Multiscale and Multiphysics Computational Frameworks for Nano- and Bio-Systems

Thesis by

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© 2009 Hyungjun Kim All Rights Reserved I dedicate this PhD thesis to God and my loving parents.

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Abstract

Multiscale and multiphysics simulation strategy is important to investigate complex problems in nature because it provides a systematic method to understand underpinning physics of the systems depending on the size. In this thesis, we discuss how such multiscale and multiphysics simulation framework can explain and rationalize the experimental observations in several nano- and biosystems. Furthermore, we exhibit the computational simulation methods that play major roles to rationally design novel materials with desired properties in next generation nano electronic devices, alternative energy materials, life science, and so on.

Chapter 1 reviews the significance of multiscale and multiphysics simulation strategy. In this chapter, we briefly discuss the multiscale and multiphysics natures in nano- and bio-systems, and detailed examples are contained in the next chapters. Chapter 2 introduces an electric field induced conformational change mechanism, which is responsible for the unique current-voltage (I-V) behavior of nano device, negative differential resistance (NDR). In Chapter 3, the on/off kinetics of the Stoddart-Heath rotaxane-based programmable molecular electronic switch is discussed in terms of the free energy quantities. Chapter 4 explores sodium diffusion through the aluminum-doped zeolite BEA system, and the effect of water uptake amount is thoroughly discussed. This has importance for the application of zeolite to proton exchange membranes for fuel cells (PEMFC). In Chapters 5 and 6, the ion mobilities of tertiary and quaternary ammonium cations (precursors for lipids), and phosphatidylcholine (PC) lipid cations are investigated, respectively. In order to compute the ion mobilities of the precursors and entire lipids, we develop a modified trajectory (TJ) method dealing with the complicated integrals of interaction terms. QM and MD simulations are performed to determine the structures and charge distributions. In Chapter 7, we study how the model lung system of lipid monolayer with surfactant protein B (SP-B) responds to ozone introduction. In parallel with the field induced droplet ionization (FIDI) mass spectrometry study, MD simulations identify the distinct ozone reaction mechanism at the interface, and the role of SP-B at the pulmonary surfactant (PS) system on the oxidative stresses.

From these studies, we suggest various multiscale and multiphysics modeling approaches depending on the characteristics of systems and objectives. These efforts allow us to overcome the limited time- and length-scales of the monoscale simulations. In addition, we expect that an establishment of such multiscale modeling procedures will invoke interdisciplinary studies by tightly combining the developments occurring independently across fields.

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Chapter 1 Introduction

Generally, a great number of chemical and physical problems in real life have multiscale and multiphysics features. Many observable physical quantities originate from multiple physical phenomena working cooperatively at different time- and length-scale. Interestingly, it is well known that different regimes are interpreted in terms of the different physics, which are inter-connected to each other through the "coarse-graining of the scale." Exemplifying, quantum mechanics (QM) governs the physics between nuclei and electrons. Classical mechanics (CM) governs the atomic or molecular dynamics on the complex energy surface, which is the outcome of the quantum mechanical interactions. The material flow is described by rheology, which coarse grains the particles into a continuum. Here, the governing parameters of such rheology are determined by the inter-molecular interactions.

Computational simulation methods, along with statistical mechanics, have been employed as a useful tool to expand our knowledge of microscale events and connect them into macroscopic observances. Thanks to the development of many simulation methods at various scales and the combination of these methods within a multiscale and multiphysics simulation paradigm (Figure 1.1), computational simulation is now regarded as an indispensable tool for the new advancement in science and engineering. In a good number of cases, computer simulations efficiently supplement experiments in interpreting observations, otherwise research would be too expensive or dangerous. On the contrary, in many others, computer simulations are the only possible choice to probe the complicated phenomena. In this context, the tremendous quest for ever-higher levels of detail and realism in such simulations, contribute to the inexorable demand for new theory, methods, and computational tools.

Currently, an enormous amount of research is focused on nano- and bio-systems. Research on nano-systems is most often centered on predicting nanoscaled transport properties such as electron, thermo, and mass transportations for the application of next-generation electronic devices or alternative energy materials. Research on bio-systems has significant potential in life science and medical applications. In particular, such nano- or bio-systems have a strong multiscale and multiphysical nature within them, intriguing the quest for the development of an elaborated methodology to un-



Figure 1.1: Multiscale and Multiphysics paradigm simulation strategy.

derstand the scale-dependent physics. Specifically, in nano-systems (Figure 1.2), electron transport through a molecule is strongly dependent on the energy eigen states of the molecule (QM regime), which are affected by the molecular/atomic conformations and motions (CM regime). When we design an engineering process for manufacturing electronic device such as ultimate complementary metal-oxide-semiconductor (CMOS) electronics using novel materials, continuum level theory and simulations are important. In bio-systems (Figure 1.3), lipid layers encapsulate cells and control fluidity and surface tensions, which are macroscopic/hydrodynamic regime quantities. These macroscopic changes are yielded by the inter-molecular interactions at the interface (CM region). In the lower scale, such molecular interactions are often tuned by chemical reactions such as a proton transfer, which has a strong QM effect.

Within contemporary computing power, direct use of first principle computational methods is limited by an order of ~ 1000 atoms and an order of *pico* to *nano* seconds. Thus, for managing many practical issues in using computational simulation methods which often involve a large lengthand long time-span, we need to overcome the limitations in simulation scales. In this thesis, several cases of nano- and bio-systems are presented; (1) we understand them by capturing fundamental nanoscale intrinsic and extensive properties, then, (2) we define the macroscopic behavior observed from experiments based on the microscopic understandings.

The first half (Chapters 2-4) discusses the multiscale and multiphysics simulation approaches for nano-systems.

In Chapter 2, we investigate a negative differential resistance (NDR) effect observed from a metal/molecular SAM/metal junction. Amino- and nitro-substituted oligo-phenylene ethynelene



Figure 1.2: Multiscale and Multiphysics characteristics in nano electronic systems. At electron size scale, electrical conductivity depends on the quantum states of the molecules. At molecular size scale, classical interactions determine the molecular conformation, which affects its quantum state. At device size scale, hundreds of molecules are assembled to build a mesoscale junction and these are packaged into a device component.

(OPE) molecules in the self-assembled monolayer (SAM) have a large molecular dipole moment, which responds to the external electric field. Hence, applying the bias voltage induces the conformational changes of the individual molecules and thereby yield a structural transition of the SAM. Such a conformational change is in the regime where the molecular dynamics (MD) simulation is useful. However, the kinetics during the structural relaxation of the SAM requires larger scale simulation methods. On the other hand, electrical conductivities on the total *I-V* curve are rooted in QM. In order to manage such a complicated problem, we design a nearest neighbor (NN) model with lattice Monte Carlo (MC) simulation, whose parameters are obtained by coarse-graining QM and MD simulation results. The electrical conductivities depending on the conformations are parameterized using non-equilibrium green functional theory combined with QM.

