenyl rings, an additional steepest-descent minimization from Avogadro was initially ran with the conformer-defining Ge-Ge dihedral angles locked in place. Additionally, a visual inspection of the phenyl rings and manual adjustments were utilized on Avogadro to reduce the chance of a relatively high energy local minima conformer. The phenyl rings usually were settled in a form of pi stacking or some kind of perpendicular ring interaction, based on relative energy stability according to the immediate simple minimization available.

To further avoid backbone rotation restrictions, variations of the bulky molecules were also produced. These included versions where the phenyl rings were replaced by methyl groups and also where the isopropyl ends were additionally replaced by methyl groups. Their intention in these designs were to observe the shift in relative energy between the sets of conformers to determine how significant of a role the phenyl rings and isopropyl groups played. These variations, along with the original form structures, were subject to the same calculations as in the first design: Gaussian 09, B3LYP hybrid functional, STO-3G basis set, no angle restrictions, single particle in a vacuum, otherwise default parameters. The results of these calculations are tabulated

in tables 3.2 and 3.3.

Immediately obvious in the table are the considerable number of nonconverged results. An unexpected bulkiness trend followed that a fully methylated variation of the structure was most likely to converge to a stable state, while the fully internal phenyl structures with methyl ends slightly reduced convergence and the original fully internal phenyl structures with isopropyl ends drastically reduced convergence. A deeper exploration into the change of stability is a promising avenue for future investigation, but was not further explored in this work. As can be seen in table 3.3, the lowest energy conformer for each structure varied greatly, but never included the fully trans conformer and only once the collaborator-reported trans-cis-trans conformer as the most stable. Still, given the considerable amount of nonconverged conformers, a new design was necessary to further improve the scope of the lowest energy conformation search.

3.2.2.3 Design 3: Death by 1.59 Million Cuts

In the final version of the conformer generation effort, additional creation efforts were focused on the individual phenyl rings. The unfavorable interactions between the phenyl rings were a considerable hurdle in the previous designs and a potential explanation for the large number of nonconverged structures, including the possibility that the terminal isopropyl hexagermanium structures contained particularly unfavorable interactions among the phenyl rings. This third design sought to remove the uncertainty in phenyl ring bulkiness by applying the same approach as the backbone generation: create unique conformers of every backbone torsion and phenyl ring, limiting each torsion to one of three rotational positions following the Newman projection style. Unfortunately, this task proved prohibitively large.

As an explanation for the insurmountability of the problem, consider the hexagermanium structure. The germanium dihedrals represent three rotatable bonds each

Internal Species	Terminal Species	Conformer	Final Energy (Hartrees)	Δ Energy (Hartrees)	Δ Energy (kJ/mol)
methyl	methyl	60-60	-10738.91336	0.0000454	0.119
methyl	methyl	60-180	-10738.9134	0	0
methyl	methyl	60-300	-10738.91286	0.0005358	1.407
methyl	methyl	180-60	-10738.91325	0.0001533	0.402
methyl	methyl	180-180	-10738.91335	0.0000475	0.125
methyl	methyl	180-300	-10738.91336	0.0000451	0.118
methyl	methyl	300-60	-10738.91336	0.0000455	0.119
methyl	methyl	300-180	-10738.91287	0.0005357	1.406
methyl	methyl	300-300	-10738.9107	0.002703	7.097
phenyl	methyl	60-60	-11875.15183	0.0001451	0.381
phenyl	methyl	60-180	-11875.15144	0.0005304	1.393
phenyl	methyl	60-300	-11875.15197	0	0
phenyl	methyl	180-60	-11875.14282	0.0091505	24.025
phenyl	methyl	180-180	-11875.15004	0.0019354	5.081
phenyl	methyl	180-300	-11875.15064	0.0013353	3.506
phenyl	methyl	300-60	-11875.06665	0.0853257	224.023
phenyl	methyl	300-180	DNC	DNC	DNC
phenyl	methyl	300-300	-11875.1497	0.0022723	5.966
phenyl	isopropyl	60-60	DNC	DNC	DNC
phenyl	isopropyl	60-180	-12341.23176	0.0053028	13.923
phenyl	isopropyl	60-300	DNC	DNC	DNC
phenyl	isopropyl	180-60	DNC	DNC	DNC
phenyl	isopropyl	180-180	-12341.23513	0.001935	5.08
phenyl	isopropyl	180-300	DNC	DNC	DNC
phenyl	isopropyl	300-60	DNC	DNC	DNC
phenyl	isopropyl	300-180	-12341.23706	0	0
phenyl	isopropyl	300-300	DNC	DNC	DNC

Table 3.2: Data of B3LYP/STO-3G minimization of variations of pentagermane compound at various conformers. DNC denotes a failure to converge with the self-consistent field method.

Internal Species	Terminal Species	Conformer	Final Energy (Hartrees)	Δ Energy (Hartrees)	Δ Energy (kJ/mol)
methyl	methyl	60-60-60	-12870.91834	0.0009503	2.495
methyl	methyl	60-180-60	-12870.91929	0.0000004	0.001
methyl	methyl	60-180-180	-12870.91813	0.0011628	3.053
methyl	methyl	60-180-300	-12870.91869	0.0005972	1.568
methyl	methyl	60-300-300	DNC	DNC	DNC
methyl	methyl	180-60-60	-12870.91897	0.0003189	0.837
methyl	methyl	180-180-60	-12870.91833	0.0009585	2.517
methyl	methyl	180-180-180	-12870.91929	0.0000004	0.001
methyl	methyl	180-180-300	-12870.91929	0.0000003	0.001
methyl	methyl	180-300-60	-12870.91897	0.0003192	0.838
methyl	methyl	300-60-180	DNC	DNC	DNC
methyl	methyl	300-180-60	-12870.91929	0	0
methyl	methyl	300-180-180	DNC	DNC	DNC
methyl	methyl	300-180-300	-12870.91814	0.0011527	3.026
phenyl	methyl	60-60-60	DNC	DNC	DNC
phenyl	methyl	60-60-180	-14385.89674	0.0052183	13.701
phenyl	methyl	60-60-300	-14385.89487	0.0070829	18.596
phenyl	methyl	60-180-60	DNC	DNC	DNC
phenyl	methyl	180-60-60	DNC	DNC	DNC
phenyl	methyl	180-60-180	-14385.90195	0	0
phenyl	methyl	180-60-300	-14385.89855	0.0033998	8.926
phenyl	methyl	180-180-180	-14385.83838	0.0635763	166.92
phenyl	methyl	180-300-180	-14385.79233	0.1096251	287.821
phenyl	methyl	300-60-60	DNC	DNC	DNC
phenyl	methyl	300-60-180	-14385.89836	0.003597	9.444
phenyl	methyl	300-60-300	-14385.89836	0.0035979	9.446
phenyl	methyl	300-180-60	DNC	DNC	DNC
phenyl	methyl	300-300-300	DNC	DNC	DNC
phenyl	isopropyl	60-180-180	-14851.9865	0	0
phenyl	isopropyl	60-300-60	DNC	DNC	DNC
phenyl	isopropyl	60-300-180	DNC	DNC	DNC
phenyl	isopropyl	180-300-60	DNC	DNC	DNC
phenyl	isopropyl	180-300-180	DNC	DNC	DNC
phenyl	isopropyl	180-300-300	DNC	DNC	DNC
phenyl	isopropyl	300-300-60	DNC	DNC	DNC
phenyl	isopropyl	300-300-180	DNC	DNC	DNC
phenyl	isopropyl	300-300-300	DNC	DNC	DNC

Table 3.3: Data of B3LYP/STO-3G minimization of variations of hexagermane compound at various conformers. DNC denotes a failure to converge with the self-consistent field method.

with three initial positions. To include the phenyl rings would require the inclusion of eight new rotatable bonds each with three initial positions. Additionally, considering each terminal germanium's rotation while ignoring each isopropyl's rotatable bonds adds two initial positions each with three initial positions. Together, this creates a structure with 13 rotatable bonds each with three initial positions. The number of conformers follows as $3^{13} = 1,594,323$ initial conformers. Now we must consider the computational aspect of this many conformers. At 10 conformers rotated and generated per second and 16 KB per conformer, the initial conformers would require 44.3 hours and generate 25.49 GB of data just in the initial structures. At an average of 72 minutes per computation and 73.7 MB produced at B3LYP hybrid functional and STO-3G basis set and access to all 255 regular nodes of Oklahoma State University's Cowboy cluster running in parallel, the complete computation would generate 117.5 TB of data and require 312 days of continuous computation to determine a possible lowest energy conformer of this one molecule at a relatively low level basis set and theory. A request to utilize 100% of university supercomputer resources for nearly a year for the sake of determining the lowest energy conformer of one molecule would likely be rejected, so this task would likely require a time scale of years or even decades to produce with shared access to university resources. While conventionally considered a small molecule, the scale of conformers and computational requirements pushes this problem into the realm of Levinthal's paradox.

While this third design would have likely revealed the lowest energy conformer, or at least one considerably close the the exactly lowest energy conformer, the effort ultimate fails under its own weight. Even with efforts to truncate duplicate forms, the problem of scale remains. A reduction by 50% still requires a computation effort in the timescale of years or decades for the calculation of a single molecule. For an effective computational outlook, this system needs to be reduced by several orders of magnitude.

3.2.3 Scale Reduction Efforts

For a system with conformers on the millions scale and computations on the hour scale, a magnitude reduction in either aspect would improve the practicality of this design approach. For example, by simplifying the computational method from 72 minutes on average to 5 minutes on average, the overall computational requirement would be reduced by 92%, a full order of magnitude. Unfortunately, reducing the complexity of the method sacrifices the reliability of data. A potential solution here would be to create rounds of calculations at different complexities, where each sequential round restricts the pool of potential conformers. Ideally, the balance of the increasing computational complexity and the decreasing pool size would maintain a consistent computational requirement. For example, a new round using a higher functional theory and basis set at 5x computational requirement would ideally be paired with a reduction in conformer pool size by a factor of 5. This would produce a series of calculation sets with additive computational requirement instead of a magnitudinal expansion.

The natural next question lies within the reliability of basis sets and functional theories. It naturally follows that a less-accurate method should not be relied on while better methods exist. However, considering the scale of the conformer pool, it follows that a less accurate method would still produce energy values with a roughly similar internal consistency. For example, a 180-0-180 form of the hexagermanium compound with parallel phenyl rings as modeled in figure 3.4 will have intense syn interactions between some phenyl rings and will likely not yield a desirable energy value at any level of calculation while a fully trans form with perfect pi stacking phenyl rings will likely have a lower energy value at all levels of calculation. It follows that, at lower levels of accuracy, the extremely high energy conformers can be pruned from the pool early and drastically reduce overall computational requirements. A generic effort at producing a method in this style is detailed in chapter 4, while the remainder of this

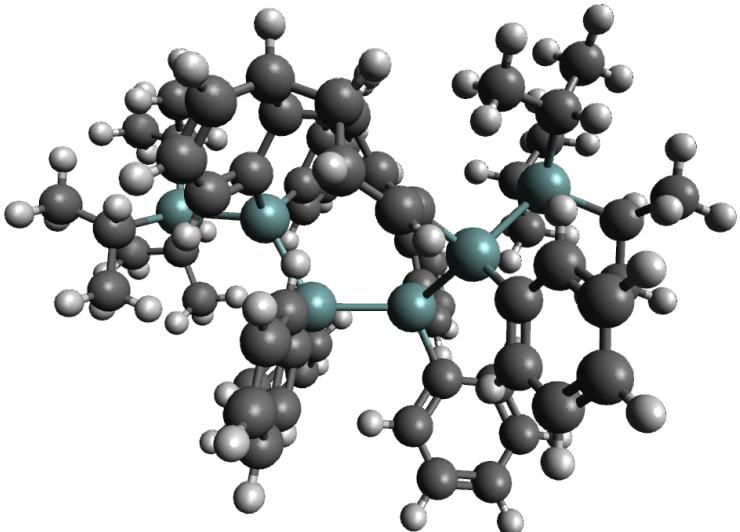


Figure 3.4: Visualization of a trans-cis-trans hexagermane structure.

chapter details additional efforts of calculating these germanium compounds.

3.2.4 Efforts at Simplification

One potential avenue of simplifying the process is computing the energy minimizations of lower-period atoms (e.g. a carbon backbone instead of germanium) and then applying a correction factor for a net reduction in computation time. As a period 4 element, germanium exhibits computational qualities similar to but more complicated than both carbon and silicon. Using tested samples, an energy minimization of a carbon-backbone molecule instead of the germanium represented a 92% increase in computation speed. Assuming a nominal correction factor exists and can be applied, this represents an order of magnitude reduction in computation time with one simplification. Potentially, this would allow investigators to much more quickly eliminate high energy conformers and more rapidly reduce the scope of the search.

The approach to acquiring sufficient data for a possible correction factor involved running an extremely simplified form of the germanium compounds, specifically a butagermanium backbone with hydrogens occupying all terminal and internal bonds. This reduced the complication and complexity of bulkiness and allowed for quick full

torsion rotations about the single Ge-Ge-Ge-Ge dihedral. By operating at intervals of 5°, a full torsion drive provides a glimpse at relative energies of the molecule at 72 discrete states.

The extended round of torsion drive calculations included an alteration in representation of the data. As the focus had shifted from relative energies and intensities across multiple theories and basis sets to a focus on graph smoothness and internal relative energies, the energy axis of plots were reduced to a unitless scale ranging 0 to 1, where 0 represents the minimum energy and 1 represents the maximum energy in a given set of torsion drive data. This allowed for graphical representations of each torsion drive to emphasize the internal variation of torsions relative to the minimum and maximum values. This was accomplished by taking any set of data with absolute scale energy unit, identifying the minimum and maximum values, and scaling each data point according to equation 3.1. The script to collect and scale data points is detailed in Appendix B.

$$E_{i,red} = \frac{E_{i,abs} - E_{min,abs}}{E_{max,abs} - E_{min,abs}} \quad (3.1)$$

An example plot of this torsion drive is shown in figure 3.5 Once multiple torsion drives had completed in multiple group four elements (butane, butasilane, and butagermane were all built and tested), the energies could be compared and analyzed for any relative or absolute scaling at the additive or multiplicative reference.

For a full comparative set, 3456 points of analyzed data were generated for each reference molecule's free energy in comparison with the others. Unsurprisingly, no simple correction factor arose by method of a simple additive or multiplicative term applied toward all torsion points. To expand on the comparative set, a set of butyl-group IV conformers were generated with every possible permutation of C, Si, and Ge, each then rotated about the torsion in 5° increments to produce a total 5832 conformers. These were then subject to the same data comparison method as before,

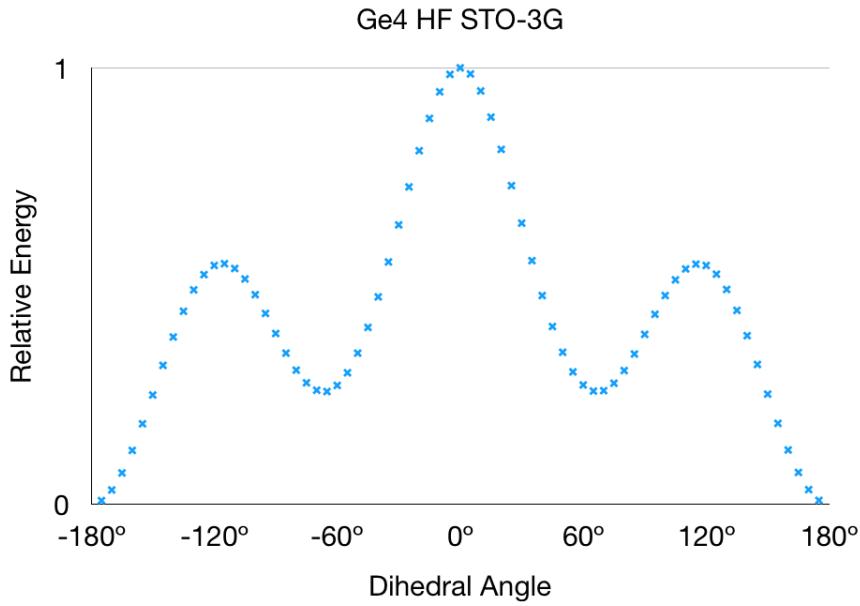
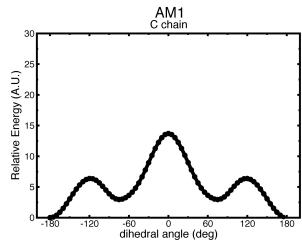
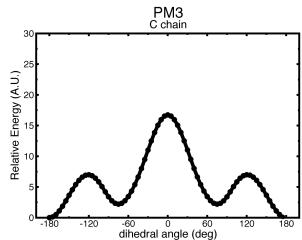
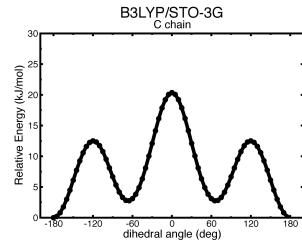
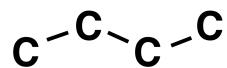
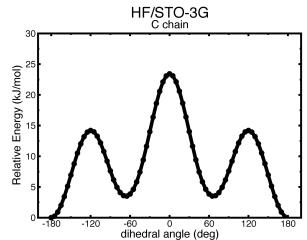


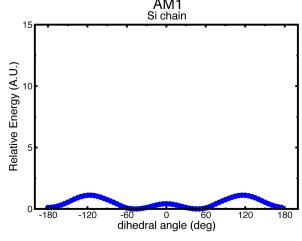
Figure 3.5: Sample torsion plot at reduced energy scale.

again to no noticeable trend. A future avenue of research could be to further explore this with depressive or polynomial terms to discover whether a simple corrective function might exist with specific molecules.

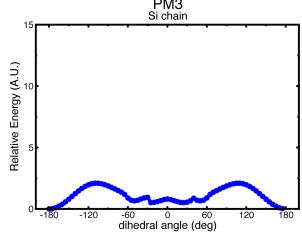
While this approach likewise did not find any simple correction factor, a graphical representation of multiple functionals across the butyl C, Si, and Ge show an interesting trend, as visualized by a graph provided by Dr. Christopher Fennell and shown in figure 3.6. A common theme of these graphs is that the relative energies follow the expected energetic barrier of a Newman projection, with local maxima at the 120° and 240° (or -120°) angles and local minima at the 60° and 300° (or -60°). The global maximum and minimum were consistently at 0° and 180° angles, respectively. As expected by different types of calculations, the torsion graphs hold different internal relative energies. For carbon, all four functionals produced a clean curve. The AM1 and PM3 functionals produced unexpected results for both Si and Ge graphs. In each, the expected highest energy 0° torsion angle was instead the most favorable of the three eclipsed angles. Additionally, the Si PM3 and the Ge AM1 and PM3 functionals showed strong spikes along the expectedly smooth curve, with the Ge PM3

AM1**PM3****B3LYP/STO-3G****HF/STO-3G**

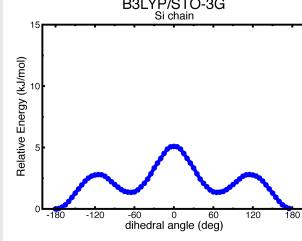
AM1



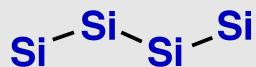
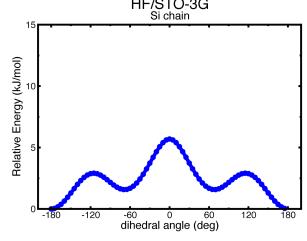
PM3



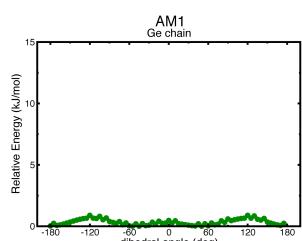
B3LYP/STO-3G



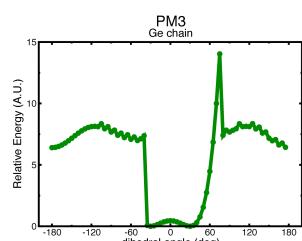
HF/STO-3G



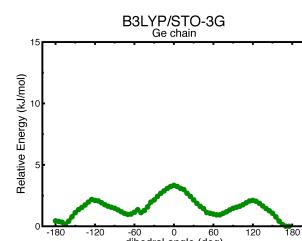
AM1



PM3



B3LYP/STO-3G



HF/STO-3G

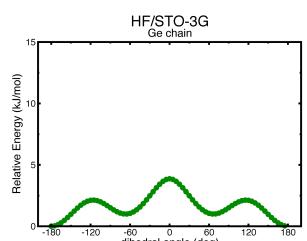


Figure 3.6: Visualization of a multiple pure group IV torsions at various theories and basis sets

being noticeably broken.

While the Si graphs smoothed out for the B3LYP and HF functionals at STO-3G basis set, the Ge B3LYP showed significant spikes and only the HF STO-3G exhibited a smooth curve. Effectively, this discovery of spikes along torsion drives led to the realization that the validity of a basis set could possibly be determined by the smoothness of a torsion drive. For example, any calculation of a germanium-containing molecule will likely not produce reliable results with a B3LYP hybrid functional and STO-3G basis set, while the Hartree Fock STO-3G calculation would at least be tentatively reliable for comparative energy levels at various conformations.

3.3 Discovery of a Consistent Inconsistency

The next natural step was to calculate and plot additional functional theories and basis sets with the butagermanium chain. While effectively a lightly guided meandering through the available calculation types, the first effort was to observe relative differences across multiple basis sets of the Hartree Fock theory and to examine the relative computational requirements of each. This plan was quickly redirected, however, when a curiosity within the data was revealed.

While running additional torsion drives of butagermane at differing basis sets and functional theories, an inverted energy was discovered. As can be seen in figure 3.7, the B3LYP theory with 6-31G(d) basis set appears flipped upon a cursory glance. After a more careful observation, the minima and maxima are at the "wrong" angles and cannot be a simple flip of the minima and maxima. Instead, the data is simply junk.

Naturally, the focus shifted toward discovering the source of the bad data. A repeat of the trial yielded the same data. A repeat of the system with a freshly created butagermane yielded the same data. A trial with data from a butagermane trial with the 6-31G(d,p) basis set yielded the same data. Each attempt at a 6-31G(d)

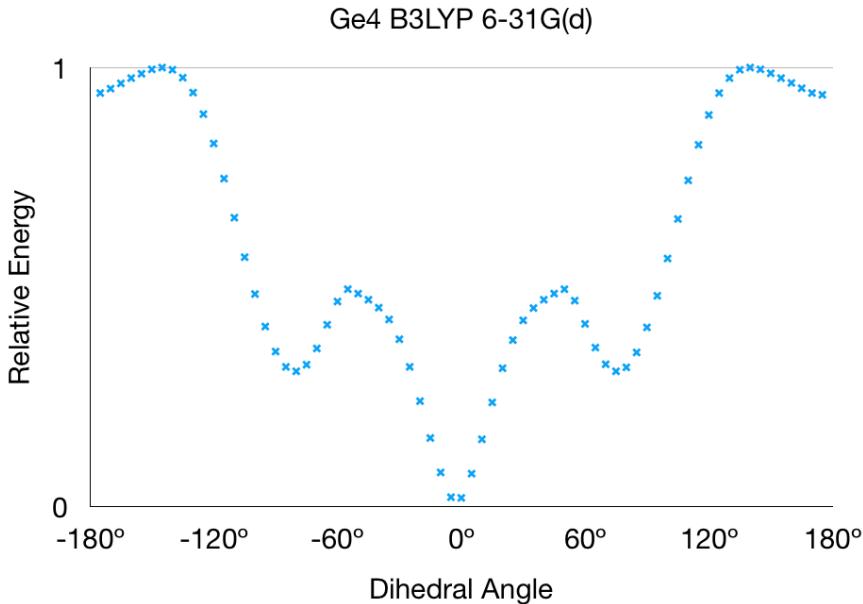


Figure 3.7: A curious seemingly-inverted torsion plot of butagermane.

basis set with the B3LYP theory yielded junk data, while other basis sets within the theory produced expected data. Next, the butagermane torsions were run with an identical basis set group with the Hartree-Fock theory, the results of which are shown in table 3.8.

Surprisingly, the 6-31G(d) result was also strangely inverted. This process was repeated for several more theories, with the 6-31G(d) basis set results plotted in figure 3.9. Curious to see if the germanium atom's basis set data or if the entire basis set method was the source, a similar run with butasilane was made and graphed in figure 3.10, to expected results. A quick run confirmed the problem to also exist on Gaussian 03 as well as Gaussian 09. The final effort was to check whether this error was isolated to Gaussian 09 or to all QM programs. A simplified test to calculate the energy of the expected global minimum (180°) and maximum (0°) of a Hartree Fock theory with the suspect 6-31G(d) basis set was prepared and executed, with the results tabulated in 3.4. As can be seen, critical energetic difference was negative for Gaussian 09 and positive for both GAMESS and NWChem. Since the expected conformations should yield a positive difference, it was concluded that both Gaussian

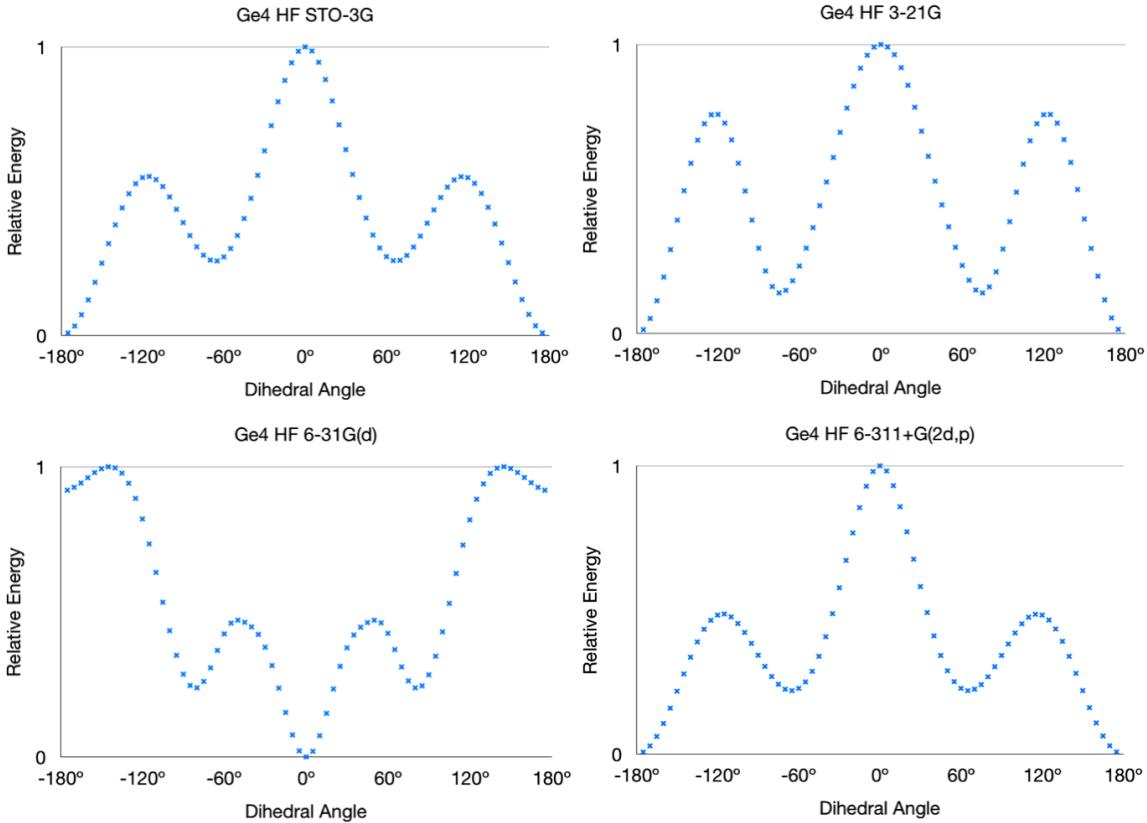


Figure 3.8: Hartree Fock energy minimization of butagermane torsion run at varying basis sets.

03 and 09 contain bad 6-31G(d) basis set data for germanium.

3.4 Final Thoughts

Unfortunately, a trend for simplifying the computation requirements of germanium was not discovered. While it may exist among the data as a more involved function or as some other representation, there also may very well be no simple trend for

Program	Trans Energy (Hartree)	Cis Energy (Hartree)	Δ Energy trans - cis (Hartree)	Δ Energy trans - cis (kJ / mol)
Gaussian	-8298.8259	-8298.8268	-0.0009	-2.4163
GAMESS	-8306.1290	-8306.1250	0.0040	10.4495
NWChem	-8306.1290	-8306.1250	0.0040	10.4495

Table 3.4: Energy comparison of HF theory with 6-31G(d) basis set across multiple computational programs. The expected ΔE should be positive.

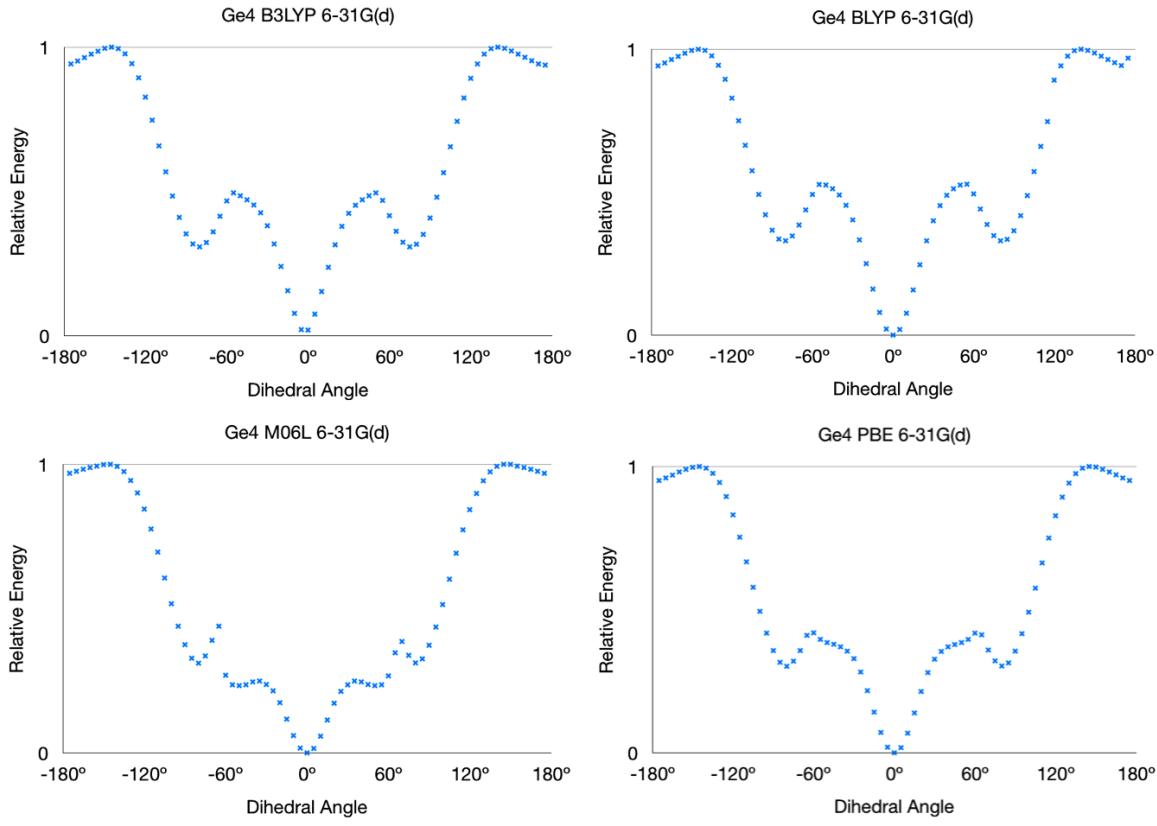


Figure 3.9: Minimization of butagermane torsion run at varying theories and the 6-31G(d) basis set.

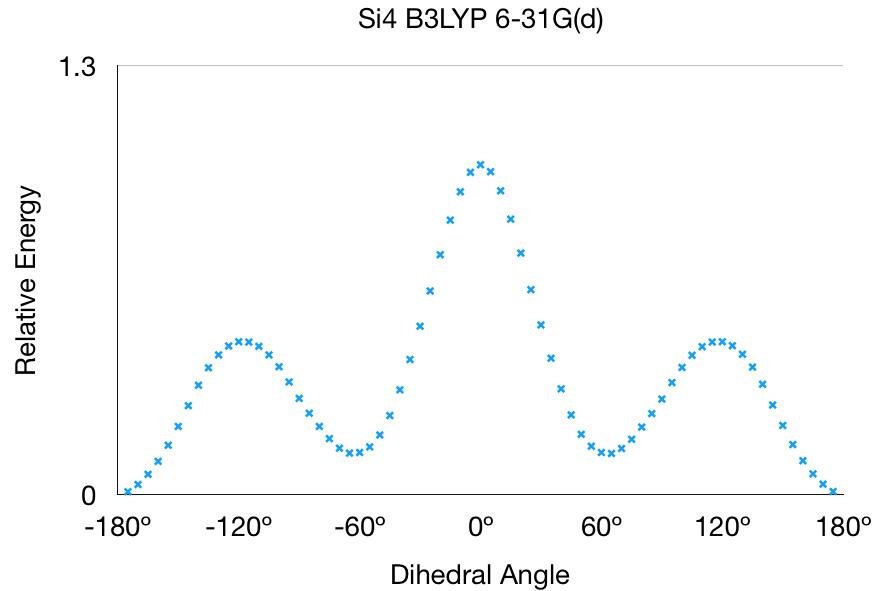


Figure 3.10: B3LYP energy minimization of butasilane torsion run at 6-31G(d) basis set.

switching between germanium and another group IV element.

On a much more interesting note, the results of the torsion drives revealed that Gaussian 03 and 09 contain some mistake within the 6-31G(d) basis set data for germanium. Considering the popularity of Gaussian software in computational chemistry, there are concerning implications about reliability of data for any germanium energy data with the 6-31G(d) basis set. Given that the torsion tests produced expected data for 6-31G(d) data subsequently run through a higher or lower basis set, only reported data with 6-31G(d) as the final calculated energy need be considered. It is recommended that any investigator into computational aspects of germanium either replace the basis set data, use another basis set, or instead use a program like GAMESS or NWChem for that final computation.

CHAPTER 4

Sampling Conformation Landscapes by Rotatable Bond Degrees of Freedom

4.1 A Brief History on Conformation Landscapes

4.1.1 Levinthal's Paradox

In 1969, a molecular biologist by the name of Cyrus Levinthal proposed a thought experiment regarding protein formation²⁷:

Consider a relatively small 150-residue peptide chain completely unfolded. This protein will have 149 peptide bonds and therefore 149 rotatable bonds, 149 phi angles, and 149 psi angles. Assuming three possible angle positions each, the number of possible folds of this protein follows as 3^{447} . How does this peptide chain fold into the appropriate secondary and tertiary structures? Even at attosecond rates of rotating and folding, this peptide chain would likely not fold into the correct structure for many times the age of the universe! Obviously, this is not the case, since proteins fold on the timescale of microseconds to milliseconds.²⁸ How, then, do proteins fold so quickly and efficiently? The answer lies in energy cascades through a visualization tool called a golf course.

4.1.2 Levinthal Golf Courses

If one imagines the energy landscape of a peptide chain like a golf course, interesting similarities arise. For example, the lowest point could be considered "the hole" of the course with the lowest energy conformer. When starting at the "tee off" point,

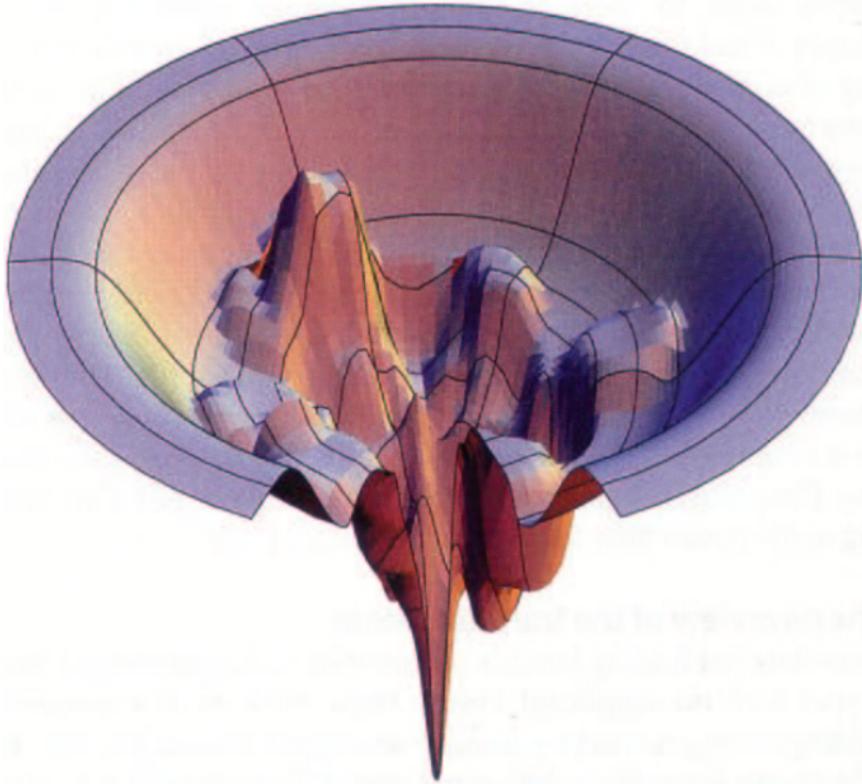


Figure 4.1: Example Levinthal Golf Course taken from reference 11997Dill and ChanDill, and Chan.

there may not be a clean pathway of energetic difference for the ball to throw. Therefore, the ball must be "struck" toward the hole in a series of motions where the ball is removed from one local minima and placed in another hopefully closer to the hole. Like the image shown in figure 4.1, the course is not always an easy, natural cascade toward the global minima. Most often, investigators will initiate several searches in several locations of this conformation landscape in hopes that one will discover a clear minima that is hopefully the true global minima.

4.2 Purpose of Project

As introduced in chapter 3, there may be a generic solution toward discovering the tetrahedral lowest energy conformer by roughly sampling the full "golf course" and procedurally focusing in on hot spots using automated methods. Ideally, the

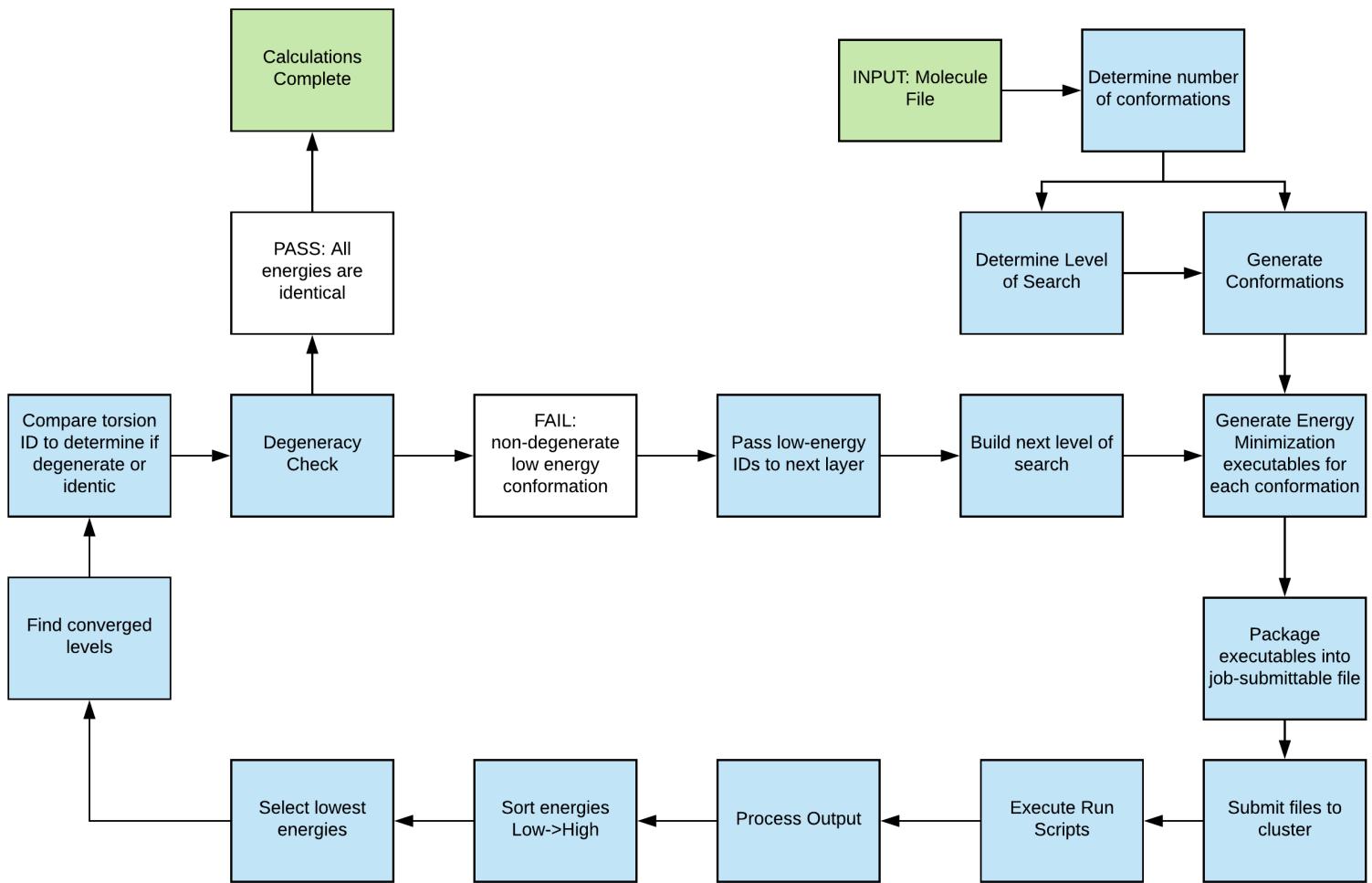


Figure 4.2: Flow of method design for variable resolution conformation landscape search.

tool would work through the seemingly infinite possibilities and quickly remove the impossible or duplicate conformers. The tool would roughly take shape though the following pattern. Run through a set of dihedral positions at a constant interval. Selection of lowest-energy optimization organized on dihedral values. Quick determination of importance of dihedral based on how heavily it impacts internal energy. Splitting "best" dihedral(s) into smaller interval to repeat the process.

An overview of system flow given in figure 4.2. This method produces an interesting multilayered visual plot with a zooming effect toward the lowest energy conformer. An example of how this might look for a two-dihedral molecule is given in figure 4.3.

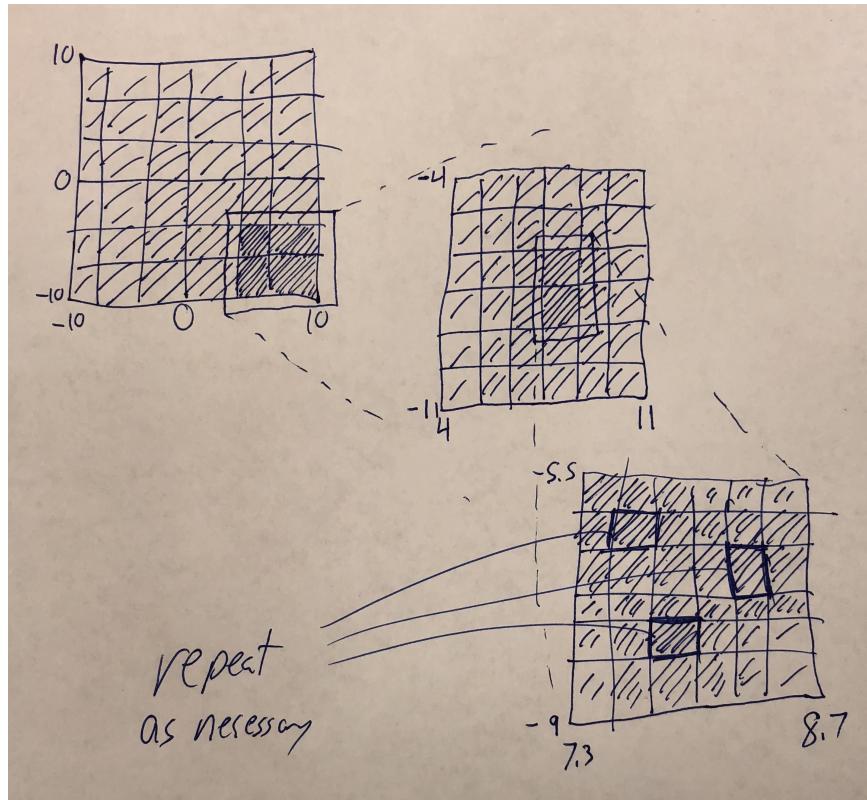


Figure 4.3: Example variable resolution chart (hand-drafted, CGI pending)

4.3 Design of System

This system designed in Python for ease of development and compiled via Cython for computational efficiency. While it currently utilizes Gaussian 09 for energy minimization and UCSF Chimera for conformer generation, it can be redesigned for any computational programs that accomplish the desired tasks.