In Chapter 3, on/off kinetics of the molecular switch, bistable [2]rotaxane is discussed. The rotaxane has been intensively studied because of its interesting properties, which are attributed to the molecular recognition between charge donor and acceptor. The shuttling motion of electron accepting cyclobis-(paraquat-p-phenylene) (CBPQT⁴⁺) between the charge donating stations such as tetrathiafulvalene (TTF) and 1,5-dioxynaphthalene (DNP) moieties, has brought many applications such as molecular switch in nanoelectronics and artificial muscle in nanomechanics. Therefore, comprehensive understanding of the free energy barrier required for this shuttling motion is essential. In addition, the fine control of the free energy barrier can open an application of the rotaxane system



Figure 1.3: Multiscale and Multiphysics characteristics in bio systems. At electron size scale, chemical reactions, which are governed by huge QM effects (e.g., electron/proton transfer), regulate the molecular architecture of the protein for an effective functionality. At molecular scale, CM decribes the interactions, such as hydrophobic interaction, among the bio components of proteins, lipids, etc. Large scale motion of the membrane, such as endo- or exo-vesiculation, is in the regime of hydrodynamic descriptions, and this affects the dynamics of a cell.

toward non-volatile flash memory devices, which has not yet achieved. Since the ring and backbone form a charge transfer complex, the local charge distribution (QM effect) strongly determines the free energy profiles for the rings shuttling. However, the time scale for the shuttling is order of μ s, which is beyond the available time scale of atomistic simulations. To handle such difficulties, we perform a "blue moon sampling technique" with MD simulations, which allows an effective sampling using a series of constraint MD simulations. The change of potential energy surface depending on the charge transfer amount is reflected on the MD simulations using various Mulliken charge populations from QM calculations according to the ring's location. The free energy barrier from the TTF station to the DNP station is evaluated as 19 kcal/mol when the system is neutral and 8 - 9 kcal/mol for the oxidation states +1 and +2, and the the free energy barrier from the DNP station to the TTF station is 18 kcal/mol, 22 - 23 kcal/mol, and 32 - 33 kcal/mol for the neutral and the oxidation states +1 and +2, respectively. These values are quite comparable to the values that were obtained from various prior experiments, and greatly explain the microscopic ground for the on/off switching kinetics of the molecular switch.

In Chapter 4, the diffusion process of sodium ion in the aluminum-doped zeolite BEA system is studied. Understanding the ionic diffusion through a percolated pore of the zeolite is important for the application of the zeolite to proton exchange membranes for fuel cells (PEMFC). Especially, investigating the role of the confined water is vital because it provides a medium for transport of the ions. The amount of water swelled into the PEMFC depends on the macroscopic variables, such as pressure and temperature, where the PEMFC is working. Thus, combining the grand canonical Monte Carlo (GCMC) simulations (for the study of water uptake amount) with MD simulations (for the study of confined water structure), we investigate the effect of water on the sodium diffusion. We observe a first-order-like transition from the absorption isotherm, inferring that zeolite provides a hydrophobic environment. From MD trajectories, we observe the sodium ions diffused via a hopping mechanism among aluminum-doped sites (which are Brönsted acid sites). We figure out that, above 15 wt % hydration (good solvation regime), the solvation cage is easily formed, and dramatically increases sodium diffusion by reducing the hopping energy barrier by 25 % from the value of 3.8 kcal/mol observed in the poor solvation regime.

The second half (Chapters 5-7) discusses the multiscale and multiphysics simulation approaches for bio-systems. In particular, we scrutinize lipid systems, which have critical roles in cell structure, energy storage and metabolic control, using computational methods in collaboration with gas-phase experiments.

In Chapter 5, we study the ion mobility of a number of tertiary amine and quaternary ammonium cations in gas-phase. These tertiary amine and quaternary ammonium cations are related to the choline and its derivatives, which are precursors for lipids such as a phosphatidlcholine and sphingomyelin. For example, choline is oxidized to betaine, which is readily demethylated to yield N, N-dimethylglycine. Decomposition of choline yields trimethylamine and dimethylamine. Ion mobility in gas phase is determined by the collision of the ion with drift gas molecules. Utilizing the kinetic theory under the assumption of binary collision, the ion mobility in gas-phase is formulated as a complex integration of interaction terms between the ion and the drift gas molecule. We develop a methodology (referred to as modified trajectory (TJ) method) for the numerical integrations of complex interaction terms for the case where the ion drifts within the N_2 buffer gas. Since the interaction terms depend on the electron distribution and molecular conformation, the gas phase structures and the charge distributions are investigated using QM calculations. Then, ion mobilities are calculated using the modified TJ method. The calculated ion mobility is in agreement with the experimental value, and it well explains the observed mass-mobility correlation of tertiary amine and quaternary ammonium cations, in terms of the asymmetry of the shape. In addition, computational numerical study allows us to identify the role of each interaction term (van der Waals interaction, ion-induced dipole interaction, ion-quadrupole interaction, charge-charge interaction) on the ion mobility at the border-line regime, which lies between the regime where the long-range interactions are dominant (small ion size) and the regime where the short-range interactions are dominant (large ion size).

In Chapter 6, we expand the ion mobility study of lipid precursors in Chapter 5 into the study of the intact lipids of phophatidycholines (PC). Since the PC contains a flexible acyl chain, the molecular fluctuation changes the mobility of the PC cation. Taking the molecular fluctuation effect into account, 200 conformations are sampled from the MD simulations, then, the average collision cross-section is computed using the modified TJ method for the calculation of ion mobility. Here, for the experimental section, a commercial traveling wave ion mobility spectrometry (TWIMS) has been employed. Our simulation results exhibit a good agreement with the experimental values. In particular, we reveal that the traveling wave applied in the experiments excites the ions. Since this excitation yields a less compact form of saturated PCs, while unsaturated PCs can not form such a stretched conformation due to the rigid double bonds, we observe distinct mass-mobility correlation lines for the saturated PC cations and for the unsaturated PC cations.

In Chapter 7, a model lung surfactant system composed of lipid monolayer with surfactant protein B (SP-B) is examined. Lung disease is the third leading cause of death in United States, and concerns about chronic respiratory tract disease increase significantly as the level of air pollution increases. Thus, chemical and physical comprehensions about the response of pulmonary surfactant (PS) system to ozone (O_3), one of the most common air pollutants, are required. Due to the interfacial characteristic of PS, the ozonolysis of PS can undergo different pathways according to the reaction environment, especially, depending on whether or not the reaction occurs under waterrich conditions. From the multiscale/multiphysics point of view, the ozonolysis is the result of the QM effect, but the reaction environment is determined by the location of each component,

which is the outcome of the CM interactions among the molecules. In addition, the change of physical properties of PS (e.g., surface tension) is in the regime of larger-scale physics such as hydrodynamics. In this chapter, a complete study on the response of lipid monolayer to O_3 is achieved at the air-liquid interface when O_3 is introduced from the air. The chemical composition changes during the heterogeneous O_3 reaction are analyzed using field induced droplet ionization (FIDI) mass spectrometry, which exhibits quite a different reaction pathway to the bulk-phase ozone reaction. Our MD simulation provides molecular level understanding and rationalization for the observed distinct reaction pathways.

Depending on the characteristics of systems and the objectives that we want to figure out, as exemplified in this thesis, distinct approaches are required to explain the actual observations from experiments. Based on the cases discussed here, we suggest various systematic strategies to overcome the limitations in time- and length-scales of the traditional monoscale approaches. In addition, due to the nature of multiscale and multiphysics phenomena, we expect that a concrete establishment of the fundamental multiscale modeling procedures will invoke interdisciplinary studies by tightly combining the developments occurring independently across fields.

Chapter 2

Negative Differential Resistance of Oligo (Phenylene Ethynylene) Self-Assembled Monolayer Systems: The Electric Field Induced Conformational Change Mechanism

2.1 Abstract

We investigate here a possible mechanism for the room temperature Negative Differential Resistance (NDR) in the Au/AN-OPE/RS/Hg self-assembled monolayer (SAM) system, where AN-OPE = 2'amino, 5'-nitro oligo (phenylene ethynylene) and RS is a C14 alkyl thiolate. Kiehl and co-workers showed that this molecular system leads to NDR with hysteresis and sweep-rate-dependent position and amplitude in the NDR peak. To investigate a molecular basis for this interesting behavior, we combine first principles quantum mechanics (QM) and meso-scale lattice Monte Carlo (MC) methods to simulate the switching as a function of voltage and voltage rate, leading to results consistent with experimental observations. This simulation shows how the structural changes at the microscopic level lead to the NDR and sweep-rate dependent macroscopic I-V curve observed experimentally, suggesting a microscopic model that might aid in designing improved NDR systems.

2.2 Introduction

Esaki's discovery of the negative differential resistance (NDR) in Ge p-n diodes opened a new phase in semiconductor devices [1]. Since the NDR devices enable faster and more efficient circuits

by reducing the number of transistors required, they have many applications such as high-speed integrated circuits and low-power memories. As the scale of electronic devices is reduced toward nano-scale sizes, it would be useful to demonstrate NDR in molecular electronic systems [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13].

Derivatives of oligo (phenylene ethynylene) (OPE) have been identified as a good candidate for the molecular junctions due to its rigid and good conducting (fully conjugated) characteristics [9, 11, 12, 13, 14, 15, 16, 17, 18, 19]. Chen *et al.* reported that a SAM of amino-nitro substituted OPE (AN-OPE) between two Au electrodes exhibits NDR at 60 K with an applied voltage of ~ 2 V. The current-voltage (*I-V*) curve is fully reversible, but the NDR peak decays as the temperature increases. This NDR has been rationalized by the electrochemical oxidation/reduction or resonant-tunneling mechanism [15, 16, 17]. Support for this oxidation/reduction mechanism was the correspondence between the threshold potential for the electrical conductance (2.09 V) and the electrochemical potential (1.67 V) [15, 19].

The device showing NDR at room temperature (RT) is important for many practical applications [20, 21]. However, the poor reproducibility in device construction and the limited device stability have hampered extensive study on NDR. Kiehl and co-workers showed that a SAM of AN-OPE deposited on an Au electrode coupled to a Hg electrode covered with a tetradecane-thiolate (RS) leads to a well-defined and stable NDR at RT [9]. In this system, a distinct sweeping-rate-dependency in the NDR hysteresis loop was observed for a bias voltage near ~ 0.6 V. The presence of hysteresis rules out the resonant tunneling mechanism [5, 6, 7, 8, 10]. Based on the observed hysteresis and a variety of detailed features of the characteristics, they proposed a charge capture (QC) mechanism to explain the macroscopic *I-V* behavior. However, an atomistic level analysis of a charge capture process and other possible mechanisms has not yet been established.

Several studies suggest that the conformational change would be a plausible mechanism to explain hysteretic I-V curve [14, 22], and the external electric field can induce conformational change of the molecule in the junction [14, 23, 24, 25, 26]. Especially, Donhauser *et al.* reported STM studies in which isolated AN-OPE molecules contained in a dodecane-thiolate SAM on the Au substrate show at least two states having different conductances [14]. They showed that the transition from the high-conductance state to the low-conductance state is switched by applying external electric field. However no detailed atomic level description of the mechanism was provided.

In this chapter, we use first principle theory to analyze the sweeping-rate-dependent hysteresis of NDR observed in Kiehl's system, focusing on the possibility of electric field based conformational changes. We find that this system has two states:

- a high-conductance phase stable at low field (planar structure) and
- a low-conductance phase stable at high field (twisted structure).

The transition between the two phases is driven by the interaction between the external field and the molecular dipole moment of the middle phenylene ring in AN-OPE. This leads to consistent results with the charge capturing mechanism of Kiehl. Using coarse-grained Monte Carlo simulations, we investigated how such a molecular conformational change results in a sweep-rate-dependent hysteresis in the NDR as well as the detailed kinetics of transition.

2.3 Simulation Details

2.3.1 Computational Details of QM Calculations

To obtain the structures and energies of planar (P) and twisted (T) structures, we carried out QM calculations for a (1×1) periodic unit cell. We employed the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation exchange-correlation density-functional with a plane wave basis set (540 eV cutoff), using the Vienna Ab initio Simulation Package (VASP) [27]. Only the gamma point is sampled in reciprocal space to reduce computational cost for this large system (67 atoms per periodic cell). For the electrodes, we used 3-layer of Au (111) surface with all gold atoms fixed at their bulk value (a = 2.8838 Å) during the geometry optimization steps. The OPE molecules were anchored on the 3×3 Au (111) surface through sulfur atoms with hexagonal packing.

To understand the local electronic structure and local interactions of the AN-OPE part, we performed non-periodic QM calculations of the isolated OPE with 3 connected Au atoms, using Jaguar package [28] with PBE exchange-correlation functional and LACVP** basis set. Using the geometries from VASP calculations, we carried out the single point calculations.

2.3.2 Conductivities of P and T Conformations (NEGF Calculations)

The I-V performance of each conformation is calculated by combining Green's function theory with the DFT Hamiltonian that are determined from the SeqQuest calculation with PBE functional [29, 30]. The current is calculated using following equation:

$$I(v) = \frac{2e}{h} \int_{-\infty}^{\infty} T(E, V) \left[f_1(E, V) - f_2(E, V_2) \right] dE,$$
(2.1)

where T(E, V) is the transmission function for the AN-OPE SAM part.