4.3.1 Variation of Theory and Basis Set Usage by System Size and largest atom type

Given that computational requirements increase with the number of atoms in a molecule and both the accuracy of the theory and basis set used, an initial focus on a manageable amount of conformers with a sufficiently simple theory and basis set is essential to success. The system should estimate quantity and cost of calculations based on physical computational constraints for various theory-basis set pairings. Sys-

tem optimizes calculation types for the scope of the landscape. Effectively, it balances between running the first broad-scope search at relatively low accuracy and a final near-final conformation space with relatively high accuracy methods.

4.3.2 Computational Optimization by Varying Resolution

A common problem in all works on this topic is that the scale of truly searching the conformation landscape is expansive in even the most restrictive designs. The manual efforts in the design of this tool are to build checkers for impossible conformations, including overlapping atom spaces. Additional considerations are that only the most bare, three conformations per rotatable bond angle be considered initially. After the first round of calculations, the scope of candidates should be reduced by several orders of magnitude by refining the search about lower energy regions in the landscape.

4.3.3 Inherent Complications

The single greatest complication of this and any energy landscape tool is the number of rotatable bonds in the target molecule and, to a lesser extent, the elements contained. Consider the hexagermane molecule of interest in chapter 3 and the general focus of this work. One can focus on the number of torsions available to be adjusted in the energy landscape, as shown in figure 4.4. Even with the minimal three rotations per bond, these 19 rotatable bonds produce $3^{19} = 1,162,261,467$ conformers, which is realistically impossible to explore even with a computational method requiring five seconds to compute as 184 years of computation time would be required. This is where the balance between recognizing impossible conformations comes in. Especially with bulky molecules like this hexagermane, many conformations could be eliminated by way of checking for overlapping atoms.

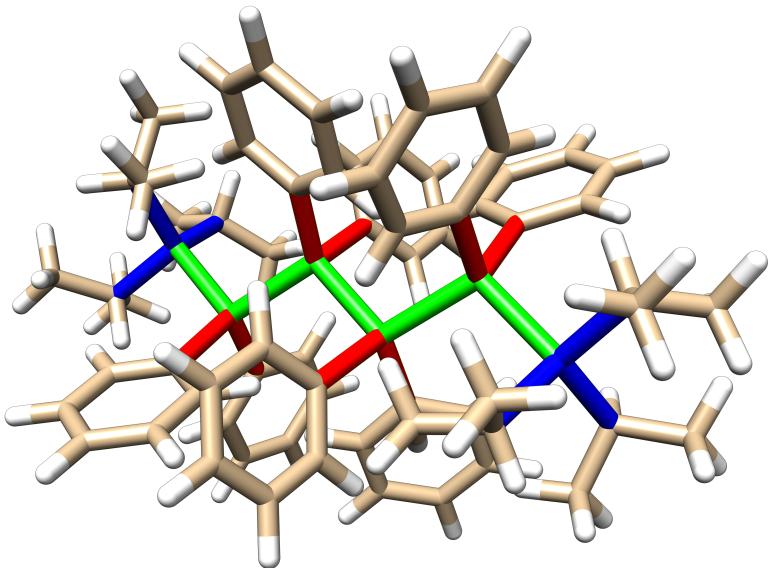


Figure 4.4: Highlighted torsions of the hexagermane molecule by type of bond, where green, red, and blue represent Ge-Ge, Ge-phenyl, and Ge-isopropyl torsion centers, respectively.

4.4 Results

Due to the scale of the hexagermane molecule, a clear answer has not yet been discovered. However, a much more simple run with o-nitrophenol, with only two rotatable bonds, was successful in finding the known lowest energy conformer shown in figures 4.5 and 4.6.

While these would have ideally been produced through a self-perpetuating system at increasing precisions and computation accuracy, the automated tool remains to be realized.

4.4.1 Difficulties and Anticipated Future Approaches

A key difficulty in automation of this tool is defining an abstract computation level based on arbitrary hardware limitations. While currently limited to the Cowboy cluster at Oklahoma State University, the goal is that this tool be made available for chemists everywhere one day. A potential solution for this abstract definition would be a small series of test runs to determine computational cost and general resource

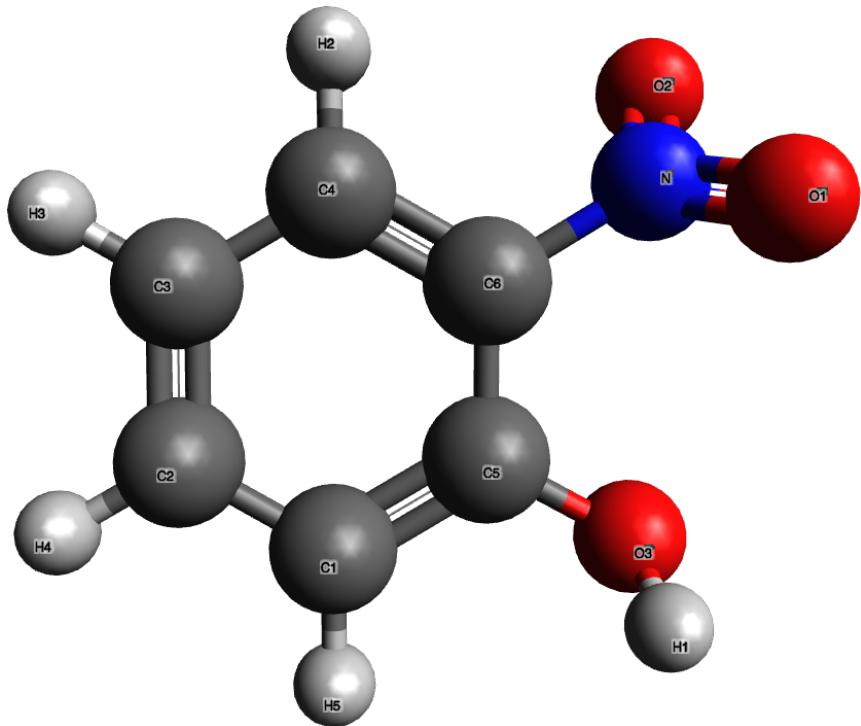


Figure 4.5: Highest energy conformer of o-nitrophenol, ignoring any ring strain conformations. Noticably was unable to rotate and form the hydrogen bond between ortho nitrogen and hydrogen.

availability.

Additionally, the number of rotatable bonds yields the single largest barrier to searching the full conformation space. With continued investigation and the inclusiveness with other works, it seems feasible that the insurmountable barrier to entry may yet be simplified in an objective way that does not perturb the system from finding the lowest energy conformer in any reasonably small molecule.

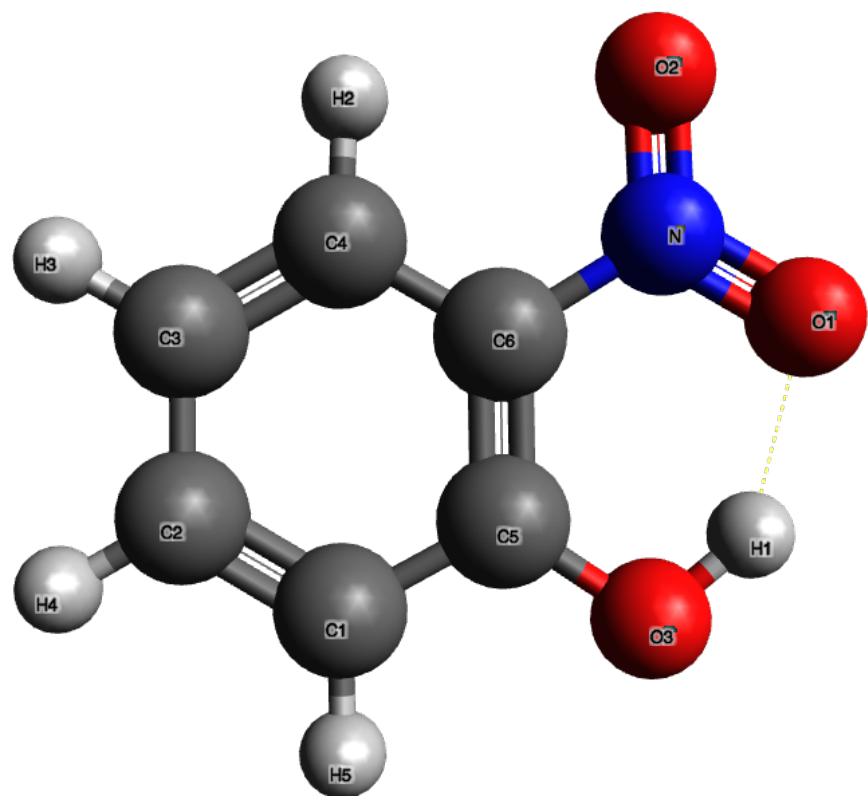


Figure 4.6: Lowest energy conformer of o-nitrophenol. Formed the expected hydrogen bond between the ortho nitrogen and hydrogen.

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APPENDIX A

Ice Ih to Ice XI Conversion

Listed below is the source code utilized in the conversion of a .pdb Ice Ice I_h structure into an Ice XI structure. This code is functional in a Python 2.7 environment with the included packages: NumPy version 1.14.3 and SciPy version 1.1.0.

A.1 Code: Crystal Disorganizer Tool

```
1  #!/usr/bin/python
2
3
4 # Author = Gentry Smith
5 # Copyright 2016, all rights reserved
6
7 # this reads in a .PDB file , takes an argument for deformities per
8 # molecules , and randomly organizes the crystal
9 # structure into a disordered proton formation
10
11 # import sample: python PDBDisorganize.py arg1 arg2 arg3
12 # where:
13 # arg1 = source pdb file to be read (ex: acetone.pdb or acetone)
14 # arg2 = number of defects per molecule (in H2O, num of non-hydrogen-
15 # bonds. from 0 to 4)
16 # arg3 = desired output pdb file name
17
18 import sys
19 print sys.path
20 import string
21 import numpy as np
22 import math
23 import random
24
25
26 pdbIN = file(sys.argv[1])      # source PDB file
27 maxErr = int(sys.argv[2])       # max errors allowed
28 pdbOUT = str(sys.argv[3])       # output file name
29 finalData = [ [ [ 0 for i in range(3) ] for j in range(3) ] for k in
30               range(300) ]
31
32 # looks at args validity
33 def checkArgs(arg1, arg2, arg3):
34     returnBool = False
```

```

34     if type(arg1) != file: # check arg1
35         print"Bad arg", arg1, " must be a file "
36         returnBool = True
37     if type(arg3) != str: # check arg3
38         print"Bad arg", arg3, ", must be a file name"
39         checkPDBSuffix(arg3)
40         print arg3
41         returnBool = True
42     if type(arg2) != int: # check arg2 type
43         print "Bad arg2: ", arg2, " is not an int."
44         returnBool = True
45     elif type(arg2) == int:
46         if arg2 < 0 or arg2 > 4: # check arg2 range
47             print "arg2 is not in a valid range 0 <= arg2 <= 4"
48             returnBool = True
49     return returnBool
50
51 def checkPDBSuffix(pdbFile):
52     if string.find(pdbFile, '.pdb', 0, len(pdbFile)) == -1:
53         print("did not find 'pdb' in ", pdbFile, ". Appending...")
54         pdbFile += '.pdb'
55
56
57
58 # reads in file ,
59 def readFile(fileName):
60     print "Reading file..."
61     # gets number of atoms
62     atoms = 0
63     for line in fileName:
64         data = line.split()
65         if len(data) > 0:
66             if data[0] != "CONECT" and data[0] != "END":
67                 atoms += 1
68     # print "atoms: ", atoms
69     numMol = atoms / 3 # assumes 3-atom water molecule
70     dataTable = [ [ [ 0 for i in range(3) ] for j in range(3) ] for k in
71     range(numMol) ]
72     fileName.seek(0)
73     iter0 = 0
74     iter1 = 0
75     pdbType = -1
76     for line in fileName:
77         data = line.split()
78         if pdbType == -1:
79             if data[0] == "ATOM":
80                 pdbType = 0
81             elif data[0] == "HETATM":
82                 pdbType = 1
83             # print "LineTuple= ", data
84             if len(data) > 1 and ( data[0] == "ATOM" or data[0] == "HETATM"
85             ):
86                 if data[0] == "ATOM":
87                     newData = getDataATOM( data )

```

```

86         for i in range(3):
87             #data[molecule][atom][X/Y/Z]
88             dataTable[iter0][iter1 % 3][i] = newData[i]
89     elif data[0] == "HETATM":
90         dataTable[iter0][iter1 % 3] = getDataHETATM(data)
91     if iter1 == 2:
92         iter0 += 1
93         iter1 = 0
94     elif iter1 != 2:
95         iter1 += 1
96 # print "DataTable: ", dataTable
97 print "File read"
98 return dataTable, pdbType
99
100
101 # Split by index
102 # if having a problem with reading data, check .pdb to see if data
103 # has a space between each value
104
105 # reads XYZ coordinate data from ATOM-type pdb
106 def getDataATOM(strLine):
107     # print "Getting ATOM Data..."
108     dataLine = strLine[5:8]
109     # print "dataline: ", dataLine
110     i = 0
111     while i < 3:
112         # print "dataline[", i, "]: ", dataLine[i]
113         dataLine[i] = float(dataLine[i])
114         # print "dataline[", i, "] type: ", type(dataLine[i])
115         i += 1
116     return dataLine
117
118 # reads XYZ coordinate data from HETATM-type pdb
119 def getDataHETATM(strLine):
120     # print "Getting HETATM Data..."
121     dataLine = strLine[5:8]
122     # print "dataline: ", dataLine
123     i = 0
124     while i < 3:
125         # print "dataline[", i, "]: ", dataLine[i]
126         dataLine[i] = float(dataLine[i])
127         # print "dataline[", i, "] type: ", type(dataLine[i])
128         i += 1
129     return dataLine
130
131
132 # gets all four position vectors of hydrogen/lone pair as offset of
133 # oxygen molecule
134 def getOrientations( molecule ):
135     # 120 degrees = ( 2 * pi ) / 3 radians
136     theta = ( ( 2 * math.pi ) / 3 )
137     newMol = zeroOrientation(molecule)
138     returnInt1 = rotateMolecule(newMol[1], newMol[2], theta)

```

```

138     returnInt2 = rotateMolecule(newMol[1], newMol[2], (-1 * theta) )
139     return [returnInt1, returnInt2]
140
141
142 # randomly selects new orientation, returns two unique ints, from 0 to 3
143 # inclusively
144 def newRandOrientation( positions ):
145     # print "Changing orientation"
146     randVal1 = random.randint(0,3)
147     randVal2 = random.randint(0,3)
148     while randVal1 == randVal2:
149         randVal2 = random.randint(0,3)
150     newMol = [ [ 0, 0, 0 ],
151                positions[ randVal1 ] ,
152                positions[ randVal2 ] ]
153     return newMol
154
155 # selects new orientation from list. Reduces computational overhead in
156 # re-orientation option traversal
157 def newSetOrientation( positions, pos1, pos2 ):
158     newMol = [ [ 0, 0, 0 ],
159                positions[ pos1 ],
160                positions[ pos2 ] ]
161     return newMol
162
163 # sets molecule coordinates so that oxygen is the origin
164 def zeroOrientation(source):
165     # print "Zeroing Molecule..."
166
167     oxy = source[0]
168     hyd1 = source[1]
169     hyd2 = source[2]
170
171     # print "Oxygen pos: ", oxy
172     # print "Hydrogen 1: ", hyd1
173     # print "Hydrogen 2: ", hyd2
174
175     zeroedOrigin = [0, 0, 0]
176     zeroedHyd1 = [0, 0, 0]
177     zeroedHyd2 = [0, 0, 0]
178     for i in range(3):
179         zeroedHyd1[i] = hyd1[i] - oxy[i]
180         zeroedHyd2[i] = hyd2[i] - oxy[i]
181
182     # print "Zeroed Hydrogen 1: ", zeroedHyd1
183     # print "Zeroed Hydrogen 2: ", zeroedHyd2
184
185     # return new molecule position
186     newMol = [zeroedOrigin, zeroedHyd1, zeroedHyd2]
187     return newMol
188
189 # resets the zeroed molecule to the original oxygen position
190 def resetOrientation(oxygenPos, molecule):

```

```

190 # print "Resetting molecule..."
191 rO = oxygenPos
192 rH1 =[0 ,0 ,0]
193 rH2 =[0 ,0 ,0]
194 newMol = []
195 for i in range(3):
196     rH1[i] = molecule[1][i] + rO[i]
197     rH2[i] = molecule[2][i] + rO[i]
198     newMol = [rO, rH1, rH2]
199 # print "Rebuilt Molecule: ", newMol
200 return newMol
201
202 # rotates vector about axis for theta degrees
203 # Handler for rotationMatrix function below
204 def rotateMolecule(vector, axis, theta):
205     rotMatx = rotationMatrix(axis, theta)
206     return np.dot(rotMatx, vector)
207
208
209 # Creates Rotation matrix for a given axis and theta
210 # from stackoverflow user unutbu
211 # page: http://stackoverflow.com/questions/6802577/python-rotation-of-3d
212 -vector
212 def rotationMatrix(axis, theta):
213     """
214
215     :type axis: list
216     :type theta: union
217     """
218     axis = np.asarray(axis)
219     theta = np.asarray(theta)
220     axis /= math.sqrt(np.dot(axis, axis))
221     a = math.cos(theta/2.0)
222     b, c, d = -axis*math.sin(theta/2.0)
223     aa, bb, cc, dd = (a * a), (b * b), (c * c), (d * d)
224     bc, ad, ac, ab, bd, cd = (b * c), (a * d), (a * c), (a * b), (b * d),
225     (c * d)
226     return np.array([
227         [(aa + bb - cc - dd), (2 * (bc + ad)), (2 *
228         (bd - ac))],
229         [(2 * (bc - ad)), (aa + cc - bb - dd), (2 *
230         (cd + ab))],
231         [(2 * (bd + ac)), (2 * (cd - ab)), (aa +
232         dd - bb - cc)]])
233
234
235 # gets results from rotateAboutAxis plus two Hydrogens to get the
236 # tetrahedron positions
237 def getTetrahedronPositions(molecule):
238     positions = [[0 for i in range(3)] for j in range(4)]
239     newMol = zeroOrientation(molecule) # zero molecule
240     positions[0] = newMol[1]
241     positions[1] = newMol[2]
242     newPos = getOrientations(molecule) # get final two positions
243     positions[2] = list(newPos[0])

```

```

238     positions[3] = list(newPos[1])
239     return positions # return all four positions
240
241
242 # checks distance of new positions from zero
243 def checkDist(posArray):
244     distance = [0 for i in range(len(posArray))]
245     for i in range(len(posArray)):
246         distance[i] = ( (posArray[i][0] * posArray[i][0]) +
247                         (posArray[i][1] * posArray[i][1]) +
248                         (posArray[i][2] * posArray[i][2]) )
249         # print "Distance", i, ":", distance[i]
250     avg = 0
251     for i in range(len(posArray)):
252         avg += distance[i]
253     averageDistance = ( avg / len(posArray) )
254     # print "Average Distance: ", averageDistance
255     return averageDistance
256
257
258 # prints data given a 3D table of water molecules
259 def printData(data):
260     print "Data: "
261     strData = [ "O" , "H1" , "H2" ]
262     dimData = [ "X" , "Y" , "Z" ]
263     bigAvg = 0
264     numAtoms = 0
265     for mol in range(len(data)):
266         for atom in range(len(data[mol])):
267             printStr = str(mol) + ":" + strData[atom] + ":" +
268             for dimension in range(3):
269                 printStr += dimData[atom] + ":" + "{:7.3f}".format(data[
270 mol][atom][dimension]) + "\t"
271             print printStr
272             bigAvg += checkDist(zeroOrientation(data[mol])[1:])
273             numAtoms += 1
274             print ""
275     print "total average distance: ", bigAvg / numAtoms
276
277
278 # checks validity of molecule
279 def isDefectiveCheck(err, neighborData, posData, index):
280     # find nearby molecules (avg oxygen distance??)
281     print "checking for defects at index", index, "... "
282     print "neighbor indices: ", neighborData[index]
283     returnBool = False
284     neighbors = 4
285     for i in range(4): # count real neighbors
286         if neighborData[index][1][i] == -1:
287             neighbors -= 1
288         if neighbors <= err: # de facto good if num(neighbors) <
maxErrAllowed
289             # print "Fewer neighbors than allowed errors. de facto Good
Orientation"

```



```

339     # re-rotate molecule through all positions (iterated through all
340     # orientations)
341     positions = getTetrahedronPositions(posData[index])
342     zeroedMol = newRandOrientation(positions)
343     # print "isGood CHECK", isGood
344     isGood, posData = iterThroughRotations(err, neighborData,
345     posData, index)
346     posData[index] = resetOrientation(posData[index][0], zeroedMol)
347     if timeCount >= 13: # { (1 - 1/6)^n < 0.05 } says n = 17
348         # BROKEN - need to rebuild
349         # 0. evaluated molecule has too many defects
350         # 1. reorient molecule statistically probable amount of
351         # times to cover all orientations
352         # 2. Repeat 1. with neighbor 1
353         # 2a repeat 1. with original molecule
354         # 3. Repeat 2. with neighbor 2, 3, 4, as/if necessary
355         for neighborIndex in range(4):
356             if neighborData[index][1][neighborIndex] != -1:
357                 positions = getTetrahedronPositions(posData[
358                 neighborIndex])
359                 zeroedMol = newRandOrientation(positions)
360                 posData[neighborIndex] = resetOrientation(posData[
361                 neighborIndex][0], zeroedMol)
362                 # isGood = isDefectiveCheck(err, neighborData,
363                 posData, neighborIndex)
364                 isGood = isDefectiveCheck(err, neighborData, posData, index)
365                 if not isGood:
366                     isGood, posData = rerunMolAndNeighbors(err, neighborData,
367                     posData, neighborData[index][1][neighborIndex])
368                     finalData = posData
369             return True, finalData
370
371 # iterates molecule through all possible rotations
372 def iterThroughRotations(err, neighborData, posData, index):
373     isGood = False
374     pos1 = 0 # tetrahedral position for H1
375     pos2 = 0 # tetrahedral position for H2
376     while not isGood or (pos1 != 3 and pos2 != 3): # iterates through
377         # all orientations, stops if good orientation
378         if pos1 != pos2:
379             posData[index] = newSetOrientation(posData[index][0], pos1,
380             pos2)
381             isGood = isDefectiveCheck(err, neighborData, posData, index)
382             if pos2 < 3:
383                 pos2 += 1
384             elif pos2 == 3:
385                 if pos1 < 3:
386                     pos1 += 1
387                     pos2 = 0
388     return isGood, posData
389 # determines minimum hydrogen distance between two atoms
390 def minHydrogenDistance(mol1, mol2):
391     minDist = 100
392     for first in range(2):

```

```

384     for second in range(2):
385         newDist = getDistBetweenAtoms(mol1[first+1], mol2[second+1])
386         if newDist < minDist:
387             minDist = newDist
388     return minDist
389
390
391
392
393
394 # finds neighboring molecules of each molecule
395 def getNeighbors(data):
396     returnData = [ [ [ 0 for i in range(4) ] for j in range(2) ] for k
397     in range(len(data)) ] # data[molecule][distance ,index ][ four values ]
398     for mol1 in range(len(data)):
399         minDist = [100, 100, 100, 100]
400         minIndex = [0, 0, 0, 0]
401         for mol2 in range(len(data)):
402             if mol1 != mol2:
403                 newMin = getDistBetweenAtoms(data[mol1][0], data[mol2]
404                 )[0])
405
406                 bigIndex = indexOfBiggest(minDist)
407                 if newMin < minDist[bigIndex]:
408                     minDist[bigIndex] = newMin
409                     minIndex[bigIndex] = mol2
410
411                 for i in range(4):
412                     if minDist[i] >= 9:
413                         minDist[i] = -1
414                         minIndex[i] = -1
415
416                 # print "Four smallest Distances of", mol1, ":", minDist
417                 # print "Four smallest Indices of", mol1, ":", minIndex
418                 returnData[mol1] = [minDist, minIndex]
419
420     return returnData
421
422
423
424
425 # finds distance between oxygen atoms
426 def getDistBetweenAtoms( mol1 , mol2 ):
427     distance = ( ( ( mol1[0] - mol2[0] ) * ( mol1[0] - mol2[0] ) ) +
428                 ( ( mol1[1] - mol2[1] ) * ( mol1[1] - mol2[1] ) ) +
429                 ( ( mol1[2] - mol2[2] ) * ( mol1[2] - mol2[2] ) ) )
430
431     return distance
432
433
434
435 # gets index of largest item from a list
436 def indexOfBiggest(check):
437     bigIndex = 0
438     for i in range(len(check)):
439         if check[i] > check[bigIndex]:
440             bigIndex = i
441
442     return bigIndex
443
444
445 # writes data to PDB file
446 def writeDataPDB( data , pdbType):

```

```

436 print "Writing Data to", str(pdbOUT)
437 fileName = str(pdbOUT)
438 output = open(fileName, 'w')
439 if pdbType == 0:
440     writeDataPDBATOM(data, output)
441 elif pdbType == 1:
442     writeDataPDBHETATM(data, output)
443 output.close()
444
445
446 # Writes data to PDB file style = ATOM
447 def writeDataPDBATOM(data, inFile):
448     iterator = 0
449     for molecule in range(len(data)):
450         for atom in range(3):
451             iterator += 1
452             outStr = "ATOM "
453             outStr += str(iterator)
454             while len(outStr) < 11:
455                 outStr = outStr[:6] + " " + outStr[6:]
456             outStr += " "
457             if atom == 0:
458                 outStr += " O " + " WAT"
459             elif atom == 1:
460                 outStr += " H1 " + " WAT"
461             elif atom == 2:
462                 outStr += " H2 " + " WAT"
463             outStr += str(molecule)
464             while len(outStr) < 26:
465                 outStr = outStr[:20] + " " + outStr[20:]
466             outStr += " "
467             outStr += "{:8.3f}".format(data[molecule][atom][0])
468             outStr += "{:8.3f}".format(data[molecule][atom][1])
469             outStr += "{:8.3f}".format(data[molecule][atom][2])
470             outStr += " 1.00 " + " 0.00"
471             outStr += " "
472             if atom == 0:
473                 outStr += " O "
474             elif atom == 1:
475                 outStr += " H "
476             elif atom == 2:
477                 outStr += " H "
478             outStr += "\n"
479             inFile.write(outStr)
480
481
482 # Writes data to PDB file style = HETATOM
483 def writeDataPDBHETATM(data, inFile):
484     iterator = 0
485     for molecule in range(len(data)):
486         for atom in range(3):
487             iterator += 1
488             outStr = "HETATOM"
489             outStr += str(iterator)

```

```

490     while len(outStr) < 11:
491         outStr = outStr[:6] + " " + outStr[6:]
492     outStr += " "
493     if atom == 0:
494         outStr += " O " + " WAT"
495     elif atom == 1:
496         outStr += " H1 " + " WAT"
497     elif atom == 2:
498         outStr += " H2 " + " WAT"
499     outStr += str(molecule)
500     while len(outStr) < 26:
501         outStr = outStr[:20] + " " + outStr[20:]
502     outStr += " "
503     outStr += "{:8.3f}".format(data[molecule][atom][0])
504     outStr += "{:8.3f}".format(data[molecule][atom][1])
505     outStr += "{:8.3f}".format(data[molecule][atom][2])
506     outStr += " 1.00" + " 0.00"
507     outStr += " "
508     if atom == 0:
509         outStr += " O "
510     elif atom == 1:
511         outStr += " H "
512     elif atom == 2:
513         outStr += " H "
514     outStr += "\n"
515     inFile.write(outStr)
516
517
518 # runs program
519 def testRun(inFile, err, outFile):
520     print "Running Test Version of Program..."
521
522
523 # this is the parent runner for the program
524 def runPgm(inFile, err):
525     print "Running Program..."
526     data, pdbType = readFile(inFile)
527     newData = [ [ [ 0 for i in range(3) ] for j in range(3) ] for k in
528     range(len(data)) ]
529     print "Reordering Molecules..."
530     for i in range(len(data)):
531         positions = getTetrahedronPositions(data[i])
532         zeroedMol = newRandOrientation(positions)
533         newMol = resetOrientation( data[i][0], zeroedMol )
534         newData[i] = newMol
535     print "Molecules Reordered"
536     connectedMolecules = getNeighbors(newData) # -1 index = not
537     neighboring
538     finalData = newData
539     for i in range(len(connectedMolecules)):
540         # print "check defects"
541         isFine = isDefectiveCheck(err, connectedMolecules, finalData, i)
542         # print "isFINE CHECK", isFine
543         if not isFine:

```

```

542     # print "fixing defects"
543     while not isFine:
544         # print "RerunMol"
545         isFine, finalData = rerunMolAndNeighbors(err,
546             connectedMolecules, finalData, i)
547         # print "rerunDone"
548         writeDataPDB(finalData, pdbType)
549         # printData(newData)
550
551 badArgs = checkArgs(pdbIN, maxErr, pdbOUT) # stop in case of bad
552     argument
553
554 # check input args
555 if not badArgs: # stop in case of bad argument
556     print "Good Arguments, Initializing Reorientation with", maxErr, "
557     maximum defects"
558     # testRun(pdbIN, maxErr, pdbOUT)
559     runPgm(pdbIN, maxErr)
560 elif badArgs:
561     print "Bad Arguments, Quitting..."
```

A.2 PDB: Parent Ice XI

The following shows the parent Ice XI .pdb file used. Any .pdb file of an ice structure that follows the HETATM or ATOM style and the Bernal-Fowler ice rules should also work.

1	HETATM	1	O	O	1	-10.483	-5.440	10.189
2	HETATM	2	1H1	H	1	-10.473	-4.440	10.185
3	HETATM	3	2H1	H	1	-10.015	-5.781	9.374
4	HETATM	4	O	O	2	-9.186	-6.385	7.933
5	HETATM	5	1H2	H	2	-9.655	-6.049	7.115
6	HETATM	6	2H2	H	2	-8.241	-6.059	7.931
7	HETATM	7	O	O	3	-6.569	-5.486	7.929
8	HETATM	8	1H3	H	3	-6.559	-4.486	7.925
9	HETATM	9	2H3	H	3	-6.101	-5.827	7.114
10	HETATM	10	O	O	4	-5.274	-6.412	10.193
11	HETATM	11	1H4	H	4	-5.741	-6.077	9.375
12	HETATM	12	2H4	H	4	-4.327	-6.087	10.191
13	HETATM	13	O	O	5	-6.569	-5.468	12.449
14	HETATM	14	1H5	H	5	-6.559	-4.468	12.445
15	HETATM	15	2H5	H	5	-6.101	-5.809	11.633
16	HETATM	16	O	O	6	-9.186	-6.366	12.453
17	HETATM	17	1H6	H	6	-9.655	-6.031	11.634
18	HETATM	18	2H6	H	6	-8.241	-6.041	12.451
19	HETATM	19	O	O	7	-10.526	-10.053	10.207
20	HETATM	20	1H1	H	7	-11.466	-9.710	10.206
21	HETATM	21	2H1	H	7	-10.052	-9.720	11.022
22	HETATM	22	O	O	8	-9.212	-9.151	7.944
23	HETATM	23	1H2	H	8	-9.203	-8.151	7.940
24	HETATM	24	2H2	H	8	-9.688	-9.477	8.762
25	HETATM	25	O	O	9	-6.612	-10.099	7.947
26	HETATM	26	1H3	H	9	-7.552	-9.756	7.946
27	HETATM	27	2H3	H	9	-6.138	-9.766	8.763

28	HETATM	28	O	O	10	-5.300	-9.179	10.204
29	HETATM	29	1H4	H	10	-5.290	-8.179	10.200
30	HETATM	30	2H4	H	10	-5.774	-9.504	11.021
31	HETATM	31	O	O	11	-6.612	-10.081	12.467
32	HETATM	32	1H5	H	11	-7.552	-9.738	12.466
33	HETATM	33	2H5	H	11	-6.138	-9.748	13.282
34	HETATM	34	O	O	12	-9.212	-9.133	12.464
35	HETATM	35	1H6	H	12	-9.203	-8.133	12.460
36	HETATM	36	2H6	H	12	-9.687	-9.458	13.281
37	HETATM	37	O	O	13	-2.655	-5.514	10.189
38	HETATM	38	1H1	H	13	-2.646	-4.514	10.185
39	HETATM	39	2H1	H	13	-2.187	-5.855	9.374
40	HETATM	40	O	O	14	-1.360	-6.458	7.933
41	HETATM	41	1H2	H	14	-1.828	-6.123	7.115
42	HETATM	42	2H2	H	14	-0.414	-6.133	7.931
43	HETATM	43	O	O	15	1.259	-5.560	7.929
44	HETATM	44	1H3	H	15	1.268	-4.560	7.925
45	HETATM	45	2H3	H	15	1.727	-5.900	7.114
46	HETATM	46	O	O	16	2.554	-6.486	10.193
47	HETATM	47	1H4	H	16	2.086	-6.151	9.375
48	HETATM	48	2H4	H	16	3.500	-6.161	10.191
49	HETATM	49	O	O	17	1.259	-5.542	12.449
50	HETATM	50	1H5	H	17	1.268	-4.542	12.445
51	HETATM	51	2H5	H	17	1.727	-5.882	11.633
52	HETATM	52	O	O	18	-1.360	-6.440	12.453
53	HETATM	53	1H6	H	18	-1.827	-6.105	11.634
54	HETATM	54	2H6	H	18	-0.413	-6.115	12.451
55	HETATM	55	O	O	19	-2.698	-10.127	10.207
56	HETATM	56	1H1	H	19	-3.638	-9.784	10.206
57	HETATM	57	2H1	H	19	-2.224	-9.794	11.022
58	HETATM	58	O	O	20	-1.386	-9.225	7.944
59	HETATM	59	1H2	H	20	-1.376	-8.225	7.940
60	HETATM	60	2H2	H	20	-1.860	-9.550	8.762
61	HETATM	61	O	O	21	1.215	-10.173	7.947
62	HETATM	62	1H3	H	21	0.276	-9.830	7.946
63	HETATM	63	2H3	H	21	1.690	-9.840	8.763
64	HETATM	64	O	O	22	2.528	-9.253	10.204
65	HETATM	65	1H4	H	22	2.538	-8.253	10.200
66	HETATM	66	2H4	H	22	2.054	-9.578	11.021
67	HETATM	67	O	O	23	1.216	-10.154	12.467
68	HETATM	68	1H5	H	23	0.276	-9.811	12.466
69	HETATM	69	2H5	H	23	1.690	-9.821	13.282
70	HETATM	70	O	O	24	-1.386	-9.207	12.464
71	HETATM	71	1H6	H	24	-1.376	-8.207	12.460
72	HETATM	72	2H6	H	24	-1.860	-9.532	13.281
73	HETATM	73	O	O	25	5.172	-5.587	10.189
74	HETATM	74	1H1	H	25	5.181	-4.587	10.185
75	HETATM	75	2H1	H	25	5.641	-5.928	9.374
76	HETATM	76	O	O	26	6.468	-6.532	7.933
77	HETATM	77	1H2	H	26	6.000	-6.197	7.115
78	HETATM	78	2H2	H	26	7.414	-6.207	7.931
79	HETATM	79	O	O	27	9.085	-5.633	7.929
80	HETATM	80	1H3	H	27	9.095	-4.633	7.925
81	HETATM	81	2H3	H	27	9.554	-5.974	7.114

82	HETATM	82	O	O	28	10.382	-6.559	10.193
83	HETATM	83	1H4	H	28	9.913	-6.224	9.375
84	HETATM	84	2H4	H	28	11.328	-6.234	10.191
85	HETATM	85	O	O	29	9.086	-5.615	12.449
86	HETATM	86	1H5	H	29	9.095	-4.615	12.445
87	HETATM	87	2H5	H	29	9.554	-5.956	11.633
88	HETATM	88	O	O	30	6.468	-6.514	12.453
89	HETATM	89	1H6	H	30	6.000	-6.178	11.634
90	HETATM	90	2H6	H	30	7.414	-6.188	12.451
91	HETATM	91	O	O	31	5.128	-10.200	10.207
92	HETATM	92	1H1	H	31	4.190	-9.857	10.206
93	HETATM	93	2H1	H	31	5.603	-9.867	11.022
94	HETATM	94	O	O	32	6.442	-9.299	7.944
95	HETATM	95	1H2	H	32	6.451	-8.299	7.940
96	HETATM	96	2H2	H	32	5.968	-9.624	8.762
97	HETATM	97	O	O	33	9.042	-10.246	7.947
98	HETATM	98	1H3	H	33	8.102	-9.903	7.946
99	HETATM	99	2H3	H	33	9.517	-9.913	8.763
100	HETATM	100	O	O	34	10.356	-9.326	10.204
101	HETATM	101	1H4	H	34	10.365	-8.326	10.200
102	HETATM	102	2H4	H	34	9.881	-9.652	11.021
103	HETATM	103	O	O	35	9.042	-10.228	12.467
104	HETATM	104	1H5	H	35	8.102	-9.885	12.466
105	HETATM	105	2H5	H	35	9.517	-9.895	13.282
106	HETATM	106	O	O	36	6.442	-9.280	12.464
107	HETATM	107	1H6	H	36	6.451	-8.280	12.460
108	HETATM	108	2H6	H	36	5.968	-9.606	13.281
109	HETATM	109	O	O	39	-10.483	-5.477	1.150
110	HETATM	110	1H3	H	39	-10.474	-4.477	1.146
111	HETATM	111	2H3	H	39	-10.015	-5.817	0.335
112	HETATM	112	O	O	40	-9.187	-6.403	3.414
113	HETATM	113	1H4	H	40	-9.655	-6.068	2.596
114	HETATM	114	2H4	H	40	-8.241	-6.078	3.412
115	HETATM	115	O	O	41	-10.483	-5.458	5.670
116	HETATM	116	1H5	H	41	-10.473	-4.459	5.666
117	HETATM	117	2H5	H	41	-10.015	-5.799	4.854
118	HETATM	118	O	O	45	-10.526	-10.089	1.169
119	HETATM	119	1H3	H	45	-11.466	-9.747	1.167
120	HETATM	120	2H3	H	45	-10.052	-9.757	1.984
121	HETATM	121	O	O	46	-9.213	-9.170	3.425
122	HETATM	122	1H4	H	46	-9.203	-8.170	3.421
123	HETATM	123	2H4	H	46	-9.688	-9.495	4.243
124	HETATM	124	O	O	47	-10.526	-10.071	5.688
125	HETATM	125	1H5	H	47	-11.466	-9.728	5.687
126	HETATM	126	2H5	H	47	-10.052	-9.738	6.503
127	HETATM	127	O	O	49	-6.569	-5.504	3.410
128	HETATM	128	1H1	H	49	-6.560	-4.504	3.406
129	HETATM	129	2H1	H	49	-6.101	-5.845	2.595
130	HETATM	130	O	O	50	-5.274	-6.449	1.154
131	HETATM	131	1H2	H	50	-5.742	-6.114	0.336
132	HETATM	132	2H2	H	50	-4.328	-6.124	1.152
133	HETATM	133	O	O	51	-2.655	-5.550	1.150
134	HETATM	134	1H3	H	51	-2.646	-4.550	1.146
135	HETATM	135	2H3	H	51	-2.187	-5.891	0.335

136	HETATM	136	O	O	52	-1.360	-6.476	3.414
137	HETATM	137	1H4	H	52	-1.828	-6.141	2.596
138	HETATM	138	2H4	H	52	-0.414	-6.151	3.412
139	HETATM	139	O	O	53	-2.655	-5.532	5.670
140	HETATM	140	1H5	H	53	-2.646	-4.532	5.666
141	HETATM	141	2H5	H	53	-2.187	-5.873	4.854
142	HETATM	142	O	O	54	-5.274	-6.430	5.674
143	HETATM	143	1H6	H	54	-5.742	-6.095	4.855
144	HETATM	144	2H6	H	54	-4.328	-6.105	5.672
145	HETATM	145	O	O	55	-6.612	-10.117	3.428
146	HETATM	146	1H1	H	55	-7.552	-9.774	3.427
147	HETATM	147	2H1	H	55	-6.138	-9.784	4.244
148	HETATM	148	O	O	56	-5.300	-9.216	1.165
149	HETATM	149	1H2	H	56	-5.290	-8.216	1.161
150	HETATM	150	2H2	H	56	-5.774	-9.541	1.983
151	HETATM	151	O	O	57	-2.699	-10.163	1.169
152	HETATM	152	1H3	H	57	-3.638	-9.820	1.167
153	HETATM	153	2H3	H	57	-2.225	-9.830	1.984
154	HETATM	154	O	O	58	-1.386	-9.243	3.425
155	HETATM	155	1H4	H	58	-1.377	-8.243	3.421
156	HETATM	156	2H4	H	58	-1.860	-9.568	4.243
157	HETATM	157	O	O	59	-2.698	-10.145	5.688
158	HETATM	158	1H5	H	59	-3.638	-9.802	5.687
159	HETATM	159	2H5	H	59	-2.224	-9.812	6.503
160	HETATM	160	O	O	60	-5.300	-9.197	5.685
161	HETATM	161	1H6	H	60	-5.290	-8.197	5.681
162	HETATM	162	2H6	H	60	-5.774	-9.523	6.502
163	HETATM	163	O	O	61	1.259	-5.578	3.410
164	HETATM	164	1H1	H	61	1.268	-4.578	3.406
165	HETATM	165	2H1	H	61	1.726	-5.919	2.595
166	HETATM	166	O	O	62	2.554	-6.522	1.154
167	HETATM	167	1H2	H	62	2.086	-6.187	0.336
168	HETATM	168	2H2	H	62	3.500	-6.197	1.152
169	HETATM	169	O	O	63	5.171	-5.624	1.150
170	HETATM	170	1H3	H	63	5.181	-4.624	1.146
171	HETATM	171	2H3	H	63	5.640	-5.965	0.335
172	HETATM	172	O	O	64	6.468	-6.550	3.414
173	HETATM	173	1H4	H	64	6.000	-6.215	2.596
174	HETATM	174	2H4	H	64	7.414	-6.225	3.412
175	HETATM	175	O	O	65	5.172	-5.606	5.670
176	HETATM	176	1H5	H	65	5.181	-4.606	5.666
177	HETATM	177	2H5	H	65	5.640	-5.946	4.854
178	HETATM	178	O	O	66	2.554	-6.504	5.674
179	HETATM	179	1H6	H	66	2.086	-6.169	4.855
180	HETATM	180	2H6	H	66	3.500	-6.179	5.672
181	HETATM	181	O	O	67	1.215	-10.191	3.428
182	HETATM	182	1H1	H	67	0.275	-9.848	3.427
183	HETATM	183	2H1	H	67	1.689	-9.858	4.244
184	HETATM	184	O	O	68	2.528	-9.289	1.165
185	HETATM	185	1H2	H	68	2.537	-8.289	1.161
186	HETATM	186	2H2	H	68	2.054	-9.614	1.983
187	HETATM	187	O	O	69	5.128	-10.237	1.169
188	HETATM	188	1H3	H	69	4.189	-9.894	1.167
189	HETATM	189	2H3	H	69	5.603	-9.904	1.984