2.3.3 Coarse-Grained NN Interacting Hamiltonian

The NN interacting Hamiltonian which describes the AN-OPE SAM is

$$H = \sum_{i=1}^{N} \left(E_i^{torsion} \left(\chi \right) - D_i F \right) + \sum_{NN} U_{ij}, \qquad (2.2)$$
	$[10\overline{1}0]$ pair	$[01\overline{1}0]$ pair	$[11\overline{2}0]$ pair
$\{i, j\} \subset \mathcal{P}$	-3.95	-5.00	-7.19
$\{i,j\}\subset\mathrm{T}$	-7.66	-3.12	-0.61
$\{i \in \mathbf{P}, j \in \mathbf{T}\}\$ or $\{i \in \mathbf{T}, j \in \mathbf{P}\}$	-5.70	-2.56	3.13

Table 2.1: AN-OPE Interaction Energies, U_{ij} , for Monte Carlo (MC) Calculations

*All energy values are in kcal/mol.

where $E_i^{torsion}(\chi)$ is the internal torsional energy of the *i*-th AN-OPE molecule due to twisting the AN-OPE by an angle χ , D_i is the [0001] component of the dipole moment of the *i*-th AN-OPE, F is the [0001] component of the external electric field, U_{ij} is the intermolecular interaction energy between *i*-th and *j*-th AN-OPE, and summation over NN denotes that the summation is over nearest neighbors. There are two interactions each for three directions: [1010], [0110], and [1120]. To avoid double counting, however, we used just one interaction per direction.

2.3.4 Extracting NN Model Parameters from QM/FF Energies

The U_{ij} terms when $\{i, j\} \subset P$ or $\{i, j\} \subset T$ were determined from the Jaguar calculations (vide infra). In order to extract U_{ij} when $\{i \in P, j \in T\}$ or $\{i \in T, j \in P\}$, we need to investigate inter-OPE interaction in the packed system from a larger simulation cell containing more than one OPE. Since this is too expensive for QM calculations (268 atoms), we used a simple DREIDING Force Field [31] (FF) in which the charges are based on QM. We considered six possible packings within a (2×2) unit cell:

- AP: all P's,
- AT: all T's,
- P3T1: 3 P's and 1 T,
- $P2T2_{10\overline{1}0}$: 2 P's and 2 T's aligned along [10 $\overline{1}0$],
- $P2T2_{01\overline{1}0}$: 2 P's and 2 T's aligned along $[01\overline{1}0]$,
- $P2T2_{11\overline{2}0}$: 2 P's and 2 T's aligned along [11 $\overline{2}0$],
- P1T3: 1 P and 3 T's.

The FF energies are shown at Figures 2.1a and 2.1b for when no external electric field and 1.2 V/Å external electric field is applied, respectively. Using FF energies under zero external field, the U_{ij} terms when $\{i \in \mathbf{P}, j \in \mathbf{T}\}$ or $\{i \in \mathbf{T}, j \in \mathbf{P}\}$ were fitted. Values are in Table 2.1.

The torsional energy, $E_i^{torsion}$ is estimated from the energy versus twisting angle χ curve (Figure 2.2), leading the 0.01 kcal/mol per AN-OPE when $i \in P$, and 0.23 kcal/mol when $i \in T$. The



Figure 2.1: (a) Energies of various conformations of AN-OPE relative to the AP conformation computed with a 1.2 V/Å external field from FF calculations (black histograms) and NN model calculations (orange histograms). (b) Energies of various conformations of AN-OPE relative to the AP conformation computed with no external field from FF calculations (black histograms), NN model calculations (orange histograms), and QM calculations (green histograms).



Figure 2.2: Torsional strain energy $E_i^{torsion}$ as a function of twisting angle χ from QM (PBE) on the isolated molecule. The energy at $\chi = 4^{\circ}$ (corresponding to P) is 0.01 kcal/mol higher than the ground state energy at $\chi = 0^{\circ}$. The energy at $\chi = 160^{\circ}$ (which corresponds to T) is 0.23 kcal/mol higher than the energy at $\chi = 0^{\circ}$, leading the 0.22 kcal/mol higher $E_i^{torsion}$ of T compared to $E_i^{torsion}$ of P.

 D_i values were optimized to fit the energies from Hamiltonian in Equation 2.2 to FF energies under 1.2 V/Å external field. The fitted values are $D_i = 5.48$ debye per AN-OPE for P and 7.30 Debye for T, which are quite comparable to the dipoles from Mulliken charge analysis, $D_i = 5.74$ Debye per AN-OPE for P and 7.03 debye for T.

All MD simulations with DREIDING FF were performed using LAMMPS (large-scale atomic/ molecular massively parallel simulator) MD code from Plimpton at Sandia [32, 33]. The equations of motion were integrated using the velocity-Verlet algorithm [34], with a time step of 1.0 fs.

2.3.5 Coarse-Grained MC Simulations

The 2-dimensional rhombic MC simulation cell containing (50×50) lattice points with periodic boundary conditions. The MC simulations used the Metropolis algorithm (our own code). Each Monte Carlo Step (MCS) is defined as 2500 MC trials with a fixed external field applied in the z-direction. Our MC simulations are similar to the study of an Ising model in a time-dependent magnetic field [35].

2.4 Results and Discussion

2.4.1 Two Conformations of AN-OPE

Figure 2.3a shows the minimized conformation of AN-OPE determined from the periodic DFT calculation. The three phenylene rings are coplanar, forming a well-conjugated structure, which we label as P (for planar). Here the lowest ring is connected to the Au electrode via a thiolate group. The middle ring (containing the functional groups) has a twist angle of $\chi = 4^{\circ}$ with respect to the



Figure 2.3: (a) Optimized geometry for the low field structure (P) of AN-OPE SAM. Here [0001] is the surface normal and the views are along z-axis (upper middle), y-axis (lower middle), and x-axis (lower right). The left picture is a perspective along the axis of one plane of molecules. The hydrogen bonding network is aligned along the [11 $\overline{2}0$] direction. (b) Optimized geometry for the high field structure (T) of AN-OPE SAM. Here [0001] is the surface normal and the views are along z-axis (upper middle), y-axis (lower middle), and x-axis (lower right). The left picture is a perspective along the axis of one plane of molecules. The hydrogen bonding network is aligned along the [10 $\overline{1}0$] direction.

bottom ring ($\chi = 0^{\circ}$ for the isolated OPE). This structure packs on the Au surface as (3 × 3), with the axis of the molecule along the [1100] direction, and a tilt angle $\theta = 66^{\circ}$ from the z-axis. The adjacent amino and nitro groups form hydrogen bonding (HB) networks along the [1120] direction.

To understand the local electronic structure and local interactions of the organic molecular part, we performed a single point non-periodic QM calculation of an isolated OPE. The polar amino and nitro groups lead to a large dipole moment of 9.24 (7.22) debye with the z-axis component ([0001]) of 5.74 (3.55) debye, the component along [1100] (tilt direction) of 4.44 (3.35) debye, and the component along [1120] (HB direction) of 5.72 (5.32) debye. These dipole moments were determined from the analysis of Mulliken charges, while the values in parenthesis are from quantum mechanical wavefunctions.

The inter AN-OPE interaction energies on the SAM, U_{ij} are determined from the difference between dimer energy and doubled monomer energy:

$$U_{ij} = E_{2 \times (AN - OPE \ w/ \ 3Au)} - 2 \times E_{AN - OPE \ w/ \ 3Au}, \tag{2.3}$$

where we included three Au atoms connected to the sulfur atom.

The value of U_{ij} between two P's are shown at Table 2.1, especially, U_{ij} along [11 $\overline{2}0$] direction shows the largest stabilization energy of -7.19 kcal/mol, due to the HB interaction.

Figure 2.3b shows the T (for twisted) conformation, which is 4.85 kcal/mol less stable than P. The middle and terminal phenyl rings are rotated from the bottom one by $\chi = 160^{\circ}$. Although we note that this twist angle is not stable for the isolated AN-OPE, it becomes meta-stable in the packed system (Figure 2.2). The rotation of the middle ring changes the direction of amino/nitro groups along [1010] from [1120], leading the hydrogen bond network to be aligned along [1010]. The axis of the molecule is at $\theta = 71^{\circ}$ from the z-axis, which makes the T lies more down than the P. The height of the terminal phenyl ring of T is 7.60 Å while that of P is 8.73 Å from the Au surface. The lower height of T is comparable to the Donhausers observations from the STM experiment that exhibits ~ 3 Å lower height of low conductance phase to higher conductance phase [14].

The dipole moment of T is 8.71 (6.88) debye with the component along [0001] of 7.04 (4.62) debye, a component along $[1\bar{1}00]$ (tilt direction) of -3.32 (-3.40) debye and a component along $[\bar{1}010]$ (HB direction) of 5.12 (5.10) debye.

The value of U_{ij} between two T's shown at Table 2.1. For T conformation, U_{ij} along the [1010] direction (HB network direction) is the most stable with the value of -7.66 kcal/mol.

2.4.2 Electrical Conductivities of P and T

The electrical conductivity, σ , was predicted using non-equilibrium Green's function (NEGF) theory for P and T structures with QM on the (1×1) unit cell. These calculations partition the tunnel-



Figure 2.4: Density of state (DOS) and transmission function T(E) of P structure (a) and T structure (b). The top electrode is located 12 Å above from the bottom electrode.

ing Hamiltonian using the Gaussian basis function representation. The semi-infinite electrode is calculated interactively using 3 explicit layers of Au [29].

The experiments use a top Hg electrode covered with a tetradecane-thiolate (RS), the atomic structure of which is not certain due to the amorphous character of the Hg electrode and the fluctuations in the alkyl thiol at room temperature. Instead, our calculations use a second 3-layer of Au (111) surface 12 Å above the bottom electrode. We also tested placing the top electrode in contact with the OPE, which 20 Å above the bottom electrode.

The density of states (DOS) with the transmission function T(E) were computed (Figures 2.4 and 2.6), and these are used to obtain the *I-V* curve and the σ -*V* curve (Figures 2.5 and 2.7). Over the range of 0 to 1.5 V, we see that the average ratio of σ_P to σ_T is 10 for the thickness of 12 Å, and 163 for the thickness of 20 Å. Since the experimental value is ~ 13 fold larger σ_P than σ_T , we adopted the case of 12 Å.

The calculated *I-V* curves lead correctly to a smaller σ for the high field stable phase. The difference in σ is explained by two factors:

1. the loss of π - π orbital overlap due to the rotation of the middle phenyl ring (which contributes to the conductivity through the molecules) and

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Figure 2.5: (a) Current through P conformation, I_P and current through T conformation, I_T versus the bias voltage V determined from the NEGF calculations using the DOS and T(E) of Figure 2.4. (b) Conductivity of P conformation, σ_P and conductivity of T conformation, σ_T versus the bias voltage V determined. The top electrode is located 12 Å above from the bottom electrode. σ_P is ~ 10 times larger than σ_T .



Figure 2.6: Density of state (DOS) and transmission function T(E) of P structure (a) and T structure (b). The top electrode is located 20 Å above from the bottom electrode.

2. the increase of vacuum distance due to the lower height of T phase.

Previous studies showed that the rotation of the ring by χ reduces the conductivity by factor of $\cos^4 \chi$ (Figure 2.8) [36]. Thus, using the QM minimized structures, which are twisted by 4° and 160°, yield an average ratio of σ_P to σ_T by ~ 1.3 times. However, considering the distribution of angles from the MD, we find an average ratio of σ_P to σ_T of ~ 3.5 times. (Details are discussed in Appendix B.)

The minimized structures for P and T lead semi-log plots of I-V curves (Figure 2.5) to show similar slopes for both phases, in disagreement with experiment showing a slope ratio of ~ 3.2. From previous study [36], we found that the slope of the semi-log plot of I-V curve strongly depends on the χ , and it decreases until almost zero when the molecule twisted with $\chi = 90^{\circ}$ (Figure 2.8a). This is a reasonable result since the slope of semi-log plot is related to the height of tunneling barrier, Φ_B which highly dependeds on the π - π orbital overlap. Therefore, consideration of the twisted structure from MD simulations, which has a significant population near 90°, well explains the distinct difference between the slopes of semi-log I-V plots for both structures observed in the experiment.



Figure 2.7: (a) Current through P conformation, I_P and current through T conformation, I_T versus the bias voltage V determined from the NEGF calculations using the DOS and T(E) of Figure 2.6. (b) Conductivity of P conformation, σ_P and conductivity of T conformation, σ_T versus the bias voltage V determined. The top electrode is located 20 Å above from the bottom electrode. σ_P is ~ 163 times larger than σ_T .



Figure 2.8: Conductivities depending on the twisting angle are extracted from the previous study [36], which are the results from NEGF calculations. (a) Semi-log plots of *I-V* curves shows that the slope decrease as the twist angle approaches to 90°, which means that the tunneling barrier from the bottom electrode to top electrode, Φ_B increases as the the π - π orbital overlap decreases. (b) Since the conductivity is dominated by the π - π orbital overlap, we assumed that the conductivity between two phenyl rings, $\sigma_i = 1/R_i$ is proportional to $\cos^4(\chi_i)$. From simple calculation leads the total conductivity tot to be proportional to the $\cos^4(\chi_1)\cos^4(\chi_2)/(\cos^4(\chi_1) + \cos^4(\chi_i))$, which shows good agreement with the NEGF results.

2.4.3 Response to Constant External Field

In order to describe the structural rearrangement process of the AN-OPE SAM, we use a (50×50) unit cell containing 2500 AN-OPE molecules. To describe the dynamics of such a large simulation cell, we developed a simplified nearest neighbor (NN) interaction Hamiltonian with the model parameters extracted from QM and Force Field (FF) energies (Figure 2.1). Important feature of the NN model is that the energetically favorable state changes from P to T as the external electric field increases, due to the higher dipole moment along [0001] of the T phase. In this model, the critical field for which the energies of both states are same is $F_c = 0.56 \text{ V/Å}$.