190	HETATM	190	O	O	70	6.442	-9.317	3.425
191	HETATM	191	1H4	H	70	6.451	-8.317	3.421
192	HETATM	192	2H4	H	70	5.968	-9.642	4.243
193	HETATM	193	O	O	71	5.128	-10.218	5.688
194	HETATM	194	1H5	H	71	4.189	-9.876	5.687
195	HETATM	195	2H5	H	71	5.603	-9.886	6.503
196	HETATM	196	O	O	72	2.528	-9.271	5.685
197	HETATM	197	1H6	H	72	2.537	-8.271	5.681
198	HETATM	198	2H6	H	72	2.054	-9.596	6.502
199	HETATM	199	O	O	73	9.085	-5.652	3.410
200	HETATM	200	1H1	H	73	9.095	-4.652	3.406
201	HETATM	201	2H1	H	73	9.554	-5.992	2.595
202	HETATM	202	O	O	74	10.381	-6.596	1.154
203	HETATM	203	1H2	H	74	9.913	-6.261	0.336
204	HETATM	204	2H2	H	74	11.328	-6.271	1.152
205	HETATM	205	O	O	78	10.382	-6.578	5.674
206	HETATM	206	1H6	H	78	9.913	-6.243	4.855
207	HETATM	207	2H6	H	78	11.328	-6.253	5.672
208	HETATM	208	O	O	79	9.042	-10.264	3.428
209	HETATM	209	1H1	H	79	8.102	-9.921	3.427
210	HETATM	210	2H1	H	79	9.517	-9.931	4.244
211	HETATM	211	O	O	80	10.355	-9.363	1.165
212	HETATM	212	1H2	H	80	10.365	-8.363	1.161
213	HETATM	213	2H2	H	80	9.880	-9.688	1.983
214	HETATM	214	O	O	84	10.356	-9.345	5.685
215	HETATM	215	1H6	H	84	10.365	-8.345	5.681
216	HETATM	216	2H6	H	84	9.881	-9.670	6.502
217	HETATM	217	O	O	85	-10.483	-5.495	-3.369
218	HETATM	218	1H1	H	85	-10.474	-4.495	-3.373
219	HETATM	219	2H1	H	85	-10.015	-5.836	-4.184
220	HETATM	220	O	O	86	-9.187	-6.439	-5.625
221	HETATM	221	1H2	H	86	-9.656	-6.104	-6.443
222	HETATM	222	2H2	H	86	-8.242	-6.114	-5.627
223	HETATM	223	O	O	87	-6.569	-5.541	-5.629
224	HETATM	224	1H3	H	87	-6.560	-4.541	-5.633
225	HETATM	225	2H3	H	87	-6.102	-5.881	-6.444
226	HETATM	226	O	O	88	-5.274	-6.467	-3.365
227	HETATM	227	1H4	H	88	-5.742	-6.132	-4.183
228	HETATM	228	2H4	H	88	-4.328	-6.142	-3.367
229	HETATM	229	O	O	89	-6.569	-5.523	-1.109
230	HETATM	230	1H5	H	89	-6.560	-4.523	-1.113
231	HETATM	231	2H5	H	89	-6.101	-5.863	-1.925
232	HETATM	232	O	O	90	-9.187	-6.421	-1.105
233	HETATM	233	1H6	H	90	-9.656	-6.086	-1.924
234	HETATM	234	2H6	H	90	-8.242	-6.096	-1.107
235	HETATM	235	O	O	91	-10.526	-10.108	-3.350
236	HETATM	236	1H1	H	91	-11.466	-9.765	-3.352
237	HETATM	237	2H1	H	91	-10.052	-9.775	-2.535
238	HETATM	238	O	O	92	-9.213	-9.206	-5.614
239	HETATM	239	1H2	H	92	-9.204	-8.206	-5.618
240	HETATM	240	2H2	H	92	-9.688	-9.531	-4.796
241	HETATM	241	O	O	93	-6.613	-10.154	-5.610
242	HETATM	242	1H3	H	93	-7.553	-9.811	-5.612
243	HETATM	243	2H3	H	93	-6.139	-9.821	-4.795

244	HETATM	244	O	O	94	-5.300	-9.234	-3.354
245	HETATM	245	1H4	H	94	-5.291	-8.234	-3.358
246	HETATM	246	2H4	H	94	-5.774	-9.559	-2.536
247	HETATM	247	O	O	95	-6.613	-10.135	-1.090
248	HETATM	248	1H5	H	95	-7.552	-9.792	-1.092
249	HETATM	249	2H5	H	95	-6.138	-9.802	-0.276
250	HETATM	250	O	O	96	-9.213	-9.188	-1.094
251	HETATM	251	1H6	H	96	-9.203	-8.188	-1.098
252	HETATM	252	2H6	H	96	-9.688	-9.513	-0.277
253	HETATM	253	O	O	97	-2.655	-5.568	-3.369
254	HETATM	254	1H1	H	97	-2.646	-4.569	-3.373
255	HETATM	255	2H1	H	97	-2.188	-5.909	-4.184
256	HETATM	256	O	O	98	-1.360	-6.513	-5.625
257	HETATM	257	1H2	H	98	-1.828	-6.178	-6.443
258	HETATM	258	2H2	H	98	-0.414	-6.188	-5.627
259	HETATM	259	O	O	99	1.258	-5.614	-5.629
260	HETATM	260	1H3	H	99	1.268	-4.614	-5.633
261	HETATM	261	2H3	H	99	1.726	-5.955	-6.444
262	HETATM	262	O	O	100	2.554	-6.540	-3.365
263	HETATM	263	1H4	H	100	2.086	-6.205	-4.183
264	HETATM	264	2H4	H	100	3.500	-6.215	-3.367
265	HETATM	265	O	O	101	1.258	-5.596	-1.109
266	HETATM	266	1H5	H	101	1.268	-4.596	-1.113
267	HETATM	267	2H5	H	101	1.726	-5.937	-1.925
268	HETATM	268	O	O	102	-1.360	-6.495	-1.105
269	HETATM	269	1H6	H	102	-1.828	-6.159	-1.924
270	HETATM	270	2H6	H	102	-0.414	-6.169	-1.107
271	HETATM	271	O	O	103	-2.699	-10.181	-3.350
272	HETATM	272	1H1	H	103	-3.639	-9.838	-3.352
273	HETATM	273	2H1	H	103	-2.225	-9.848	-2.535
274	HETATM	274	O	O	104	-1.386	-9.280	-5.614
275	HETATM	275	1H2	H	104	-1.377	-8.280	-5.618
276	HETATM	276	2H2	H	104	-1.860	-9.605	-4.796
277	HETATM	277	O	O	105	1.215	-10.227	-5.610
278	HETATM	278	1H3	H	105	0.275	-9.884	-5.612
279	HETATM	279	2H3	H	105	1.689	-9.894	-4.795
280	HETATM	280	O	O	106	2.528	-9.307	-3.354
281	HETATM	281	1H4	H	106	2.537	-8.307	-3.358
282	HETATM	282	2H4	H	106	2.054	-9.633	-2.536
283	HETATM	283	O	O	107	1.215	-10.209	-1.090
284	HETATM	284	1H5	H	107	0.275	-9.866	-1.092
285	HETATM	285	2H5	H	107	1.689	-9.876	-0.276
286	HETATM	286	O	O	108	-1.386	-9.261	-1.094
287	HETATM	287	1H6	H	108	-1.377	-8.261	-1.098
288	HETATM	288	2H6	H	108	-1.860	-9.587	-0.277
289	HETATM	289	O	O	109	5.171	-5.642	-3.369
290	HETATM	290	1H1	H	109	5.181	-4.642	-3.373
291	HETATM	291	2H1	H	109	5.640	-5.983	-4.184
292	HETATM	292	O	O	110	6.467	-6.586	-5.625
293	HETATM	293	1H2	H	110	6.000	-6.251	-6.443
294	HETATM	294	2H2	H	110	7.413	-6.261	-5.627
295	HETATM	295	O	O	111	9.085	-5.688	-5.629
296	HETATM	296	1H3	H	111	9.094	-4.688	-5.633
297	HETATM	297	2H3	H	111	9.554	-6.029	-6.444

298	HETATM	298	O	O	112	10.381	-6.614	-3.365
299	HETATM	299	1H4	H	112	9.912	-6.279	-4.183
300	HETATM	300	2H4	H	112	11.327	-6.289	-3.367
301	HETATM	301	O	O	113	9.085	-5.670	-1.109
302	HETATM	302	1H5	H	113	9.095	-4.670	-1.113
303	HETATM	303	2H5	H	113	9.554	-6.010	-1.925
304	HETATM	304	O	O	114	6.468	-6.568	-1.105
305	HETATM	305	1H6	H	114	6.000	-6.233	-1.924
306	HETATM	306	2H6	H	114	7.414	-6.243	-1.107
307	HETATM	307	O	O	115	5.128	-10.255	-3.350
308	HETATM	308	1H1	H	115	4.189	-9.912	-3.352
309	HETATM	309	2H1	H	115	5.603	-9.922	-2.535
310	HETATM	310	O	O	116	6.441	-9.353	-5.614
311	HETATM	311	1H2	H	116	6.451	-8.353	-5.618
312	HETATM	312	2H2	H	116	5.967	-9.678	-4.796
313	HETATM	313	O	O	117	9.042	-10.301	-5.610
314	HETATM	314	1H3	H	117	8.102	-9.958	-5.612
315	HETATM	315	2H3	H	117	9.517	-9.968	-4.795
316	HETATM	316	O	O	118	10.355	-9.381	-3.354
317	HETATM	317	1H4	H	118	10.365	-8.381	-3.358
318	HETATM	318	2H4	H	118	9.880	-9.706	-2.536
319	HETATM	319	O	O	119	9.042	-10.282	-1.090
320	HETATM	320	1H5	H	119	8.102	-9.940	-1.092
321	HETATM	321	2H5	H	119	9.517	-9.950	-0.276
322	HETATM	322	O	O	120	6.442	-9.335	-1.094
323	HETATM	323	1H6	H	120	6.451	-8.335	-1.098
324	HETATM	324	2H6	H	120	5.967	-9.660	-0.277
325	HETATM	325	O	O	123	-10.483	-5.531	-12.408
326	HETATM	326	1H3	H	123	-10.474	-4.531	-12.412
327	HETATM	327	2H3	H	123	-10.016	-5.872	-13.223
328	HETATM	328	O	O	124	-9.187	-6.457	-10.144
329	HETATM	329	1H4	H	124	-9.656	-6.122	-10.962
330	HETATM	330	2H4	H	124	-8.242	-6.132	-10.146
331	HETATM	331	O	O	125	-10.483	-5.513	-7.888
332	HETATM	332	1H5	H	125	-10.474	-4.513	-7.892
333	HETATM	333	2H5	H	125	-10.015	-5.854	-8.704
334	HETATM	334	O	O	129	-10.527	-10.144	-12.389
335	HETATM	335	1H3	H	129	-11.467	-9.801	-12.391
336	HETATM	336	2H3	H	129	-10.053	-9.811	-11.574
337	HETATM	337	O	O	130	-9.213	-9.224	-10.133
338	HETATM	338	1H4	H	130	-9.204	-8.224	-10.137
339	HETATM	339	2H4	H	130	-9.688	-9.550	-9.315
340	HETATM	340	O	O	131	-10.527	-10.126	-7.869
341	HETATM	341	1H5	H	131	-11.466	-9.783	-7.871
342	HETATM	342	2H5	H	131	-10.053	-9.793	-7.055
343	HETATM	343	O	O	133	-6.570	-5.559	-10.148
344	HETATM	344	1H1	H	133	-6.560	-4.559	-10.152
345	HETATM	345	2H1	H	133	-6.102	-5.900	-10.963
346	HETATM	346	O	O	134	-5.274	-6.503	-12.404
347	HETATM	347	1H2	H	134	-5.742	-6.168	-13.222
348	HETATM	348	2H2	H	134	-4.328	-6.178	-12.406
349	HETATM	349	O	O	135	-2.656	-5.605	-12.408
350	HETATM	350	1H3	H	135	-2.646	-4.605	-12.412
351	HETATM	351	2H3	H	135	-2.188	-5.946	-13.223

352	HETATM	352	O	O	136	-1.360	-6.531	-10.144
353	HETATM	353	1H4	H	136	-1.828	-6.196	-10.962
354	HETATM	354	2H4	H	136	-0.414	-6.206	-10.146
355	HETATM	355	O	O	137	-2.656	-5.587	-7.888
356	HETATM	356	1H5	H	137	-2.646	-4.587	-7.892
357	HETATM	357	2H5	H	137	-2.188	-5.927	-8.704
358	HETATM	358	O	O	138	-5.274	-6.485	-7.884
359	HETATM	359	1H6	H	138	-5.742	-6.150	-8.703
360	HETATM	360	2H6	H	138	-4.328	-6.160	-7.886
361	HETATM	361	O	O	139	-6.613	-10.172	-10.129
362	HETATM	362	1H1	H	139	-7.553	-9.829	-10.131
363	HETATM	363	2H1	H	139	-6.139	-9.839	-9.314
364	HETATM	364	O	O	140	-5.300	-9.270	-12.393
365	HETATM	365	1H2	H	140	-5.291	-8.270	-12.397
366	HETATM	366	2H2	H	140	-5.774	-9.595	-11.575
367	HETATM	367	O	O	141	-2.699	-10.218	-12.389
368	HETATM	368	1H3	H	141	-3.639	-9.875	-12.391
369	HETATM	369	2H3	H	141	-2.225	-9.885	-11.574
370	HETATM	370	O	O	142	-1.386	-9.298	-10.133
371	HETATM	371	1H4	H	142	-1.377	-8.298	-10.137
372	HETATM	372	2H4	H	142	-1.861	-9.623	-9.315
373	HETATM	373	O	O	143	-2.699	-10.199	-7.869
374	HETATM	374	1H5	H	143	-3.639	-9.857	-7.871
375	HETATM	375	2H5	H	143	-2.225	-9.867	-7.055
376	HETATM	376	O	O	144	-5.300	-9.252	-7.873
377	HETATM	377	1H6	H	144	-5.291	-8.252	-7.877
378	HETATM	378	2H6	H	144	-5.774	-9.577	-7.056
379	HETATM	379	O	O	145	1.258	-5.633	-10.148
380	HETATM	380	1H1	H	145	1.268	-4.633	-10.152
381	HETATM	381	2H1	H	145	1.726	-5.973	-10.963
382	HETATM	382	O	O	146	2.553	-6.577	-12.404
383	HETATM	383	1H2	H	146	2.085	-6.242	-13.222
384	HETATM	384	2H2	H	146	3.499	-6.252	-12.406
385	HETATM	385	O	O	147	5.171	-5.678	-12.408
386	HETATM	386	1H3	H	147	5.180	-4.679	-12.412
387	HETATM	387	2H3	H	147	5.640	-6.019	-13.223
388	HETATM	388	O	O	148	6.467	-6.605	-10.144
389	HETATM	389	1H4	H	148	5.999	-6.269	-10.962
390	HETATM	390	2H4	H	148	7.413	-6.279	-10.146
391	HETATM	391	O	O	149	5.171	-5.660	-7.888
392	HETATM	392	1H5	H	149	5.180	-4.660	-7.892
393	HETATM	393	2H5	H	149	5.640	-6.001	-8.704
394	HETATM	394	O	O	150	2.553	-6.559	-7.884
395	HETATM	395	1H6	H	150	2.086	-6.224	-8.703
396	HETATM	396	2H6	H	150	3.500	-6.234	-7.886
397	HETATM	397	O	O	151	1.215	-10.245	-10.129
398	HETATM	398	1H1	H	151	0.275	-9.902	-10.131
399	HETATM	399	2H1	H	151	1.689	-9.912	-9.314
400	HETATM	400	O	O	152	2.527	-9.344	-12.393
401	HETATM	401	1H2	H	152	2.537	-8.344	-12.397
402	HETATM	402	2H2	H	152	2.053	-9.669	-11.575
403	HETATM	403	O	O	153	5.127	-10.291	-12.389
404	HETATM	404	1H3	H	153	4.189	-9.948	-12.391
405	HETATM	405	2H3	H	153	5.603	-9.958	-11.574

406	HETATM	406	O	O	154	6.441	-9.371	-10.133
407	HETATM	407	1H4	H	154	6.451	-8.371	-10.137
408	HETATM	408	2H4	H	154	5.967	-9.697	-9.315
409	HETATM	409	O	O	155	5.128	-10.273	-7.869
410	HETATM	410	1H5	H	155	4.189	-9.930	-7.871
411	HETATM	411	2H5	H	155	5.603	-9.940	-7.055
412	HETATM	412	O	O	156	2.527	-9.326	-7.873
413	HETATM	413	1H6	H	156	2.537	-8.326	-7.877
414	HETATM	414	2H6	H	156	2.053	-9.651	-7.056
415	HETATM	415	O	O	157	9.085	-5.706	-10.148
416	HETATM	416	1H1	H	157	9.094	-4.706	-10.152
417	HETATM	417	2H1	H	157	9.554	-6.047	-10.963
418	HETATM	418	O	O	158	10.381	-6.650	-12.404
419	HETATM	419	1H2	H	158	9.912	-6.315	-13.222
420	HETATM	420	2H2	H	158	11.327	-6.325	-12.406
421	HETATM	421	O	O	162	10.381	-6.632	-7.884
422	HETATM	422	1H6	H	162	9.912	-6.297	-8.703
423	HETATM	423	2H6	H	162	11.327	-6.307	-7.886
424	HETATM	424	O	O	163	9.041	-10.319	-10.129
425	HETATM	425	1H1	H	163	8.102	-9.976	-10.131
426	HETATM	426	2H1	H	163	9.517	-9.986	-9.314
427	HETATM	427	O	O	164	10.355	-9.417	-12.393
428	HETATM	428	1H2	H	164	10.364	-8.417	-12.397
429	HETATM	429	2H2	H	164	9.880	-9.743	-11.575
430	HETATM	430	O	O	168	10.355	-9.399	-7.873
431	HETATM	431	1H6	H	168	10.365	-8.399	-7.877
432	HETATM	432	2H6	H	168	9.880	-9.724	-7.056
433	HETATM	433	O	O	169	-10.413	1.939	10.159
434	HETATM	434	1H1	H	169	-10.404	2.939	10.155
435	HETATM	435	2H1	H	169	-9.945	1.599	9.344
436	HETATM	436	O	O	170	-9.117	0.996	7.903
437	HETATM	437	1H2	H	170	-9.586	1.330	7.086
438	HETATM	438	2H2	H	170	-8.172	1.320	7.902
439	HETATM	439	O	O	171	-6.499	1.893	7.899
440	HETATM	440	1H3	H	171	-6.490	2.893	7.895
441	HETATM	441	2H3	H	171	-6.032	1.553	7.084
442	HETATM	442	O	O	172	-5.204	0.968	10.163
443	HETATM	443	1H4	H	172	-5.672	1.302	9.346
444	HETATM	444	2H4	H	172	-4.258	1.292	10.162
445	HETATM	445	O	O	173	-6.499	1.912	12.419
446	HETATM	446	1H5	H	173	-6.490	2.912	12.415
447	HETATM	447	2H5	H	173	-6.031	1.571	11.603
448	HETATM	448	O	O	174	-9.117	1.014	12.423
449	HETATM	449	1H6	H	174	-9.586	1.348	11.604
450	HETATM	450	2H6	H	174	-8.172	1.338	12.421
451	HETATM	451	O	O	175	-10.457	-2.672	10.178
452	HETATM	452	1H1	H	175	-11.396	-2.331	10.176
453	HETATM	453	2H1	H	175	-9.982	-2.341	10.992
454	HETATM	454	O	O	176	-9.143	-1.772	7.914
455	HETATM	455	1H2	H	176	-9.134	-0.772	7.910
456	HETATM	456	2H2	H	176	-9.618	-2.097	8.732
457	HETATM	457	O	O	177	-6.543	-2.718	7.918
458	HETATM	458	1H3	H	177	-7.483	-2.376	7.916
459	HETATM	459	2H3	H	177	-6.069	-2.386	8.733

460	HETATM	460	O	O	178	-5.230	-1.800	10.174
461	HETATM	461	1H4	H	178	-5.221	-0.800	10.170
462	HETATM	462	2H4	H	178	-5.704	-2.125	10.991
463	HETATM	463	O	O	179	-6.543	-2.700	12.438
464	HETATM	464	1H5	H	179	-7.482	-2.358	12.436
465	HETATM	465	2H5	H	179	-6.069	-2.368	13.252
466	HETATM	466	O	O	180	-9.143	-1.754	12.434
467	HETATM	467	1H6	H	180	-9.133	-0.754	12.430
468	HETATM	468	2H6	H	180	-9.618	-2.079	13.251
469	HETATM	469	O	O	181	-2.586	1.866	10.159
470	HETATM	470	1H1	H	181	-2.576	2.866	10.155
471	HETATM	471	2H1	H	181	-2.118	1.525	9.344
472	HETATM	472	O	O	182	-1.290	0.922	7.903
473	HETATM	473	1H2	H	182	-1.758	1.257	7.086
474	HETATM	474	2H2	H	182	-0.344	1.247	7.902
475	HETATM	475	O	O	183	1.328	1.820	7.899
476	HETATM	476	1H3	H	183	1.338	2.820	7.895
477	HETATM	477	2H3	H	183	1.796	1.479	7.084
478	HETATM	478	O	O	184	2.624	0.895	10.163
479	HETATM	479	1H4	H	184	2.156	1.229	9.346
480	HETATM	480	2H4	H	184	3.570	1.219	10.162
481	HETATM	481	O	O	185	1.328	1.838	12.419
482	HETATM	482	1H5	H	185	1.338	2.838	12.415
483	HETATM	483	2H5	H	185	1.796	1.497	11.603
484	HETATM	484	O	O	186	-1.290	0.941	12.423
485	HETATM	485	1H6	H	186	-1.758	1.275	11.604
486	HETATM	486	2H6	H	186	-0.344	1.265	12.421
487	HETATM	487	O	O	187	-2.629	-2.746	10.178
488	HETATM	488	1H1	H	187	-3.569	-2.404	10.176
489	HETATM	489	2H1	H	187	-2.155	-2.414	10.992
490	HETATM	490	O	O	188	-1.316	-1.845	7.914
491	HETATM	491	1H2	H	188	-1.307	-0.845	7.910
492	HETATM	492	2H2	H	188	-1.790	-2.171	8.732
493	HETATM	493	O	O	189	1.285	-2.792	7.918
494	HETATM	494	1H3	H	189	0.345	-2.450	7.916
495	HETATM	495	2H3	H	189	1.759	-2.460	8.733
496	HETATM	496	O	O	190	2.598	-1.873	10.174
497	HETATM	497	1H4	H	190	2.607	-0.873	10.170
498	HETATM	498	2H4	H	190	2.123	-2.198	10.991
499	HETATM	499	O	O	191	1.285	-2.774	12.438
500	HETATM	500	1H5	H	191	0.345	-2.432	12.436
501	HETATM	501	2H5	H	191	1.759	-2.442	13.252
502	HETATM	502	O	O	192	-1.316	-1.827	12.434
503	HETATM	503	1H6	H	192	-1.307	-0.827	12.430
504	HETATM	504	2H6	H	192	-1.790	-2.152	13.251
505	HETATM	505	O	O	193	5.241	1.792	10.159
506	HETATM	506	1H1	H	193	5.250	2.792	10.155
507	HETATM	507	2H1	H	193	5.710	1.451	9.344
508	HETATM	508	O	O	194	6.537	0.849	7.903
509	HETATM	509	1H2	H	194	6.069	1.183	7.086
510	HETATM	510	2H2	H	194	7.483	1.173	7.902
511	HETATM	511	O	O	195	9.155	1.746	7.899
512	HETATM	512	1H3	H	195	9.164	2.746	7.895
513	HETATM	513	2H3	H	195	9.624	1.406	7.084

514	HETATM	514	O	O	196	10.451	0.821	10.163
515	HETATM	515	1H4	H	196	9.982	1.155	9.346
516	HETATM	516	2H4	H	196	11.397	1.145	10.162
517	HETATM	517	O	O	197	9.155	1.764	12.419
518	HETATM	518	1H5	H	197	9.164	2.764	12.415
519	HETATM	519	2H5	H	197	9.624	1.424	11.603
520	HETATM	520	O	O	198	6.537	0.867	12.423
521	HETATM	521	1H6	H	198	6.070	1.201	11.604
522	HETATM	522	2H6	H	198	7.484	1.191	12.421
523	HETATM	523	O	O	199	5.198	-2.820	10.178
524	HETATM	524	1H1	H	199	4.259	-2.478	10.176
525	HETATM	525	2H1	H	199	5.673	-2.488	10.992
526	HETATM	526	O	O	200	6.511	-1.919	7.914
527	HETATM	527	1H2	H	200	6.521	-0.919	7.910
528	HETATM	528	2H2	H	200	6.037	-2.244	8.732
529	HETATM	529	O	O	201	9.111	-2.865	7.918
530	HETATM	530	1H3	H	201	8.172	-2.524	7.916
531	HETATM	531	2H3	H	201	9.587	-2.534	8.733
532	HETATM	532	O	O	202	10.425	-1.947	10.174
533	HETATM	533	1H4	H	202	10.435	-0.947	10.170
534	HETATM	534	2H4	H	202	9.950	-2.272	10.991
535	HETATM	535	O	O	203	9.112	-2.847	12.438
536	HETATM	536	1H5	H	203	8.172	-2.505	12.436
537	HETATM	537	2H5	H	203	9.587	-2.515	13.252
538	HETATM	538	O	O	204	6.511	-1.901	12.434
539	HETATM	539	1H6	H	204	6.521	-0.901	12.430
540	HETATM	540	2H6	H	204	6.037	-2.226	13.251
541	HETATM	541	O	O	207	-10.414	1.903	1.120
542	HETATM	542	1H3	H	207	-10.404	2.903	1.116
543	HETATM	543	2H3	H	207	-9.946	1.562	0.306
544	HETATM	544	O	O	208	-9.117	0.978	3.384
545	HETATM	545	1H4	H	208	-9.586	1.312	2.567
546	HETATM	546	2H4	H	208	-8.172	1.302	3.383
547	HETATM	547	O	O	209	-10.413	1.921	5.640
548	HETATM	548	1H5	H	209	-10.404	2.921	5.636
549	HETATM	549	2H5	H	209	-9.946	1.580	4.825
550	HETATM	550	O	O	213	-10.457	-2.709	1.139
551	HETATM	551	1H3	H	213	-11.397	-2.367	1.137
552	HETATM	552	2H3	H	213	-9.983	-2.377	1.954
553	HETATM	553	O	O	214	-9.143	-1.790	3.395
554	HETATM	554	1H4	H	214	-9.134	-0.790	3.391
555	HETATM	555	2H4	H	214	-9.618	-2.115	4.213
556	HETATM	556	O	O	215	-10.457	-2.691	5.659
557	HETATM	557	1H5	H	215	-11.397	-2.349	5.657
558	HETATM	558	2H5	H	215	-9.983	-2.359	6.473
559	HETATM	559	O	O	217	-6.500	1.875	3.380
560	HETATM	560	1H1	H	217	-6.490	2.875	3.376
561	HETATM	561	2H1	H	217	-6.032	1.535	2.566
562	HETATM	562	O	O	218	-5.204	0.932	1.124
563	HETATM	563	1H2	H	218	-5.672	1.266	0.307
564	HETATM	564	2H2	H	218	-4.258	1.256	1.123
565	HETATM	565	O	O	219	-2.586	1.829	1.120
566	HETATM	566	1H3	H	219	-2.577	2.829	1.116
567	HETATM	567	2H3	H	219	-2.118	1.489	0.306

568	HETATM	568	O	O	220	-1.291	0.904	3.384
569	HETATM	569	1H4	H	220	-1.758	1.238	2.567
570	HETATM	570	2H4	H	220	-0.344	1.228	3.383
571	HETATM	571	O	O	221	-2.586	1.848	5.640
572	HETATM	572	1H5	H	221	-2.576	2.848	5.636
573	HETATM	573	2H5	H	221	-2.118	1.507	4.825
574	HETATM	574	O	O	222	-5.204	0.950	5.644
575	HETATM	575	1H6	H	222	-5.672	1.284	4.826
576	HETATM	576	2H6	H	222	-4.258	1.274	5.643
577	HETATM	577	O	O	223	-6.543	-2.737	3.399
578	HETATM	578	1H1	H	223	-7.483	-2.395	3.397
579	HETATM	579	2H1	H	223	-6.069	-2.405	4.214
580	HETATM	580	O	O	224	-5.230	-1.836	1.135
581	HETATM	581	1H2	H	224	-5.221	-0.836	1.131
582	HETATM	582	2H2	H	224	-5.705	-2.161	1.953
583	HETATM	583	O	O	225	-2.629	-2.782	1.139
584	HETATM	584	1H3	H	225	-3.569	-2.441	1.137
585	HETATM	585	2H3	H	225	-2.155	-2.451	1.954
586	HETATM	586	O	O	226	-1.317	-1.864	3.395
587	HETATM	587	1H4	H	226	-1.307	-0.864	3.391
588	HETATM	588	2H4	H	226	-1.791	-2.189	4.213
589	HETATM	589	O	O	227	-2.629	-2.764	5.659
590	HETATM	590	1H5	H	227	-3.569	-2.422	5.657
591	HETATM	591	2H5	H	227	-2.155	-2.432	6.473
592	HETATM	592	O	O	228	-5.230	-1.818	5.655
593	HETATM	593	1H6	H	228	-5.221	-0.818	5.651
594	HETATM	594	2H6	H	228	-5.704	-2.143	6.472
595	HETATM	595	O	O	229	1.328	1.802	3.380
596	HETATM	596	1H1	H	229	1.337	2.802	3.376
597	HETATM	597	2H1	H	229	1.796	1.461	2.566
598	HETATM	598	O	O	230	2.623	0.858	1.124
599	HETATM	599	1H2	H	230	2.155	1.192	0.307
600	HETATM	600	2H2	H	230	3.569	1.182	1.123
601	HETATM	601	O	O	231	5.241	1.756	1.120
602	HETATM	602	1H3	H	231	5.250	2.756	1.116
603	HETATM	603	2H3	H	231	5.710	1.415	0.306
604	HETATM	604	O	O	232	6.537	0.831	3.384
605	HETATM	605	1H4	H	232	6.069	1.165	2.567
606	HETATM	606	2H4	H	232	7.483	1.155	3.383
607	HETATM	607	O	O	233	5.241	1.774	5.640
608	HETATM	608	1H5	H	233	5.250	2.774	5.636
609	HETATM	609	2H5	H	233	5.710	1.433	4.825
610	HETATM	610	O	O	234	2.623	0.877	5.644
611	HETATM	611	1H6	H	234	2.155	1.211	4.826
612	HETATM	612	2H6	H	234	3.569	1.201	5.643
613	HETATM	613	O	O	235	1.285	-2.810	3.399
614	HETATM	614	1H1	H	235	0.345	-2.468	3.397
615	HETATM	615	2H1	H	235	1.759	-2.478	4.214
616	HETATM	616	O	O	236	2.597	-1.910	1.135
617	HETATM	617	1H2	H	236	2.607	-0.910	1.131
618	HETATM	618	2H2	H	236	2.123	-2.235	1.953
619	HETATM	619	O	O	237	5.197	-2.856	1.139
620	HETATM	620	1H3	H	237	4.259	-2.514	1.137
621	HETATM	621	2H3	H	237	5.673	-2.524	1.954

622	HETATM	622	O	O	238	6.511	-1.937	3.395
623	HETATM	623	1H4	H	238	6.520	-0.937	3.391
624	HETATM	624	2H4	H	238	6.037	-2.262	4.213
625	HETATM	625	O	O	239	5.198	-2.838	5.659
626	HETATM	626	1H5	H	239	4.259	-2.496	5.657
627	HETATM	627	2H5	H	239	5.673	-2.506	6.473
628	HETATM	628	O	O	240	2.597	-1.891	5.655
629	HETATM	629	1H6	H	240	2.607	-0.891	5.651
630	HETATM	630	2H6	H	240	2.123	-2.217	6.472
631	HETATM	631	O	O	241	9.155	1.728	3.380
632	HETATM	632	1H1	H	241	9.164	2.728	3.376
633	HETATM	633	2H1	H	241	9.623	1.387	2.566
634	HETATM	634	O	O	242	10.451	0.785	1.124
635	HETATM	635	1H2	H	242	9.982	1.119	0.307
636	HETATM	636	2H2	H	242	11.397	1.109	1.123
637	HETATM	637	O	O	246	10.451	0.803	5.644
638	HETATM	638	1H6	H	246	9.982	1.137	4.826
639	HETATM	639	2H6	H	246	11.397	1.127	5.643
640	HETATM	640	O	O	247	9.111	-2.884	3.399
641	HETATM	641	1H1	H	247	8.171	-2.542	3.397
642	HETATM	642	2H1	H	247	9.586	-2.552	4.214
643	HETATM	643	O	O	248	10.425	-1.983	1.135
644	HETATM	644	1H2	H	248	10.434	-0.983	1.131
645	HETATM	645	2H2	H	248	9.950	-2.308	1.953
646	HETATM	646	O	O	252	10.425	-1.965	5.655
647	HETATM	647	1H6	H	252	10.434	-0.965	5.651
648	HETATM	648	2H6	H	252	9.950	-2.290	6.472
649	HETATM	649	O	O	253	-10.414	1.885	-3.399
650	HETATM	650	1H1	H	253	-10.404	2.885	-3.403
651	HETATM	651	2H1	H	253	-9.946	1.544	-4.213
652	HETATM	652	O	O	254	-9.118	0.941	-5.655
653	HETATM	653	1H2	H	254	-9.586	1.276	-6.472
654	HETATM	654	2H2	H	254	-8.172	1.266	-5.656
655	HETATM	655	O	O	255	-6.500	1.839	-5.659
656	HETATM	656	1H3	H	255	-6.491	2.839	-5.663
657	HETATM	657	2H3	H	255	-6.032	1.498	-6.473
658	HETATM	658	O	O	256	-5.205	0.914	-3.395
659	HETATM	659	1H4	H	256	-5.673	1.248	-4.212
660	HETATM	660	2H4	H	256	-4.259	1.238	-3.396
661	HETATM	661	O	O	257	-6.500	1.857	-1.139
662	HETATM	662	1H5	H	257	-6.490	2.857	-1.143
663	HETATM	663	2H5	H	257	-6.032	1.516	-1.954
664	HETATM	664	O	O	258	-9.117	0.960	-1.135
665	HETATM	665	1H6	H	258	-9.586	1.294	-1.953
666	HETATM	666	2H6	H	258	-8.172	1.284	-1.136
667	HETATM	667	O	O	259	-10.457	-2.727	-3.380
668	HETATM	668	1H1	H	259	-11.397	-2.385	-3.382
669	HETATM	669	2H1	H	259	-9.983	-2.395	-2.565
670	HETATM	670	O	O	260	-9.144	-1.826	-5.644
671	HETATM	671	1H2	H	260	-9.134	-0.827	-5.648
672	HETATM	672	2H2	H	260	-9.619	-2.152	-4.826
673	HETATM	673	O	O	261	-6.543	-2.773	-5.640
674	HETATM	674	1H3	H	261	-7.483	-2.431	-5.642
675	HETATM	675	2H3	H	261	-6.069	-2.441	-4.825

676	HETATM	676	O	O	262	-5.231	-1.854	-3.384
677	HETATM	677	1H4	H	262	-5.221	-0.854	-3.388
678	HETATM	678	2H4	H	262	-5.705	-2.179	-2.566
679	HETATM	679	O	O	263	-6.543	-2.755	-1.120
680	HETATM	680	1H5	H	263	-7.483	-2.413	-1.122
681	HETATM	681	2H5	H	263	-6.069	-2.423	-0.306
682	HETATM	682	O	O	264	-9.143	-1.808	-1.124
683	HETATM	683	1H6	H	264	-9.134	-0.808	-1.128
684	HETATM	684	2H6	H	264	-9.618	-2.133	-0.307
685	HETATM	685	O	O	265	-2.586	1.811	-3.399
686	HETATM	686	1H1	H	265	-2.577	2.811	-3.403
687	HETATM	687	2H1	H	265	-2.118	1.470	-4.213
688	HETATM	688	O	O	266	-1.291	0.868	-5.655
689	HETATM	689	1H2	H	266	-1.759	1.202	-6.472
690	HETATM	690	2H2	H	266	-0.345	1.192	-5.656
691	HETATM	691	O	O	267	1.328	1.765	-5.659
692	HETATM	692	1H3	H	267	1.337	2.765	-5.663
693	HETATM	693	2H3	H	267	1.795	1.425	-6.473
694	HETATM	694	O	O	268	2.623	0.840	-3.395
695	HETATM	695	1H4	H	268	2.155	1.174	-4.212
696	HETATM	696	2H4	H	268	3.569	1.164	-3.396
697	HETATM	697	O	O	269	1.328	1.783	-1.139
698	HETATM	698	1H5	H	269	1.337	2.783	-1.143
699	HETATM	699	2H5	H	269	1.796	1.443	-1.954
700	HETATM	700	O	O	270	-1.291	0.886	-1.135
701	HETATM	701	1H6	H	270	-1.759	1.220	-1.953
702	HETATM	702	2H6	H	270	-0.345	1.210	-1.136
703	HETATM	703	O	O	271	-2.629	-2.801	-3.380
704	HETATM	704	1H1	H	271	-3.569	-2.459	-3.382
705	HETATM	705	2H1	H	271	-2.155	-2.469	-2.565
706	HETATM	706	O	O	272	-1.317	-1.900	-5.644
707	HETATM	707	1H2	H	272	-1.308	-0.900	-5.648
708	HETATM	708	2H2	H	272	-1.791	-2.225	-4.826
709	HETATM	709	O	O	273	1.284	-2.847	-5.640
710	HETATM	710	1H3	H	273	0.344	-2.505	-5.642
711	HETATM	711	2H3	H	273	1.758	-2.515	-4.825
712	HETATM	712	O	O	274	2.597	-1.928	-3.384
713	HETATM	713	1H4	H	274	2.606	-0.928	-3.388
714	HETATM	714	2H4	H	274	2.123	-2.253	-2.566
715	HETATM	715	O	O	275	1.284	-2.828	-1.120
716	HETATM	716	1H5	H	275	0.345	-2.486	-1.122
717	HETATM	717	2H5	H	275	1.759	-2.496	-0.306
718	HETATM	718	O	O	276	-1.317	-1.882	-1.124
719	HETATM	719	1H6	H	276	-1.307	-0.882	-1.128
720	HETATM	720	2H6	H	276	-1.791	-2.207	-0.307
721	HETATM	721	O	O	277	5.241	1.738	-3.399
722	HETATM	722	1H1	H	277	5.250	2.738	-3.403
723	HETATM	723	2H1	H	277	5.709	1.397	-4.213
724	HETATM	724	O	O	278	6.537	0.794	-5.655
725	HETATM	725	1H2	H	278	6.069	1.128	-6.472
726	HETATM	726	2H2	H	278	7.483	1.118	-5.656
727	HETATM	727	O	O	279	9.154	1.692	-5.659
728	HETATM	728	1H3	H	279	9.164	2.692	-5.663
729	HETATM	729	2H3	H	279	9.623	1.351	-6.473

730	HETATM	730	O	O	280	10.451	0.767	-3.395
731	HETATM	731	1H4	H	280	9.982	1.101	-4.212
732	HETATM	732	2H4	H	280	11.397	1.091	-3.396
733	HETATM	733	O	O	281	9.154	1.710	-1.139
734	HETATM	734	1H5	H	281	9.164	2.710	-1.143
735	HETATM	735	2H5	H	281	9.623	1.369	-1.954
736	HETATM	736	O	O	282	6.537	0.812	-1.135
737	HETATM	737	1H6	H	282	6.069	1.147	-1.953
738	HETATM	738	2H6	H	282	7.483	1.137	-1.136
739	HETATM	739	O	O	283	5.197	-2.874	-3.380
740	HETATM	740	1H1	H	283	4.258	-2.532	-3.382
741	HETATM	741	2H1	H	283	5.672	-2.542	-2.565
742	HETATM	742	O	O	284	6.511	-1.974	-5.644
743	HETATM	743	1H2	H	284	6.520	-0.974	-5.648
744	HETATM	744	2H2	H	284	6.037	-2.299	-4.826
745	HETATM	745	O	O	285	9.111	-2.920	-5.640
746	HETATM	746	1H3	H	285	8.171	-2.578	-5.642
747	HETATM	747	2H3	H	285	9.586	-2.588	-4.825
748	HETATM	748	O	O	286	10.425	-2.001	-3.384
749	HETATM	749	1H4	H	286	10.434	-1.001	-3.388
750	HETATM	750	2H4	H	286	9.950	-2.327	-2.566
751	HETATM	751	O	O	287	9.111	-2.902	-1.120
752	HETATM	752	1H5	H	287	8.171	-2.560	-1.122
753	HETATM	753	2H5	H	287	9.586	-2.570	-0.306
754	HETATM	754	O	O	288	6.511	-1.955	-1.124
755	HETATM	755	1H6	H	288	6.520	-0.955	-1.128
756	HETATM	756	2H6	H	288	6.037	-2.281	-0.307
757	HETATM	757	O	O	291	-10.414	1.848	-12.438
758	HETATM	758	1H3	H	291	-10.405	2.848	-12.442
759	HETATM	759	2H3	H	291	-9.946	1.508	-13.252
760	HETATM	760	O	O	292	-9.118	0.923	-10.174
761	HETATM	761	1H4	H	292	-9.587	1.257	-10.991
762	HETATM	762	2H4	H	292	-8.173	1.247	-10.175
763	HETATM	763	O	O	293	-10.414	1.867	-7.918
764	HETATM	764	1H5	H	293	-10.405	2.866	-7.922
765	HETATM	765	2H5	H	293	-9.946	1.526	-8.733
766	HETATM	766	O	O	297	-10.457	-2.763	-12.419
767	HETATM	767	1H3	H	297	-11.397	-2.422	-12.420
768	HETATM	768	2H3	H	297	-9.983	-2.432	-11.603
769	HETATM	769	O	O	298	-9.144	-1.845	-10.163
770	HETATM	770	1H4	H	298	-9.134	-0.845	-10.167
771	HETATM	771	2H4	H	298	-9.619	-2.170	-9.345
772	HETATM	772	O	O	299	-10.457	-2.745	-7.899
773	HETATM	773	1H5	H	299	-11.397	-2.403	-7.900
774	HETATM	774	2H5	H	299	-9.983	-2.413	-7.084
775	HETATM	775	O	O	301	-6.500	1.821	-10.178
776	HETATM	776	1H1	H	301	-6.491	2.821	-10.182
777	HETATM	777	2H1	H	301	-6.032	1.480	-10.992
778	HETATM	778	O	O	302	-5.205	0.877	-12.434
779	HETATM	779	1H2	H	302	-5.673	1.211	-13.251
780	HETATM	780	2H2	H	302	-4.259	1.201	-12.435
781	HETATM	781	O	O	303	-2.586	1.775	-12.438
782	HETATM	782	1H3	H	303	-2.577	2.775	-12.442
783	HETATM	783	2H3	H	303	-2.119	1.434	-13.252

784	HETATM	784	O	O	304	-1.291	0.850	-10.174
785	HETATM	785	1H4	H	304	-1.759	1.184	-10.991
786	HETATM	786	2H4	H	304	-0.345	1.174	-10.175
787	HETATM	787	O	O	305	-2.586	1.793	-7.918
788	HETATM	788	1H5	H	305	-2.577	2.793	-7.922
789	HETATM	789	2H5	H	305	-2.118	1.452	-8.733
790	HETATM	790	O	O	306	-5.205	0.896	-7.914
791	HETATM	791	1H6	H	306	-5.673	1.230	-8.732
792	HETATM	792	2H6	H	306	-4.259	1.220	-7.915
793	HETATM	793	O	O	307	-6.544	-2.791	-10.159
794	HETATM	794	1H1	H	307	-7.483	-2.449	-10.160
795	HETATM	795	2H1	H	307	-6.069	-2.459	-9.343
796	HETATM	796	O	O	308	-5.231	-1.891	-12.423
797	HETATM	797	1H2	H	308	-5.222	-0.891	-12.427
798	HETATM	798	2H2	H	308	-5.705	-2.216	-11.604
799	HETATM	799	O	O	309	-2.630	-2.837	-12.419
800	HETATM	800	1H3	H	309	-3.570	-2.495	-12.420
801	HETATM	801	2H3	H	309	-2.156	-2.505	-11.603
802	HETATM	802	O	O	310	-1.317	-1.918	-10.163
803	HETATM	803	1H4	H	310	-1.308	-0.918	-10.167
804	HETATM	804	2H4	H	310	-1.791	-2.243	-9.345
805	HETATM	805	O	O	311	-2.630	-2.819	-7.899
806	HETATM	806	1H5	H	311	-3.569	-2.477	-7.900
807	HETATM	807	2H5	H	311	-2.155	-2.487	-7.084
808	HETATM	808	O	O	312	-5.231	-1.872	-7.903
809	HETATM	809	1H6	H	312	-5.221	-0.872	-7.907
810	HETATM	810	2H6	H	312	-5.705	-2.198	-7.086
811	HETATM	811	O	O	313	1.327	1.747	-10.178
812	HETATM	812	1H1	H	313	1.337	2.747	-10.182
813	HETATM	813	2H1	H	313	1.795	1.406	-10.992
814	HETATM	814	O	O	314	2.623	0.804	-12.434
815	HETATM	815	1H2	H	314	2.155	1.138	-13.251
816	HETATM	816	2H2	H	314	3.569	1.128	-12.435
817	HETATM	817	O	O	315	5.240	1.701	-12.438
818	HETATM	818	1H3	H	315	5.250	2.701	-12.442
819	HETATM	819	2H3	H	315	5.709	1.360	-13.252
820	HETATM	820	O	O	316	6.537	0.776	-10.174
821	HETATM	821	1H4	H	316	6.069	1.110	-10.991
822	HETATM	822	2H4	H	316	7.483	1.100	-10.175
823	HETATM	823	O	O	317	5.240	1.719	-7.918
824	HETATM	824	1H5	H	317	5.250	2.719	-7.922
825	HETATM	825	2H5	H	317	5.709	1.379	-8.733
826	HETATM	826	O	O	318	2.623	0.822	-7.914
827	HETATM	827	1H6	H	318	2.155	1.156	-8.732
828	HETATM	828	2H6	H	318	3.569	1.146	-7.915
829	HETATM	829	O	O	319	1.284	-2.865	-10.159
830	HETATM	830	1H1	H	319	0.344	-2.523	-10.160
831	HETATM	831	2H1	H	319	1.758	-2.533	-9.343
832	HETATM	832	O	O	320	2.597	-1.964	-12.423
833	HETATM	833	1H2	H	320	2.606	-0.964	-12.427
834	HETATM	834	2H2	H	320	2.123	-2.289	-11.604
835	HETATM	835	O	O	321	5.197	-2.911	-12.419
836	HETATM	836	1H3	H	321	4.258	-2.569	-12.420
837	HETATM	837	2H3	H	321	5.672	-2.579	-11.603

838	HETATM	838	O	O	322	6.511	-1.992	-10.163
839	HETATM	839	1H4	H	322	6.520	-0.992	-10.167
840	HETATM	840	2H4	H	322	6.036	-2.317	-9.345
841	HETATM	841	O	O	323	5.197	-2.892	-7.899
842	HETATM	842	1H5	H	323	4.258	-2.551	-7.900
843	HETATM	843	2H5	H	323	5.672	-2.561	-7.084
844	HETATM	844	O	O	324	2.597	-1.946	-7.903
845	HETATM	845	1H6	H	324	2.606	-0.946	-7.907
846	HETATM	846	2H6	H	324	2.123	-2.271	-7.086
847	HETATM	847	O	O	325	9.154	1.673	-10.178
848	HETATM	848	1H1	H	325	9.164	2.673	-10.182
849	HETATM	849	2H1	H	325	9.623	1.333	-10.992
850	HETATM	850	O	O	326	10.450	0.730	-12.434
851	HETATM	851	1H2	H	326	9.981	1.064	-13.251
852	HETATM	852	2H2	H	326	11.396	1.054	-12.435
853	HETATM	853	O	O	330	10.451	0.748	-7.914
854	HETATM	854	1H6	H	330	9.982	1.082	-8.732
855	HETATM	855	2H6	H	330	11.397	1.072	-7.915
856	HETATM	856	O	O	331	9.111	-2.938	-10.159
857	HETATM	857	1H1	H	331	8.171	-2.596	-10.160
858	HETATM	858	2H1	H	331	9.586	-2.606	-9.343
859	HETATM	859	O	O	332	10.424	-2.038	-12.423
860	HETATM	860	1H2	H	332	10.434	-1.038	-12.427
861	HETATM	861	2H2	H	332	9.949	-2.363	-11.604
862	HETATM	862	O	O	336	10.424	-2.020	-7.903
863	HETATM	863	1H6	H	336	10.434	-1.020	-7.907
864	HETATM	864	2H6	H	336	9.949	-2.345	-7.086
865	HETATM	865	O	O	337	-10.344	9.319	10.129
866	HETATM	866	1H1	H	337	-10.334	10.319	10.125
867	HETATM	867	2H1	H	337	-9.876	8.978	9.315
868	HETATM	868	O	O	338	-9.048	8.376	7.873
869	HETATM	869	1H2	H	338	-9.517	8.710	7.056
870	HETATM	870	2H2	H	338	-8.103	8.700	7.872
871	HETATM	871	O	O	339	-6.430	9.273	7.869
872	HETATM	872	1H3	H	339	-6.421	10.273	7.865
873	HETATM	873	2H3	H	339	-5.962	8.932	7.055
874	HETATM	874	O	O	340	-5.135	8.348	10.133
875	HETATM	875	1H4	H	340	-5.603	8.682	9.316
876	HETATM	876	2H4	H	340	-4.189	8.672	10.132
877	HETATM	877	O	O	341	-6.430	9.291	12.389
878	HETATM	878	1H5	H	341	-6.421	10.291	12.385
879	HETATM	879	2H5	H	341	-5.962	8.951	11.574
880	HETATM	880	O	O	342	-9.047	8.394	12.393
881	HETATM	881	1H6	H	342	-9.516	8.728	11.575
882	HETATM	882	2H6	H	342	-8.102	8.718	12.392
883	HETATM	883	O	O	343	-10.387	4.707	10.148
884	HETATM	884	1H1	H	343	-11.327	5.049	10.147
885	HETATM	885	2H1	H	343	-9.913	5.039	10.963
886	HETATM	886	O	O	344	-9.074	5.608	7.884
887	HETATM	887	1H2	H	344	-9.064	6.608	7.880
888	HETATM	888	2H2	H	344	-9.549	5.283	8.703
889	HETATM	889	O	O	345	-6.473	4.661	7.888
890	HETATM	890	1H3	H	345	-7.413	5.003	7.887
891	HETATM	891	2H3	H	345	-5.999	4.993	8.704

892	HETATM	892	O	O	346	-5.161	5.580	10.144
893	HETATM	893	1H4	H	346	-5.151	6.580	10.140
894	HETATM	894	2H4	H	346	-5.635	5.255	10.962
895	HETATM	895	O	O	347	-6.473	4.680	12.408
896	HETATM	896	1H5	H	347	-7.413	5.021	12.407
897	HETATM	897	2H5	H	347	-5.999	5.011	13.223
898	HETATM	898	O	O	348	-9.074	5.626	12.404
899	HETATM	899	1H6	H	348	-9.064	6.626	12.400
900	HETATM	900	2H6	H	348	-9.549	5.301	13.222
901	HETATM	901	O	O	349	-2.516	9.245	10.129
902	HETATM	902	1H1	H	349	-2.507	10.245	10.125
903	HETATM	903	2H1	H	349	-2.048	8.905	9.315
904	HETATM	904	O	O	350	-1.221	8.302	7.873
905	HETATM	905	1H2	H	350	-1.689	8.636	7.056
906	HETATM	906	2H2	H	350	-0.275	8.626	7.872
907	HETATM	907	O	O	351	1.398	9.199	7.869
908	HETATM	908	1H3	H	351	1.407	10.199	7.865
909	HETATM	909	2H3	H	351	1.865	8.859	7.055
910	HETATM	910	O	O	352	2.693	8.274	10.133
911	HETATM	911	1H4	H	352	2.225	8.608	9.316
912	HETATM	912	2H4	H	352	3.639	8.598	10.132
913	HETATM	913	O	O	353	1.398	9.218	12.389
914	HETATM	914	1H5	H	353	1.407	10.218	12.385
915	HETATM	915	2H5	H	353	1.866	8.877	11.574
916	HETATM	916	O	O	354	-1.221	8.320	12.393
917	HETATM	917	1H6	H	354	-1.689	8.654	11.575
918	HETATM	918	2H6	H	354	-0.275	8.644	12.392
919	HETATM	919	O	O	355	-2.560	4.634	10.148
920	HETATM	920	1H1	H	355	-3.499	4.975	10.147
921	HETATM	921	2H1	H	355	-2.085	4.965	10.963
922	HETATM	922	O	O	356	-1.247	5.534	7.884
923	HETATM	923	1H2	H	356	-1.238	6.534	7.880
924	HETATM	924	2H2	H	356	-1.721	5.209	8.703
925	HETATM	925	O	O	357	1.354	4.588	7.888
926	HETATM	926	1H3	H	357	0.414	4.930	7.887
927	HETATM	927	2H3	H	357	1.828	4.920	8.704
928	HETATM	928	O	O	358	2.667	5.507	10.144
929	HETATM	929	1H4	H	358	2.676	6.506	10.140
930	HETATM	930	2H4	H	358	2.193	5.181	10.962
931	HETATM	931	O	O	359	1.354	4.606	12.408
932	HETATM	932	1H5	H	359	0.415	4.948	12.407
933	HETATM	933	2H5	H	359	1.829	4.938	13.223
934	HETATM	934	O	O	360	-1.247	5.552	12.404
935	HETATM	935	1H6	H	360	-1.237	6.552	12.400
936	HETATM	936	2H6	H	360	-1.721	5.227	13.222
937	HETATM	937	O	O	361	5.310	9.172	10.129
938	HETATM	938	1H1	H	361	5.320	10.172	10.125
939	HETATM	939	2H1	H	361	5.779	8.831	9.315
940	HETATM	940	O	O	362	6.607	8.228	7.873
941	HETATM	941	1H2	H	362	6.139	8.563	7.056
942	HETATM	942	2H2	H	362	7.553	8.553	7.872
943	HETATM	943	O	O	363	9.224	9.126	7.869
944	HETATM	944	1H3	H	363	9.234	10.126	7.865
945	HETATM	945	2H3	H	363	9.693	8.785	7.055

946	HETATM	946	O	O	364	10.521	8.201	10.133
947	HETATM	947	1H4	H	364	10.052	8.535	9.316
948	HETATM	948	2H4	H	364	11.467	8.525	10.132
949	HETATM	949	O	O	365	9.224	9.144	12.389
950	HETATM	950	1H5	H	365	9.234	10.144	12.385
951	HETATM	951	2H5	H	365	9.693	8.803	11.574
952	HETATM	952	O	O	366	6.607	8.247	12.393
953	HETATM	953	1H6	H	366	6.139	8.581	11.575
954	HETATM	954	2H6	H	366	7.553	8.571	12.392
955	HETATM	955	O	O	367	5.267	4.560	10.148
956	HETATM	956	1H1	H	367	4.328	4.902	10.147
957	HETATM	957	2H1	H	367	5.742	4.892	10.963
958	HETATM	958	O	O	368	6.581	5.461	7.884
959	HETATM	959	1H2	H	368	6.590	6.461	7.880
960	HETATM	960	2H2	H	368	6.107	5.135	8.703
961	HETATM	961	O	O	369	9.181	4.514	7.888
962	HETATM	962	1H3	H	369	8.241	4.856	7.887
963	HETATM	963	2H3	H	369	9.656	4.846	8.704
964	HETATM	964	O	O	370	10.495	5.433	10.144
965	HETATM	965	1H4	H	370	10.504	6.433	10.140
966	HETATM	966	2H4	H	370	10.019	5.108	10.962
967	HETATM	967	O	O	371	9.181	4.532	12.408
968	HETATM	968	1H5	H	371	8.241	4.874	12.407
969	HETATM	969	2H5	H	371	9.656	4.864	13.223
970	HETATM	970	O	O	372	6.581	5.479	12.404
971	HETATM	971	1H6	H	372	6.590	6.479	12.400
972	HETATM	972	2H6	H	372	6.107	5.154	13.222
973	HETATM	973	O	O	375	-10.344	9.283	1.090
974	HETATM	974	1H3	H	375	-10.335	10.283	1.086
975	HETATM	975	2H3	H	375	-9.876	8.942	0.276
976	HETATM	976	O	O	376	-9.048	8.357	3.354
977	HETATM	977	1H4	H	376	-9.517	8.692	2.537
978	HETATM	978	2H4	H	376	-8.103	8.682	3.353
979	HETATM	979	O	O	377	-10.344	9.301	5.610
980	HETATM	980	1H5	H	377	-10.335	10.301	5.606
981	HETATM	981	2H5	H	377	-9.876	8.960	4.795
982	HETATM	982	O	O	381	-10.388	4.671	1.109
983	HETATM	983	1H3	H	381	-11.327	5.013	1.108
984	HETATM	984	2H3	H	381	-9.913	5.003	1.925
985	HETATM	985	O	O	382	-9.074	5.590	3.365
986	HETATM	986	1H4	H	382	-9.064	6.590	3.361
987	HETATM	987	2H4	H	382	-9.549	5.264	4.184
988	HETATM	988	O	O	383	-10.387	4.689	5.629
989	HETATM	989	1H5	H	383	-11.327	5.031	5.628
990	HETATM	990	2H5	H	383	-9.913	5.021	6.444
991	HETATM	991	O	O	385	-6.430	9.255	3.350
992	HETATM	992	1H1	H	385	-6.421	10.255	3.346
993	HETATM	993	2H1	H	385	-5.962	8.914	2.536
994	HETATM	994	O	O	386	-5.135	8.312	1.094
995	HETATM	995	1H2	H	386	-5.603	8.646	0.277
996	HETATM	996	2H2	H	386	-4.189	8.636	1.093
997	HETATM	997	O	O	387	-2.517	9.209	1.090
998	HETATM	998	1H3	H	387	-2.507	10.209	1.086
999	HETATM	999	2H3	H	387	-2.049	8.868	0.276

1000	HETATM	1000	O	O	388	-1.221	8.284	3.354
1001	HETATM	1001	1H4	H	388	-1.689	8.618	2.537
1002	HETATM	1002	2H4	H	388	-0.275	8.608	3.353
1003	HETATM	1003	O	O	389	-2.516	9.227	5.610
1004	HETATM	1004	1H5	H	389	-2.507	10.227	5.606
1005	HETATM	1005	2H5	H	389	-2.049	8.886	4.795
1006	HETATM	1006	O	O	390	-5.135	8.330	5.614
1007	HETATM	1007	1H6	H	390	-5.603	8.664	4.796
1008	HETATM	1008	2H6	H	390	-4.189	8.654	5.613
1009	HETATM	1009	O	O	391	-6.474	4.643	3.369
1010	HETATM	1010	1H1	H	391	-7.413	4.985	3.368
1011	HETATM	1011	2H1	H	391	-5.999	4.975	4.185
1012	HETATM	1012	O	O	392	-5.161	5.544	1.105
1013	HETATM	1013	1H2	H	392	-5.152	6.544	1.101
1014	HETATM	1014	2H2	H	392	-5.635	5.218	1.924
1015	HETATM	1015	O	O	393	-2.560	4.597	1.109
1016	HETATM	1016	1H3	H	393	-3.500	4.939	1.108
1017	HETATM	1017	2H3	H	393	-2.086	4.929	1.925
1018	HETATM	1018	O	O	394	-1.247	5.516	3.365
1019	HETATM	1019	1H4	H	394	-1.238	6.516	3.361
1020	HETATM	1020	2H4	H	394	-1.721	5.191	4.184
1021	HETATM	1021	O	O	395	-2.560	4.615	5.629
1022	HETATM	1022	1H5	H	395	-3.500	4.957	5.628
1023	HETATM	1023	2H5	H	395	-2.086	4.947	6.444
1024	HETATM	1024	O	O	396	-5.161	5.562	5.625
1025	HETATM	1025	1H6	H	396	-5.152	6.562	5.621
1026	HETATM	1026	2H6	H	396	-5.635	5.237	6.443
1027	HETATM	1027	O	O	397	1.397	9.181	3.350
1028	HETATM	1028	1H1	H	397	1.407	10.181	3.346
1029	HETATM	1029	2H1	H	397	1.865	8.841	2.536
1030	HETATM	1030	O	O	398	2.693	8.238	1.094
1031	HETATM	1031	1H2	H	398	2.225	8.572	0.277
1032	HETATM	1032	2H2	H	398	3.639	8.562	1.093
1033	HETATM	1033	O	O	399	5.310	9.135	1.090
1034	HETATM	1034	1H3	H	399	5.320	10.135	1.086
1035	HETATM	1035	2H3	H	399	5.779	8.795	0.276
1036	HETATM	1036	O	O	400	6.606	8.210	3.354
1037	HETATM	1037	1H4	H	400	6.139	8.544	2.537
1038	HETATM	1038	2H4	H	400	7.553	8.534	3.353
1039	HETATM	1039	O	O	401	5.310	9.154	5.610
1040	HETATM	1040	1H5	H	401	5.320	10.154	5.606
1041	HETATM	1041	2H5	H	401	5.779	8.813	4.795
1042	HETATM	1042	O	O	402	2.693	8.256	5.614
1043	HETATM	1043	1H6	H	402	2.225	8.590	4.796
1044	HETATM	1044	2H6	H	402	3.639	8.580	5.613
1045	HETATM	1045	O	O	403	1.354	4.570	3.369
1046	HETATM	1046	1H1	H	403	0.414	4.911	3.368
1047	HETATM	1047	2H1	H	403	1.828	4.901	4.185
1048	HETATM	1048	O	O	404	2.667	5.470	1.105
1049	HETATM	1049	1H2	H	404	2.676	6.470	1.101
1050	HETATM	1050	2H2	H	404	2.192	5.145	1.924
1051	HETATM	1051	O	O	405	5.267	4.524	1.109
1052	HETATM	1052	1H3	H	405	4.328	4.865	1.108
1053	HETATM	1053	2H3	H	405	5.742	4.855	1.925

1054	HETATM	1054	O	O	406	6.580	5.442	3.365
1055	HETATM	1055	1H4	H	406	6.590	6.442	3.361
1056	HETATM	1056	2H4	H	406	6.106	5.117	4.184
1057	HETATM	1057	O	O	407	5.267	4.542	5.629
1058	HETATM	1058	1H5	H	407	4.328	4.884	5.628
1059	HETATM	1059	2H5	H	407	5.742	4.874	6.444
1060	HETATM	1060	O	O	408	2.667	5.488	5.625
1061	HETATM	1061	1H6	H	408	2.676	6.488	5.621
1062	HETATM	1062	2H6	H	408	2.193	5.163	6.443
1063	HETATM	1063	O	O	409	9.224	9.108	3.350
1064	HETATM	1064	1H1	H	409	9.233	10.108	3.346
1065	HETATM	1065	2H1	H	409	9.693	8.767	2.536
1066	HETATM	1066	O	O	410	10.520	8.164	1.094
1067	HETATM	1067	1H2	H	410	10.051	8.499	0.277
1068	HETATM	1068	2H2	H	410	11.466	8.488	1.093
1069	HETATM	1069	O	O	414	10.520	8.183	5.614
1070	HETATM	1070	1H6	H	414	10.052	8.517	4.796
1071	HETATM	1071	2H6	H	414	11.466	8.507	5.613
1072	HETATM	1072	O	O	415	9.181	4.496	3.369
1073	HETATM	1073	1H1	H	415	8.241	4.838	3.368
1074	HETATM	1074	2H1	H	415	9.656	4.828	4.185
1075	HETATM	1075	O	O	416	10.494	5.397	1.105
1076	HETATM	1076	1H2	H	416	10.504	6.396	1.101
1077	HETATM	1077	2H2	H	416	10.019	5.071	1.924
1078	HETATM	1078	O	O	420	10.494	5.415	5.625
1079	HETATM	1079	1H6	H	420	10.504	6.415	5.621
1080	HETATM	1080	2H6	H	420	10.019	5.089	6.443
1081	HETATM	1081	O	O	421	-10.344	9.264	-3.428
1082	HETATM	1082	1H1	H	421	-10.335	10.264	-3.433
1083	HETATM	1083	2H1	H	421	-9.877	8.924	-4.243
1084	HETATM	1084	O	O	422	-9.048	8.321	-5.685
1085	HETATM	1085	1H2	H	422	-9.517	8.655	-6.502
1086	HETATM	1086	2H2	H	422	-8.103	8.645	-5.686
1087	HETATM	1087	O	O	423	-6.431	9.218	-5.688
1088	HETATM	1088	1H3	H	423	-6.421	10.218	-5.693
1089	HETATM	1089	2H3	H	423	-5.963	8.878	-6.503
1090	HETATM	1090	O	O	424	-5.135	8.293	-3.425
1091	HETATM	1091	1H4	H	424	-5.603	8.627	-4.242
1092	HETATM	1092	2H4	H	424	-4.189	8.617	-3.426
1093	HETATM	1093	O	O	425	-6.430	9.237	-1.169
1094	HETATM	1094	1H5	H	425	-6.421	10.237	-1.173
1095	HETATM	1095	2H5	H	425	-5.963	8.896	-1.984
1096	HETATM	1096	O	O	426	-9.048	8.339	-1.165
1097	HETATM	1097	1H6	H	426	-9.517	8.673	-1.983
1098	HETATM	1098	2H6	H	426	-8.103	8.663	-1.166
1099	HETATM	1099	O	O	427	-10.388	4.653	-3.410
1100	HETATM	1100	1H1	H	427	-11.328	4.994	-3.411
1101	HETATM	1101	2H1	H	427	-9.914	4.984	-2.594
1102	HETATM	1102	O	O	428	-9.074	5.553	-5.674
1103	HETATM	1103	1H2	H	428	-9.065	6.553	-5.678
1104	HETATM	1104	2H2	H	428	-9.549	5.228	-4.855
1105	HETATM	1105	O	O	429	-6.474	4.607	-5.670
1106	HETATM	1106	1H3	H	429	-7.414	4.949	-5.671
1107	HETATM	1107	2H3	H	429	-6.000	4.939	-4.854

1108	HETATM	1108	O	O	430	-5.161	5.525	-3.414
1109	HETATM	1109	1H4	H	430	-5.152	6.525	-3.418
1110	HETATM	1110	2H4	H	430	-5.635	5.200	-2.595
1111	HETATM	1111	O	O	431	-6.474	4.625	-1.150
1112	HETATM	1112	1H5	H	431	-7.414	4.967	-1.151
1113	HETATM	1113	2H5	H	431	-6.000	4.957	-0.335
1114	HETATM	1114	O	O	432	-9.074	5.571	-1.154
1115	HETATM	1115	1H6	H	432	-9.065	6.571	-1.158
1116	HETATM	1116	2H6	H	432	-9.549	5.246	-0.336
1117	HETATM	1117	O	O	433	-2.517	9.191	-3.428
1118	HETATM	1118	1H1	H	433	-2.507	10.191	-3.433
1119	HETATM	1119	2H1	H	433	-2.049	8.850	-4.243
1120	HETATM	1120	O	O	434	-1.222	8.247	-5.685
1121	HETATM	1121	1H2	H	434	-1.689	8.582	-6.502
1122	HETATM	1122	2H2	H	434	-0.275	8.572	-5.686
1123	HETATM	1123	O	O	435	1.397	9.145	-5.688
1124	HETATM	1124	1H3	H	435	1.406	10.145	-5.693
1125	HETATM	1125	2H3	H	435	1.865	8.804	-6.503
1126	HETATM	1126	O	O	436	2.692	8.220	-3.425
1127	HETATM	1127	1H4	H	436	2.225	8.554	-4.242
1128	HETATM	1128	2H4	H	436	3.638	8.544	-3.426
1129	HETATM	1129	O	O	437	1.397	9.163	-1.169
1130	HETATM	1130	1H5	H	437	1.407	10.163	-1.173
1131	HETATM	1131	2H5	H	437	1.865	8.822	-1.984
1132	HETATM	1132	O	O	438	-1.221	8.266	-1.165
1133	HETATM	1133	1H6	H	438	-1.689	8.600	-1.983
1134	HETATM	1134	2H6	H	438	-0.275	8.590	-1.166
1135	HETATM	1135	O	O	439	-2.560	4.579	-3.410
1136	HETATM	1136	1H1	H	439	-3.500	4.921	-3.411
1137	HETATM	1137	2H1	H	439	-2.086	4.911	-2.594
1138	HETATM	1138	O	O	440	-1.248	5.480	-5.674
1139	HETATM	1139	1H2	H	440	-1.238	6.480	-5.678
1140	HETATM	1140	2H2	H	440	-1.722	5.154	-4.855
1141	HETATM	1141	O	O	441	1.354	4.533	-5.670
1142	HETATM	1142	1H3	H	441	0.414	4.875	-5.671
1143	HETATM	1143	2H3	H	441	1.828	4.865	-4.854
1144	HETATM	1144	O	O	442	2.666	5.452	-3.414
1145	HETATM	1145	1H4	H	442	2.676	6.452	-3.418
1146	HETATM	1146	2H4	H	442	2.192	5.127	-2.595
1147	HETATM	1147	O	O	443	1.354	4.551	-1.150
1148	HETATM	1148	1H5	H	443	0.414	4.893	-1.151
1149	HETATM	1149	2H5	H	443	1.828	4.883	-0.335
1150	HETATM	1150	O	O	444	-1.247	5.498	-1.154
1151	HETATM	1151	1H6	H	444	-1.238	6.498	-1.158
1152	HETATM	1152	2H6	H	444	-1.721	5.173	-0.336
1153	HETATM	1153	O	O	445	5.310	9.117	-3.428
1154	HETATM	1154	1H1	H	445	5.319	10.117	-3.433
1155	HETATM	1155	2H1	H	445	5.779	8.776	-4.243
1156	HETATM	1156	O	O	446	6.606	8.174	-5.685
1157	HETATM	1157	1H2	H	446	6.138	8.508	-6.502
1158	HETATM	1158	2H2	H	446	7.552	8.498	-5.686
1159	HETATM	1159	O	O	447	9.224	9.071	-5.688
1160	HETATM	1160	1H3	H	447	9.233	10.071	-5.693
1161	HETATM	1161	2H3	H	447	9.693	8.731	-6.503

1162	HETATM	1162	O	O	448	10.520	8.146	-3.425
1163	HETATM	1163	1H4	H	448	10.051	8.480	-4.242
1164	HETATM	1164	2H4	H	448	11.466	8.470	-3.426
1165	HETATM	1165	O	O	449	9.224	9.089	-1.169
1166	HETATM	1166	1H5	H	449	9.233	10.089	-1.173
1167	HETATM	1167	2H5	H	449	9.693	8.749	-1.984
1168	HETATM	1168	O	O	450	6.606	8.192	-1.165
1169	HETATM	1169	1H6	H	450	6.138	8.526	-1.983
1170	HETATM	1170	2H6	H	450	7.552	8.516	-1.166
1171	HETATM	1171	O	O	451	5.267	4.505	-3.410
1172	HETATM	1172	1H1	H	451	4.328	4.847	-3.411
1173	HETATM	1173	2H1	H	451	5.742	4.837	-2.594
1174	HETATM	1174	O	O	452	6.580	5.406	-5.674
1175	HETATM	1175	1H2	H	452	6.590	6.406	-5.678
1176	HETATM	1176	2H2	H	452	6.106	5.081	-4.855
1177	HETATM	1177	O	O	453	9.180	4.460	-5.670
1178	HETATM	1178	1H3	H	453	8.241	4.801	-5.671
1179	HETATM	1179	2H3	H	453	9.655	4.791	-4.854
1180	HETATM	1180	O	O	454	10.494	5.378	-3.414
1181	HETATM	1181	1H4	H	454	10.503	6.378	-3.418
1182	HETATM	1182	2H4	H	454	10.019	5.053	-2.595
1183	HETATM	1183	O	O	455	9.181	4.478	-1.150
1184	HETATM	1184	1H5	H	455	8.241	4.820	-1.151
1185	HETATM	1185	2H5	H	455	9.656	4.810	-0.335
1186	HETATM	1186	O	O	456	6.580	5.424	-1.154
1187	HETATM	1187	1H6	H	456	6.590	6.424	-1.158
1188	HETATM	1188	2H6	H	456	6.106	5.099	-0.336
1189	HETATM	1189	O	O	459	-10.345	9.228	-12.467
1190	HETATM	1190	1H3	H	459	-10.335	10.228	-12.471
1191	HETATM	1191	2H3	H	459	-9.877	8.887	-13.282
1192	HETATM	1192	O	O	460	-9.048	8.303	-10.204
1193	HETATM	1193	1H4	H	460	-9.517	8.637	-11.021
1194	HETATM	1194	2H4	H	460	-8.103	8.627	-10.205
1195	HETATM	1195	O	O	461	-10.345	9.246	-7.947
1196	HETATM	1196	1H5	H	461	-10.335	10.246	-7.951
1197	HETATM	1197	2H5	H	461	-9.877	8.905	-8.763
1198	HETATM	1198	O	O	465	-10.388	4.616	-12.449
1199	HETATM	1199	1H3	H	465	-11.328	4.958	-12.450
1200	HETATM	1200	2H3	H	465	-9.914	4.948	-11.633
1201	HETATM	1201	O	O	466	-9.074	5.535	-10.193
1202	HETATM	1202	1H4	H	466	-9.065	6.535	-10.197
1203	HETATM	1203	2H4	H	466	-9.549	5.210	-9.374
1204	HETATM	1204	O	O	467	-10.388	4.634	-7.929
1205	HETATM	1205	1H5	H	467	-11.328	4.976	-7.930
1206	HETATM	1206	2H5	H	467	-9.914	4.966	-7.114
1207	HETATM	1207	O	O	469	-6.431	9.200	-10.207
1208	HETATM	1208	1H1	H	469	-6.421	10.200	-10.211
1209	HETATM	1209	2H1	H	469	-5.963	8.860	-11.022
1210	HETATM	1210	O	O	470	-5.136	8.257	-12.464
1211	HETATM	1211	1H2	H	470	-5.603	8.591	-13.281
1212	HETATM	1212	2H2	H	470	-4.190	8.581	-12.465
1213	HETATM	1213	O	O	471	-2.517	9.154	-12.467
1214	HETATM	1214	1H3	H	471	-2.508	10.154	-12.471
1215	HETATM	1215	2H3	H	471	-2.049	8.814	-13.282

1216	HETATM	1216	O	O	472	-1.222	8.229	-10.204
1217	HETATM	1217	1H4	H	472	-1.690	8.563	-11.021
1218	HETATM	1218	2H4	H	472	-0.276	8.553	-10.205
1219	HETATM	1219	O	O	473	-2.517	9.173	-7.947
1220	HETATM	1220	1H5	H	473	-2.507	10.173	-7.951
1221	HETATM	1221	2H5	H	473	-2.049	8.832	-8.763
1222	HETATM	1222	O	O	474	-5.135	8.275	-7.944
1223	HETATM	1223	1H6	H	474	-5.603	8.609	-8.762
1224	HETATM	1224	2H6	H	474	-4.189	8.599	-7.945
1225	HETATM	1225	O	O	475	-6.474	4.588	-10.189
1226	HETATM	1226	1H1	H	475	-7.414	4.930	-10.190
1227	HETATM	1227	2H1	H	475	-6.000	4.920	-9.373
1228	HETATM	1228	O	O	476	-5.162	5.489	-12.453
1229	HETATM	1229	1H2	H	476	-5.152	6.489	-12.457
1230	HETATM	1230	2H2	H	476	-5.636	5.164	-11.634
1231	HETATM	1231	O	O	477	-2.560	4.543	-12.449
1232	HETATM	1232	1H3	H	477	-3.500	4.884	-12.450
1233	HETATM	1233	2H3	H	477	-2.086	4.874	-11.633
1234	HETATM	1234	O	O	478	-1.248	5.461	-10.193
1235	HETATM	1235	1H4	H	478	-1.238	6.461	-10.197
1236	HETATM	1236	2H4	H	478	-1.722	5.136	-9.374
1237	HETATM	1237	O	O	479	-2.560	4.561	-7.929
1238	HETATM	1238	1H5	H	479	-3.500	4.903	-7.930
1239	HETATM	1239	2H5	H	479	-2.086	4.893	-7.114
1240	HETATM	1240	O	O	480	-5.161	5.507	-7.933
1241	HETATM	1241	1H6	H	480	-5.152	6.507	-7.937
1242	HETATM	1242	2H6	H	480	-5.636	5.182	-7.115
1243	HETATM	1243	O	O	481	1.397	9.127	-10.207
1244	HETATM	1244	1H1	H	481	1.406	10.127	-10.211
1245	HETATM	1245	2H1	H	481	1.865	8.786	-11.022
1246	HETATM	1246	O	O	482	2.692	8.183	-12.464
1247	HETATM	1247	1H2	H	482	2.224	8.517	-13.281
1248	HETATM	1248	2H2	H	482	3.638	8.507	-12.465
1249	HETATM	1249	O	O	483	5.310	9.081	-12.467
1250	HETATM	1250	1H3	H	483	5.319	10.081	-12.471
1251	HETATM	1251	2H3	H	483	5.778	8.740	-13.282
1252	HETATM	1252	O	O	484	6.606	8.156	-10.204
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1254	HETATM	1254	2H4	H	484	7.552	8.480	-10.205
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1258	HETATM	1258	O	O	486	2.692	8.202	-7.944
1259	HETATM	1259	1H6	H	486	2.224	8.536	-8.762
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1267	HETATM	1267	O	O	489	5.266	4.469	-12.449
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1273	HETATM	1273	O	O	491	5.266	4.487	-7.929
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1275	HETATM	1275	2H5	H	491	5.742	4.819	-7.114
1276	HETATM	1276	O	O	492	2.666	5.434	-7.933
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1278	HETATM	1278	2H6	H	492	2.192	5.108	-7.115
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1280	HETATM	1280	1H1	H	493	9.233	10.053	-10.211
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1285	HETATM	1285	O	O	498	10.520	8.128	-7.944
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A.3 PDB: Sample Generated Ice I_h

The following details a generated Ice I_h .pdb file from the above parent.

1	HETATM	1	O	WAT	0	-10.483	-5.440	10.189	1.00	0.00
			O							
2	HETATM	2	H1	WAT	0	-10.015	-5.781	9.374	1.00	0.00
			H							
3	HETATM	3	H2	WAT	0	-11.429	-5.764	10.190	1.00	0.00
			H							
4	HETATM	4	O	WAT	1	-9.186	-6.385	7.933	1.00	0.00
			O							
5	HETATM	5	H1	WAT	1	-9.655	-6.049	7.115	1.00	0.00
			H							
6	HETATM	6	H2	WAT	1	-9.192	-7.386	7.935	1.00	0.00
			H							
7	HETATM	7	O	WAT	2	-6.569	-5.486	7.929	1.00	0.00
			O							
8	HETATM	8	H1	WAT	2	-6.559	-4.486	7.925	1.00	0.00
			H							
9	HETATM	9	H2	WAT	2	-6.101	-5.821	8.747	1.00	0.00
			H							
10	HETATM	10	O	WAT	3	-5.274	-6.412	10.193	1.00	0.00
			O							

11	HETATM	11	H1	WAT	3	-5.740	-6.070	11.009	1.00	0.00
12	HETATM	12	H2	WAT	3	-5.281	-7.412	10.197	1.00	0.00
13	HETATM	13	O	WAT	4	-6.569	-5.468	12.449	1.00	0.00
14	HETATM	14	H1	WAT	4	-6.559	-4.468	12.445	1.00	0.00
15	HETATM	15	H2	WAT	4	-6.100	-5.803	13.266	1.00	0.00
16	HETATM	16	O	WAT	5	-9.186	-6.366	12.453	1.00	0.00
17	HETATM	17	H1	WAT	5	-9.654	-6.024	13.270	1.00	0.00
18	HETATM	18	H2	WAT	5	-9.194	-7.367	12.457	1.00	0.00
19	HETATM	19	O	WAT	6	-10.526	-10.053	10.207	1.00	0.00
20	HETATM	20	H1	WAT	6	-11.466	-9.710	10.206	1.00	0.00
21	HETATM	21	H2	WAT	6	-10.535	-11.054	10.213	1.00	0.00
22	HETATM	22	O	WAT	7	-9.212	-9.151	7.944	1.00	0.00
23	HETATM	23	H1	WAT	7	-9.203	-8.151	7.940	1.00	0.00
24	HETATM	24	H2	WAT	7	-9.688	-9.477	8.762	1.00	0.00
25	HETATM	25	O	WAT	8	-6.612	-10.099	7.947	1.00	0.00
26	HETATM	26	H1	WAT	8	-6.138	-9.766	8.763	1.00	0.00
27	HETATM	27	H2	WAT	8	-6.135	-9.773	7.130	1.00	0.00
28	HETATM	28	O	WAT	9	-5.300	-9.179	10.204	1.00	0.00
29	HETATM	29	H1	WAT	9	-5.774	-9.504	11.021	1.00	0.00
30	HETATM	30	H2	WAT	9	-5.290	-8.179	10.200	1.00	0.00
31	HETATM	31	O	WAT	10	-6.612	-10.081	12.467	1.00	0.00
32	HETATM	32	H1	WAT	10	-6.136	-9.755	11.649	1.00	0.00
33	HETATM	33	H2	WAT	10	-6.621	-11.082	12.473	1.00	0.00
34	HETATM	34	O	WAT	11	-9.212	-9.133	12.464	1.00	0.00
35	HETATM	35	H1	WAT	11	-9.687	-9.458	13.281	1.00	0.00
36	HETATM	36	H2	WAT	11	-9.686	-9.466	11.649	1.00	0.00
37	HETATM	37	O	WAT	12	-2.655	-5.514	10.189	1.00	0.00

38	HETATM	38	H1	WAT	12	-2.187	-5.848	11.007	1.00	0.00
39	HETATM	39	H2	WAT	12	-3.601	-5.839	10.191	1.00	0.00
40	HETATM	40	O	WAT	13	-1.360	-6.458	7.933	1.00	0.00
41	HETATM	41	H1	WAT	13	-1.368	-7.458	7.937	1.00	0.00
42	HETATM	42	H2	WAT	13	-0.414	-6.133	7.931	1.00	0.00
43	HETATM	43	O	WAT	14	1.259	-5.560	7.929	1.00	0.00
44	HETATM	44	H1	WAT	14	1.727	-5.900	7.114	1.00	0.00
45	HETATM	45	H2	WAT	14	0.313	-5.885	7.930	1.00	0.00
46	HETATM	46	O	WAT	15	2.554	-6.486	10.193	1.00	0.00
47	HETATM	47	H1	WAT	15	2.087	-6.145	11.009	1.00	0.00
48	HETATM	48	H2	WAT	15	2.546	-7.486	10.197	1.00	0.00
49	HETATM	49	O	WAT	16	1.259	-5.542	12.449	1.00	0.00
50	HETATM	50	H1	WAT	16	1.729	-5.877	13.266	1.00	0.00
51	HETATM	51	H2	WAT	16	1.268	-4.542	12.445	1.00	0.00
52	HETATM	52	O	WAT	17	-1.360	-6.440	12.453	1.00	0.00
53	HETATM	53	H1	WAT	17	-0.413	-6.115	12.451	1.00	0.00
54	HETATM	54	H2	WAT	17	-1.367	-7.441	12.458	1.00	0.00
55	HETATM	55	O	WAT	18	-2.698	-10.127	10.207	1.00	0.00
56	HETATM	56	H1	WAT	18	-3.638	-9.784	10.206	1.00	0.00
57	HETATM	57	H2	WAT	18	-2.222	-9.801	9.389	1.00	0.00
58	HETATM	58	O	WAT	19	-1.386	-9.225	7.944	1.00	0.00
59	HETATM	59	H1	WAT	19	-1.862	-9.557	7.129	1.00	0.00
60	HETATM	60	H2	WAT	19	-0.447	-9.568	7.945	1.00	0.00
61	HETATM	61	O	WAT	20	1.215	-10.173	7.947	1.00	0.00
62	HETATM	62	H1	WAT	20	1.690	-9.848	7.130	1.00	0.00
63	HETATM	63	H2	WAT	20	1.690	-9.840	8.763	1.00	0.00
64	HETATM	64	O	WAT	21	2.528	-9.253	10.204	1.00	0.00

65	HETATM	65	H1	WAT	21	2.053	-9.585	9.389	1.00	0.00
66	HETATM	66	H2	WAT	21	2.538	-8.253	10.200	1.00	0.00
67	HETATM	67	O	WAT	22	1.216	-10.154	12.467	1.00	0.00
68	HETATM	68	H1	WAT	22	0.276	-9.811	12.466	1.00	0.00
69	HETATM	69	H2	WAT	22	1.207	-11.155	12.473	1.00	0.00
70	HETATM	70	O	WAT	23	-1.386	-9.207	12.464	1.00	0.00
71	HETATM	71	H1	WAT	23	-1.861	-9.539	11.649	1.00	0.00
72	HETATM	72	H2	WAT	23	-1.860	-9.532	13.281	1.00	0.00
73	HETATM	73	O	WAT	24	5.172	-5.587	10.189	1.00	0.00
74	HETATM	74	H1	WAT	24	4.226	-5.912	10.190	1.00	0.00
75	HETATM	75	H2	WAT	24	5.640	-5.921	11.007	1.00	0.00
76	HETATM	76	O	WAT	25	6.468	-6.532	7.933	1.00	0.00
77	HETATM	77	H1	WAT	25	7.414	-6.207	7.931	1.00	0.00
78	HETATM	78	H2	WAT	25	6.001	-6.191	8.749	1.00	0.00
79	HETATM	79	O	WAT	26	9.085	-5.633	7.929	1.00	0.00
80	HETATM	80	H1	WAT	26	8.139	-5.957	7.929	1.00	0.00
81	HETATM	81	H2	WAT	26	9.553	-5.968	8.747	1.00	0.00
82	HETATM	82	O	WAT	27	10.382	-6.559	10.193	1.00	0.00
83	HETATM	83	H1	WAT	27	9.914	-6.218	11.009	1.00	0.00
84	HETATM	84	H2	WAT	27	9.913	-6.224	9.375	1.00	0.00
85	HETATM	85	O	WAT	28	9.086	-5.615	12.449	1.00	0.00
86	HETATM	86	H1	WAT	28	9.095	-4.615	12.445	1.00	0.00
87	HETATM	87	H2	WAT	28	8.140	-5.940	12.451	1.00	0.00
88	HETATM	88	O	WAT	29	6.468	-6.514	12.453	1.00	0.00
89	HETATM	89	H1	WAT	29	6.000	-6.178	11.634	1.00	0.00
90	HETATM	90	H2	WAT	29	7.414	-6.188	12.451	1.00	0.00
91	HETATM	91	O	WAT	30	5.128	-10.200	10.207	1.00	0.00