We simulated the response of the SAM of the P's to the 1.2 V/Å external field during 1.2×10^6 Monte Carlo steps (MCS) at T = 300 K. Figures 2.9a and 2.9b show the time evolution of the system starting with all P's and ending with all T's and the population change with the electrical conductivity change during this P-to-T transition, respectively. There were no T states until just before 55, 184 MCS, but within the next 15 steps, half of the neighbors along [11 $\overline{2}0$] have transformed, and after another 15 steps the entire [11 $\overline{2}0$] line is transformed to the T. Then, by 405, 907 MCS, totally 19 [11 $\overline{2}0$] lines have transformed, which are all neighbors to the original one. Then, at 486, 389 MCS, we see that a second [11 $\overline{2}0$] swath has nucleated. By 697, 272 MCS, these two have grown to 28 and 7 adjacent lines but still just two swathes, and from 697, 273 MCS, they are merged into one swath. Finally, by 1,008,706 MCS the full system is transformed to T. Along with the decrease of the P population, the total conductivity through the SAM also decreases.

The analysis of the snapshots demonstrates that the time to complete the transformation of each line in [11 $\overline{2}0$] after initiation is 26.32 MCS, leading to the rate constant of propagation, $k_{[11\overline{2}0]} = 5.48$ Å/MCS. The $k_{[11\overline{2}0]}$ shows almost no dependence on the temperature (Figure 2.10a, top), which infers that the energy barrier for the propagation is zero or quite negligible. Thus, once one AN-OPE is switched as a nucleation, the transformation propagates quickly along the [11 $\overline{2}0$] line, which is quite reasonable in terms of the energetic stability of P2T2_{11\overline{2}0} (Figure 2.1). Then, another nucleation occurs for subsequent transformation of another [11 $\overline{2}0$] line. Typically this subsequent transformation takes place right next to the precedent transformed line in the [1 $\overline{1}00$] direction.

Therefore, the nucleation is the key step governing the time scale of the transition. The middle panel of Figure 2.10a shows the probability, P(t) of exhibiting no nucleation until time t. To obtain the nucleation time (τ) when we have a transformed [11 $\overline{2}0$] line already, the nucleation events initiated next to [11 $\overline{2}0$] line are analyzed among the snapshots. The nucleation process is found to be a Poisson process, in which P(t) decays exponentially with time. The value of τ was obtained as 5,583 MCS by fitting of P(t).

To obtain the nucleation time (τ_0) in the absence of $[11\overline{2}0]$ line, we carried out additional 50 simulations to find when the first P transforms to the T, showing that this process proceeds as a Poisson process with $\tau_0 = 274,193$ MCS that is ~ 50 time larger than τ (Figure 2.10a, bottom



Figure 2.9: (a) Snapshots during P-to-T transition from MC simulation with 1.2 V/Å external field. The first nucleation is occurred at 55, 184 MCS, then, the [1120] line propagates until 55, 214 MCS. More nucleation and propagation along [1120] are taken place, and finally, the full system is transformed by 1,008, 706 MCS. We note that increased bias voltage yields a faster P-to-T transition. (b) Time dependence of P and T populations and electrical conductivity through the SAM during P-to-T transition. (c) Snapshots during T-to-P transition from MC simulation without an external field. The first nucleation is occurred at 486,389 MCS, then, the [1120] line propagates until 486,410 MCS. More nucleation and propagation along [1120] are taken place, and finally, the full system is transformed by 2,377,335 MCS. (d) Time dependence of P and T populations and electrical conductivity through the SAM during T-to-P transition.



Figure 2.10: (a) P-to-T transition; (b) T-to-P transition; Top panels show the temperature dependence of the propagation rate along [11 $\overline{2}0$], $k_{[11\overline{2}0]}$. Middle panels show the probability, P(t) of exhibiting no nucleation by time, t for the case when the nucleation is initiated next to another [11 $\overline{2}0$] line. The dotted lines is an exponential fit of P(t). This leads to a nucleation rate of $\tau = 5,583$ MCS for the P-to-T transition and $\tau = 72,926$ MCS for the T-to-P transition. Bottom panels show the probability, P(t) of exhibiting no nucleation by time, t for the case when the nucleation is initiated in the absence of next [11 $\overline{2}0$] line. The exponential fit leads to a nucleation rate of $\tau_0 = 274,193$ MCS for the P-to-T transition and $\tau_0 = 357,135$ MCS for the T-to-P transition.

panel).

Figures 2.9c and 2.9d show the time evolution of the system with no external field starting with all T's and ending with all P's and the population change with the electrical conductivity change during this T-to-P transition, respectively. The overall process is quite similar to that of P-to-T transition except for the detailed numbers. The first nucleation occurred at 486, 389 MCS, and then, the neighbors along $[11\overline{2}0]$ showed fast transition to P within 21 MCS. While this swath is growing along $[1\overline{1}00]$ direction, the second and the third nucleation without next transformed line occurred at 1, 174, 624 MCS and 1, 239, 313 MCS, respectively. Finally, the full system is transformed to P by 2, 377, 335 MCS. During the transition, the total conductivity through the SAM increases along with the decrease of the P population.

During T-to-P transition, the average time to complete each line of [11 $\overline{2}0$] growth is 25.38 MCS, leading to $k_{[11\overline{2}0]} = 5.68$ Å/MCS with no temperature dependency (Figure 2.10b, top panel).

The nucleation times are studied in the same manner with the P-to-T transition. The nucleation process follows Poisson process with the $\tau = 72,926$ MCS and $\tau_0 = 357,135$ MCS in the presence and the absence of the next transformed [1120] line, respectively (Figure 2.10b, middle and bottom panels).

The interaction between P-T is smaller than the interaction between P-P or T-T by ~ 8.6 kcal/mol in average (Table 1), due to the loss of HB or less-favorable van der Waals interaction caused by the packing of two different conformations. This infers that the boundary of $[11\bar{2}0]$ line is energetically less stable, leading a fast transformation at the boundary. This well explains the smaller τ than τ_0 .

We also found τ during P-to-T transition is smaller than τ during T-to-P transition (which is responsible to that NDR is not shown during the backward sweep). This is because the formation of T-T HB network is accompanied with the expansion of [1120] swath along [1100] during the P-to-T transition, while the loss of T-T HB network is accompanied during the T-to-P transition.