92	HETATM	92	H1	WAT	30	4.190	-9.857	10.206	1.00	0.00
93	HETATM	93	H2	WAT	30	5.603	-9.876	9.390	1.00	0.00
94	HETATM	94	O	WAT	31	6.442	-9.299	7.944	1.00	0.00
95	HETATM	95	H1	WAT	31	7.382	-9.642	7.946	1.00	0.00
96	HETATM	96	H2	WAT	31	5.967	-9.632	7.130	1.00	0.00
97	HETATM	97	O	WAT	32	9.042	-10.246	7.947	1.00	0.00
98	HETATM	98	H1	WAT	32	9.033	-11.247	7.952	1.00	0.00
99	HETATM	99	H2	WAT	32	9.517	-9.913	8.763	1.00	0.00
100	HETATM	100	O	WAT	33	10.356	-9.326	10.204	1.00	0.00
101	HETATM	101	H1	WAT	33	11.296	-9.668	10.206	1.00	0.00
102	HETATM	102	H2	WAT	33	10.365	-8.326	10.200	1.00	0.00
103	HETATM	103	O	WAT	34	9.042	-10.228	12.467	1.00	0.00
104	HETATM	104	H1	WAT	34	9.517	-9.895	13.282	1.00	0.00
105	HETATM	105	H2	WAT	34	9.033	-11.229	12.473	1.00	0.00
106	HETATM	106	O	WAT	35	6.442	-9.280	12.464	1.00	0.00
107	HETATM	107	H1	WAT	35	5.968	-9.612	11.648	1.00	0.00
108	HETATM	108	H2	WAT	35	5.968	-9.606	13.281	1.00	0.00
109	HETATM	109	O	WAT	36	-10.483	-5.477	1.150	1.00	0.00
110	HETATM	110	H1	WAT	36	-11.429	-5.802	1.151	1.00	0.00
111	HETATM	111	H2	WAT	36	-10.015	-5.817	0.335	1.00	0.00
112	HETATM	112	O	WAT	37	-9.187	-6.403	3.414	1.00	0.00
113	HETATM	113	H1	WAT	37	-9.195	-7.403	3.418	1.00	0.00
114	HETATM	114	H2	WAT	37	-9.654	-6.062	4.230	1.00	0.00
115	HETATM	115	O	WAT	38	-10.483	-5.458	5.670	1.00	0.00
116	HETATM	116	H1	WAT	38	-10.015	-5.799	4.854	1.00	0.00
117	HETATM	117	H2	WAT	38	-10.015	-5.793	6.486	1.00	0.00
118	HETATM	118	O	WAT	39	-10.526	-10.089	1.169	1.00	0.00

119	HETATM	119	H1	WAT	39	-10.535	-11.089	1.173	1.00	0.00
120	HETATM	120	H2	WAT	39	-10.051	-9.763	0.351	1.00	0.00
121	HETATM	121	O	WAT	40	-9.213	-9.170	3.425	1.00	0.00
122	HETATM	122	H1	WAT	40	-8.274	-9.513	3.427	1.00	0.00
123	HETATM	123	H2	WAT	40	-9.688	-9.495	4.243	1.00	0.00
124	HETATM	124	O	WAT	41	-10.526	-10.071	5.688	1.00	0.00
125	HETATM	125	H1	WAT	41	-10.050	-9.745	4.870	1.00	0.00
126	HETATM	126	H2	WAT	41	-11.466	-9.728	5.687	1.00	0.00
127	HETATM	127	O	WAT	42	-6.569	-5.504	3.410	1.00	0.00
128	HETATM	128	H1	WAT	42	-6.101	-5.845	2.595	1.00	0.00
129	HETATM	129	H2	WAT	42	-7.515	-5.829	3.412	1.00	0.00
130	HETATM	130	O	WAT	43	-5.274	-6.449	1.154	1.00	0.00
131	HETATM	131	H1	WAT	43	-5.741	-6.108	1.970	1.00	0.00
132	HETATM	132	H2	WAT	43	-4.328	-6.124	1.152	1.00	0.00
133	HETATM	133	O	WAT	44	-2.655	-5.550	1.150	1.00	0.00
134	HETATM	134	H1	WAT	44	-2.187	-5.884	1.968	1.00	0.00
135	HETATM	135	H2	WAT	44	-3.601	-5.875	1.152	1.00	0.00
136	HETATM	136	O	WAT	45	-1.360	-6.476	3.414	1.00	0.00
137	HETATM	137	H1	WAT	45	-1.368	-7.476	3.418	1.00	0.00
138	HETATM	138	H2	WAT	45	-1.828	-6.141	2.596	1.00	0.00
139	HETATM	139	O	WAT	46	-2.655	-5.532	5.670	1.00	0.00
140	HETATM	140	H1	WAT	46	-2.646	-4.532	5.666	1.00	0.00
141	HETATM	141	H2	WAT	46	-2.186	-5.866	6.487	1.00	0.00
142	HETATM	142	O	WAT	47	-5.274	-6.430	5.674	1.00	0.00
143	HETATM	143	H1	WAT	47	-4.328	-6.105	5.672	1.00	0.00
144	HETATM	144	H2	WAT	47	-5.741	-6.088	6.491	1.00	0.00
145	HETATM	145	O	WAT	48	-6.612	-10.117	3.428	1.00	0.00

146	HETATM	146	H1	WAT	48	-7.552	-9.774	3.427	1.00	0.00
		H								
147	HETATM	147	H2	WAT	48	-6.620	-11.118	3.434	1.00	0.00
		H								
148	HETATM	148	O	WAT	49	-5.300	-9.216	1.165	1.00	0.00
		O								
149	HETATM	149	H1	WAT	49	-5.776	-9.548	0.350	1.00	0.00
		H								
150	HETATM	150	H2	WAT	49	-4.361	-9.559	1.166	1.00	0.00
		H								
151	HETATM	151	O	WAT	50	-2.699	-10.163	1.169	1.00	0.00
		O								
152	HETATM	152	H1	WAT	50	-2.223	-9.839	0.352	1.00	0.00
		H								
153	HETATM	153	H2	WAT	50	-2.709	-11.163	1.175	1.00	0.00
		H								
154	HETATM	154	O	WAT	51	-1.386	-9.243	3.425	1.00	0.00
		O								
155	HETATM	155	H1	WAT	51	-1.377	-8.243	3.421	1.00	0.00
		H								
156	HETATM	156	H2	WAT	51	-1.860	-9.568	4.243	1.00	0.00
		H								
157	HETATM	157	O	WAT	52	-2.698	-10.145	5.688	1.00	0.00
		O								
158	HETATM	158	H1	WAT	52	-2.224	-9.812	6.503	1.00	0.00
		H								
159	HETATM	159	H2	WAT	52	-3.638	-9.802	5.687	1.00	0.00
		H								
160	HETATM	160	O	WAT	53	-5.300	-9.197	5.685	1.00	0.00
		O								
161	HETATM	161	H1	WAT	53	-5.774	-9.528	4.869	1.00	0.00
		H								
162	HETATM	162	H2	WAT	53	-5.290	-8.197	5.681	1.00	0.00
		H								
163	HETATM	163	O	WAT	54	1.259	-5.578	3.410	1.00	0.00
		O								
164	HETATM	164	H1	WAT	54	1.726	-5.919	2.595	1.00	0.00
		H								
165	HETATM	165	H2	WAT	54	1.268	-4.578	3.406	1.00	0.00
		H								
166	HETATM	166	O	WAT	55	2.554	-6.522	1.154	1.00	0.00
		O								
167	HETATM	167	H1	WAT	55	2.546	-7.522	1.158	1.00	0.00
		H								
168	HETATM	168	H2	WAT	55	2.087	-6.181	1.970	1.00	0.00
		H								
169	HETATM	169	O	WAT	56	5.171	-5.624	1.150	1.00	0.00
		O								
170	HETATM	170	H1	WAT	56	4.225	-5.948	1.150	1.00	0.00
		H								
171	HETATM	171	H2	WAT	56	5.181	-4.624	1.146	1.00	0.00
		H								
172	HETATM	172	O	WAT	57	6.468	-6.550	3.414	1.00	0.00
		O								

173	HETATM	173	H1	WAT	57	7.414	-6.225	3.412	1.00	0.00
		H								
174	HETATM	174	H2	WAT	57	6.460	-7.550	3.418	1.00	0.00
		H								
175	HETATM	175	O	WAT	58	5.172	-5.606	5.670	1.00	0.00
		O								
176	HETATM	176	H1	WAT	58	5.181	-4.606	5.666	1.00	0.00
		H								
177	HETATM	177	H2	WAT	58	4.226	-5.932	5.671	1.00	0.00
		H								
178	HETATM	178	O	WAT	59	2.554	-6.504	5.674	1.00	0.00
		O								
179	HETATM	179	H1	WAT	59	3.500	-6.179	5.672	1.00	0.00
		H								
180	HETATM	180	H2	WAT	59	2.547	-7.505	5.678	1.00	0.00
		H								
181	HETATM	181	O	WAT	60	1.215	-10.191	3.428	1.00	0.00
		O								
182	HETATM	182	H1	WAT	60	1.692	-9.865	2.611	1.00	0.00
		H								
183	HETATM	183	H2	WAT	60	1.689	-9.858	4.244	1.00	0.00
		H								
184	HETATM	184	O	WAT	61	2.528	-9.289	1.165	1.00	0.00
		O								
185	HETATM	185	H1	WAT	61	2.053	-9.622	0.351	1.00	0.00
		H								
186	HETATM	186	H2	WAT	61	2.537	-8.289	1.161	1.00	0.00
		H								
187	HETATM	187	O	WAT	62	5.128	-10.237	1.169	1.00	0.00
		O								
188	HETATM	188	H1	WAT	62	5.603	-9.913	0.351	1.00	0.00
		H								
189	HETATM	189	H2	WAT	62	5.603	-9.904	1.984	1.00	0.00
		H								
190	HETATM	190	O	WAT	63	6.442	-9.317	3.425	1.00	0.00
		O								
191	HETATM	191	H1	WAT	63	5.967	-9.650	2.611	1.00	0.00
		H								
192	HETATM	192	H2	WAT	63	7.382	-9.660	3.427	1.00	0.00
		H								
193	HETATM	193	O	WAT	64	5.128	-10.218	5.688	1.00	0.00
		O								
194	HETATM	194	H1	WAT	64	5.603	-9.886	6.503	1.00	0.00
		H								
195	HETATM	195	H2	WAT	64	4.189	-9.876	5.687	1.00	0.00
		H								
196	HETATM	196	O	WAT	65	2.528	-9.271	5.685	1.00	0.00
		O								
197	HETATM	197	H1	WAT	65	2.537	-8.271	5.681	1.00	0.00
		H								
198	HETATM	198	H2	WAT	65	3.468	-9.613	5.687	1.00	0.00
		H								
199	HETATM	199	O	WAT	66	9.085	-5.652	3.410	1.00	0.00
		O								

200	HETATM	200	H1	WAT	66	8.139	-5.977	3.409	1.00	0.00
201	HETATM	201	H2	WAT	66	9.553	-5.988	4.227	1.00	0.00
202	HETATM	202	O	WAT	67	10.381	-6.596	1.154	1.00	0.00
203	HETATM	203	H1	WAT	67	9.914	-6.254	1.970	1.00	0.00
204	HETATM	204	H2	WAT	67	11.328	-6.271	1.152	1.00	0.00
205	HETATM	205	O	WAT	68	10.382	-6.578	5.674	1.00	0.00
206	HETATM	206	H1	WAT	68	11.328	-6.253	5.672	1.00	0.00
207	HETATM	207	H2	WAT	68	9.914	-6.236	6.491	1.00	0.00
208	HETATM	208	O	WAT	69	9.042	-10.264	3.428	1.00	0.00
209	HETATM	209	H1	WAT	69	9.033	-11.265	3.433	1.00	0.00
210	HETATM	210	H2	WAT	69	8.102	-9.921	3.427	1.00	0.00
211	HETATM	211	O	WAT	70	10.355	-9.363	1.165	1.00	0.00
212	HETATM	212	H1	WAT	70	11.294	-9.706	1.167	1.00	0.00
213	HETATM	213	H2	WAT	70	9.880	-9.688	1.983	1.00	0.00
214	HETATM	214	O	WAT	71	10.356	-9.345	5.685	1.00	0.00
215	HETATM	215	H1	WAT	71	9.882	-9.678	4.870	1.00	0.00
216	HETATM	216	H2	WAT	71	11.296	-9.687	5.688	1.00	0.00
217	HETATM	217	O	WAT	72	-10.483	-5.495	-3.369	1.00	0.00
218	HETATM	218	H1	WAT	72	-10.015	-5.829	-2.551	1.00	0.00
219	HETATM	219	H2	WAT	72	-11.429	-5.820	-3.367	1.00	0.00
220	HETATM	220	O	WAT	73	-9.187	-6.439	-5.625	1.00	0.00
221	HETATM	221	H1	WAT	73	-8.242	-6.114	-5.627	1.00	0.00
222	HETATM	222	H2	WAT	73	-9.195	-7.440	-5.621	1.00	0.00
223	HETATM	223	O	WAT	74	-6.569	-5.541	-5.629	1.00	0.00
224	HETATM	224	H1	WAT	74	-6.102	-5.881	-6.444	1.00	0.00
225	HETATM	225	H2	WAT	74	-7.515	-5.866	-5.627	1.00	0.00
226	HETATM	226	O	WAT	75	-5.274	-6.467	-3.365	1.00	0.00

227	HETATM	227	H1	WAT	75	-5.742	-6.132	-4.183	1.00	0.00
228	HETATM	228	H	WAT	75	-4.328	-6.142	-3.367	1.00	0.00
229	HETATM	229	O	WAT	76	-6.569	-5.523	-1.109	1.00	0.00
230	HETATM	230	H	WAT	76	-6.099	-5.858	-0.292	1.00	0.00
231	HETATM	231	H	WAT	76	-6.101	-5.863	-1.925	1.00	0.00
232	HETATM	232	O	WAT	77	-9.187	-6.421	-1.105	1.00	0.00
233	HETATM	233	H	WAT	77	-8.242	-6.096	-1.107	1.00	0.00
234	HETATM	234	H	WAT	77	-9.655	-6.079	-0.288	1.00	0.00
235	HETATM	235	O	WAT	78	-10.526	-10.108	-3.350	1.00	0.00
236	HETATM	236	H	WAT	78	-10.535	-11.109	-3.344	1.00	0.00
237	HETATM	237	H	WAT	78	-10.050	-9.783	-4.168	1.00	0.00
238	HETATM	238	O	WAT	79	-9.213	-9.206	-5.614	1.00	0.00
239	HETATM	239	H	WAT	79	-9.688	-9.539	-6.429	1.00	0.00
240	HETATM	240	H	WAT	79	-8.273	-9.549	-5.611	1.00	0.00
241	HETATM	241	O	WAT	80	-6.613	-10.154	-5.610	1.00	0.00
242	HETATM	242	H	WAT	80	-6.622	-11.155	-5.604	1.00	0.00
243	HETATM	243	H	WAT	80	-6.139	-9.821	-4.795	1.00	0.00
244	HETATM	244	O	WAT	81	-5.300	-9.234	-3.354	1.00	0.00
245	HETATM	245	H	WAT	81	-5.774	-9.559	-2.536	1.00	0.00
246	HETATM	246	H	WAT	81	-5.291	-8.234	-3.358	1.00	0.00
247	HETATM	247	O	WAT	82	-6.613	-10.135	-1.090	1.00	0.00
248	HETATM	248	H	WAT	82	-7.552	-9.792	-1.092	1.00	0.00
249	HETATM	249	H	WAT	82	-6.138	-9.802	-0.276	1.00	0.00
250	HETATM	250	O	WAT	83	-9.213	-9.188	-1.094	1.00	0.00
251	HETATM	251	H	WAT	83	-8.274	-9.531	-1.092	1.00	0.00
252	HETATM	252	H	WAT	83	-9.203	-8.188	-1.098	1.00	0.00
253	HETATM	253	O	WAT	84	-2.655	-5.568	-3.369	1.00	0.00

254	HETATM	254	H1	WAT	84	-3.600	-5.892	-3.366	1.00	0.00
255	HETATM	255	H	WAT	84	-2.646	-4.569	-3.373	1.00	0.00
256	HETATM	256	O	WAT	85	-1.360	-6.513	-5.625	1.00	0.00
257	HETATM	257	H	WAT	85	-0.414	-6.188	-5.627	1.00	0.00
258	HETATM	258	H	WAT	85	-1.827	-6.172	-4.809	1.00	0.00
259	HETATM	259	O	WAT	86	1.258	-5.614	-5.629	1.00	0.00
260	HETATM	260	H	WAT	86	1.268	-4.614	-5.633	1.00	0.00
261	HETATM	261	H	WAT	86	0.312	-5.938	-5.628	1.00	0.00
262	HETATM	262	O	WAT	87	2.554	-6.540	-3.365	1.00	0.00
263	HETATM	263	H	WAT	87	2.086	-6.205	-4.183	1.00	0.00
264	HETATM	264	H	WAT	87	2.546	-7.540	-3.361	1.00	0.00
265	HETATM	265	O	WAT	88	1.258	-5.596	-1.109	1.00	0.00
266	HETATM	266	H	WAT	88	1.727	-5.931	-0.292	1.00	0.00
267	HETATM	267	H	WAT	88	1.268	-4.596	-1.113	1.00	0.00
268	HETATM	268	O	WAT	89	-1.360	-6.495	-1.105	1.00	0.00
269	HETATM	269	H	WAT	89	-0.414	-6.169	-1.107	1.00	0.00
270	HETATM	270	H	WAT	89	-1.826	-6.154	-0.287	1.00	0.00
271	HETATM	271	O	WAT	90	-2.699	-10.181	-3.350	1.00	0.00
272	HETATM	272	H	WAT	90	-2.225	-9.848	-2.535	1.00	0.00
273	HETATM	273	H	WAT	90	-2.708	-11.182	-3.344	1.00	0.00
274	HETATM	274	O	WAT	91	-1.386	-9.280	-5.614	1.00	0.00
275	HETATM	275	H	WAT	91	-1.861	-9.613	-6.428	1.00	0.00
276	HETATM	276	H	WAT	91	-1.377	-8.280	-5.618	1.00	0.00
277	HETATM	277	O	WAT	92	1.215	-10.227	-5.610	1.00	0.00
278	HETATM	278	H	WAT	92	0.275	-9.884	-5.612	1.00	0.00
279	HETATM	279	H	WAT	92	1.691	-9.902	-6.428	1.00	0.00
280	HETATM	280	O	WAT	93	2.528	-9.307	-3.354	1.00	0.00

281	HETATM	281	H1	WAT	93	2.054	-9.633	-2.536	1.00	0.00
282	HETATM	282	H	WAT	93	2.537	-8.307	-3.358	1.00	0.00
283	HETATM	283	O	WAT	94	1.215	-10.209	-1.090	1.00	0.00
284	HETATM	284	H1	WAT	94	0.275	-9.866	-1.092	1.00	0.00
285	HETATM	285	H	WAT	94	1.690	-9.885	-1.909	1.00	0.00
286	HETATM	286	O	WAT	95	-1.386	-9.261	-1.094	1.00	0.00
287	HETATM	287	H	WAT	95	-1.377	-8.261	-1.098	1.00	0.00
288	HETATM	288	H	WAT	95	-1.860	-9.593	-1.910	1.00	0.00
289	HETATM	289	O	WAT	96	5.171	-5.642	-3.369	1.00	0.00
290	HETATM	290	H	WAT	96	5.639	-5.977	-2.551	1.00	0.00
291	HETATM	291	H2	WAT	96	5.640	-5.983	-4.184	1.00	0.00
292	HETATM	292	O	WAT	97	6.467	-6.586	-5.625	1.00	0.00
293	HETATM	293	H	WAT	97	6.460	-7.586	-5.621	1.00	0.00
294	HETATM	294	H	WAT	97	6.000	-6.251	-6.443	1.00	0.00
295	HETATM	295	O	WAT	98	9.085	-5.688	-5.629	1.00	0.00
296	HETATM	296	H	WAT	98	9.094	-4.688	-5.633	1.00	0.00
297	HETATM	297	H	WAT	98	9.553	-6.022	-4.811	1.00	0.00
298	HETATM	298	O	WAT	99	10.381	-6.614	-3.365	1.00	0.00
299	HETATM	299	H	WAT	99	9.912	-6.279	-4.183	1.00	0.00
300	HETATM	300	H	WAT	99	11.327	-6.289	-3.367	1.00	0.00
301	HETATM	301	O	WAT	100	9.085	-5.670	-1.109	1.00	0.00
302	HETATM	302	H	WAT	100	9.554	-6.010	-1.925	1.00	0.00
303	HETATM	303	H	WAT	100	9.554	-6.006	-0.292	1.00	0.00
304	HETATM	304	O	WAT	101	6.468	-6.568	-1.105	1.00	0.00
305	HETATM	305	H	WAT	101	7.414	-6.243	-1.107	1.00	0.00
306	HETATM	306	H	WAT	101	6.000	-6.233	-1.924	1.00	0.00
307	HETATM	307	O	WAT	102	5.128	-10.255	-3.350	1.00	0.00

308	HETATM	308	H1	WAT	102		5.603	-9.922	-2.535	1.00	0.00
309	HETATM	309	H2	WAT	102		5.118	-11.255	-3.345	1.00	0.00
310	HETATM	310	O	WAT	103		6.441	-9.353	-5.614	1.00	0.00
311	HETATM	311	H1	WAT	103		5.967	-9.678	-4.796	1.00	0.00
312	HETATM	312	H2	WAT	103		6.451	-8.353	-5.618	1.00	0.00
313	HETATM	313	O	WAT	104		9.042	-10.301	-5.610	1.00	0.00
314	HETATM	314	H1	WAT	104		9.517	-9.968	-4.795	1.00	0.00
315	HETATM	315	H2	WAT	104		8.102	-9.958	-5.612	1.00	0.00
316	HETATM	316	O	WAT	105		10.355	-9.381	-3.354	1.00	0.00
317	HETATM	317	H1	WAT	105		9.880	-9.706	-2.536	1.00	0.00
318	HETATM	318	H2	WAT	105		11.294	-9.724	-3.352	1.00	0.00
319	HETATM	319	O	WAT	106		9.042	-10.282	-1.090	1.00	0.00
320	HETATM	320	H1	WAT	106		8.102	-9.940	-1.092	1.00	0.00
321	HETATM	321	H2	WAT	106		9.517	-9.950	-0.276	1.00	0.00
322	HETATM	322	O	WAT	107		6.442	-9.335	-1.094	1.00	0.00
323	HETATM	323	H1	WAT	107		6.451	-8.335	-1.098	1.00	0.00
324	HETATM	324	H2	WAT	107		5.967	-9.660	-0.277	1.00	0.00
325	HETATM	325	O	WAT	108		-10.483	-5.531	-12.408	1.00	0.00
326	HETATM	326	H1	WAT	108		-10.016	-5.872	-13.223	1.00	0.00
327	HETATM	327	H2	WAT	108		-11.429	-5.855	-12.405	1.00	0.00
328	HETATM	328	O	WAT	109		-9.187	-6.457	-10.144	1.00	0.00
329	HETATM	329	H1	WAT	109		-9.195	-7.458	-10.140	1.00	0.00
330	HETATM	330	H2	WAT	109		-8.242	-6.132	-10.146	1.00	0.00
331	HETATM	331	O	WAT	110		-10.483	-5.513	-7.888	1.00	0.00
332	HETATM	332	H1	WAT	110		-10.474	-4.513	-7.892	1.00	0.00
333	HETATM	333	H2	WAT	110		-10.015	-5.854	-8.704	1.00	0.00
334	HETATM	334	O	WAT	111		-10.527	-10.144	-12.389	1.00	0.00

335	HETATM	335	H1	WAT	111	-10.051	-9.819	-13.207	1.00	0.00
			H							
336	HETATM	336	H2	WAT	111	-10.536	-11.145	-12.383	1.00	0.00
			H							
337	HETATM	337	O	WAT	112	-9.213	-9.224	-10.133	1.00	0.00
			O							
338	HETATM	338	H1	WAT	112	-9.688	-9.550	-9.315	1.00	0.00
			H							
339	HETATM	339	H2	WAT	112	-8.273	-9.566	-10.131	1.00	0.00
			H							
340	HETATM	340	O	WAT	113	-10.527	-10.126	-7.869	1.00	0.00
			O							
341	HETATM	341	H1	WAT	113	-10.052	-9.802	-8.687	1.00	0.00
			H							
342	HETATM	342	H2	WAT	113	-11.466	-9.783	-7.871	1.00	0.00
			H							
343	HETATM	343	O	WAT	114	-6.570	-5.559	-10.148	1.00	0.00
			O							
344	HETATM	344	H1	WAT	114	-6.560	-4.559	-10.152	1.00	0.00
			H							
345	HETATM	345	H2	WAT	114	-6.102	-5.894	-9.330	1.00	0.00
			H							
346	HETATM	346	O	WAT	115	-5.274	-6.503	-12.404	1.00	0.00
			O							
347	HETATM	347	H1	WAT	115	-5.741	-6.162	-11.588	1.00	0.00
			H							
348	HETATM	348	H2	WAT	115	-4.328	-6.178	-12.406	1.00	0.00
			H							
349	HETATM	349	O	WAT	116	-2.656	-5.605	-12.408	1.00	0.00
			O							
350	HETATM	350	H1	WAT	116	-2.188	-5.940	-11.590	1.00	0.00
			H							
351	HETATM	351	H2	WAT	116	-2.646	-4.605	-12.412	1.00	0.00
			H							
352	HETATM	352	O	WAT	117	-1.360	-6.531	-10.144	1.00	0.00
			O							
353	HETATM	353	H1	WAT	117	-1.827	-6.190	-9.328	1.00	0.00
			H							
354	HETATM	354	H2	WAT	117	-1.828	-6.196	-10.962	1.00	0.00
			H							
355	HETATM	355	O	WAT	118	-2.656	-5.587	-7.888	1.00	0.00
			O							
356	HETATM	356	H1	WAT	118	-2.646	-4.587	-7.892	1.00	0.00
			H							
357	HETATM	357	H2	WAT	118	-2.186	-5.923	-7.072	1.00	0.00
			H							
358	HETATM	358	O	WAT	119	-5.274	-6.485	-7.884	1.00	0.00
			O							
359	HETATM	359	H1	WAT	119	-5.742	-6.150	-8.703	1.00	0.00
			H							
360	HETATM	360	H2	WAT	119	-5.281	-7.486	-7.880	1.00	0.00
			H							
361	HETATM	361	O	WAT	120	-6.613	-10.172	-10.129	1.00	0.00
			O							

362	HETATM	362	H1	WAT	120	-6.139	-9.839	-9.314	1.00	0.00
		H								
363	HETATM	363	H2	WAT	120	-6.137	-9.847	-10.947	1.00	0.00
		H								
364	HETATM	364	O	WAT	121	-5.300	-9.270	-12.393	1.00	0.00
		O								
365	HETATM	365	H1	WAT	121	-4.360	-9.613	-12.391	1.00	0.00
		H								
366	HETATM	366	H2	WAT	121	-5.291	-8.270	-12.397	1.00	0.00
		H								
367	HETATM	367	O	WAT	122	-2.699	-10.218	-12.389	1.00	0.00
		O								
368	HETATM	368	H1	WAT	122	-3.639	-9.875	-12.391	1.00	0.00
		H								
369	HETATM	369	H2	WAT	122	-2.223	-9.893	-13.207	1.00	0.00
		H								
370	HETATM	370	O	WAT	123	-1.386	-9.298	-10.133	1.00	0.00
		O								
371	HETATM	371	H1	WAT	123	-0.446	-9.641	-10.130	1.00	0.00
		H								
372	HETATM	372	H2	WAT	123	-1.377	-8.298	-10.137	1.00	0.00
		H								
373	HETATM	373	O	WAT	124	-2.699	-10.199	-7.869	1.00	0.00
		O								
374	HETATM	374	H1	WAT	124	-2.225	-9.874	-8.688	1.00	0.00
		H								
375	HETATM	375	H2	WAT	124	-2.709	-11.199	-7.865	1.00	0.00
		H								
376	HETATM	376	O	WAT	125	-5.300	-9.252	-7.873	1.00	0.00
		O								
377	HETATM	377	H1	WAT	125	-5.291	-8.252	-7.877	1.00	0.00
		H								
378	HETATM	378	H2	WAT	125	-5.774	-9.577	-7.056	1.00	0.00
		H								
379	HETATM	379	O	WAT	126	1.258	-5.633	-10.148	1.00	0.00
		O								
380	HETATM	380	H1	WAT	126	0.312	-5.958	-10.148	1.00	0.00
		H								
381	HETATM	381	H2	WAT	126	1.726	-5.973	-10.963	1.00	0.00
		H								
382	HETATM	382	O	WAT	127	2.553	-6.577	-12.404	1.00	0.00
		O								
383	HETATM	383	H1	WAT	127	3.499	-6.252	-12.406	1.00	0.00
		H								
384	HETATM	384	H2	WAT	127	2.085	-6.242	-13.222	1.00	0.00
		H								
385	HETATM	385	O	WAT	128	5.171	-5.678	-12.408	1.00	0.00
		O								
386	HETATM	386	H1	WAT	128	5.180	-4.679	-12.412	1.00	0.00
		H								
387	HETATM	387	H2	WAT	128	4.226	-6.002	-12.407	1.00	0.00
		H								
388	HETATM	388	O	WAT	129	6.467	-6.605	-10.144	1.00	0.00
		O								

389	HETATM	389	H1	WAT	129	6.001	-6.264	-9.327	1.00	0.00
390	HETATM	390	H2	WAT	129	5.999	-6.269	-10.962	1.00	0.00
391	HETATM	391	O	WAT	130	5.171	-5.660	-7.888	1.00	0.00
392	HETATM	392	H1	WAT	130	5.640	-6.001	-8.704	1.00	0.00
393	HETATM	393	H2	WAT	130	4.225	-5.985	-7.887	1.00	0.00
394	HETATM	394	O	WAT	131	2.553	-6.559	-7.884	1.00	0.00
395	HETATM	395	H1	WAT	131	2.546	-7.560	-7.879	1.00	0.00
396	HETATM	396	H2	WAT	131	3.500	-6.234	-7.886	1.00	0.00
397	HETATM	397	O	WAT	132	1.215	-10.245	-10.129	1.00	0.00
398	HETATM	398	H1	WAT	132	1.691	-9.920	-10.947	1.00	0.00
399	HETATM	399	H2	WAT	132	0.275	-9.902	-10.131	1.00	0.00
400	HETATM	400	O	WAT	133	2.527	-9.344	-12.393	1.00	0.00
401	HETATM	401	H1	WAT	133	3.466	-9.687	-12.392	1.00	0.00
402	HETATM	402	H2	WAT	133	2.053	-9.669	-11.575	1.00	0.00
403	HETATM	403	O	WAT	134	5.127	-10.291	-12.389	1.00	0.00
404	HETATM	404	H1	WAT	134	5.600	-9.968	-13.207	1.00	0.00
405	HETATM	405	H2	WAT	134	5.116	-11.290	-12.384	1.00	0.00
406	HETATM	406	O	WAT	135	6.441	-9.371	-10.133	1.00	0.00
407	HETATM	407	H1	WAT	135	5.966	-9.702	-10.948	1.00	0.00
408	HETATM	408	H2	WAT	135	6.451	-8.371	-10.137	1.00	0.00
409	HETATM	409	O	WAT	136	5.128	-10.273	-7.869	1.00	0.00
410	HETATM	410	H1	WAT	136	5.117	-11.273	-7.863	1.00	0.00
411	HETATM	411	H2	WAT	136	4.189	-9.930	-7.871	1.00	0.00
412	HETATM	412	O	WAT	137	2.527	-9.326	-7.873	1.00	0.00
413	HETATM	413	H1	WAT	137	2.052	-9.658	-8.688	1.00	0.00
414	HETATM	414	H2	WAT	137	2.537	-8.326	-7.877	1.00	0.00
415	HETATM	415	O	WAT	138	9.085	-5.706	-10.148	1.00	0.00

416	HETATM	416	H1	WAT	138	8.139	-6.031	-10.147	1.00	0.00
			H							
417	HETATM	417	H2	WAT	138	9.553	-6.040	-9.330	1.00	0.00
			H							
418	HETATM	418	O	WAT	139	10.381	-6.650	-12.404	1.00	0.00
			O							
419	HETATM	419	H1	WAT	139	9.913	-6.309	-11.588	1.00	0.00
			H							
420	HETATM	420	H2	WAT	139	11.327	-6.325	-12.406	1.00	0.00
			H							
421	HETATM	421	O	WAT	140	10.381	-6.632	-7.884	1.00	0.00
			O							
422	HETATM	422	H1	WAT	140	10.373	-7.633	-7.880	1.00	0.00
			H							
423	HETATM	423	H2	WAT	140	9.912	-6.297	-8.703	1.00	0.00
			H							
424	HETATM	424	O	WAT	141	9.041	-10.319	-10.129	1.00	0.00
			O							
425	HETATM	425	H1	WAT	141	8.102	-9.976	-10.131	1.00	0.00
			H							
426	HETATM	426	H2	WAT	141	9.515	-9.996	-10.948	1.00	0.00
			H							
427	HETATM	427	O	WAT	142	10.355	-9.417	-12.393	1.00	0.00
			O							
428	HETATM	428	H1	WAT	142	9.880	-9.743	-11.575	1.00	0.00
			H							
429	HETATM	429	H2	WAT	142	11.295	-9.759	-12.391	1.00	0.00
			H							
430	HETATM	430	O	WAT	143	10.355	-9.399	-7.873	1.00	0.00
			O							
431	HETATM	431	H1	WAT	143	9.881	-9.731	-8.688	1.00	0.00
			H							
432	HETATM	432	H2	WAT	143	11.294	-9.742	-7.871	1.00	0.00
			H							
433	HETATM	433	O	WAT	144	-10.413	1.939	10.159	1.00	0.00
			O							
434	HETATM	434	H1	WAT	144	-9.944	1.604	10.976	1.00	0.00
			H							
435	HETATM	435	H2	WAT	144	-9.945	1.599	9.344	1.00	0.00
			H							
436	HETATM	436	O	WAT	145	-9.117	0.996	7.903	1.00	0.00
			O							
437	HETATM	437	H1	WAT	145	-8.172	1.320	7.902	1.00	0.00
			H							
438	HETATM	438	H2	WAT	145	-9.586	1.336	8.717	1.00	0.00
			H							
439	HETATM	439	O	WAT	146	-6.499	1.893	7.899	1.00	0.00
			O							
440	HETATM	440	H1	WAT	146	-6.029	1.558	8.716	1.00	0.00
			H							
441	HETATM	441	H2	WAT	146	-7.445	1.568	7.901	1.00	0.00
			H							
442	HETATM	442	O	WAT	147	-5.204	0.968	10.163	1.00	0.00
			O							

443	HETATM	443	H1	WAT	147	-5.672	1.302	9.346	1.00	0.00
444	HETATM	444	H2	WAT	147	-5.215	-0.031	10.167	1.00	0.00
445	HETATM	445	O	WAT	148	-6.499	1.912	12.419	1.00	0.00
446	HETATM	446	H1	WAT	148	-6.490	2.912	12.415	1.00	0.00
447	HETATM	447	H2	WAT	148	-7.445	1.587	12.421	1.00	0.00
448	HETATM	448	O	WAT	149	-9.117	1.014	12.423	1.00	0.00
449	HETATM	449	H1	WAT	149	-9.585	1.356	13.239	1.00	0.00
450	HETATM	450	H2	WAT	149	-9.127	0.013	12.428	1.00	0.00
451	HETATM	451	O	WAT	150	-10.457	-2.672	10.178	1.00	0.00
452	HETATM	452	H1	WAT	150	-9.985	-2.347	9.359	1.00	0.00
453	HETATM	453	H2	WAT	150	-9.982	-2.341	10.992	1.00	0.00
454	HETATM	454	O	WAT	151	-9.143	-1.772	7.914	1.00	0.00
455	HETATM	455	H1	WAT	151	-8.203	-2.115	7.917	1.00	0.00
456	HETATM	456	H2	WAT	151	-9.134	-0.772	7.910	1.00	0.00
457	HETATM	457	O	WAT	152	-6.543	-2.718	7.918	1.00	0.00
458	HETATM	458	H1	WAT	152	-6.552	-3.718	7.922	1.00	0.00
459	HETATM	459	H2	WAT	152	-7.483	-2.376	7.916	1.00	0.00
460	HETATM	460	O	WAT	153	-5.230	-1.800	10.174	1.00	0.00
461	HETATM	461	H1	WAT	153	-4.290	-2.142	10.176	1.00	0.00
462	HETATM	462	H2	WAT	153	-5.705	-2.133	9.359	1.00	0.00
463	HETATM	463	O	WAT	154	-6.543	-2.700	12.438	1.00	0.00
464	HETATM	464	H1	WAT	154	-6.069	-2.368	13.252	1.00	0.00
465	HETATM	465	H2	WAT	154	-6.069	-2.375	11.620	1.00	0.00
466	HETATM	466	O	WAT	155	-9.143	-1.754	12.434	1.00	0.00
467	HETATM	467	H1	WAT	155	-8.204	-2.097	12.436	1.00	0.00
468	HETATM	468	H2	WAT	155	-9.133	-0.754	12.430	1.00	0.00
469	HETATM	469	O	WAT	156	-2.586	1.866	10.159	1.00	0.00

470	HETATM	470	H1	WAT	156	-2.118	1.525	9.344	1.00	0.00
		H								
471	HETATM	471	H2	WAT	156	-2.576	2.866	10.155	1.00	0.00
		H								
472	HETATM	472	O	WAT	157	-1.290	0.922	7.903	1.00	0.00
		O								
473	HETATM	473	H1	WAT	157	-1.758	1.257	7.086	1.00	0.00
		H								
474	HETATM	474	H2	WAT	157	-1.758	1.262	8.718	1.00	0.00
		H								
475	HETATM	475	O	WAT	158	1.328	1.820	7.899	1.00	0.00
		O								
476	HETATM	476	H1	WAT	158	0.382	1.496	7.900	1.00	0.00
		H								
477	HETATM	477	H2	WAT	158	1.796	1.479	7.084	1.00	0.00
		H								
478	HETATM	478	O	WAT	159	2.624	0.895	10.163	1.00	0.00
		O								
479	HETATM	479	H1	WAT	159	2.613	-0.104	10.167	1.00	0.00
		H								
480	HETATM	480	H2	WAT	159	3.570	1.219	10.162	1.00	0.00
		H								
481	HETATM	481	O	WAT	160	1.328	1.838	12.419	1.00	0.00
		O								
482	HETATM	482	H1	WAT	160	1.338	2.838	12.415	1.00	0.00
		H								
483	HETATM	483	H2	WAT	160	1.796	1.497	11.603	1.00	0.00
		H								
484	HETATM	484	O	WAT	161	-1.290	0.941	12.423	1.00	0.00
		O								
485	HETATM	485	H1	WAT	161	-1.758	1.284	13.238	1.00	0.00
		H								
486	HETATM	486	H2	WAT	161	-0.344	1.265	12.421	1.00	0.00
		H								
487	HETATM	487	O	WAT	162	-2.629	-2.746	10.178	1.00	0.00
		O								
488	HETATM	488	H1	WAT	162	-2.639	-3.746	10.182	1.00	0.00
		H								
489	HETATM	489	H2	WAT	162	-3.569	-2.404	10.176	1.00	0.00
		H								
490	HETATM	490	O	WAT	163	-1.316	-1.845	7.914	1.00	0.00
		O								
491	HETATM	491	H1	WAT	163	-0.376	-2.187	7.915	1.00	0.00
		H								
492	HETATM	492	H2	WAT	163	-1.791	-2.177	7.099	1.00	0.00
		H								
493	HETATM	493	O	WAT	164	1.285	-2.792	7.918	1.00	0.00
		O								
494	HETATM	494	H1	WAT	164	1.759	-2.460	8.733	1.00	0.00
		H								
495	HETATM	495	H2	WAT	164	1.760	-2.466	7.100	1.00	0.00
		H								
496	HETATM	496	O	WAT	165	2.598	-1.873	10.174	1.00	0.00
		O								

497	HETATM	497	H1	WAT	165	2.123	-2.198	10.991	1.00	0.00
498	HETATM	498	H2	WAT	165	3.538	-2.215	10.177	1.00	0.00
499	HETATM	499	O	WAT	166	1.285	-2.774	12.438	1.00	0.00
500	HETATM	500	H1	WAT	166	1.275	-3.774	12.442	1.00	0.00
501	HETATM	501	H2	WAT	166	0.345	-2.432	12.436	1.00	0.00
502	HETATM	502	O	WAT	167	-1.316	-1.827	12.434	1.00	0.00
503	HETATM	503	H1	WAT	167	-1.307	-0.827	12.430	1.00	0.00
504	HETATM	504	H2	WAT	167	-1.790	-2.152	13.251	1.00	0.00
505	HETATM	505	O	WAT	168	5.241	1.792	10.159	1.00	0.00
506	HETATM	506	H1	WAT	168	5.250	2.792	10.155	1.00	0.00
507	HETATM	507	H2	WAT	168	5.710	1.451	9.344	1.00	0.00
508	HETATM	508	O	WAT	169	6.537	0.849	7.903	1.00	0.00
509	HETATM	509	H1	WAT	169	6.526	-0.150	7.907	1.00	0.00
510	HETATM	510	H2	WAT	169	6.068	1.190	8.717	1.00	0.00
511	HETATM	511	O	WAT	170	9.155	1.746	7.899	1.00	0.00
512	HETATM	512	H1	WAT	170	8.209	1.420	7.899	1.00	0.00
513	HETATM	513	H2	WAT	170	9.624	1.406	7.084	1.00	0.00
514	HETATM	514	O	WAT	171	10.451	0.821	10.163	1.00	0.00
515	HETATM	515	H1	WAT	171	10.440	-0.178	10.167	1.00	0.00
516	HETATM	516	H2	WAT	171	9.982	1.161	10.977	1.00	0.00
517	HETATM	517	O	WAT	172	9.155	1.764	12.419	1.00	0.00
518	HETATM	518	H1	WAT	172	9.164	2.764	12.415	1.00	0.00
519	HETATM	519	H2	WAT	172	9.624	1.429	13.236	1.00	0.00
520	HETATM	520	O	WAT	173	6.537	0.867	12.423	1.00	0.00
521	HETATM	521	H1	WAT	173	6.070	1.211	13.238	1.00	0.00
522	HETATM	522	H2	WAT	173	7.484	1.191	12.421	1.00	0.00
523	HETATM	523	O	WAT	174	5.198	-2.820	10.178	1.00	0.00

524	HETATM	524	H1	WAT	174	4.259	-2.478	10.176	1.00	0.00
525	HETATM	525	H2	WAT	174	5.671	-2.496	9.359	1.00	0.00
526	HETATM	526	O	WAT	175	6.511	-1.919	7.914	1.00	0.00
527	HETATM	527	H1	WAT	175	6.521	-0.919	7.910	1.00	0.00
528	HETATM	528	H2	WAT	175	7.450	-2.262	7.915	1.00	0.00
529	HETATM	529	O	WAT	176	9.111	-2.865	7.918	1.00	0.00
530	HETATM	530	H1	WAT	176	9.100	-3.864	7.918	1.00	0.00
531	HETATM	531	H2	WAT	176	9.587	-2.534	8.733	1.00	0.00
532	HETATM	532	O	WAT	177	10.425	-1.947	10.174	1.00	0.00
533	HETATM	533	H1	WAT	177	10.435	-0.947	10.170	1.00	0.00
534	HETATM	534	H2	WAT	177	11.364	-2.290	10.176	1.00	0.00
535	HETATM	535	O	WAT	178	9.112	-2.847	12.438	1.00	0.00
536	HETATM	536	H1	WAT	178	9.587	-2.515	13.252	1.00	0.00
537	HETATM	537	H2	WAT	178	9.101	-3.847	12.441	1.00	0.00
538	HETATM	538	O	WAT	179	6.511	-1.901	12.434	1.00	0.00
539	HETATM	539	H1	WAT	179	6.037	-2.226	13.251	1.00	0.00
540	HETATM	540	H2	WAT	179	6.521	-0.901	12.430	1.00	0.00
541	HETATM	541	O	WAT	180	-10.414	1.903	1.120	1.00	0.00
542	HETATM	542	H1	WAT	180	-9.946	1.568	1.938	1.00	0.00
543	HETATM	543	H2	WAT	180	-10.404	2.903	1.116	1.00	0.00
544	HETATM	544	O	WAT	181	-9.117	0.978	3.384	1.00	0.00
545	HETATM	545	H1	WAT	181	-8.172	1.302	3.383	1.00	0.00
546	HETATM	546	H2	WAT	181	-9.586	1.318	4.198	1.00	0.00
547	HETATM	547	O	WAT	182	-10.413	1.921	5.640	1.00	0.00
548	HETATM	548	H1	WAT	182	-11.359	1.597	5.643	1.00	0.00
549	HETATM	549	H2	WAT	182	-9.944	1.587	6.458	1.00	0.00
550	HETATM	550	O	WAT	183	-10.457	-2.709	1.139	1.00	0.00

551	HETATM	551	H1	WAT	183	-9.983	-2.377	1.954	1.00	0.00
552	HETATM	552	H2	WAT	183	-9.982	-2.383	0.321	1.00	0.00
553	HETATM	553	O	WAT	184	-9.143	-1.790	3.395	1.00	0.00
554	HETATM	554	H1	WAT	184	-9.134	-0.790	3.391	1.00	0.00
555	HETATM	555	H2	WAT	184	-8.203	-2.133	3.398	1.00	0.00
556	HETATM	556	O	WAT	185	-10.457	-2.691	5.659	1.00	0.00
557	HETATM	557	H1	WAT	185	-9.983	-2.366	4.840	1.00	0.00
558	HETATM	558	H2	WAT	185	-11.397	-2.349	5.657	1.00	0.00
559	HETATM	559	O	WAT	186	-6.500	1.875	3.380	1.00	0.00
560	HETATM	560	H1	WAT	186	-6.490	2.875	3.376	1.00	0.00
561	HETATM	561	H2	WAT	186	-6.032	1.535	2.566	1.00	0.00
562	HETATM	562	O	WAT	187	-5.204	0.932	1.124	1.00	0.00
563	HETATM	563	H1	WAT	187	-5.215	-0.067	1.128	1.00	0.00
564	HETATM	564	H2	WAT	187	-4.258	1.256	1.123	1.00	0.00
565	HETATM	565	O	WAT	188	-2.586	1.829	1.120	1.00	0.00
566	HETATM	566	H1	WAT	188	-2.118	1.489	0.306	1.00	0.00
567	HETATM	567	H2	WAT	188	-3.532	1.504	1.121	1.00	0.00
568	HETATM	568	O	WAT	189	-1.291	0.904	3.384	1.00	0.00
569	HETATM	569	H1	WAT	189	-1.758	1.238	2.567	1.00	0.00
570	HETATM	570	H2	WAT	189	-0.344	1.228	3.383	1.00	0.00
571	HETATM	571	O	WAT	190	-2.586	1.848	5.640	1.00	0.00
572	HETATM	572	H1	WAT	190	-2.118	1.507	4.825	1.00	0.00
573	HETATM	573	H2	WAT	190	-2.576	2.848	5.636	1.00	0.00
574	HETATM	574	O	WAT	191	-5.204	0.950	5.644	1.00	0.00
575	HETATM	575	H1	WAT	191	-5.214	-0.050	5.649	1.00	0.00
576	HETATM	576	H2	WAT	191	-4.258	1.274	5.643	1.00	0.00
577	HETATM	577	O	WAT	192	-6.543	-2.737	3.399	1.00	0.00

578	HETATM	578	H1	WAT	192	-6.068	-2.411	2.581	1.00	0.00
		H								
579	HETATM	579	H2	WAT	192	-6.552	-3.737	3.403	1.00	0.00
		H								
580	HETATM	580	O	WAT	193	-5.230	-1.836	1.135	1.00	0.00
		O								
581	HETATM	581	H1	WAT	193	-5.705	-2.161	1.953	1.00	0.00
		H								
582	HETATM	582	H2	WAT	193	-4.290	-2.179	1.138	1.00	0.00
		H								
583	HETATM	583	O	WAT	194	-2.629	-2.782	1.139	1.00	0.00
		O								
584	HETATM	584	H1	WAT	194	-2.639	-3.782	1.140	1.00	0.00
		H								
585	HETATM	585	H2	WAT	194	-3.569	-2.441	1.137	1.00	0.00
		H								
586	HETATM	586	O	WAT	195	-1.317	-1.864	3.395	1.00	0.00
		O								
587	HETATM	587	H1	WAT	195	-1.307	-0.864	3.391	1.00	0.00
		H								
588	HETATM	588	H2	WAT	195	-1.793	-2.196	2.580	1.00	0.00
		H								
589	HETATM	589	O	WAT	196	-2.629	-2.764	5.659	1.00	0.00
		O								
590	HETATM	590	H1	WAT	196	-2.639	-3.764	5.663	1.00	0.00
		H								
591	HETATM	591	H2	WAT	196	-2.155	-2.439	4.840	1.00	0.00
		H								
592	HETATM	592	O	WAT	197	-5.230	-1.818	5.655	1.00	0.00
		O								
593	HETATM	593	H1	WAT	197	-5.221	-0.818	5.651	1.00	0.00
		H								
594	HETATM	594	H2	WAT	197	-5.704	-2.143	6.472	1.00	0.00
		H								
595	HETATM	595	O	WAT	198	1.328	1.802	3.380	1.00	0.00
		O								
596	HETATM	596	H1	WAT	198	1.796	1.461	2.566	1.00	0.00
		H								
597	HETATM	597	H2	WAT	198	1.796	1.468	4.198	1.00	0.00
		H								
598	HETATM	598	O	WAT	199	2.623	0.858	1.124	1.00	0.00
		O								
599	HETATM	599	H1	WAT	199	3.569	1.182	1.123	1.00	0.00
		H								
600	HETATM	600	H2	WAT	199	2.154	1.199	1.938	1.00	0.00
		H								
601	HETATM	601	O	WAT	200	5.241	1.756	1.120	1.00	0.00
		O								
602	HETATM	602	H1	WAT	200	5.710	1.415	0.306	1.00	0.00
		H								
603	HETATM	603	H2	WAT	200	4.295	1.432	1.121	1.00	0.00
		H								
604	HETATM	604	O	WAT	201	6.537	0.831	3.384	1.00	0.00
		O								

605	HETATM	605	H1	WAT	201	6.526	-0.168	3.388	1.00	0.00
606	HETATM	606	H2	WAT	201	7.483	1.155	3.383	1.00	0.00
607	HETATM	607	O	WAT	202	5.241	1.774	5.640	1.00	0.00
608	HETATM	608	H1	WAT	202	5.710	1.433	4.825	1.00	0.00
609	HETATM	609	H2	WAT	202	5.709	1.440	6.458	1.00	0.00
610	HETATM	610	O	WAT	203	2.623	0.877	5.644	1.00	0.00
611	HETATM	611	H1	WAT	203	2.154	1.218	6.458	1.00	0.00
612	HETATM	612	H2	WAT	203	2.155	1.211	4.826	1.00	0.00
613	HETATM	613	O	WAT	204	1.285	-2.810	3.399	1.00	0.00
614	HETATM	614	H1	WAT	204	0.345	-2.468	3.397	1.00	0.00
615	HETATM	615	H2	WAT	204	1.276	-3.810	3.403	1.00	0.00
616	HETATM	616	O	WAT	205	2.597	-1.910	1.135	1.00	0.00
617	HETATM	617	H1	WAT	205	2.607	-0.910	1.131	1.00	0.00
618	HETATM	618	H2	WAT	205	3.536	-2.253	1.136	1.00	0.00
619	HETATM	619	O	WAT	206	5.197	-2.856	1.139	1.00	0.00
620	HETATM	620	H1	WAT	206	5.673	-2.524	1.954	1.00	0.00
621	HETATM	621	H2	WAT	206	5.669	-2.533	0.321	1.00	0.00
622	HETATM	622	O	WAT	207	6.511	-1.937	3.395	1.00	0.00
623	HETATM	623	H1	WAT	207	6.037	-2.262	4.213	1.00	0.00
624	HETATM	624	H2	WAT	207	6.520	-0.937	3.391	1.00	0.00
625	HETATM	625	O	WAT	208	5.198	-2.838	5.659	1.00	0.00
626	HETATM	626	H1	WAT	208	5.671	-2.514	4.840	1.00	0.00
627	HETATM	627	H2	WAT	208	5.673	-2.506	6.473	1.00	0.00
628	HETATM	628	O	WAT	209	2.597	-1.891	5.655	1.00	0.00
629	HETATM	629	H1	WAT	209	2.123	-2.217	6.472	1.00	0.00
630	HETATM	630	H2	WAT	209	3.537	-2.233	5.655	1.00	0.00
631	HETATM	631	O	WAT	210	9.155	1.728	3.380	1.00	0.00

632	HETATM	632	H1	WAT	210	9.164	2.728	3.376	1.00	0.00
			H							
633	HETATM	633	H2	WAT	210	8.209	1.404	3.382	1.00	0.00
			H							
634	HETATM	634	O	WAT	211	10.451	0.785	1.124	1.00	0.00
			O							
635	HETATM	635	H1	WAT	211	10.440	-0.214	1.128	1.00	0.00
			H							
636	HETATM	636	H2	WAT	211	11.397	1.109	1.123	1.00	0.00
			H							
637	HETATM	637	O	WAT	212	10.451	0.803	5.644	1.00	0.00
			O							
638	HETATM	638	H1	WAT	212	9.982	1.137	4.826	1.00	0.00
			H							
639	HETATM	639	H2	WAT	212	11.397	1.127	5.643	1.00	0.00
			H							
640	HETATM	640	O	WAT	213	9.111	-2.884	3.399	1.00	0.00
			O							
641	HETATM	641	H1	WAT	213	9.586	-2.552	4.214	1.00	0.00
			H							
642	HETATM	642	H2	WAT	213	9.101	-3.884	3.402	1.00	0.00
			H							
643	HETATM	643	O	WAT	214	10.425	-1.983	1.135	1.00	0.00
			O							
644	HETATM	644	H1	WAT	214	10.434	-0.983	1.131	1.00	0.00
			H							
645	HETATM	645	H2	WAT	214	9.950	-2.316	0.320	1.00	0.00
			H							
646	HETATM	646	O	WAT	215	10.425	-1.965	5.655	1.00	0.00
			O							
647	HETATM	647	H1	WAT	215	10.434	-0.965	5.651	1.00	0.00
			H							
648	HETATM	648	H2	WAT	215	11.365	-2.307	5.658	1.00	0.00
			H							
649	HETATM	649	O	WAT	216	-10.414	1.885	-3.399	1.00	0.00
			O							
650	HETATM	650	H1	WAT	216	-10.404	2.885	-3.403	1.00	0.00
			H							
651	HETATM	651	H2	WAT	216	-11.360	1.561	-3.398	1.00	0.00
			H							
652	HETATM	652	O	WAT	217	-9.118	0.941	-5.655	1.00	0.00
			O							
653	HETATM	653	H1	WAT	217	-9.127	-0.058	-5.652	1.00	0.00
			H							
654	HETATM	654	H2	WAT	217	-9.586	1.276	-6.472	1.00	0.00
			H							
655	HETATM	655	O	WAT	218	-6.500	1.839	-5.659	1.00	0.00
			O							
656	HETATM	656	H1	WAT	218	-7.446	1.515	-5.657	1.00	0.00
			H							
657	HETATM	657	H2	WAT	218	-6.491	2.839	-5.663	1.00	0.00
			H							
658	HETATM	658	O	WAT	219	-5.205	0.914	-3.395	1.00	0.00
			O							

659	HETATM	659	H1	WAT	219	-4.259	1.238	-3.396	1.00	0.00
		H								
660	HETATM	660	H2	WAT	219	-5.216	-0.085	-3.391	1.00	0.00
		H								
661	HETATM	661	O	WAT	220	-6.500	1.857	-1.139	1.00	0.00
		O								
662	HETATM	662	H1	WAT	220	-6.490	2.857	-1.143	1.00	0.00
		H								
663	HETATM	663	H2	WAT	220	-6.032	1.522	-0.321	1.00	0.00
		H								
664	HETATM	664	O	WAT	221	-9.117	0.960	-1.135	1.00	0.00
		O								
665	HETATM	665	H1	WAT	221	-9.128	-0.040	-1.131	1.00	0.00
		H								
666	HETATM	666	H2	WAT	221	-8.172	1.284	-1.136	1.00	0.00
		H								
667	HETATM	667	O	WAT	222	-10.457	-2.727	-3.380	1.00	0.00
		O								
668	HETATM	668	H1	WAT	222	-10.466	-3.727	-3.376	1.00	0.00
		H								
669	HETATM	669	H2	WAT	222	-11.397	-2.385	-3.382	1.00	0.00
		H								
670	HETATM	670	O	WAT	223	-9.144	-1.826	-5.644	1.00	0.00
		O								
671	HETATM	671	H1	WAT	223	-9.134	-0.827	-5.648	1.00	0.00
		H								
672	HETATM	672	H2	WAT	223	-8.205	-2.168	-5.643	1.00	0.00
		H								
673	HETATM	673	O	WAT	224	-6.543	-2.773	-5.640	1.00	0.00
		O								
674	HETATM	674	H1	WAT	224	-6.069	-2.441	-4.825	1.00	0.00
		H								
675	HETATM	675	H2	WAT	224	-7.483	-2.431	-5.642	1.00	0.00
		H								
676	HETATM	676	O	WAT	225	-5.231	-1.854	-3.384	1.00	0.00
		O								
677	HETATM	677	H1	WAT	225	-4.292	-2.197	-3.383	1.00	0.00
		H								
678	HETATM	678	H2	WAT	225	-5.221	-0.854	-3.388	1.00	0.00
		H								
679	HETATM	679	O	WAT	226	-6.543	-2.755	-1.120	1.00	0.00
		O								
680	HETATM	680	H1	WAT	226	-6.069	-2.423	-0.306	1.00	0.00
		H								
681	HETATM	681	H2	WAT	226	-6.553	-3.755	-1.116	1.00	0.00
		H								
682	HETATM	682	O	WAT	227	-9.143	-1.808	-1.124	1.00	0.00
		O								
683	HETATM	683	H1	WAT	227	-9.134	-0.808	-1.128	1.00	0.00
		H								
684	HETATM	684	H2	WAT	227	-9.618	-2.133	-0.307	1.00	0.00
		H								
685	HETATM	685	O	WAT	228	-2.586	1.811	-3.399	1.00	0.00
		O								

686	HETATM	686	H1	WAT	228	-2.118	1.470	-4.213	1.00	0.00
		H								
687	HETATM	687	H2	WAT	228	-3.532	1.487	-3.397	1.00	0.00
		H								
688	HETATM	688	O	WAT	229	-1.291	0.868	-5.655	1.00	0.00
		O								
689	HETATM	689	H1	WAT	229	-1.760	1.209	-4.841	1.00	0.00
		H								
690	HETATM	690	H2	WAT	229	-1.302	-0.131	-5.651	1.00	0.00
		H								
691	HETATM	691	O	WAT	230	1.328	1.765	-5.659	1.00	0.00
		O								
692	HETATM	692	H1	WAT	230	0.382	1.440	-5.657	1.00	0.00
		H								
693	HETATM	693	H2	WAT	230	1.797	1.430	-4.842	1.00	0.00
		H								
694	HETATM	694	O	WAT	231	2.623	0.840	-3.395	1.00	0.00
		O								
695	HETATM	695	H1	WAT	231	2.155	1.174	-4.212	1.00	0.00
		H								
696	HETATM	696	H2	WAT	231	2.612	-0.159	-3.391	1.00	0.00
		H								
697	HETATM	697	O	WAT	232	1.328	1.783	-1.139	1.00	0.00
		O								
698	HETATM	698	H1	WAT	232	1.337	2.783	-1.143	1.00	0.00
		H								
699	HETATM	699	H2	WAT	232	1.796	1.443	-1.954	1.00	0.00
		H								
700	HETATM	700	O	WAT	233	-1.291	0.886	-1.135	1.00	0.00
		O								
701	HETATM	701	H1	WAT	233	-1.301	-0.114	-1.130	1.00	0.00
		H								
702	HETATM	702	H2	WAT	233	-0.345	1.210	-1.136	1.00	0.00
		H								
703	HETATM	703	O	WAT	234	-2.629	-2.801	-3.380	1.00	0.00
		O								
704	HETATM	704	H1	WAT	234	-2.154	-2.475	-4.198	1.00	0.00
		H								
705	HETATM	705	H2	WAT	234	-2.638	-3.801	-3.376	1.00	0.00
		H								
706	HETATM	706	O	WAT	235	-1.317	-1.900	-5.644	1.00	0.00
		O								
707	HETATM	707	H1	WAT	235	-1.792	-2.233	-6.458	1.00	0.00
		H								
708	HETATM	708	H2	WAT	235	-1.791	-2.225	-4.826	1.00	0.00
		H								
709	HETATM	709	O	WAT	236	1.284	-2.847	-5.640	1.00	0.00
		O								
710	HETATM	710	H1	WAT	236	1.759	-2.521	-6.458	1.00	0.00
		H								
711	HETATM	711	H2	WAT	236	1.275	-3.847	-5.636	1.00	0.00
		H								
712	HETATM	712	O	WAT	237	2.597	-1.928	-3.384	1.00	0.00
		O								

713	HETATM	713	H1	WAT	237	3.537	-2.271	-3.382	1.00	0.00
		H								
714	HETATM	714	H2	WAT	237	2.123	-2.253	-2.566	1.00	0.00
		H								
715	HETATM	715	O	WAT	238	1.284	-2.828	-1.120	1.00	0.00
		O								
716	HETATM	716	H1	WAT	238	1.273	-3.827	-1.117	1.00	0.00
		H								
717	HETATM	717	H2	WAT	238	1.757	-2.504	-1.939	1.00	0.00
		H								
718	HETATM	718	O	WAT	239	-1.317	-1.882	-1.124	1.00	0.00
		O								
719	HETATM	719	H1	WAT	239	-1.791	-2.207	-0.307	1.00	0.00
		H								
720	HETATM	720	H2	WAT	239	-0.378	-2.225	-1.123	1.00	0.00
		H								
721	HETATM	721	O	WAT	240	5.241	1.738	-3.399	1.00	0.00
		O								
722	HETATM	722	H1	WAT	240	5.250	2.738	-3.403	1.00	0.00
		H								
723	HETATM	723	H2	WAT	240	5.709	1.404	-2.581	1.00	0.00
		H								
724	HETATM	724	O	WAT	241	6.537	0.794	-5.655	1.00	0.00
		O								
725	HETATM	725	H1	WAT	241	6.526	-0.205	-5.651	1.00	0.00
		H								
726	HETATM	726	H2	WAT	241	6.068	1.135	-4.841	1.00	0.00
		H								
727	HETATM	727	O	WAT	242	9.154	1.692	-5.659	1.00	0.00
		O								
728	HETATM	728	H1	WAT	242	8.208	1.368	-5.659	1.00	0.00
		H								
729	HETATM	729	H2	WAT	242	9.623	1.351	-6.473	1.00	0.00
		H								
730	HETATM	730	O	WAT	243	10.451	0.767	-3.395	1.00	0.00
		O								
731	HETATM	731	H1	WAT	243	10.440	-0.232	-3.391	1.00	0.00
		H								
732	HETATM	732	H2	WAT	243	11.397	1.091	-3.396	1.00	0.00
		H								
733	HETATM	733	O	WAT	244	9.154	1.710	-1.139	1.00	0.00
		O								
734	HETATM	734	H1	WAT	244	9.623	1.369	-1.954	1.00	0.00
		H								
735	HETATM	735	H2	WAT	244	8.208	1.386	-1.139	1.00	0.00
		H								
736	HETATM	736	O	WAT	245	6.537	0.812	-1.135	1.00	0.00
		O								
737	HETATM	737	H1	WAT	245	7.483	1.137	-1.136	1.00	0.00
		H								
738	HETATM	738	H2	WAT	245	6.529	-0.188	-1.132	1.00	0.00
		H								
739	HETATM	739	O	WAT	246	5.197	-2.874	-3.380	1.00	0.00
		O								

740	HETATM	740	H1	WAT	246	5.670	-2.549	-4.198	1.00	0.00
		H								
741	HETATM	741	H2	WAT	246	5.672	-2.542	-2.565	1.00	0.00
		H								
742	HETATM	742	O	WAT	247	6.511	-1.974	-5.644	1.00	0.00
		O								
743	HETATM	743	H1	WAT	247	6.520	-0.974	-5.648	1.00	0.00
		H								
744	HETATM	744	H2	WAT	247	7.451	-2.317	-5.642	1.00	0.00
		H								
745	HETATM	745	O	WAT	248	9.111	-2.920	-5.640	1.00	0.00
		O								
746	HETATM	746	H1	WAT	248	9.101	-3.920	-5.637	1.00	0.00
		H								
747	HETATM	747	H2	WAT	248	9.585	-2.595	-6.459	1.00	0.00
		H								
748	HETATM	748	O	WAT	249	10.425	-2.001	-3.384	1.00	0.00
		O								
749	HETATM	749	H1	WAT	249	11.365	-2.343	-3.382	1.00	0.00
		H								
750	HETATM	750	H2	WAT	249	9.951	-2.333	-4.199	1.00	0.00
		H								
751	HETATM	751	O	WAT	250	9.111	-2.902	-1.120	1.00	0.00
		O								
752	HETATM	752	H1	WAT	250	9.100	-3.902	-1.117	1.00	0.00
		H								
753	HETATM	753	H2	WAT	250	9.584	-2.578	-1.939	1.00	0.00
		H								
754	HETATM	754	O	WAT	251	6.511	-1.955	-1.124	1.00	0.00
		O								
755	HETATM	755	H1	WAT	251	6.037	-2.281	-0.307	1.00	0.00
		H								
756	HETATM	756	H2	WAT	251	7.451	-2.296	-1.123	1.00	0.00
		H								
757	HETATM	757	O	WAT	252	-10.414	1.848	-12.438	1.00	0.00
		O								
758	HETATM	758	H1	WAT	252	-9.945	1.513	-11.620	1.00	0.00
		H								
759	HETATM	759	H2	WAT	252	-11.360	1.523	-12.437	1.00	0.00
		H								
760	HETATM	760	O	WAT	253	-9.118	0.923	-10.174	1.00	0.00
		O								
761	HETATM	761	H1	WAT	253	-8.173	1.247	-10.175	1.00	0.00
		H								
762	HETATM	762	H2	WAT	253	-9.129	-0.076	-10.170	1.00	0.00
		H								
763	HETATM	763	O	WAT	254	-10.414	1.867	-7.918	1.00	0.00
		O								
764	HETATM	764	H1	WAT	254	-11.359	1.543	-7.916	1.00	0.00
		H								
765	HETATM	765	H2	WAT	254	-10.405	2.866	-7.922	1.00	0.00
		H								
766	HETATM	766	O	WAT	255	-10.457	-2.763	-12.419	1.00	0.00
		O								

767	HETATM	767	H1	WAT	255	-9.983	-2.435	-13.236	1.00	0.00
768	HETATM	768	H2	WAT	255	-11.397	-2.422	-12.420	1.00	0.00
769	HETATM	769	O	WAT	256	-9.144	-1.845	-10.163	1.00	0.00
770	HETATM	770	H1	WAT	256	-9.134	-0.845	-10.167	1.00	0.00
771	HETATM	771	H2	WAT	256	-9.619	-2.177	-10.978	1.00	0.00
772	HETATM	772	O	WAT	257	-10.457	-2.745	-7.899	1.00	0.00
773	HETATM	773	H1	WAT	257	-9.982	-2.419	-8.717	1.00	0.00
774	HETATM	774	H2	WAT	257	-11.397	-2.403	-7.900	1.00	0.00
775	HETATM	775	O	WAT	258	-6.500	1.821	-10.178	1.00	0.00
776	HETATM	776	H1	WAT	258	-6.032	1.480	-10.992	1.00	0.00
777	HETATM	777	H2	WAT	258	-6.491	2.821	-10.182	1.00	0.00
778	HETATM	778	O	WAT	259	-5.205	0.877	-12.434	1.00	0.00
779	HETATM	779	H1	WAT	259	-5.674	1.218	-11.620	1.00	0.00
780	HETATM	780	H2	WAT	259	-4.259	1.201	-12.435	1.00	0.00
781	HETATM	781	O	WAT	260	-2.586	1.775	-12.438	1.00	0.00
782	HETATM	782	H1	WAT	260	-3.532	1.451	-12.435	1.00	0.00
783	HETATM	783	H2	WAT	260	-2.119	1.434	-13.252	1.00	0.00
784	HETATM	784	O	WAT	261	-1.291	0.850	-10.174	1.00	0.00
785	HETATM	785	H1	WAT	261	-1.759	1.184	-10.991	1.00	0.00
786	HETATM	786	H2	WAT	261	-1.760	1.191	-9.360	1.00	0.00
787	HETATM	787	O	WAT	262	-2.586	1.793	-7.918	1.00	0.00
788	HETATM	788	H1	WAT	262	-2.577	2.793	-7.922	1.00	0.00
789	HETATM	789	H2	WAT	262	-2.118	1.459	-7.100	1.00	0.00
790	HETATM	790	O	WAT	263	-5.205	0.896	-7.914	1.00	0.00
791	HETATM	791	H1	WAT	263	-5.673	1.230	-8.732	1.00	0.00
792	HETATM	792	H2	WAT	263	-5.674	1.237	-7.100	1.00	0.00
793	HETATM	793	O	WAT	264	-6.544	-2.791	-10.159	1.00	0.00

794	HETATM	794	H1	WAT	264	-6.070	-2.465	-10.976	1.00	0.00
795	HETATM	795	H	WAT	264	-6.553	-3.790	-10.155	1.00	0.00
796	HETATM	796	O	WAT	265	-5.231	-1.891	-12.423	1.00	0.00
797	HETATM	797	H	WAT	265	-4.292	-2.234	-12.421	1.00	0.00
798	HETATM	798	H	WAT	265	-5.705	-2.216	-11.604	1.00	0.00
799	HETATM	799	O	WAT	266	-2.630	-2.837	-12.419	1.00	0.00
800	HETATM	800	H	WAT	266	-2.155	-2.510	-13.236	1.00	0.00
801	HETATM	801	H	WAT	266	-2.156	-2.505	-11.603	1.00	0.00
802	HETATM	802	O	WAT	267	-1.317	-1.918	-10.163	1.00	0.00
803	HETATM	803	H	WAT	267	-0.377	-2.261	-10.161	1.00	0.00
804	HETATM	804	H	WAT	267	-1.308	-0.918	-10.167	1.00	0.00
805	HETATM	805	O	WAT	268	-2.630	-2.819	-7.899	1.00	0.00
806	HETATM	806	H	WAT	268	-2.156	-2.494	-8.717	1.00	0.00
807	HETATM	807	H	WAT	268	-3.569	-2.477	-7.900	1.00	0.00
808	HETATM	808	O	WAT	269	-5.231	-1.872	-7.903	1.00	0.00
809	HETATM	809	H	WAT	269	-4.291	-2.214	-7.903	1.00	0.00
810	HETATM	810	H	WAT	269	-5.705	-2.203	-8.719	1.00	0.00
811	HETATM	811	O	WAT	270	1.327	1.747	-10.178	1.00	0.00
812	HETATM	812	H	WAT	270	1.795	1.412	-9.360	1.00	0.00
813	HETATM	813	H	WAT	270	1.795	1.406	-10.992	1.00	0.00
814	HETATM	814	O	WAT	271	2.623	0.804	-12.434	1.00	0.00
815	HETATM	815	H	WAT	271	2.155	1.138	-13.251	1.00	0.00
816	HETATM	816	H	WAT	271	2.612	-0.195	-12.430	1.00	0.00
817	HETATM	817	O	WAT	272	5.240	1.701	-12.438	1.00	0.00
818	HETATM	818	H	WAT	272	5.709	1.360	-13.252	1.00	0.00
819	HETATM	819	H	WAT	272	5.707	1.366	-11.620	1.00	0.00
820	HETATM	820	O	WAT	273	6.537	0.776	-10.174	1.00	0.00

821	HETATM	821	H1	WAT	273	6.068	1.117	-9.360	1.00	0.00
			H							
822	HETATM	822	H2	WAT	273	6.069	1.110	-10.991	1.00	0.00
			H							
823	HETATM	823	O	WAT	274	5.240	1.719	-7.918	1.00	0.00
			O							
824	HETATM	824	H1	WAT	274	5.709	1.379	-8.733	1.00	0.00
			H							
825	HETATM	825	H2	WAT	274	4.294	1.394	-7.919	1.00	0.00
			H							
826	HETATM	826	O	WAT	275	2.623	0.822	-7.914	1.00	0.00
			O							
827	HETATM	827	H1	WAT	275	2.154	1.163	-7.100	1.00	0.00
			H							
828	HETATM	828	H2	WAT	275	2.155	1.156	-8.732	1.00	0.00
			H							
829	HETATM	829	O	WAT	276	1.284	-2.865	-10.159	1.00	0.00
			O							
830	HETATM	830	H1	WAT	276	1.276	-3.865	-10.155	1.00	0.00
			H							
831	HETATM	831	H2	WAT	276	1.758	-2.533	-9.343	1.00	0.00
			H							
832	HETATM	832	O	WAT	277	2.597	-1.964	-12.423	1.00	0.00
			O							
833	HETATM	833	H1	WAT	277	2.123	-2.289	-11.604	1.00	0.00
			H							
834	HETATM	834	H2	WAT	277	3.536	-2.307	-12.421	1.00	0.00
			H							
835	HETATM	835	O	WAT	278	5.197	-2.911	-12.419	1.00	0.00
			O							
836	HETATM	836	H1	WAT	278	5.188	-3.910	-12.415	1.00	0.00
			H							
837	HETATM	837	H2	WAT	278	4.258	-2.569	-12.420	1.00	0.00
			H							
838	HETATM	838	O	WAT	279	6.511	-1.992	-10.163	1.00	0.00
			O							
839	HETATM	839	H1	WAT	279	6.036	-2.317	-9.345	1.00	0.00
			H							
840	HETATM	840	H2	WAT	279	7.451	-2.335	-10.160	1.00	0.00
			H							
841	HETATM	841	O	WAT	280	5.197	-2.892	-7.899	1.00	0.00
			O							
842	HETATM	842	H1	WAT	280	4.258	-2.551	-7.900	1.00	0.00
			H							
843	HETATM	843	H2	WAT	280	5.669	-2.566	-8.717	1.00	0.00
			H							
844	HETATM	844	O	WAT	281	2.597	-1.946	-7.903	1.00	0.00
			O							
845	HETATM	845	H1	WAT	281	2.122	-2.279	-8.718	1.00	0.00
			H							
846	HETATM	846	H2	WAT	281	2.606	-0.946	-7.907	1.00	0.00
			H							
847	HETATM	847	O	WAT	282	9.154	1.673	-10.178	1.00	0.00
			O							

848	HETATM	848	H1	WAT	282	9.622	1.337	-9.360	1.00	0.00
		H								
849	HETATM	849	H2	WAT	282	9.164	2.673	-10.182	1.00	0.00
		H								
850	HETATM	850	O	WAT	283	10.450	0.730	-12.434	1.00	0.00
		O								
851	HETATM	851	H1	WAT	283	10.439	-0.269	-12.430	1.00	0.00
		H								
852	HETATM	852	H2	WAT	283	9.981	1.064	-13.251	1.00	0.00
		H								
853	HETATM	853	O	WAT	284	10.451	0.748	-7.914	1.00	0.00
		O								
854	HETATM	854	H1	WAT	284	10.440	-0.252	-7.910	1.00	0.00
		H								
855	HETATM	855	H2	WAT	284	9.981	1.089	-7.099	1.00	0.00
		H								
856	HETATM	856	O	WAT	285	9.111	-2.938	-10.159	1.00	0.00
		O								
857	HETATM	857	H1	WAT	285	9.585	-2.612	-10.977	1.00	0.00
		H								
858	HETATM	858	H2	WAT	285	9.102	-3.938	-10.156	1.00	0.00
		H								
859	HETATM	859	O	WAT	286	10.424	-2.038	-12.423	1.00	0.00
		O								
860	HETATM	860	H1	WAT	286	10.434	-1.038	-12.427	1.00	0.00
		H								
861	HETATM	861	H2	WAT	286	9.948	-2.371	-13.237	1.00	0.00
		H								
862	HETATM	862	O	WAT	287	10.424	-2.020	-7.903	1.00	0.00
		O								
863	HETATM	863	H1	WAT	287	9.949	-2.345	-7.086	1.00	0.00
		H								
864	HETATM	864	H2	WAT	287	9.950	-2.352	-8.718	1.00	0.00
		H								
865	HETATM	865	O	WAT	288	-10.344	9.319	10.129	1.00	0.00
		O								
866	HETATM	866	H1	WAT	288	-11.290	8.995	10.130	1.00	0.00
		H								
867	HETATM	867	H2	WAT	288	-10.334	10.319	10.125	1.00	0.00
		H								
868	HETATM	868	O	WAT	289	-9.048	8.376	7.873	1.00	0.00
		O								
869	HETATM	869	H1	WAT	289	-9.517	8.710	7.056	1.00	0.00
		H								
870	HETATM	870	H2	WAT	289	-8.103	8.700	7.872	1.00	0.00
		H								
871	HETATM	871	O	WAT	290	-6.430	9.273	7.869	1.00	0.00
		O								
872	HETATM	872	H1	WAT	290	-5.962	8.932	7.055	1.00	0.00
		H								
873	HETATM	873	H2	WAT	290	-7.376	8.949	7.871	1.00	0.00
		H								
874	HETATM	874	O	WAT	291	-5.135	8.348	10.133	1.00	0.00
		O								

875	HETATM	875	H1	WAT	291	-5.604	8.689	10.947	1.00	0.00
		H								
876	HETATM	876	H2	WAT	291	-5.146	7.349	10.137	1.00	0.00
		H								
877	HETATM	877	O	WAT	292	-6.430	9.291	12.389	1.00	0.00
		O								
878	HETATM	878	H1	WAT	292	-6.421	10.291	12.385	1.00	0.00
		H								
879	HETATM	879	H2	WAT	292	-7.376	8.966	12.390	1.00	0.00
		H								
880	HETATM	880	O	WAT	293	-9.047	8.394	12.393	1.00	0.00
		O								
881	HETATM	881	H1	WAT	293	-9.516	8.728	11.575	1.00	0.00
		H								
882	HETATM	882	H2	WAT	293	-9.517	8.735	13.208	1.00	0.00
		H								
883	HETATM	883	O	WAT	294	-10.387	4.707	10.148	1.00	0.00
		O								
884	HETATM	884	H1	WAT	294	-10.396	3.707	10.152	1.00	0.00
		H								
885	HETATM	885	H2	WAT	294	-9.913	5.039	10.963	1.00	0.00
		H								
886	HETATM	886	O	WAT	295	-9.074	5.608	7.884	1.00	0.00
		O								
887	HETATM	887	H1	WAT	295	-9.549	5.283	8.703	1.00	0.00
		H								
888	HETATM	888	H2	WAT	295	-8.135	5.265	7.886	1.00	0.00
		H								
889	HETATM	889	O	WAT	296	-6.473	4.661	7.888	1.00	0.00
		O								
890	HETATM	890	H1	WAT	296	-7.413	5.003	7.887	1.00	0.00
		H								
891	HETATM	891	H2	WAT	296	-6.481	3.661	7.892	1.00	0.00
		H								
892	HETATM	892	O	WAT	297	-5.161	5.580	10.144	1.00	0.00
		O								
893	HETATM	893	H1	WAT	297	-5.635	5.255	10.962	1.00	0.00
		H								
894	HETATM	894	H2	WAT	297	-4.222	5.237	10.145	1.00	0.00
		H								
895	HETATM	895	O	WAT	298	-6.473	4.680	12.408	1.00	0.00
		O								
896	HETATM	896	H1	WAT	298	-5.999	5.007	11.590	1.00	0.00
		H								
897	HETATM	897	H2	WAT	298	-7.413	5.021	12.407	1.00	0.00
		H								
898	HETATM	898	O	WAT	299	-9.074	5.626	12.404	1.00	0.00
		O								
899	HETATM	899	H1	WAT	299	-9.064	6.626	12.400	1.00	0.00
		H								
900	HETATM	900	H2	WAT	299	-9.549	5.294	11.589	1.00	0.00
		H								
901	HETATM	901	O	WAT	300	-2.516	9.245	10.129	1.00	0.00
		O								

902	HETATM	902	H1	WAT	300	-2.048	8.905	9.315	1.00	0.00
903	HETATM	903	H2	WAT	300	-2.507	10.245	10.125	1.00	0.00
904	HETATM	904	O	WAT	301	-1.221	8.302	7.873	1.00	0.00
905	HETATM	905	H	WAT	301	-1.232	7.303	7.877	1.00	0.00
906	HETATM	906	H2	WAT	301	-1.689	8.636	7.056	1.00	0.00
907	HETATM	907	O	WAT	302	1.398	9.199	7.869	1.00	0.00
908	HETATM	908	H	WAT	302	1.867	8.864	8.686	1.00	0.00
909	HETATM	909	H2	WAT	302	1.865	8.859	7.055	1.00	0.00
910	HETATM	910	O	WAT	303	2.693	8.274	10.133	1.00	0.00
911	HETATM	911	H	WAT	303	2.682	7.275	10.137	1.00	0.00
912	HETATM	912	H2	WAT	303	2.225	8.608	9.316	1.00	0.00
913	HETATM	913	O	WAT	304	1.398	9.218	12.389	1.00	0.00
914	HETATM	914	H	WAT	304	1.866	8.877	11.574	1.00	0.00
915	HETATM	915	H2	WAT	304	0.452	8.893	12.391	1.00	0.00
916	HETATM	916	O	WAT	305	-1.221	8.320	12.393	1.00	0.00
917	HETATM	917	H	WAT	305	-1.231	7.320	12.398	1.00	0.00
918	HETATM	918	H2	WAT	305	-0.275	8.644	12.392	1.00	0.00
919	HETATM	919	O	WAT	306	-2.560	4.634	10.148	1.00	0.00
920	HETATM	920	H	WAT	306	-2.088	4.960	9.330	1.00	0.00
921	HETATM	921	H2	WAT	306	-3.499	4.975	10.147	1.00	0.00
922	HETATM	922	O	WAT	307	-1.247	5.534	7.884	1.00	0.00
923	HETATM	923	H	WAT	307	-0.308	5.191	7.886	1.00	0.00
924	HETATM	924	H2	WAT	307	-1.721	5.209	8.703	1.00	0.00
925	HETATM	925	O	WAT	308	1.354	4.588	7.888	1.00	0.00
926	HETATM	926	H	WAT	308	1.346	3.588	7.892	1.00	0.00
927	HETATM	927	H2	WAT	308	0.414	4.930	7.887	1.00	0.00
928	HETATM	928	O	WAT	309	2.667	5.507	10.144	1.00	0.00

929	HETATM	929	H1	WAT	309	2.676	6.506	10.140	1.00	0.00
		H								
930	HETATM	930	H2	WAT	309	2.193	5.181	10.962	1.00	0.00
		H								
931	HETATM	931	O	WAT	310	1.354	4.606	12.408	1.00	0.00
		O								
932	HETATM	932	H1	WAT	310	0.415	4.948	12.407	1.00	0.00
		H								
933	HETATM	933	H2	WAT	310	1.829	4.938	13.223	1.00	0.00
		H								
934	HETATM	934	O	WAT	311	-1.247	5.552	12.404	1.00	0.00
		O								
935	HETATM	935	H1	WAT	311	-0.308	5.209	12.405	1.00	0.00
		H								
936	HETATM	936	H2	WAT	311	-1.723	5.220	11.589	1.00	0.00
		H								
937	HETATM	937	O	WAT	312	5.310	9.172	10.129	1.00	0.00
		O								
938	HETATM	938	H1	WAT	312	5.320	10.172	10.125	1.00	0.00
		H								
939	HETATM	939	H2	WAT	312	5.777	8.837	10.947	1.00	0.00
		H								
940	HETATM	940	O	WAT	313	6.607	8.228	7.873	1.00	0.00
		O								
941	HETATM	941	H1	WAT	313	6.139	8.563	7.056	1.00	0.00
		H								
942	HETATM	942	H2	WAT	313	6.598	7.229	7.876	1.00	0.00
		H								
943	HETATM	943	O	WAT	314	9.224	9.126	7.869	1.00	0.00
		O								
944	HETATM	944	H1	WAT	314	9.234	10.126	7.865	1.00	0.00
		H								
945	HETATM	945	H2	WAT	314	9.693	8.785	7.055	1.00	0.00
		H								
946	HETATM	946	O	WAT	315	10.521	8.201	10.133	1.00	0.00
		O								
947	HETATM	947	H1	WAT	315	11.467	8.525	10.132	1.00	0.00
		H								
948	HETATM	948	H2	WAT	315	10.052	8.535	9.316	1.00	0.00
		H								
949	HETATM	949	O	WAT	316	9.224	9.144	12.389	1.00	0.00
		O								
950	HETATM	950	H1	WAT	316	9.693	8.803	11.574	1.00	0.00
		H								
951	HETATM	951	H2	WAT	316	9.692	8.809	13.207	1.00	0.00
		H								
952	HETATM	952	O	WAT	317	6.607	8.247	12.393	1.00	0.00
		O								
953	HETATM	953	H1	WAT	317	6.597	7.247	12.398	1.00	0.00
		H								
954	HETATM	954	H2	WAT	317	7.553	8.571	12.392	1.00	0.00
		H								
955	HETATM	955	O	WAT	318	5.267	4.560	10.148	1.00	0.00
		O								

956	HETATM	956	H1	WAT	318	4.328	4.902	10.147	1.00	0.00
		H								
957	HETATM	957	H2	WAT	318	5.741	4.885	9.330	1.00	0.00
		H								
958	HETATM	958	O	WAT	319	6.581	5.461	7.884	1.00	0.00
		O								
959	HETATM	959	H1	WAT	319	6.107	5.135	8.703	1.00	0.00
		H								
960	HETATM	960	H2	WAT	319	7.521	5.119	7.885	1.00	0.00
		H								
961	HETATM	961	O	WAT	320	9.181	4.514	7.888	1.00	0.00
		O								
962	HETATM	962	H1	WAT	320	9.655	4.840	7.070	1.00	0.00
		H								
963	HETATM	963	H2	WAT	320	8.241	4.856	7.887	1.00	0.00
		H								
964	HETATM	964	O	WAT	321	10.495	5.433	10.144	1.00	0.00
		O								
965	HETATM	965	H1	WAT	321	11.434	5.090	10.148	1.00	0.00
		H								
966	HETATM	966	H2	WAT	321	10.504	6.433	10.140	1.00	0.00
		H								
967	HETATM	967	O	WAT	322	9.181	4.532	12.408	1.00	0.00
		O								
968	HETATM	968	H1	WAT	322	9.172	3.532	12.411	1.00	0.00
		H								
969	HETATM	969	H2	WAT	322	8.241	4.874	12.407	1.00	0.00
		H								
970	HETATM	970	O	WAT	323	6.581	5.479	12.404	1.00	0.00
		O								
971	HETATM	971	H1	WAT	323	7.521	5.136	12.406	1.00	0.00
		H								
972	HETATM	972	H2	WAT	323	6.590	6.479	12.400	1.00	0.00
		H								
973	HETATM	973	O	WAT	324	-10.344	9.283	1.090	1.00	0.00
		O								
974	HETATM	974	H1	WAT	324	-10.335	10.283	1.086	1.00	0.00
		H								
975	HETATM	975	H2	WAT	324	-9.876	8.949	1.908	1.00	0.00
		H								
976	HETATM	976	O	WAT	325	-9.048	8.357	3.354	1.00	0.00
		O								
977	HETATM	977	H1	WAT	325	-9.517	8.696	4.169	1.00	0.00
		H								
978	HETATM	978	H2	WAT	325	-9.057	7.357	3.357	1.00	0.00
		H								
979	HETATM	979	O	WAT	326	-10.344	9.301	5.610	1.00	0.00
		O								
980	HETATM	980	H1	WAT	326	-9.876	8.960	4.795	1.00	0.00
		H								
981	HETATM	981	H2	WAT	326	-10.335	10.301	5.606	1.00	0.00
		H								
982	HETATM	982	O	WAT	327	-10.388	4.671	1.109	1.00	0.00
		O								