2.4.4 NDR for Time Dependent Electric Field

Applying a time dependent external field, we calculated the response of the system to voltage sweeps at various sweep rates. For each sweep, the magnitude of the external field was increased linearly until F = 1.4 V/Å (corresponding to 1.5 V bias voltage in forward sweep) and then it was decreased at the same rate until the field was 0 V/Å (corresponding to 0 V bias voltage in backward sweep). (Appendix D discusses the conversion factor between the external electic field and the bias voltage.) The sweep rates were $1 \times 10^{-8} \text{ V/MCS}$, 4^{-8} V/MCS , and $2 \times 10^{-7} \text{ V/MCS}$. The resultant *I*-*V* curves are shown in Figure 2.11a. Although the current drops dramatically at sufficiently high voltage, similar for all cases, we found that faster sweep let the systems stay in the P phase at higher voltage, which is in a good agreement with the experimental observation. Clearly, the simulations



Figure 2.11: (a) Current-voltage (I-V) curves calculated at 300 K from MC simulations combined with the *I-V* results of the Green's function calculations. Results for three sweeping rates are shown: S (blue line): 1×10^{-8} V/MCS, M (red line): 4×10^{-8} V/MCS, and F (black line): 2×10^{-7} V/MCS. Inset is the experimental *I-V* curves from the reference [9] with 3 different sweeping rates: S (blue line) : 21 mV/sec, M (red line) : 83 mV/sec, and F (black line) : 415 mV/sec. (b) The sweep rate dependence of the integral of the current from the peak to the valley during NDR, Q_F from current simulation (left panel) and experiment [9] (right panel).

show both the NDR phenomena and hysteretic behavior with sweep rate dependence as observed experimentally.

We found that the P-to-T transition voltage is located at 1.1 - 1.4 V, depending on sweep rate. This can be compared to the experimental results in which the transition is completed by 0.6 to 1.0 V. During the backward sweep, the simulations found that the T state transforms back to P at ~ 0.2 V bias voltage with slower sweep rates.

To determine the total charge associated with the NDR region, we integrated the current from the peak to the valley in Figure 2.11a. This amount of charge (Q_F) flowing through the junction during NDR, is an important physical quantity that characterizes the QC model [9]. The calculated Q_F values are

- $Q_F = 4.34 \times 10^4 \ \mu \text{A} \cdot \text{MCS/\AA}^2$ (~ $1.76 \times 10^6 \text{ e/AN-OPE}$), for sweep rates of $1 \times 10^{-8} \text{ V/MCS}$,
- $Q_F = 1.87 \times 10^4 \ \mu \text{A} \cdot \text{MCS/\AA}^2$ (~ 7.57 × 10⁵ e/AN-OPE), for sweep rates of 4 × 10⁻⁸ V/MCS, and
- $Q_F = 1.03 \times 10^4 \ \mu \text{A} \cdot \text{MCS/\AA}^2$ (~ 4.17 × 10⁵ e/AN-OPE), for sweep rates of 2 × 10⁻⁷ V/MCS.

Figure 2.11b shows the sweep rate versus Q_F plots from the simulation (left panel) and from the experiment (right panel). The simulations reproduce the experimental observation that Q_F decreases with increasing sweep rate. Additionally, we find that changing the sweep rate by 20 times only changes the Q_F by 4.2 times, which is comparable to the experimental observation that the Q_F varies 2.5 times while the sweep rate changes by ~ 20 times [9].

The NDR peak from the MC simulations leads to a voltage range of ~ 0.15 V while the experimental NDR range is ~ 0.25 V. One issue is the time scale. Our MC sweep frequency was ~ 10^{-7} V/MCS whereas experimental sweep frequency is ~ 10^{-1} V/s. To convert from MCS to second, we compared the initial nucleation rate expressed in MCS to that expected from the transition state theory using the predicted barrier in kcal/mol. The result is 1 MCS equals ~ 10^{-13} s (see Appendix A.), indicating the theoretical sweep frequency ~ 10^6 times the experimental sweep frequency. This faster sweep should decrease the NDR range. In addition, the small size of our periodic cell, 1620 nm², compared to the experiment of $O(\text{cm}^2)$ would also tend to decrease the NDR range.

A limitation in our MC simulations is that we idealized the degrees of freedom for the molecules into two states, which consider as the perfectly crystallized phases where an infinite AN-OPEs are connected through the HB network. In order to investigate the effect of molecular fluctuations, we performed a series of MD simulations with a (10×10) unit cell (100 independent AN-OPE molecules). The MD simulations account for two aspects missing from the MC simulations:

1. The AN-OPE is allowed to have a distribution of conformations, accounting for the much lower current for χ near 90° while losing the HB network at high fields. This distribution in χ leads

to decreased current at a given voltage, leading to a lower slope in the higher-field due to the larger $\Delta \Phi_B$.

2. The AN-OPE forms a partially disordered phase with some HB along [1010] in the low field (Appendix B). The loss of the HB network at high field decreases the hysteresis during the backward sweep since the loss of HB in the high field decreases the T-to-P transition barrier.

In addition, we found that once a disordered area is developed, it does not easily recover the P phase; hence, the development of a disordered part on the SAM yields less dramatic changes in conductivity. The experimental observation of slight current decrease with successive sweeps may result from the expansion of the disordered area during the sweep cycles.

In order to validate the suggested mechanism for NDR for AN-OPE, we investigated the possibility of NDR from the system N-OPE which contains no NH_2 group and the bare B-OPE containing no functional group. We found that the N-OPE system shows NDR behavior very similar to AN-OPE, in agreement with experiment [37]. However, we found no NDR behavior for B-OPE, also in agreement with experiment (Appendix C).

2.5 Conclusions

Summarizing, we find that a coarse-grained model based on parameters from first principles calculations leads to a mechanism for room temperature hysteretic NDR that is in qualitative agreement with experiments on AN-OPE, N-OPE, and B-OPE. This provide a plausible mechanism for understanding this phenomena which maybe useful in developing new NDR systems.

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Chapter 3

Free Energy Barrier for Molecular Motions in Bistable [2]Rotaxane Molecular Electronic Devices

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3.1 Abstract

Donor-acceptor binding of the π -electron-poor cyclophane cyclobis(paraquat-*p*-phenylene) (CBPQT ⁴⁺) with the π -electron-rich tetrathiafulvalene (TTF) and 1,5-dioxynaphthalene (DNP) stations provides the basis for electrochemically switchable, bistable [2]rotaxanes, which have been incorporated and operated within solid state devices to form ultradense memory circuits [1, 2] and nanoelectromechanical systems. The rate of CBPQT⁴⁺ shuttling at each oxidation state of the [2]rotaxane dictates critical write-and-retention time parameters within the devices, which can be tuned through chemical synthesis. To validate how well computational chemistry methods can estimate these rates for use in designing new devices, we used molecular dynamics simulations to calculate the free energy barrier for the shuttling of the CBPQT⁴⁺ ring between the TTF and the DNP. The approach used here was to calculate the potential of mean force along the switching pathway, from which we calculated free energy barriers. These calculations find a turn-on time after the rotaxane is doubly oxidized of ~ 10⁻⁷ s (suggesting that the much longer experimental turn-on time is determined by the time scale of oxidization). The return barrier from the DNP to the TTF leads to a predicted lifetime of 2.1 s, which is compatible with experiments.