983	HETATM	983	H1	WAT	327	-9.913	5.003	1.925	1.00	0.00
984	HETATM	984	H2	WAT	327	-9.914	4.997	0.292	1.00	0.00
985	HETATM	985	O	WAT	328	-9.074	5.590	3.365	1.00	0.00
986	HETATM	986	H1	WAT	328	-9.549	5.258	2.550	1.00	0.00
987	HETATM	987	H2	WAT	328	-9.549	5.264	4.184	1.00	0.00
988	HETATM	988	O	WAT	329	-10.387	4.689	5.629	1.00	0.00
989	HETATM	989	H1	WAT	329	-9.913	5.021	6.444	1.00	0.00
990	HETATM	990	H2	WAT	329	-11.327	5.031	5.628	1.00	0.00
991	HETATM	991	O	WAT	330	-6.430	9.255	3.350	1.00	0.00
992	HETATM	992	H1	WAT	330	-7.376	8.931	3.352	1.00	0.00
993	HETATM	993	H2	WAT	330	-5.962	8.914	2.536	1.00	0.00
994	HETATM	994	O	WAT	331	-5.135	8.312	1.094	1.00	0.00
995	HETATM	995	H1	WAT	331	-5.604	8.653	1.908	1.00	0.00
996	HETATM	996	H2	WAT	331	-4.189	8.636	1.093	1.00	0.00
997	HETATM	997	O	WAT	332	-2.517	9.209	1.090	1.00	0.00
998	HETATM	998	H1	WAT	332	-2.049	8.868	0.276	1.00	0.00
999	HETATM	999	H2	WAT	332	-2.507	10.209	1.086	1.00	0.00
1000	HETATM	1000	O	WAT	333	-1.221	8.284	3.354	1.00	0.00
1001	HETATM	1001	H1	WAT	333	-1.232	7.285	3.358	1.00	0.00
1002	HETATM	1002	H2	WAT	333	-1.689	8.618	2.537	1.00	0.00
1003	HETATM	1003	O	WAT	334	-2.516	9.227	5.610	1.00	0.00
1004	HETATM	1004	H1	WAT	334	-2.049	8.886	4.795	1.00	0.00
1005	HETATM	1005	H2	WAT	334	-3.462	8.903	5.613	1.00	0.00
1006	HETATM	1006	O	WAT	335	-5.135	8.330	5.614	1.00	0.00
1007	HETATM	1007	H1	WAT	335	-4.189	8.654	5.613	1.00	0.00
1008	HETATM	1008	H2	WAT	335	-5.145	7.330	5.619	1.00	0.00
1009	HETATM	1009	O	WAT	336	-6.474	4.643	3.369	1.00	0.00

1010	HETATM	1010	H1	WAT	336	-7.413	4.985	3.368	1.00	0.00
		H								
1011	HETATM	1011	H2	WAT	336	-6.000	4.969	2.552	1.00	0.00
		H								
1012	HETATM	1012	O	WAT	337	-5.161	5.544	1.105	1.00	0.00
		O								
1013	HETATM	1013	H1	WAT	337	-4.221	5.202	1.106	1.00	0.00
		H								
1014	HETATM	1014	H2	WAT	337	-5.152	6.544	1.101	1.00	0.00
		H								
1015	HETATM	1015	O	WAT	338	-2.560	4.597	1.109	1.00	0.00
		O								
1016	HETATM	1016	H1	WAT	338	-3.500	4.939	1.108	1.00	0.00
		H								
1017	HETATM	1017	H2	WAT	338	-2.085	4.924	0.292	1.00	0.00
		H								
1018	HETATM	1018	O	WAT	339	-1.247	5.516	3.365	1.00	0.00
		O								
1019	HETATM	1019	H1	WAT	339	-0.308	5.173	3.367	1.00	0.00
		H								
1020	HETATM	1020	H2	WAT	339	-1.238	6.516	3.361	1.00	0.00
		H								
1021	HETATM	1021	O	WAT	340	-2.560	4.615	5.629	1.00	0.00
		O								
1022	HETATM	1022	H1	WAT	340	-2.569	3.615	5.633	1.00	0.00
		H								
1023	HETATM	1023	H2	WAT	340	-2.085	4.941	4.811	1.00	0.00
		H								
1024	HETATM	1024	O	WAT	341	-5.161	5.562	5.625	1.00	0.00
		O								
1025	HETATM	1025	H1	WAT	341	-4.221	5.219	5.627	1.00	0.00
		H								
1026	HETATM	1026	H2	WAT	341	-5.152	6.562	5.621	1.00	0.00
		H								
1027	HETATM	1027	O	WAT	342	1.397	9.181	3.350	1.00	0.00
		O								
1028	HETATM	1028	H1	WAT	342	1.865	8.841	2.536	1.00	0.00
		H								
1029	HETATM	1029	H2	WAT	342	0.451	8.856	3.350	1.00	0.00
		H								
1030	HETATM	1030	O	WAT	343	2.693	8.238	1.094	1.00	0.00
		O								
1031	HETATM	1031	H1	WAT	343	2.224	8.579	1.908	1.00	0.00
		H								
1032	HETATM	1032	H2	WAT	343	2.225	8.572	0.277	1.00	0.00
		H								
1033	HETATM	1033	O	WAT	344	5.310	9.135	1.090	1.00	0.00
		O								
1034	HETATM	1034	H1	WAT	344	5.779	8.795	0.276	1.00	0.00
		H								
1035	HETATM	1035	H2	WAT	344	5.778	8.799	1.908	1.00	0.00
		H								
1036	HETATM	1036	O	WAT	345	6.606	8.210	3.354	1.00	0.00
		O								

1037	HETATM	1037	H1	WAT	345	6.139	8.544	2.537	1.00	0.00
1038	HETATM	1038	H2	WAT	345	6.138	8.551	4.168	1.00	0.00
1039	HETATM	1039	O	WAT	346	5.310	9.154	5.610	1.00	0.00
1040	HETATM	1040	H1	WAT	346	5.778	8.819	6.428	1.00	0.00
1041	HETATM	1041	H2	WAT	346	4.364	8.830	5.610	1.00	0.00
1042	HETATM	1042	O	WAT	347	2.693	8.256	5.614	1.00	0.00
1043	HETATM	1043	H	WAT	347	2.224	8.597	6.428	1.00	0.00
1044	HETATM	1044	H2	WAT	347	2.225	8.590	4.796	1.00	0.00
1045	HETATM	1045	O	WAT	348	1.354	4.570	3.369	1.00	0.00
1046	HETATM	1046	H1	WAT	348	1.828	4.901	4.185	1.00	0.00
1047	HETATM	1047	H2	WAT	348	1.828	4.898	2.552	1.00	0.00
1048	HETATM	1048	O	WAT	349	2.667	5.470	1.105	1.00	0.00
1049	HETATM	1049	H	WAT	349	3.606	5.127	1.108	1.00	0.00
1050	HETATM	1050	H2	WAT	349	2.192	5.145	1.924	1.00	0.00
1051	HETATM	1051	O	WAT	350	5.267	4.524	1.109	1.00	0.00
1052	HETATM	1052	H1	WAT	350	5.258	3.525	1.110	1.00	0.00
1053	HETATM	1053	H2	WAT	350	5.740	4.851	0.292	1.00	0.00
1054	HETATM	1054	O	WAT	351	6.580	5.442	3.365	1.00	0.00
1055	HETATM	1055	H	WAT	351	6.106	5.117	4.184	1.00	0.00
1056	HETATM	1056	H2	WAT	351	6.590	6.442	3.361	1.00	0.00
1057	HETATM	1057	O	WAT	352	5.267	4.542	5.629	1.00	0.00
1058	HETATM	1058	H1	WAT	352	5.741	4.867	4.811	1.00	0.00
1059	HETATM	1059	H2	WAT	352	5.742	4.874	6.444	1.00	0.00
1060	HETATM	1060	O	WAT	353	2.667	5.488	5.625	1.00	0.00
1061	HETATM	1061	H1	WAT	353	2.192	5.155	4.811	1.00	0.00
1062	HETATM	1062	H2	WAT	353	2.193	5.163	6.443	1.00	0.00
1063	HETATM	1063	O	WAT	354	9.224	9.108	3.350	1.00	0.00

1064	HETATM	1064	H1	WAT	354	9.693	8.767	2.536	1.00	0.00
		H								
1065	HETATM	1065	H2	WAT	354	8.278	8.784	3.351	1.00	0.00
		H								
1066	HETATM	1066	O	WAT	355	10.520	8.164	1.094	1.00	0.00
		O								
1067	HETATM	1067	H1	WAT	355	10.509	7.164	1.097	1.00	0.00
		H								
1068	HETATM	1068	H2	WAT	355	10.051	8.499	0.277	1.00	0.00
		H								
1069	HETATM	1069	O	WAT	356	10.520	8.183	5.614	1.00	0.00
		O								
1070	HETATM	1070	H1	WAT	356	10.051	8.524	6.428	1.00	0.00
		H								
1071	HETATM	1071	H2	WAT	356	11.466	8.507	5.613	1.00	0.00
		H								
1072	HETATM	1072	O	WAT	357	9.181	4.496	3.369	1.00	0.00
		O								
1073	HETATM	1073	H1	WAT	357	9.172	3.496	3.372	1.00	0.00
		H								
1074	HETATM	1074	H2	WAT	357	9.655	4.822	2.551	1.00	0.00
		H								
1075	HETATM	1075	O	WAT	358	10.494	5.397	1.105	1.00	0.00
		O								
1076	HETATM	1076	H1	WAT	358	10.020	5.066	0.291	1.00	0.00
		H								
1077	HETATM	1077	H2	WAT	358	11.433	5.055	1.106	1.00	0.00
		H								
1078	HETATM	1078	O	WAT	359	10.494	5.415	5.625	1.00	0.00
		O								
1079	HETATM	1079	H1	WAT	359	10.020	5.084	4.809	1.00	0.00
		H								
1080	HETATM	1080	H2	WAT	359	10.504	6.415	5.621	1.00	0.00
		H								
1081	HETATM	1081	O	WAT	360	-10.344	9.264	-3.428	1.00	0.00
		O								
1082	HETATM	1082	H1	WAT	360	-9.873	8.929	-2.612	1.00	0.00
		H								
1083	HETATM	1083	H2	WAT	360	-10.335	10.264	-3.433	1.00	0.00
		H								
1084	HETATM	1084	O	WAT	361	-9.048	8.321	-5.685	1.00	0.00
		O								
1085	HETATM	1085	H1	WAT	361	-9.059	7.322	-5.681	1.00	0.00
		H								
1086	HETATM	1086	H2	WAT	361	-9.517	8.655	-6.502	1.00	0.00
		H								
1087	HETATM	1087	O	WAT	362	-6.431	9.218	-5.688	1.00	0.00
		O								
1088	HETATM	1088	H1	WAT	362	-5.963	8.878	-6.503	1.00	0.00
		H								
1089	HETATM	1089	H2	WAT	362	-5.961	8.882	-4.872	1.00	0.00
		H								
1090	HETATM	1090	O	WAT	363	-5.135	8.293	-3.425	1.00	0.00
		O								

1091	HETATM	1091	H1	WAT	363	-5.603	8.627	-4.242	1.00	0.00
		H								
1092	HETATM	1092	H2	WAT	363	-5.604	8.634	-2.611	1.00	0.00
		H								
1093	HETATM	1093	O	WAT	364	-6.430	9.237	-1.169	1.00	0.00
		O								
1094	HETATM	1094	H1	WAT	364	-7.376	8.913	-1.166	1.00	0.00
		H								
1095	HETATM	1095	H2	WAT	364	-5.963	8.896	-1.984	1.00	0.00
		H								
1096	HETATM	1096	O	WAT	365	-9.048	8.339	-1.165	1.00	0.00
		O								
1097	HETATM	1097	H1	WAT	365	-9.517	8.673	-1.983	1.00	0.00
		H								
1098	HETATM	1098	H2	WAT	365	-9.059	7.339	-1.161	1.00	0.00
		H								
1099	HETATM	1099	O	WAT	366	-10.388	4.653	-3.410	1.00	0.00
		O								
1100	HETATM	1100	H1	WAT	366	-11.328	4.994	-3.411	1.00	0.00
		H								
1101	HETATM	1101	H2	WAT	366	-9.914	4.984	-2.594	1.00	0.00
		H								
1102	HETATM	1102	O	WAT	367	-9.074	5.553	-5.674	1.00	0.00
		O								
1103	HETATM	1103	H1	WAT	367	-9.065	6.553	-5.678	1.00	0.00
		H								
1104	HETATM	1104	H2	WAT	367	-9.549	5.220	-6.488	1.00	0.00
		H								
1105	HETATM	1105	O	WAT	368	-6.474	4.607	-5.670	1.00	0.00
		O								
1106	HETATM	1106	H1	WAT	368	-7.414	4.949	-5.671	1.00	0.00
		H								
1107	HETATM	1107	H2	WAT	368	-6.000	4.939	-4.854	1.00	0.00
		H								
1108	HETATM	1108	O	WAT	369	-5.161	5.525	-3.414	1.00	0.00
		O								
1109	HETATM	1109	H1	WAT	369	-4.222	5.182	-3.412	1.00	0.00
		H								
1110	HETATM	1110	H2	WAT	369	-5.152	6.525	-3.418	1.00	0.00
		H								
1111	HETATM	1111	O	WAT	370	-6.474	4.625	-1.150	1.00	0.00
		O								
1112	HETATM	1112	H1	WAT	370	-5.999	4.951	-1.968	1.00	0.00
		H								
1113	HETATM	1113	H2	WAT	370	-6.000	4.957	-0.335	1.00	0.00
		H								
1114	HETATM	1114	O	WAT	371	-9.074	5.571	-1.154	1.00	0.00
		O								
1115	HETATM	1115	H1	WAT	371	-9.549	5.246	-0.336	1.00	0.00
		H								
1116	HETATM	1116	H2	WAT	371	-9.065	6.571	-1.158	1.00	0.00
		H								
1117	HETATM	1117	O	WAT	372	-2.517	9.191	-3.428	1.00	0.00
		O								

1118	HETATM	1118	H1	WAT	372	-2.507	10.191	-3.433	1.00	0.00
		H								
1119	HETATM	1119	H2	WAT	372	-2.048	8.856	-2.611	1.00	0.00
		H								
1120	HETATM	1120	O	WAT	373	-1.222	8.247	-5.685	1.00	0.00
		O								
1121	HETATM	1121	H1	WAT	373	-0.275	8.572	-5.686	1.00	0.00
		H								
1122	HETATM	1122	H2	WAT	373	-1.689	8.582	-6.502	1.00	0.00
		H								
1123	HETATM	1123	O	WAT	374	1.397	9.145	-5.688	1.00	0.00
		O								
1124	HETATM	1124	H1	WAT	374	1.865	8.804	-6.503	1.00	0.00
		H								
1125	HETATM	1125	H2	WAT	374	0.451	8.820	-5.687	1.00	0.00
		H								
1126	HETATM	1126	O	WAT	375	2.692	8.220	-3.425	1.00	0.00
		O								
1127	HETATM	1127	H1	WAT	375	2.682	7.221	-3.421	1.00	0.00
		H								
1128	HETATM	1128	H2	WAT	375	2.224	8.561	-2.611	1.00	0.00
		H								
1129	HETATM	1129	O	WAT	376	1.397	9.163	-1.169	1.00	0.00
		O								
1130	HETATM	1130	H1	WAT	376	1.865	8.822	-1.984	1.00	0.00
		H								
1131	HETATM	1131	H2	WAT	376	0.451	8.839	-1.168	1.00	0.00
		H								
1132	HETATM	1132	O	WAT	377	-1.221	8.266	-1.165	1.00	0.00
		O								
1133	HETATM	1133	H1	WAT	377	-1.689	8.600	-1.983	1.00	0.00
		H								
1134	HETATM	1134	H2	WAT	377	-0.275	8.590	-1.166	1.00	0.00
		H								
1135	HETATM	1135	O	WAT	378	-2.560	4.579	-3.410	1.00	0.00
		O								
1136	HETATM	1136	H1	WAT	378	-2.085	4.906	-4.227	1.00	0.00
		H								
1137	HETATM	1137	H2	WAT	378	-2.086	4.911	-2.594	1.00	0.00
		H								
1138	HETATM	1138	O	WAT	379	-1.248	5.480	-5.674	1.00	0.00
		O								
1139	HETATM	1139	H1	WAT	379	-1.723	5.149	-6.489	1.00	0.00
		H								
1140	HETATM	1140	H2	WAT	379	-0.308	5.138	-5.674	1.00	0.00
		H								
1141	HETATM	1141	O	WAT	380	1.354	4.533	-5.670	1.00	0.00
		O								
1142	HETATM	1142	H1	WAT	380	0.414	4.875	-5.671	1.00	0.00
		H								
1143	HETATM	1143	H2	WAT	380	1.828	4.865	-4.854	1.00	0.00
		H								
1144	HETATM	1144	O	WAT	381	2.666	5.452	-3.414	1.00	0.00
		O								

1145	HETATM	1145	H1	WAT	381	2.190	5.120	-4.228	1.00	0.00
		H								
1146	HETATM	1146	H2	WAT	381	2.192	5.127	-2.595	1.00	0.00
		H								
1147	HETATM	1147	O	WAT	382	1.354	4.551	-1.150	1.00	0.00
		O								
1148	HETATM	1148	H1	WAT	382	1.828	4.883	-0.335	1.00	0.00
		H								
1149	HETATM	1149	H2	WAT	382	1.829	4.877	-1.968	1.00	0.00
		H								
1150	HETATM	1150	O	WAT	383	-1.247	5.498	-1.154	1.00	0.00
		O								
1151	HETATM	1151	H1	WAT	383	-1.238	6.498	-1.158	1.00	0.00
		H								
1152	HETATM	1152	H2	WAT	383	-0.307	5.155	-1.152	1.00	0.00
		H								
1153	HETATM	1153	O	WAT	384	5.310	9.117	-3.428	1.00	0.00
		O								
1154	HETATM	1154	H1	WAT	384	4.364	8.791	-3.428	1.00	0.00
		H								
1155	HETATM	1155	H2	WAT	384	5.319	10.117	-3.433	1.00	0.00
		H								
1156	HETATM	1156	O	WAT	385	6.606	8.174	-5.685	1.00	0.00
		O								
1157	HETATM	1157	H1	WAT	385	7.552	8.498	-5.686	1.00	0.00
		H								
1158	HETATM	1158	H2	WAT	385	6.138	8.508	-6.502	1.00	0.00
		H								
1159	HETATM	1159	O	WAT	386	9.224	9.071	-5.688	1.00	0.00
		O								
1160	HETATM	1160	H1	WAT	386	9.233	10.071	-5.693	1.00	0.00
		H								
1161	HETATM	1161	H2	WAT	386	9.693	8.731	-6.503	1.00	0.00
		H								
1162	HETATM	1162	O	WAT	387	10.520	8.146	-3.425	1.00	0.00
		O								
1163	HETATM	1163	H1	WAT	387	10.509	7.147	-3.421	1.00	0.00
		H								
1164	HETATM	1164	H2	WAT	387	10.051	8.486	-2.611	1.00	0.00
		H								
1165	HETATM	1165	O	WAT	388	9.224	9.089	-1.169	1.00	0.00
		O								
1166	HETATM	1166	H1	WAT	388	9.233	10.089	-1.173	1.00	0.00
		H								
1167	HETATM	1167	H2	WAT	388	8.278	8.763	-1.169	1.00	0.00
		H								
1168	HETATM	1168	O	WAT	389	6.606	8.192	-1.165	1.00	0.00
		O								
1169	HETATM	1169	H1	WAT	389	6.138	8.526	-1.983	1.00	0.00
		H								
1170	HETATM	1170	H2	WAT	389	7.552	8.516	-1.166	1.00	0.00
		H								
1171	HETATM	1171	O	WAT	390	5.267	4.505	-3.410	1.00	0.00
		O								

1172	HETATM	1172	H1	WAT	390	5.258	3.506	-3.406	1.00	0.00
		H								
1173	HETATM	1173	H2	WAT	390	5.741	4.831	-4.227	1.00	0.00
		H								
1174	HETATM	1174	O	WAT	391	6.580	5.406	-5.674	1.00	0.00
		O								
1175	HETATM	1175	H1	WAT	391	6.106	5.081	-4.855	1.00	0.00
		H								
1176	HETATM	1176	H2	WAT	391	6.104	5.074	-6.488	1.00	0.00
		H								
1177	HETATM	1177	O	WAT	392	9.180	4.460	-5.670	1.00	0.00
		O								
1178	HETATM	1178	H1	WAT	392	9.171	3.461	-5.669	1.00	0.00
		H								
1179	HETATM	1179	H2	WAT	392	9.655	4.791	-4.854	1.00	0.00
		H								
1180	HETATM	1180	O	WAT	393	10.494	5.378	-3.414	1.00	0.00
		O								
1181	HETATM	1181	H1	WAT	393	10.019	5.045	-4.228	1.00	0.00
		H								
1182	HETATM	1182	H2	WAT	393	11.433	5.035	-3.411	1.00	0.00
		H								
1183	HETATM	1183	O	WAT	394	9.181	4.478	-1.150	1.00	0.00
		O								
1184	HETATM	1184	H1	WAT	394	9.172	3.478	-1.147	1.00	0.00
		H								
1185	HETATM	1185	H2	WAT	394	9.656	4.810	-0.335	1.00	0.00
		H								
1186	HETATM	1186	O	WAT	395	6.580	5.424	-1.154	1.00	0.00
		O								
1187	HETATM	1187	H1	WAT	395	6.590	6.424	-1.158	1.00	0.00
		H								
1188	HETATM	1188	H2	WAT	395	6.104	5.092	-1.969	1.00	0.00
		H								
1189	HETATM	1189	O	WAT	396	-10.345	9.228	-12.467	1.00	0.00
		O								
1190	HETATM	1190	H1	WAT	396	-10.335	10.228	-12.471	1.00	0.00
		H								
1191	HETATM	1191	H2	WAT	396	-11.291	8.904	-12.466	1.00	0.00
		H								
1192	HETATM	1192	O	WAT	397	-9.048	8.303	-10.204	1.00	0.00
		O								
1193	HETATM	1193	H1	WAT	397	-9.517	8.643	-9.390	1.00	0.00
		H								
1194	HETATM	1194	H2	WAT	397	-9.059	7.304	-10.200	1.00	0.00
		H								
1195	HETATM	1195	O	WAT	398	-10.345	9.246	-7.947	1.00	0.00
		O								
1196	HETATM	1196	H1	WAT	398	-9.877	8.905	-8.763	1.00	0.00
		H								
1197	HETATM	1197	H2	WAT	398	-11.291	8.922	-7.946	1.00	0.00
		H								
1198	HETATM	1198	O	WAT	399	-10.388	4.616	-12.449	1.00	0.00
		O								

1199	HETATM	1199	H1	WAT	399	-11.328	4.958	-12.450	1.00	0.00
1200	HETATM	1200	H	WAT	399	-9.914	4.948	-11.633	1.00	0.00
1201	HETATM	1201	O	WAT	400	-9.074	5.535	-10.193	1.00	0.00
1202	HETATM	1202	H	WAT	400	-9.549	5.210	-9.374	1.00	0.00
1203	HETATM	1203	H	WAT	400	-9.065	6.535	-10.197	1.00	0.00
1204	HETATM	1204	O	WAT	401	-10.388	4.634	-7.929	1.00	0.00
1205	HETATM	1205	H	WAT	401	-10.397	3.634	-7.925	1.00	0.00
1206	HETATM	1206	H	WAT	401	-9.914	4.966	-7.114	1.00	0.00
1207	HETATM	1207	O	WAT	402	-6.431	9.200	-10.207	1.00	0.00
1208	HETATM	1208	H	WAT	402	-7.377	8.875	-10.207	1.00	0.00
1209	HETATM	1209	H	WAT	402	-5.963	8.860	-11.022	1.00	0.00
1210	HETATM	1210	O	WAT	403	-5.136	8.257	-12.464	1.00	0.00
1211	HETATM	1211	H	WAT	403	-5.603	8.591	-13.281	1.00	0.00
1212	HETATM	1212	H	WAT	403	-5.146	7.258	-12.460	1.00	0.00
1213	HETATM	1213	O	WAT	404	-2.517	9.154	-12.467	1.00	0.00
1214	HETATM	1214	H	WAT	404	-2.049	8.814	-13.282	1.00	0.00
1215	HETATM	1215	H	WAT	404	-2.508	10.154	-12.471	1.00	0.00
1216	HETATM	1216	O	WAT	405	-1.222	8.229	-10.204	1.00	0.00
1217	HETATM	1217	H	WAT	405	-1.691	8.570	-9.390	1.00	0.00
1218	HETATM	1218	H	WAT	405	-1.233	7.230	-10.200	1.00	0.00
1219	HETATM	1219	O	WAT	406	-2.517	9.173	-7.947	1.00	0.00
1220	HETATM	1220	H	WAT	406	-3.463	8.849	-7.946	1.00	0.00
1221	HETATM	1221	H	WAT	406	-2.049	8.832	-8.763	1.00	0.00
1222	HETATM	1222	O	WAT	407	-5.135	8.275	-7.944	1.00	0.00
1223	HETATM	1223	H	WAT	407	-5.145	7.275	-7.939	1.00	0.00
1224	HETATM	1224	H	WAT	407	-5.604	8.616	-7.130	1.00	0.00
1225	HETATM	1225	O	WAT	408	-6.474	4.588	-10.189	1.00	0.00

1226	HETATM	1226	H1	WAT	408	-7.414	4.930	-10.190	1.00	0.00
		H								
1227	HETATM	1227	H2	WAT	408	-6.482	3.588	-10.185	1.00	0.00
		H								
1228	HETATM	1228	O	WAT	409	-5.162	5.489	-12.453	1.00	0.00
		O								
1229	HETATM	1229	H1	WAT	409	-5.636	5.164	-11.634	1.00	0.00
		H								
1230	HETATM	1230	H2	WAT	409	-5.152	6.489	-12.457	1.00	0.00
		H								
1231	HETATM	1231	O	WAT	410	-2.560	4.543	-12.449	1.00	0.00
		O								
1232	HETATM	1232	H1	WAT	410	-2.568	3.543	-12.447	1.00	0.00
		H								
1233	HETATM	1233	H2	WAT	410	-2.086	4.871	-13.266	1.00	0.00
		H								
1234	HETATM	1234	O	WAT	411	-1.248	5.461	-10.193	1.00	0.00
		O								
1235	HETATM	1235	H1	WAT	411	-1.724	5.129	-11.007	1.00	0.00
		H								
1236	HETATM	1236	H2	WAT	411	-1.722	5.136	-9.374	1.00	0.00
		H								
1237	HETATM	1237	O	WAT	412	-2.560	4.561	-7.929	1.00	0.00
		O								
1238	HETATM	1238	H1	WAT	412	-2.085	4.887	-8.747	1.00	0.00
		H								
1239	HETATM	1239	H2	WAT	412	-2.569	3.561	-7.925	1.00	0.00
		H								
1240	HETATM	1240	O	WAT	413	-5.161	5.507	-7.933	1.00	0.00
		O								
1241	HETATM	1241	H1	WAT	413	-5.152	6.507	-7.937	1.00	0.00
		H								
1242	HETATM	1242	H2	WAT	413	-5.636	5.182	-7.115	1.00	0.00
		H								
1243	HETATM	1243	O	WAT	414	1.397	9.127	-10.207	1.00	0.00
		O								
1244	HETATM	1244	H1	WAT	414	1.865	8.793	-9.389	1.00	0.00
		H								
1245	HETATM	1245	H2	WAT	414	1.406	10.127	-10.211	1.00	0.00
		H								
1246	HETATM	1246	O	WAT	415	2.692	8.183	-12.464	1.00	0.00
		O								
1247	HETATM	1247	H1	WAT	415	2.681	7.184	-12.460	1.00	0.00
		H								
1248	HETATM	1248	H2	WAT	415	2.223	8.524	-11.650	1.00	0.00
		H								
1249	HETATM	1249	O	WAT	416	5.310	9.081	-12.467	1.00	0.00
		O								
1250	HETATM	1250	H1	WAT	416	5.778	8.747	-11.649	1.00	0.00
		H								
1251	HETATM	1251	H2	WAT	416	4.364	8.756	-12.465	1.00	0.00
		H								
1252	HETATM	1252	O	WAT	417	6.606	8.156	-10.204	1.00	0.00
		O								

1253	HETATM	1253	H1	WAT	417	6.595	7.157	-10.200	1.00	0.00
		H								
1254	HETATM	1254	H2	WAT	417	6.137	8.497	-9.390	1.00	0.00
		H								
1255	HETATM	1255	O	WAT	418	5.310	9.099	-7.947	1.00	0.00
		O								
1256	HETATM	1256	H1	WAT	418	5.319	10.099	-7.951	1.00	0.00
		H								
1257	HETATM	1257	H2	WAT	418	5.778	8.765	-7.129	1.00	0.00
		H								
1258	HETATM	1258	O	WAT	419	2.692	8.202	-7.944	1.00	0.00
		O								
1259	HETATM	1259	H1	WAT	419	3.638	8.526	-7.945	1.00	0.00
		H								
1260	HETATM	1260	H2	WAT	419	2.223	8.543	-7.130	1.00	0.00
		H								
1261	HETATM	1261	O	WAT	420	1.354	4.515	-10.189	1.00	0.00
		O								
1262	HETATM	1262	H1	WAT	420	1.829	4.842	-11.006	1.00	0.00
		H								
1263	HETATM	1263	H2	WAT	420	0.414	4.857	-10.190	1.00	0.00
		H								
1264	HETATM	1264	O	WAT	421	2.666	5.415	-12.453	1.00	0.00
		O								
1265	HETATM	1265	H1	WAT	421	2.675	6.415	-12.457	1.00	0.00
		H								
1266	HETATM	1266	H2	WAT	421	2.192	5.090	-11.634	1.00	0.00
		H								
1267	HETATM	1267	O	WAT	422	5.266	4.469	-12.449	1.00	0.00
		O								
1268	HETATM	1268	H1	WAT	422	5.741	4.801	-11.633	1.00	0.00
		H								
1269	HETATM	1269	H2	WAT	422	5.257	3.470	-12.445	1.00	0.00
		H								
1270	HETATM	1270	O	WAT	423	6.580	5.388	-10.193	1.00	0.00
		O								
1271	HETATM	1271	H1	WAT	423	6.589	6.388	-10.197	1.00	0.00
		H								
1272	HETATM	1272	H2	WAT	423	6.104	5.055	-11.007	1.00	0.00
		H								
1273	HETATM	1273	O	WAT	424	5.266	4.487	-7.929	1.00	0.00
		O								
1274	HETATM	1274	H1	WAT	424	4.328	4.829	-7.930	1.00	0.00
		H								
1275	HETATM	1275	H2	WAT	424	5.742	4.819	-7.114	1.00	0.00
		H								
1276	HETATM	1276	O	WAT	425	2.666	5.434	-7.933	1.00	0.00
		O								
1277	HETATM	1277	H1	WAT	425	2.192	5.108	-7.115	1.00	0.00
		H								
1278	HETATM	1278	H2	WAT	425	3.606	5.092	-7.933	1.00	0.00
		H								
1279	HETATM	1279	O	WAT	426	9.224	9.053	-10.207	1.00	0.00
		O								

1280	HETATM	1280	H1	WAT	426	9.233	10.053	-10.211	1.00	0.00
			H							
1281	HETATM	1281	H2	WAT	426	9.692	8.712	-11.022	1.00	0.00
			H							
1282	HETATM	1282	O	WAT	427	10.520	8.110	-12.464	1.00	0.00
			O							
1283	HETATM	1283	H1	WAT	427	11.466	8.434	-12.465	1.00	0.00
			H							
1284	HETATM	1284	H2	WAT	427	10.509	7.111	-12.460	1.00	0.00
			H							
1285	HETATM	1285	O	WAT	428	10.520	8.128	-7.944	1.00	0.00
			O							
1286	HETATM	1286	H1	WAT	428	11.466	8.452	-7.945	1.00	0.00
			H							
1287	HETATM	1287	H2	WAT	428	10.509	7.128	-7.940	1.00	0.00
			H							
1288	HETATM	1288	O	WAT	429	9.180	4.441	-10.189	1.00	0.00
			O							
1289	HETATM	1289	H1	WAT	429	9.654	4.767	-11.007	1.00	0.00
			H							
1290	HETATM	1290	H2	WAT	429	9.655	4.773	-9.373	1.00	0.00
			H							
1291	HETATM	1291	O	WAT	430	10.494	5.342	-12.453	1.00	0.00
			O							
1292	HETATM	1292	H1	WAT	430	10.019	5.009	-13.267	1.00	0.00
			H							
1293	HETATM	1293	H2	WAT	430	10.019	5.017	-11.634	1.00	0.00
			H							
1294	HETATM	1294	O	WAT	431	10.494	5.360	-7.933	1.00	0.00
			O							
1295	HETATM	1295	H1	WAT	431	10.503	6.360	-7.937	1.00	0.00
			H							
1296	HETATM	1296	H2	WAT	431	10.019	5.035	-7.115	1.00	0.00
			H							

APPENDIX B

Germanium Landscape

B.1 Sample Gaussian 09 Germanium File

Command files like the one below were built using Dr. Fennell's Gaussian 09 run builder script and proved very effective in producing command files.

41	H	-4.1260000000000	-0.8790000000000	-2.3610000000000
42	H	-5.4330000000000	0.3560000000000	-2.3850000000000
43	H	-5.7540000000000	-1.3310000000000	-2.9170000000000
44	H	-7.3270000000000	-1.4620000000000	0.4590000000000
45	H	-7.5880000000000	-1.6770000000000	-1.2900000000000
46	H	-7.4380000000000	-0.0190000000000	-0.6080000000000
47	C	5.1710000000000	-1.2860000000000	3.1080000000000
48	C	6.7030000000000	-3.1420000000000	3.8230000000000
49	H	4.6120000000000	-3.3360000000000	3.4560000000000
50	H	7.6170000000000	-2.6600000000000	3.4250000000000
51	H	6.8340000000000	-4.2420000000000	3.8350000000000
52	H	6.5690000000000	-2.8200000000000	4.8770000000000
53	H	6.0030000000000	-0.6730000000000	2.7150000000000
54	H	4.9880000000000	-0.9950000000000	4.1640000000000
55	H	4.2810000000000	-1.0550000000000	2.5110000000000
56	C	6.8810000000000	-2.4910000000000	-1.3860000000000
57	C	8.0000000000000	-1.6920000000000	0.6950000000000
58	H	6.0930000000000	-1.0840000000000	0.0270000000000
59	H	8.6630000000000	-2.5690000000000	0.7760000000000
60	H	7.8710000000000	-1.2570000000000	1.7000000000000
61	H	8.5270000000000	-0.9270000000000	0.0850000000000
62	H	7.5310000000000	-3.3840000000000	-1.4160000000000
63	H	7.3870000000000	-1.6900000000000	-1.9660000000000
64	H	5.9290000000000	-2.7200000000000	-1.8880000000000
65	C	6.0420000000000	-5.8440000000000	-0.3400000000000
66	H	5.9120000000000	-5.7470000000000	1.8170000000000
67	C	7.8820000000000	-5.1770000000000	1.1930000000000
68	H	8.3970000000000	-4.6880000000000	0.3460000000000
69	H	8.2400000000000	-6.2280000000000	1.2290000000000
70	H	8.1890000000000	-4.6900000000000	2.1340000000000
71	H	4.9590000000000	-5.9050000000000	-0.5140000000000
72	H	6.4360000000000	-6.8830000000000	-0.3370000000000
73	H	6.4870000000000	-5.3110000000000	-1.1990000000000
74	H	-6.3620000000000	1.5630000000000	1.3030000000000
75	C	-5.6460000000000	2.4560000000000	-0.4830000000000
76	C	-4.5230000000000	2.5900000000000	1.7560000000000
77	H	-4.3490000000000	2.0800000000000	2.7250000000000
78	H	-5.0420000000000	3.5500000000000	1.9600000000000
79	H	-3.5480000000000	2.8210000000000	1.2850000000000
80	H	-6.3580000000000	1.8940000000000	-1.1100000000000
81	H	-4.7250000000000	2.6290000000000	-1.0570000000000
82	H	-6.1170000000000	3.4400000000000	-0.2730000000000
83	C	-0.5320000000000	2.4210000000000	0.8170000000000
84	C	-1.5290000000000	1.2580000000000	2.6840000000000
85	H	-2.1290000000000	0.4690000000000	3.0880000000000
86	C	-0.9960000000000	2.2060000000000	3.5610000000000
87	C	-0.0010000000000	3.3710000000000	1.6940000000000
88	C	-0.2370000000000	3.2670000000000	3.0660000000000
89	H	0.5960000000000	4.1880000000000	1.3100000000000
90	H	-1.1800000000000	2.1220000000000	4.6240000000000
91	H	0.1740000000000	4.0020000000000	3.7450000000000
92	C	-1.7770000000000	-4.3220000000000	1.7250000000000
93	C	-0.2170000000000	-3.3920000000000	-2.1750000000000
94	C	-2.2320000000000	-5.0370000000000	2.8380000000000

95	H	-1.775000000000	-4.812000000000	0.763000000000
96	C	-1.348000000000	-2.404000000000	3.134000000000
97	C	-0.568000000000	-4.133000000000	-3.309000000000
98	H	0.799000000000	-3.079000000000	-2.038000000000
99	C	-2.513000000000	-3.435000000000	-1.440000000000
100	C	-2.250000000000	-4.433000000000	4.097000000000
101	H	-2.571000000000	-6.058000000000	2.723000000000
102	C	-1.802000000000	-3.118000000000	4.246000000000
103	H	-1.007000000000	-1.394000000000	3.262000000000
104	C	-2.868000000000	-4.180000000000	-2.567000000000
105	H	-3.268000000000	-3.168000000000	-0.721000000000
106	C	-1.893000000000	-4.529000000000	-3.504000000000
107	H	0.183000000000	-4.395000000000	-4.040000000000
108	H	-3.896000000000	-4.482000000000	-2.715000000000
109	H	-2.164000000000	-5.101000000000	-4.381000000000
110	H	-2.602000000000	-4.985000000000	4.958000000000
111	H	-1.809000000000	-2.651000000000	5.222000000000
112	C	3.101000000000	-6.123000000000	1.997000000000
113	C	2.378000000000	-5.604000000000	-1.315000000000
114	C	3.370000000000	-3.619000000000	-2.281000000000
115	H	2.025000000000	-6.170000000000	-0.467000000000
116	C	2.272000000000	-6.169000000000	-2.590000000000
117	C	1.513000000000	-4.525000000000	2.832000000000
118	C	2.686000000000	-7.047000000000	2.960000000000
119	H	3.865000000000	-6.421000000000	1.310000000000
120	C	1.687000000000	-6.704000000000	3.869000000000
121	H	3.142000000000	-8.028000000000	3.002000000000
122	C	1.100000000000	-5.441000000000	3.804000000000
123	H	1.054000000000	-3.568000000000	2.784000000000
124	C	2.720000000000	-5.462000000000	-3.708000000000
125	H	1.844000000000	-7.156000000000	-2.710000000000
126	C	3.263000000000	-4.184000000000	-3.554000000000
127	H	3.780000000000	-2.628000000000	-2.178000000000
128	H	3.599000000000	-3.631000000000	-4.421000000000
129	H	2.636000000000	-5.900000000000	-4.694000000000
130	H	1.366000000000	-7.414000000000	4.620000000000
131	H	0.327000000000	-5.175000000000	4.510000000000
132	C	1.504000000000	-0.326000000000	-2.095000000000
133	C	1.670000000000	-0.714000000000	3.412000000000
134	C	3.620000000000	-0.040000000000	-0.992000000000
135	C	1.987000000000	0.362000000000	-3.212000000000
136	H	0.510000000000	-0.709000000000	-2.093000000000
137	C	2.402000000000	1.008000000000	1.889000000000
138	C	1.890000000000	0.147000000000	4.490000000000
139	H	1.314000000000	-1.696000000000	3.632000000000
140	C	4.114000000000	0.652000000000	-2.102000000000
141	H	4.233000000000	-0.179000000000	-0.124000000000
142	C	3.296000000000	0.851000000000	-3.216000000000
143	H	1.348000000000	0.514000000000	-4.073000000000
144	H	5.127000000000	1.034000000000	-2.095000000000
145	H	3.673000000000	1.385000000000	-4.079000000000
146	C	2.374000000000	1.435000000000	4.270000000000
147	H	1.691000000000	-0.189000000000	5.500000000000
148	C	2.630000000000	1.865000000000	2.969000000000

```

149 H 2.603000000000 1.384000000000 0.900000000000
150 H 3.001000000000 2.867000000000 2.795000000000
151 H 2.548000000000 2.101000000000 5.105000000000
152 C -2.041000000000 0.841000000000 -1.709000000000
153 C -1.767000000000 0.059000000000 -2.841000000000
154 C -2.300000000000 2.209000000000 -1.888000000000
155 C -1.732000000000 0.632000000000 -4.115000000000
156 H -1.595000000000 -0.996000000000 -2.753000000000
157 C -2.263000000000 2.785000000000 -3.160000000000
158 H -2.521000000000 2.839000000000 -1.039000000000
159 C -1.977000000000 1.997000000000 -4.275000000000
160 H -1.519000000000 0.016000000000 -4.979000000000
161 H -2.458000000000 3.843000000000 -3.281000000000
162 H -1.950000000000 2.441000000000 -5.262000000000
163 H -0.322000000000 2.526000000000 -0.236000000000
164
165 EOF
166 formchk B3LYP_STO-3G_1_hexagermane_transall_first_reorder.chk
167 newzmat -ichk -opdb -step 999 B3LYP_STO-3
    G_1_hexagermane_transall_first_reorder.chk final_B3LYP_STO-3
    G_1_hexagermane_transall_first_reorder.pdb
168 echo
169 echo "Job done"

```

B.2 Building Group 4 Chains

While briefly mentioned and the subject of research for some time, the butyl-IV chain builder is detailed below. Ultimately unsuccessful in the initial trials, these scripts may serve a purpose in further work.

This first script builds a parent set of all possible C, Si, and Ge butylalkyl chains.

```

1 #!/usr/bin/python
2
3 import sys
4 import subprocess
5
6 # argument: sys.argv[1]
7 # Replacement: sed -i -e 's/IN/OUT/g' FILE > NEWFILE
8
9 inFile = file(sys.argv[1])
10
11 def DoIT():
12     for first in { 'C', 'Si', 'Ge' }:
13         name1 = "%s" % (first.lstrip(' '))
14         out1 = open(name1, "w")
15         cmdStr = "sed -e 's/1 GE/1 %s/g' ./%s >> ./%s.pdb" % (first,
16         inFile, name1)
17         # subprocess.call(cmdStr, shell=True, stdout=out1)
18         subprocess.Popen(cmdStr, shell=True, executable='/bin/bash')
19         out1.close()
20         for second in { 'C', 'Si', 'Ge' }:
21             name2 = name1 + "%s" % (second.lstrip(' '))
22             out2 = open(name2, "w")

```

```

22     cmdStr = "sed -e 's/2 GE/2 %s/g' ./%s.pdb >> ./%s.pdb" % (
23         second, name1, name2)
24         # subprocess.call(cmdStr, shell=True, stdout=out2)
25         subprocess.Popen(cmdStr, shell=True, executable='/bin/bash')
26         out2.close()
27         for third in {'C', 'Si', 'Ge'}:
28             name3 = name2 + "%s" % (third.lstrip(' '))
29             out3 = open(name3, "w")
30             cmdStr = "sed -e 's/3 GE/3 %s/g' ./%s.pdb >> ./%s.pdb" %
31             (third, name2, name3)
32             # subprocess.call(cmdStr, shell=True, stdout=out3)
33             subprocess.Popen(cmdStr, shell=True, executable='/bin/
34             bash')
35             out3.close()
36             for fourth in {'C', 'Si', 'Ge'}:
37                 name4 = name3 + "%s" % (fourth.lstrip(' '))
38                 out4 = open(name4, "w")
39                 cmdStr = "sed -e 's/4 GE/4 %s/g' ./%s.pdb >> ./%s.
40                 pdb" % (fourth, name3, name4)
41                 # subprocess.call(cmdStr, shell=True, stdout=out4)
42                 subprocess.Popen(cmdStr, shell=True, executable='/
43                 bin/bash')
44                 out4.close()
45
46 DoIT()

```

This second script takes the original trans-all butyl chain and enumerates 72 torsional rotations into a folder.

```

1 from chimera import runCommand as rc
2 from chimera import replyobj
3 import sys
4 import os
5
6 #standard sys.argv[] for script args?
7 # sys.argv[0] = directory
8 os.chdir(sys.argv[0])
9
10 file_names = [fn for fn in os.listdir(".") if fn.endswith(".pdb")]
11 fn = file_names[0]
12 # inPDB = chimera.openModels.open('/Users/gentry/Desktop/test/testmol.
13     pdb', type="PDB")
14
15 rc("open " + fn)
16 rc("rotation 1 reverse #0:1.HET@/serialNumber=2 #0:1.HET@/serialNumber=3
17 ")
18 for i in range(72):
19     #replyobj.status("Processing " + fn)
20     #rc("open " + fn)
21     #rc("rotation 1 reverse #0:1.HET@/serialNumber=2 #0:1.HET@/
22     serialNumber=3")
23     rc("rotation 1 5")
24     newName = (fn[:-3] + str((i*5)) + ".pdb")

```

```

24 rc("write format pdb 0 " + newName)
25 #rc("close ")
26
27
28 # chimera.runCommand("rotation 2 3 5")
29 # newName = ( inPDB[:-3] + i*5 + ".pdb" )
30 # chimera.runCommand("write format pdb " + newName)

```

B.3 Collecting and Comparing Torsional Data

These two scripts were utilized to reduce the output data into an energy value with normalized intensity from 0 to 1. The third script compares two of these files and looks for any additive or multiplicative trend.

This first file reads energy data and creates a list of absolute energy values per torsion degree.

```

1#!/usr/bin/python
2
3### Author: Gentry Smith, Oklahoma State University
4### Created: August 7, 2017, 3PM
5### Last Edited: August 7, 2017
6
7### Takes a stationary_points.txt file and will copy .pdb files of the
8### same name from a split_conformers.pdb/ folder
9### into a new folder "stationary_conformers"
10# This does not use any args and instead relies on the stationary points
11# file being "stationary_points.txt" and the
12# conformers residing in a "split_conformers.pdb/" directory on the same
13# level. It will create the new folder "stationary_conformers"
14
15import os
16
17def IOValidator():
18    returnBool = [False, False]
19    try:
20        file1 = open('stationary_points.txt', 'r')
21        file1.close()
22        returnBool[0] = True
23    except IOError:
24        print("Did not find 'stationary_points.txt' file. Quitting...")
25        quit()
26    try:
27        wkdir = os.getcwd()
28        file2 = os.chdir('split_conformers.pdb')
29        os.chdir(wkdir)
30        returnBool[1] = True
31    except OSError:
32        print("Did not find 'split_conformers.pdb' folder. Quitting...")
33        quit()
34    if returnBool[0] & returnBool[1]:
35        return True
36    else:

```

```

35         return False
36
37
38 def GetPDBs():
39     pdbNames = []
40     inFile = open('stationary_points.txt', 'r')
41     for line in inFile:
42         pdbNames.append(line.split()[1])
43     return pdbNames
44
45
46 def CopyPDBs(pdbList):
47     wkdir = os.getcwd()
48     for i in range(len(pdbList)):
49         pstring = ('cp ' + 'split_conformers.pdb/' + str(pdbList[i]) +
50         ' stationary_conformers/')
51         os.popen(pstring)
52
53 def Runner():
54     if IOValidator():
55         print('Valid Args. Running... ')
56         pdbList = GetPDBs()
57         try:
58             os.mkdir('stationary_conformers')
59             CopyPDBs(pdbList)
60         except OSError:
61             print("stationary_conformers' directory already exists.
62 Erase directory and run again. Quitting... ")
63             quit()
64
65 Runner()

```

This second file converts the first file into a relative scale from 0 to 1.

```

1#!/usr/bin/python
2
3### Author: Gentry Smith, Oklahoma State University
4### Created: July 31, 2017, 12PM
5### Last Edited: July 31, 2017
6
7### takes file arg with format [ [energy] [pdb_name] ], alters to [ [
8    energy] [torsion] ], and creates copy with
9    [ [relative energy] [torsion] ].
10
11
12
13 def IOValidator():
14     isValid = False
15     try:
16         inFile = sys.argv[1]
17         isValid = True
18     except IOError:

```

```

19     print("Input arg is not a file.\nQuitting...")
20     exit()
21 return isValid
22
23
24 def GetFileData():
25     inData = []
26     inFile = open(sys.argv[1], 'r')
27     iter = 0
28     for line in inFile:
29         inLine = line.split()
30         inData.append(float(inLine[0]))
31         iter = iter + 1
32     inFile.close()
33 return inData
34
35
36 def Relativize(energies):
37     minimum = min(energies)
38     # print("Relativize: minimum=" + str(minimum))
39     newEnergies = []
40     for i in range(len(energies)):
41         # print("Relativize: index=" + str(i))
42         # print("Relativize: energy=" + str(energies[i]))
43         newMin = (float(energies[i]) - float(minimum))
44         # print("Relativize: newMin=" + str(newMin))
45         newEnergies.append((newMin))
46         # print("Relativize: newEnergies=" + str(newEnergies))
47     return newEnergies
48
49
50 def UnifiedScale(energies):
51     # print("unifying scale...")
52     maxi = max(energies)
53     # print("Unify: max=" + str(maxi))
54     newEnergies = []
55     for i in range(len(energies)):
56         # print("Unify: energy=" + str(energies[i]))
57         newEner = (float(energies[i]) / maxi)
58         # print("Unify: scaled energy=" + str(newEner))
59         newEnergies.append(newEner)
60     return newEnergies
61
62
63 def CriticalHit(energies, torsions):
64     isIncreasing = True
65     crits = []
66     tors = []
67     prev = 0
68     for i in range(len(energies)):
69         if (energies[i] == 0):
70             crits.append(energies[i])
71             tors.append(torsions[i])
72         if ((isIncreasing) & (energies[i] < prev)) or ((not

```

```

    isIncreasing) & (energies[i] > prev) ):
73        crits.append(energies[i-1])
74        tors.append(torsions[i-1])
75        isIncreasing = not isIncreasing
76        prev = float(energies[i])
77    returnThing = [crits, tors]
78    return returnThing
79
80
81 def MakeFile(energies, torsions, fileName):
82     outFile = open(fileName, 'w')
83     for i in range(len(energies)):
84         strOut = ('{:.11e}'.format(energies[i]) + " " + str(torsions[i])
85         + "\n")
86         outFile.write(strOut)
87     outFile.close()
88
89 def Runner():
90     if IOValidator():
91         energies = GetFileData()
92         torsions = [180]
93         i = 185
94         while i != 180:
95             if i == 360:
96                 i = 0
97             torsions.append(i)
98             i = i + 5
99         MakeFile(energies, torsions, 'abs_energ.txt')
100        relativeEnergies = Relativize(energies)
101        MakeFile(relativeEnergies, torsions, 'rel_energ.txt')
102        MakeFile(UnifiedScale(relativeEnergies), torsions, 'uni_energ.
103        txt')
104        crits = CriticalHit(relativeEnergies, torsions)
105        MakeFile(crits[0], crits[1], 'crit_pts.txt')
106
107 Runner()

```

This third script compares two generated files using the prior scripts. It can compare the generated absolute energy with the relative energy files. It was often run as a loop through every permutation of the group 4 builder.

```

1#!/usr/bin/python
2
3### Author: Gentry Smith, Oklahoma State University
4### Created: July 31, 2017, 3PM
5### Last Edited: August 1, 2017
6
7### Takes data created by teatAbsEnergies and compares values via
8### additive and multiplicative comparison
9###      with abs or rel data. Math in terms of File 2 sub/div File 1.
10# sys.argv[1] = file 1, working directory here.
11# sys.argv[2] = file 2, compared with file 1.

```

```

12
13
14 import sys
15 import numpy
16 import math
17
18 def IOValidator():
19     isValid1 = False
20     isValid2 = False
21     try:
22         inFile1 = open(sys.argv[1])
23         isValid1 = True
24     except IOError:
25         print("Arg File 1 is invalid.")
26         isValid1 = False
27     try:
28         inFile1 = open(sys.argv[2])
29         isValid2 = True
30     except IOError:
31         print("Arg File 2 is invalid.")
32         isValid2 = False
33     if (isValid1 & isValid2 & (sys.argv[1] != sys.argv[2])):
34         print('Valid Args. Running... ')
35         return True
36     else:
37         if (sys.argv[1] == sys.argv[2]):
38             print ('args are indentical. Skipping... ')
39         else:
40             print("Invalid args. Quitting... ")
41         exit()
42
43
44 def ExtractData(data):
45     inFile = open(data, 'r')
46     inData = []
47     inTorsions = []
48     # print('Extracting Data... ')
49     for line in inFile:
50         # print('line=' + str(line))
51         # print('line.split()=' + str(line.split()))
52         # print('line.split()[1]=' + str(line.split()[1]))
53         inData.append(float(line.split()[0]))
54         inTorsions.append(int(line.split()[1]))
55     # print(str(inTorsions))
56     # print('Done. ')
57     return [inData, inTorsions]
58
59
60 def Comparator(data1, data2, func):
61     # func: 0=add, 1=mult
62     newData = []
63     if func == 0:
64         for i in range(len(data2)):
65             newData.append(float(data2[i] - data1[i]))

```

```

66     elif func == 1:
67         for i in range(len(data2)):
68             try:
69                 newData.append(float(data2[i] / data1[i]))
70             except ZeroDivisionError:
71                 newData.append(0.0)
72     return newData
73
74
75 def WriteFile(data1, data2, tors, compData, comp, sigs):
76     # writes data of comparison. Format:
77     #   File1 = {file1}
78     #   File2 = {file2}
79     #   Source: {absolute, relative}
80     #   Comparison: {additive, multiplicative}
81     #   comp: {min/max/avg/stdev of all comp values}
82     #   Raw Data: {includes header of File1, File2, Torsions, Comp
83     # defining each column}
84     # print("Writing file...")
85     # print('File2=' + str((sys.argv[2]).split("/")))
86     source = ""
87     if str(sys.argv[1])[:3] == "abs":
88         source = "absolute"
89     elif str(sys.argv[1])[:3] == "rel":
90         source = "relative"
91     elif str(sys.argv[1])[:3] == "uni":
92         source = "unified relative scale"
93     else:
94         print(str(sys.argv[1])[:2])
95     comparison = ""
96     if comp == 0:
97         comparison = "additive"
98     elif comp == 1:
99         comparison = "multiplicative"
100    headerLines = [0]*10
101    headerLines[0] = ('File1 = ' + sys.argv[1] + '\n')
102    headerLines[1] = ('File2 = ' + sys.argv[2] + '\n')
103    headerLines[2] = ('Source: ' + source + '\n')
104    headerLines[3] = ('Comparison: ' + comparison + '\n')
105    headerLines[4] = ('Comparison min: ' + str(sigs[0]) + '\n')
106    headerLines[5] = ('Comparison max: ' + str(sigs[1]) + '\n')
107    headerLines[6] = ('Comparison avg: ' + str(sigs[2]) + '\n')
108    headerLines[7] = ('Comparison stdev: ' + str(sigs[3]) + '\n')
109    headerLines[8] = ('Raw Data: ' + '\n')
110    f1ColSize = len(str(data1[0]))
111    f2ColSize = len(str(data2[0]))
112    headerLines[9] = ('File1'.ljust(18) + 'File2'.ljust(18) + 'Tors'.
113    ljust(5) + 'Comp'.ljust(18) + '\n')
114    fileName = (str((sys.argv[2]).split("/"))[-2]) + "_" + str(sys.argv
115    [1])[:3] + "_" + comparison + ".txt")
116    outFile = open(fileName, 'w')
117    for i in range(len(headerLines)):
118        outFile.write(str(headerLines[i]))
119    for i in range(len(data1)):

```

```
117     # print('str(tors[i]).ljust(5)=' + str(tors[i]).ljust(5))
118     string = (str(data1[i])[:17].ljust(18) + ',' + str(data2[i]))
119     [:17].ljust(18) + str(tors[i]).ljust(5) + str(compData[i])[:17].
120     ljust(18) + '\n')
121     outFile.write(string)
122
123 def GetCompSigs(data):
124     sigs = []
125     sigs.append(min(data))
126     sigs.append(max(data))
127     sigs.append((float(sum(data))/float(len(data))))
128     sigs.append(numpy.std(data, axis=0))
129
130
131 def Runner():
132     if IOValidator():
133         [data1, torsions1] = ExtractData(sys.argv[1])
134         [data2, torsions2] = ExtractData(sys.argv[2])
135         if (len(data1) == len(data2)) & (len(torsions1) == len(torsions2)):
136             aData = Comparator(data1, data2, 0)
137             aSigs = GetCompSigs(aData)
138             WriteFile(data1, data2, torsions1, aData, 0, aSigs)
139             mData = Comparator(data1, data2, 1)
140             mSigs = GetCompSigs(mData)
141             WriteFile(data1, data2, torsions1, mData, 1, mSigs)
142             print('Complete.')
143 Runner()
```

APPENDIX C

Conformation Landscapes

Listed below are two example Germanium PDB files. The first is for the end-goal hexagermane in the trans-trans-trans conformation with isopropyl groups on the terminal Ge atoms. The second is for the simplified butagermane with fully protonated Germanium atoms.

C.1 Code: hexagermane-transall.pdb

```
1 HEADER
2 REMARK Title: hexagermane_transall system
3 HETATM    1  Ge          1      -4.399   0.008   0.355   0.00   0.00
4           Ge
5 HETATM    2  Ge          1      -1.965   0.138   -0.022   0.00   0.00
6           Ge
7 HETATM    3  C          1      -4.822   1.886   0.961   0.00   0.00
8           C
9 HETATM    4  C          1      -5.008   -1.297   1.715   0.00   0.00
10          C
11 HETATM   5  C          1      -5.256   -0.261   -1.445   0.00   0.00
12          C
13 HETATM   6  C          1      -1.213   1.435   1.157   0.00   0.00
14          C
15 HETATM   7  Ge         1      -0.756   -1.988   0.223   0.00   0.00
16           Ge
17 HETATM   8  C          1      -1.297   -2.917   1.805   0.00   0.00
18           C
19 HETATM   9  Ge         1      1.647   -1.496   0.371   0.00   0.00
20           Ge
21 HETATM  10  C          1      -1.182   -3.010   -1.339   0.00   0.00
22           C
23 HETATM  11  C          1      2.131   -0.425   1.877   0.00   0.00
24           C
25 HETATM  12  C          1      2.111   -0.634   -1.269   0.00   0.00
26           C
27 HETATM  13  Ge         1      2.889   -3.585   0.738   0.00   0.00
28           Ge
29 HETATM  14  C          1      2.287   -4.358   2.378   0.00   0.00
30           C
31 HETATM  15  Ge         1      5.327   -3.386   1.080   0.00   0.00
32           Ge
33 HETATM  16  C          1      2.766   -4.685   -0.813   0.00   0.00
34           C
35 HETATM  17  C          1      5.688   -2.615   2.887   0.00   0.00
36           C
```

20	HETATM	18	C		1	6.239	-2.415	-0.417	0.00	0.00
			C							
21	HETATM	19	C		1	5.893	-5.324	0.888	0.00	0.00
			C							
22	HETATM	20	C		1	-3.527	2.543	1.328	0.00	0.00
			C							
23	HETATM	21	C		1	-5.754	1.844	2.133	0.00	0.00
			C							
24	HETATM	22	H		1	-5.303	2.355	0.072	0.00	0.00
			H							
25	HETATM	23	H		1	-5.269	1.358	2.999	0.00	0.00
			H							
26	HETATM	24	H		1	-6.679	1.287	1.913	0.00	0.00
			H							
27	HETATM	25	H		1	-6.047	2.856	2.449	0.00	0.00
			H							
28	HETATM	26	H		1	-3.043	2.019	2.171	0.00	0.00
			H							
29	HETATM	27	H		1	-3.683	3.585	1.642	0.00	0.00
			H							
30	HETATM	28	H		1	-2.818	2.559	0.490	0.00	0.00
			H							
31	HETATM	29	H		1	-4.336	-1.167	2.589	0.00	0.00
			H							
32	HETATM	30	C		1	-4.907	-2.680	1.154	0.00	0.00
			C							
33	HETATM	31	C		1	-6.417	-0.909	2.051	0.00	0.00
			C							
34	HETATM	32	H		1	-3.858	-2.985	0.982	0.00	0.00
			H							
35	HETATM	33	H		1	-5.433	-2.773	0.187	0.00	0.00
			H							
36	HETATM	34	H		1	-5.349	-3.420	1.836	0.00	0.00
			H							
37	HETATM	35	H		1	-6.488	0.167	2.302	0.00	0.00
			H							
38	HETATM	36	H		1	-6.802	-1.477	2.909	0.00	0.00
			H							
39	HETATM	37	H		1	-7.103	-1.094	1.205	0.00	0.00
			H							
40	HETATM	38	C		1	5.200	-6.127	1.944	0.00	0.00
			C							
41	HETATM	39	C		1	7.384	-5.453	0.966	0.00	0.00
			C							
42	HETATM	40	H		1	5.523	-5.590	-0.126	0.00	0.00
			H							
43	HETATM	41	H		1	7.790	-4.974	1.874	0.00	0.00
			H							
44	HETATM	42	H		1	7.885	-4.994	0.099	0.00	0.00
			H							
45	HETATM	43	H		1	7.691	-6.509	0.992	0.00	0.00
			H							
46	HETATM	44	H		1	5.502	-5.821	2.960	0.00	0.00
			H							

47	HETATM	45	H		1	5.436	-7.197	1.849	0.00	0.00
			H							
48	HETATM	46	H		1	4.106	-6.027	1.879	0.00	0.00
			H							
49	HETATM	47	C		1	6.243	-1.232	2.746	0.00	0.00
			C							
50	HETATM	48	C		1	6.612	-3.524	3.636	0.00	0.00
			C							
51	HETATM	49	H		1	4.684	-2.582	3.376	0.00	0.00
			H							
52	HETATM	50	H		1	7.535	-3.731	3.068	0.00	0.00
			H							
53	HETATM	51	H		1	6.139	-4.497	3.853	0.00	0.00
			H							
54	HETATM	52	H		1	6.913	-3.088	4.599	0.00	0.00
			H							
55	HETATM	53	H		1	7.243	-1.234	2.279	0.00	0.00
			H							
56	HETATM	54	H		1	6.347	-0.742	3.725	0.00	0.00
			H							
57	HETATM	55	H		1	5.589	-0.589	2.128	0.00	0.00
			H							
58	HETATM	56	C		1	5.630	-1.055	-0.555	0.00	0.00
			C							
59	HETATM	57	H		1	6.024	-3.039	-1.315	0.00	0.00
			H							
60	HETATM	58	C		1	7.712	-2.342	-0.145	0.00	0.00
			C							
61	HETATM	59	H		1	7.923	-1.890	0.839	0.00	0.00
			H							
62	HETATM	60	H		1	8.227	-1.728	-0.898	0.00	0.00
			H							
63	HETATM	61	H		1	8.188	-3.335	-0.163	0.00	0.00
			H							
64	HETATM	62	H		1	4.573	-1.106	-0.861	0.00	0.00
			H							
65	HETATM	63	H		1	6.155	-0.455	-1.314	0.00	0.00
			H							
66	HETATM	64	H		1	5.675	-0.486	0.391	0.00	0.00
			H							
67	HETATM	65	H		1	-5.890	-1.163	-1.302	0.00	0.00
			H							
68	HETATM	66	C		1	-4.220	-0.487	-2.505	0.00	0.00
			C							
69	HETATM	67	C		1	-6.093	0.945	-1.729	0.00	0.00
			C							
70	HETATM	68	H		1	-6.841	1.122	-0.939	0.00	0.00
			H							
71	HETATM	69	H		1	-6.644	0.838	-2.676	0.00	0.00
			H							
72	HETATM	70	H		1	-5.478	1.858	-1.818	0.00	0.00
			H							
73	HETATM	71	H		1	-3.754	-1.481	-2.414	0.00	0.00
			H							

74	HETATM	72	H		1	-3.411	0.262	-2.459	0.00	0.00
			H							
75	HETATM	73	H		1	-4.659	-0.429	-3.512	0.00	0.00
			H							
76	HETATM	74	C		1	-1.706	1.681	2.429	0.00	0.00
			C							
77	HETATM	75	C		1	-0.128	2.155	0.679	0.00	0.00
			C							
78	HETATM	76	H		1	0.268	1.941	-0.323	0.00	0.00
			H							
79	HETATM	77	C		1	0.451	3.147	1.465	0.00	0.00
			C							
80	HETATM	78	C		1	-1.134	2.678	3.216	0.00	0.00
			C							
81	HETATM	79	C		1	-0.058	3.415	2.731	0.00	0.00
			C							
82	HETATM	80	H		1	-1.525	2.873	4.219	0.00	0.00
			H							
83	HETATM	81	H		1	1.306	3.716	1.086	0.00	0.00
			H							
84	HETATM	82	H		1	0.391	4.199	3.349	0.00	0.00
			H							
85	HETATM	83	C		1	-1.557	-4.274	1.694	0.00	0.00
			C							
86	HETATM	84	C		1	-0.365	-3.088	-2.455	0.00	0.00
			C							
87	HETATM	85	C		1	-2.027	-4.985	2.796	0.00	0.00
			C							
88	HETATM	86	H		1	-1.378	-4.792	0.742	0.00	0.00
			H							
89	HETATM	87	C		1	-1.446	-2.277	3.025	0.00	0.00
			C							
90	HETATM	88	C		1	-0.752	-3.866	-3.544	0.00	0.00
			C							
91	HETATM	89	H		1	0.592	-2.548	-2.482	0.00	0.00
			H							
92	HETATM	90	C		1	-2.386	-3.699	-1.304	0.00	0.00
			C							
93	HETATM	91	C		1	-2.219	-4.336	4.011	0.00	0.00
			C							
94	HETATM	92	H		1	-2.237	-6.056	2.707	0.00	0.00
			H							
95	HETATM	93	C		1	-1.915	-2.983	4.130	0.00	0.00
			C							
96	HETATM	94	H		1	-1.159	-1.217	3.132	0.00	0.00
			H							
97	HETATM	95	C		1	-2.771	-4.484	-2.388	0.00	0.00
			C							
98	HETATM	96	H		1	-3.043	-3.610	-0.422	0.00	0.00
			H							
99	HETATM	97	C		1	-1.952	-4.568	-3.509	0.00	0.00
			C							
100	HETATM	98	H		1	-0.105	-3.928	-4.425	0.00	0.00
			H							

101	HETATM	99	H		1	-3.721	-5.027	-2.358	0.00	0.00
			H							
102	HETATM	100	H		1	-2.253	-5.182	-4.364	0.00	0.00
			H							
103	HETATM	101	H		1	-2.596	-4.891	4.876	0.00	0.00
			H							
104	HETATM	102	H		1	-2.041	-2.474	5.091	0.00	0.00
			H							
105	HETATM	103	C		1	2.487	-3.679	3.571	0.00	0.00
			C							
106	HETATM	104	C		1	1.701	-5.563	-0.935	0.00	0.00
			C							
107	HETATM	105	C		1	3.733	-4.618	-1.807	0.00	0.00
			C							
108	HETATM	106	H		1	0.940	-5.615	-0.140	0.00	0.00
			H							
109	HETATM	107	C		1	1.598	-6.382	-2.057	0.00	0.00
			C							
110	HETATM	108	C		1	1.690	-5.609	2.382	0.00	0.00
			C							
111	HETATM	109	C		1	2.102	-4.259	4.776	0.00	0.00
			C							
112	HETATM	110	H		1	2.956	-2.680	3.567	0.00	0.00
			H							
113	HETATM	111	C		1	1.520	-5.523	4.784	0.00	0.00
			C							
114	HETATM	112	H		1	2.260	-3.721	5.716	0.00	0.00
			H							
115	HETATM	113	C		1	1.311	-6.197	3.585	0.00	0.00
			C							
116	HETATM	114	H		1	1.504	-6.131	1.431	0.00	0.00
			H							
117	HETATM	115	C		1	2.562	-6.313	-3.057	0.00	0.00
			C							
118	HETATM	116	H		1	0.754	-7.074	-2.153	0.00	0.00
			H							
119	HETATM	117	C		1	3.630	-5.430	-2.933	0.00	0.00
			C							
120	HETATM	118	H		1	4.590	-3.931	-1.700	0.00	0.00
			H							
121	HETATM	119	H		1	4.391	-5.376	-3.718	0.00	0.00
			H							
122	HETATM	120	H		1	2.481	-6.954	-3.941	0.00	0.00
			H							
123	HETATM	121	H		1	1.223	-5.984	5.731	0.00	0.00
			H							
124	HETATM	122	H		1	0.844	-7.187	3.587	0.00	0.00
			H							
125	HETATM	123	C		1	1.878	0.732	-1.306	0.00	0.00
			C							
126	HETATM	124	C		1	1.530	-0.534	3.120	0.00	0.00
			C							
127	HETATM	125	C		1	2.642	-1.289	-2.370	0.00	0.00
			C							

128	HETATM	126	C		1	2.179	1.455	-2.458	0.00	0.00
		C								
129	HETATM	127	H		1	1.444	1.239	-0.432	0.00	0.00
		H								
130	HETATM	128	C		1	3.179	0.461	1.679	0.00	0.00
		C								
131	HETATM	129	C		1	2.005	0.227	4.186	0.00	0.00
		C								
132	HETATM	130	H		1	0.661	-1.197	3.265	0.00	0.00
		H								
133	HETATM	131	C		1	2.940	-0.568	-3.524	0.00	0.00
		C								
134	HETATM	132	H		1	2.840	-2.370	-2.334	0.00	0.00
		H								
135	HETATM	133	C		1	2.710	0.804	-3.567	0.00	0.00
		C								
136	HETATM	134	H		1	1.989	2.533	-2.491	0.00	0.00
		H								
137	HETATM	135	H		1	3.358	-1.081	-4.396	0.00	0.00
		H								
138	HETATM	136	H		1	2.944	1.370	-4.475	0.00	0.00
		H								
139	HETATM	137	C		1	3.067	1.105	3.998	0.00	0.00
		C								
140	HETATM	138	H		1	1.534	0.140	5.170	0.00	0.00
		H								
141	HETATM	139	C		1	3.650	1.229	2.740	0.00	0.00
		C								
142	HETATM	140	H		1	3.633	0.553	0.682	0.00	0.00
		H								
143	HETATM	141	H		1	4.480	1.926	2.585	0.00	0.00
		H								
144	HETATM	142	H		1	3.439	1.703	4.836	0.00	0.00
		H								
145	HETATM	143	C		1	-2.039	0.838	-1.804	0.00	0.00
		C								
146	HETATM	144	C		1	-1.525	0.195	-2.916	0.00	0.00
		C								
147	HETATM	145	C		1	-2.655	2.077	-1.927	0.00	0.00
		C								
148	HETATM	146	C		1	-1.618	0.802	-4.168	0.00	0.00
		C								
149	HETATM	147	H		1	-1.048	-0.789	-2.818	0.00	0.00
		H								
150	HETATM	148	C		1	-2.746	2.686	-3.175	0.00	0.00
		C								
151	HETATM	149	H		1	-3.084	2.566	-1.036	0.00	0.00
		H								
152	HETATM	150	C		1	-2.223	2.047	-4.296	0.00	0.00
		C								
153	HETATM	151	H		1	-1.210	0.296	-5.049	0.00	0.00
		H								
154	HETATM	152	H		1	-3.229	3.663	-3.275	0.00	0.00
		H								

155	HETATM	153	H		1	-2.292	2.524	-5.279	0.00	0.00
		H								
156	HETATM	154	H		1	-2.539	1.081	2.827	0.00	0.00
		H								
157	CONECT	3	1	20	21	22				
158	CONECT	4	1	29	30	31				
159	CONECT	5	1	65	66	67				
160	CONECT	6	74	75	2					
161	CONECT	8	83	87	7					
162	CONECT	10	84	90	7					
163	CONECT	11	124	128	9					
164	CONECT	12	123	125	9					
165	CONECT	14	103	108	13					
166	CONECT	16	104	105	13					
167	CONECT	17	15	47	48	49				
168	CONECT	18	56	57	58	15				
169	CONECT	19	15	38	39	40				
170	CONECT	20	3	26	27	28				
171	CONECT	21	3	23	24	25				
172	CONECT	30	4	34	32	33				
173	CONECT	31	4	35	36	37				
174	CONECT	38	19	44	45	46				
175	CONECT	39	19	41	42	43				
176	CONECT	47	54	55	17	53				
177	CONECT	48	17	50	51	52				
178	CONECT	56	62	63	64	18				
179	CONECT	58	59	60	61	18				
180	CONECT	66	71	72	73	5				
181	CONECT	67	68	69	70	5				
182	CONECT	74	78	154	6					
183	CONECT	75	76	77	6					
184	CONECT	77	75	79	81					
185	CONECT	78	74	79	80					
186	CONECT	79	77	78	82					
187	CONECT	83	85	86	8					
188	CONECT	84	88	89	10					
189	CONECT	85	83	91	92					
190	CONECT	87	93	94	8					
191	CONECT	88	84	97	98					
192	CONECT	90	95	96	10					
193	CONECT	91	85	93	101					
194	CONECT	93	87	91	102					
195	CONECT	95	90	97	99					
196	CONECT	97	88	95	100					
197	CONECT	103	109	110	14					
198	CONECT	104	106	107	16					
199	CONECT	105	117	118	16					
200	CONECT	107	104	115	116					
201	CONECT	108	113	114	14					
202	CONECT	109	103	111	112					
203	CONECT	111	109	113	121					
204	CONECT	113	108	111	122					
205	CONECT	115	107	117	120					
206	CONECT	117	105	115	119					

207	CONECT	123	126	127	12
208	CONECT	124	129	130	11
209	CONECT	125	131	132	12
210	CONECT	126	123	133	134
211	CONECT	128	139	140	11
212	CONECT	129	124	137	138
213	CONECT	131	125	133	135
214	CONECT	133	126	131	136
215	CONECT	137	129	139	142
216	CONECT	139	128	137	141
217	CONECT	143	144	145	2
218	CONECT	144	143	146	147
219	CONECT	145	143	148	149
220	CONECT	146	144	150	151
221	CONECT	148	145	150	152
222	CONECT	150	146	148	153
223	CONECT	1	2	3	4
224	CONECT	2	1	143	6
225	CONECT	7	2	8	9
226	CONECT	9	7	11	12
227	CONECT	13	9	14	15
228	CONECT	15	13	17	18
229	CONECT	22	3		
230	CONECT	23	21		
231	CONECT	24	21		
232	CONECT	25	21		
233	CONECT	26	20		
234	CONECT	27	20		
235	CONECT	28	20		
236	CONECT	29	4		
237	CONECT	32	30		
238	CONECT	33	30		
239	CONECT	34	30		
240	CONECT	35	31		
241	CONECT	36	31		
242	CONECT	37	31		
243	CONECT	40	19		
244	CONECT	41	39		
245	CONECT	42	39		
246	CONECT	43	39		
247	CONECT	44	38		
248	CONECT	45	38		
249	CONECT	46	38		
250	CONECT	49	17		
251	CONECT	50	48		
252	CONECT	51	48		
253	CONECT	52	48		
254	CONECT	53	47		
255	CONECT	54	47		
256	CONECT	55	47		
257	CONECT	57	18		
258	CONECT	59	58		
259	CONECT	60	58		
260	CONECT	61	58		

```
261 CONECT  62   56
262 CONECT  63   56
263 CONECT  64   56
264 CONECT  65    5
265 CONECT  68   67
266 CONECT  69   67
267 CONECT  70   67
268 CONECT  71   66
269 CONECT  72   66
270 CONECT  73   66
271 CONECT  76   75
272 CONECT  80   78
273 CONECT  81   77
274 CONECT  82   79
275 CONECT  86   83
276 CONECT  89   84
277 CONECT  92   85
278 CONECT  94   87
279 CONECT  96   90
280 CONECT  98   88
281 CONECT  99   95
282 CONECT 100   97
283 CONECT 101   91
284 CONECT 102   93
285 CONECT 106  104
286 CONECT 110  103
287 CONECT 112  109
288 CONECT 114  108
289 CONECT 116  107
290 CONECT 118  105
291 CONECT 119  117
292 CONECT 120  115
293 CONECT 121  111
294 CONECT 122  113
295 CONECT 127  123
296 CONECT 130  124
297 CONECT 132  125
298 CONECT 134  126
299 CONECT 135  131
300 CONECT 136  133
301 CONECT 138  129
302 CONECT 140  128
303 CONECT 141  139
304 CONECT 142  137
305 CONECT 147  144
306 CONECT 149  145
307 CONECT 151  146
308 CONECT 152  148
309 CONECT 153  150
310 CONECT 154   74
311 END
```

The above molecule contains 154 atoms and 153 bonds, making it extremely computationally expensive for regular QM calculations. This made utilizing the large

molecule as a trial system unreasonable due to the prohibitively long computation time for each conformation, assuming the conformation calculation would complete at all.

The below PDB file is the simplified butagermane with fully protonated Germanium atoms. As a significantly smaller system with only 14 atoms and 13 bonds, the relatively short computation time allowed the trial system to move with relative ease.

C.2 Code: ge4h.pdb

```

1 COMPND      UNNAMED
2 AUTHOR      GENERATED BY OPEN BABEL 2.3.90
3 HETATM      1  GE   UNL    1     -3.520   1.842  -0.078   1.00   0.00
4           Ge3-
5 HETATM      2  GE   UNL    1     -1.368   2.888  -0.034   1.00   0.00
6           Ge2-
7 HETATM      3  GE   UNL    1      0.324   1.200   0.059   1.00   0.00
8           Ge3-
9 HETATM      4  GE   UNL    1      2.475   2.248   0.099   1.00   0.00
10          Ge
11 HETATM     5   H    UNL    1     -4.622   2.930  -0.135   1.00   0.00
12          H
13 HETATM     6   H    UNL    1     -3.699   0.985   1.202   1.00   0.00
14          H
15 HETATM     7   H    UNL    1     -3.621   0.932  -1.328   1.00   0.00
16          H
17 HETATM     8   H    UNL    1     -1.258   3.797   1.217   1.00   0.00
18          H
19 HETATM     9   H    UNL    1     -1.178   3.740  -1.314   1.00   0.00
20          H
21 HETATM    10   H    UNL    1      0.213   0.288  -1.189   1.00   0.00
22          H
23 HETATM    11   H    UNL    1      0.135   0.352   1.342   1.00   0.00
24          H
25 HETATM    12   H    UNL    1      2.655   3.095  -1.186   1.00   0.00
26          H
27 HETATM    13   H    UNL    1      3.578   1.161   0.165   1.00   0.00
28          H
29 HETATM    14   H    UNL    1      2.574   3.167   1.343   1.00   0.00
30          H
31 CONECT     1     2     5     6     7
32 CONECT     2     1     3     8     9
33 CONECT     3     2     4    10    11
34 CONECT     4     3    12    13    14
35 CONECT     5     1
36 CONECT     6     1
37 CONECT     7     1
38 CONECT     8     2
39 CONECT     9     2
40 CONECT    10     3
41 CONECT    11     3
42 CONECT    12     4
43 CONECT    13     4
44 CONECT    14     4

```

31	MASTER	0	0	0	0	0	0	0	14	0	14	0
32	END											

C.3 Progress on Torsion Minimizer System

While incomplete and largely nonfunctioning, this code is the current progress toward the implementation of the torsion minimizer system as outlined in 4.2.

```

1  ### Author: Gentry Smith
2  ### Date: April 22, 2017
3  ### Description: This is the runner file that is the primary executable
4  ###      for the torsion minimizer. Currently is the
5  ###      only file utilized.
6
7  # Inputs:
8  # Arg1: the molecule file to be minimized (currently only accepts a pdb
9  #       file)
10
11 import sys
12 import subprocess
13 import math
14
15 # IO Validator: validates user-submitted molecule.
16 def IOValidator():
17     isValid = False
18     # Check for valid length of args (2)
19     if len(sys.argv) == 2:
20         # Check arg to make sure it's a file.
21         argFile = sys.argv[1]
22         try:
23             inputFile = open(argFile)
24             # Finally, make sure the file is a .pdb
25             if inputFile[-4:] == ".pdb":
26                 isValid = True
27             else:
28                 print("This is not a .pdb file. Please try again with a
29 .pdb file.\n")
30                 inputFile.close()
31             except IOError:
32                 print("System was not able to open '", str(argFile), "'")
33             # too long
34             elif len(sys.argv) > 2:
35                 print("You have too many arguments. Call the file as 'Runner.py
36 [molecule file]' and try again.\n")
37             # too short
38             else:
39                 print("You do not have enough arguments. Start the program as '
40 Runner.py [molecule file]' and try again.\n")
41             # return validity boolean
42             return isValid
43
44 # Get Torsions: initiates function to get user-specified torsion bonds.
45 # Returns bonds as int[[a,b],[a,b]] list
46 def getTorsions():
47     torsions = [[0, 0]]

```

```

42     newTorsion = "first"
43     firstTime = True
44     doneCheck = ""
45     badIn = False
46
47     # loop for all torsions until user types "done"
48     while newTorsion != "":
49         if firstTime:
50             print("It's time to define the torsions of the molecule and")
51             print("declare which bonds you would like to rotate.\n")
52             print("Before going any further, it's important to note at")
53             print("this time that version 0.2 (current) will assume the torsions you")
54             print("enter are completely correct. You'll see a bunch of error messages")
55             print("soon if it isn't correct.\n")
56             print("Open the .pdb file and identify the numbers of the")
57             print("atoms on the .pdb that will make the bond (the first number on the")
58             print("line of each atom)\n\n")
59             print("Now it's time to enter in the numbers of the two")
60             print("atoms. We'll do it one at a time.")
61
62             firstTor = raw_input("Type in the number of the first atom")
63             in the bond and hit enter. \nEx: type 3 and then hit enter.\n")
64
65             try:
66                 confFirstTor = int(firstTor)
67             except ValueError:
68                 print("You typed in '", firstTor, "'", which is not a")
69                 print("number. Let's start again.")
70                 badIn = True
71
72             secondTor = raw_input("Type in the number of the second atom")
73             in the bond and hit enter. \nEx: type 3 and then hit enter.\n")
74
75             try:
76                 confSecondTor = int(secondTor)
77             except ValueError:
78                 print("You typed in '", secondTor, "'", which is not a")
79                 print("number. Let's start again.")
80                 badIn = True
81                 firstTime = False
82
83             else:
84                 print("Open the .pdb file and identify the numbers of the")
85                 print("atoms on the .pdb that will make the bond (the first number on the")
86                 print("line of each atom)\n\n")
87
88             firstTor = raw_input("Type in the number of the first atom")
89             in the bond and hit enter. \nEx: type 3 and then hit enter.\n")
90
91             try:
92                 confFirstTor = int(firstTor)
93             except ValueError:
94                 print("You typed in '", firstTor, "'", which is not a")
95                 print("number. Let's start again.")

```

```

81         badIn = True
82
83     secondTor = raw_input("Type in the number of the second atom
84     in the bond and hit enter. \nEx: type 3 and then hit enter.\n")
85
86     try:
87         confSecondTor = int(secondTor)
88     except ValueError:
89         print("You typed in '", secondTor, "' , which is not a
90     number. Let's start again.")
91         badIn = True
92         firstTime = False
93
94     if badIn == False:
95         newTorsion = [confFirstTor, confSecondTor]
96         if torsions == [[0, 0]]:
97             print("You added a new torsion: ", newTorsion, "\n")
98             torsions = newTorsion
99         else:
100             torsions.append(newTorsion)
101             print("The current torsions you have created are:\n")
102             for each in torsions:
103                 print(each, "\n")
104             doneCheck = raw_input("If you would like to add another
105             torsion, press enter. If you are finished adding torsions, type
106             'done' and press enter\n")
107
108             if str(doneCheck) == "done":
109                 print("Finished entering torsions. Beginning the work.\n")
110             else:
111                 newTorsion = "first"
112
113
114     return torsions
115
116 # Get Conformation Count: determines conformations needed. Returns list
117 # in form: [#conf, rotDeg, rotRng]
118 def getConformationInfo(depth, torsions):
119     # rotates 60 degrees on the first search, then logarithmic decrease
120     # from 10 for each subsequent search.
121     rotDeg = [60, 10]
122     # full torsion range for first search, logarithmic decrease from 50
123     # for each subsequent search
124     rotRng = [360, 50]
125     # number of conformations needed
126     numConf = 0
127     # degrees per rotation
128     deg = 0
129     # rotation range

```

```

127     rng = 0
128     # number of rotations per torsion
129     rotTick = 0
130
131     # determine counts from depth
132     if depth >= 2:
133         deg = math.pow(10, (2-depth))
134         rng = deg*5
135     elif depth <2:
136         deg = rotDeg[depth]
137         rng = rotRng[depth]
138     if depth == 1:
139         rotTick = 6
140     elif depth >= 1:
141         rotTick = 11
142
143     numConf = math.pow(torsions, rotTick)
144
145     return [numConf, deg, rng]
146
147
148
149
150
151
152
153
154 def Launcher():
155     valid = IOValidator()
156     if valid:
157         # do everything
158         depth = 0
159
160         InitWD()
161
162     else:
163         print("There was a problem while reading in the molecule file.
164             Please try again.\n")
165         exit()
166
167
168 # Initiates proper working directory.
169 def InitWD():
170
171
172
173
174 # Recursive search through molecule torsions
175 def RecursiveSearch(depth):
176
177     torsions = getTorsions()
178
179

```

180
181 Launcher()

VITA

Gentry H. Smith

Candidate for the Degree of

Master of Science

Thesis: EXPLORING CRITICAL CONFORMATIONS

Major Field: Chemistry

Biographical:

Personal Information: Born in Olathe, KS in November 1993.

Education:

Received a Bachelors of Science in Chemistry at Southern Nazarene University in May 2016.

Completed the requirements for the degree of Master of Science with a major in Chemistry at Oklahoma State University in December 2018.

Experience:

Teaching Assistant, various undergraduate chemistry courses, Southern Nazarene University, Aug. 2014 - May 2016

Graduate Teaching Assistant, CHEM 1314, 1414 at Oklahoma State University, Aug. 2016 - Dec. 2018

Professional Affiliations:

American Chemical Society

Awards

Colonel Andre Whitely Scholarship in Chemistry