3.2 Introduction

The electrochemically switchable, bistable $\frac{2}{rotaxanes}$ [1] (Figure 3.1) developed in recent years by Stoddart and co-workers exhibit two distinct co-conformations [3, 4, 5, 6, 7]: the ground-state co-conformation, in which the cyclobis (paraquat-p-phenylene) (CBPQT⁴⁺) encircles the tetrathiafulvalene (TTF) station, and the metastable state co-conformation, in which the $CBPQT^{4+}$ encircles the 1,5-dioxynaphthalene (DNP) station [2, 8, 9, 10, 11, 12, 13, 14, 15]. The population of the two co-conformations may be shifted away from equilibrium by temporarily oxidizing one or two electrons from the TTF units. This switching process forms the basis of using these compounds as storage elements in molecular electronic devices. Consequently, significant experimental efforts have been made to investigate the switching behavior of molecular switches [5, 6, 16, 17, 18, 19, 20, 21, 22, 23] and molecular machines [24, 25, 26, 27, 28, 29] in various environments, such as solution [5, 6, 30, 31, 32, 33, 34, 35, 36, 37], polymer electrolyte gels [38], metal surfaces [39, 40, 41] and devices [7, 16, 17]. Important experimental evidence [15] for molecular switching in these devices was the correlation of the kinetics of relaxation from the DNP to the TTF, across each of these environments. However, the rate of this process is also a function of the molecular structure, suggesting that longer storage times, or even nonvolatile memory, might be possible with the appropriate molecular design.

Computation chemistry calculations could provide an effective approach for optimizing the performance of such molecular switches, but such applications require that the accuracy of the theory be validated by comparing to well-documented experimental results. The purpose of this paper is to provide such validation. Previously, we investigated these compounds using a multiscale first principles approach combining quantum mechanics (QM) and atomistic force field (FF) methods [42, 43, 44, 45, 46, 47]. First we considered the molecules as individual species, and then we examined self-assembled monolayers bound to gold surfaces or compressed into Langmuir monolayers at the air-water interface. These studies successfully predicted a number of phenomena that were confirmed later experimentally, including the higher conductivity [47] of the DNP relative to the TTF, and the increased stability of the TTF relative to the DNP (by 2.0 kcal/mol from QM, 2.3 kcal/mol from the FF, and 1.4 - 1.6 kcal/mol from experiment) [15, 43]. In addition, on the basis of the predicted footprint of the 115 Å²/molecule for the self-assembled structure, we predicted that the surface tension of the TTF is 32 % lower than that of the DNP, an observation that was confirmed in subsequent experiments [43, 44].

In this study, we evaluated the free energy profile of the shuttling motion of the CBPQT⁴⁺ ring between the TTF and the DNP stations to determine how the nature of the rotaxane affects the switching and relaxation rates. These rates have been determined experimentally in various environments [15, 35, 40, 48], and we now want to understand the structural contributions to these



Figure 3.1: Structural formula of the two co-conformations of a bistable [2]rotaxane fragment used in this study.

rates. We seek to find a level for theoretical calculations of these rates that is both accurate and fast so that we can use theory to optimize the structural characteristics to achieve desired rates.

Rather than finding the energy barrier for a minimized reaction path connecting the two states, we used potential of mean force (PMF) to evaluate the change of free energy along the shuttling pathway of the CBPQT⁴⁺ ring between the TTF and the DNP so that we can determine the rates at the experimental temperature. We carried out these calculations for three oxidation states of the molecule relevant to the switching and thermally activated relaxation process.

3.3 Simulation Details

3.3.1 Potential of Mean Force from Constrained Molecular Dynamics Simulation

The experimental time scale for the ring to relax back from the DNP to the TTF is $10^{-1} - 10^3$ seconds [15, 34, 49], suggesting that simple molecular dynamics (MD) simulation of a few hundred nanoseconds might not be sufficiently ergodic to provide an accurate transition rate. Hence, we adopted the "Blue Moon sampling" technique [50, 51] of constrained MD simulations using holonomic constraints that fix the systems along the reaction coordinate. To determine the free energy barrier, we used the reaction-coordinate (*R*)-dependent potential of mean force (PMF), F_{TXR} (*R*) defined as the integration of the mean force (MF) along the reaction coordinate, $-dF_{\text{TXR}}$ (*R*) d*R* [52],

$$F_{\text{rxn}}(R) = F_{\text{rxn}}(\infty) + \int_{\infty}^{R} \frac{\mathrm{d}F_{\text{rxn}}(R')}{\mathrm{d}R'} \mathrm{d}R'.$$
(3.1)

Here, the MF is a measurable quantity from our simulations. To calculate the MF, we assumed that the CBPQT⁴⁺ ring moves between the TTF and the DNP along the backbone of the rotaxane (Figure 3.2a), which we assume to be in an extended conformation but with the minimized structure. This extended conformation should provide the fastest shuttling motion of the CBPQT⁴⁺ ring, being governed mainly by its interaction with the backbone. This MF does not account for the presence of folded chain conformations, so that the PMF may lack some contributions from conformational entropy.

First, we prepared the extended rotaxane backbone without the CBPQT⁴⁺ ring using quantum mechanical geometry optimization at the level of B3LYP/6-31G* (Figure 3.2a). Then, we added and optimized the CBPQT⁴⁺ ring at various fixed points on the fixed extended backbone (Figure 3.2b) using quantum mechanics. Thus, the atomic partial charges of all atoms are allowed to readjust, depending on the relative position of the charge acceptor (CBPQT⁴⁺) with respect to the charge donor (TTF and DNP).

To obtain the change of the PMF during the shuttling process, we first evaluated the MF as a



Figure 3.2: (a) Backbone of the rotaxane molecule simulated in this study. (b) $CBPQT^{4+}$ ring positions along the backbone (unit: Å).

function of the position of the CBPQT⁴⁺ ring. Because the length of the backbone is 54.7 Å and the distance between the TTF and the DNP is 36.9 Å, we chose to sample the dynamics for nine independent samples, each of which has the z-coordinate (along the backbone) of the center of mass (COM) of the CBPQT⁴⁺ ring at a different position along the extended backbone, as schematically presented in Figure 3.3. Using quantum mechanics, the geometry and atomic charges were obtained from each of these nine cases.

After preparing these nine initial structures, we prepared two more structures beyond each station of the TTF and the DNP with identical charges to the CBPQT⁴⁺@TTF case and the CBPQT⁴⁺@DNP case, respectively. In addition, we constructed another ten structures in which the position and charges of the CBPQT⁴⁺ ring were calculated by arithmetically averaging the coordinates and charges of two consecutive structures in the eleven structures. Thus, a total of 21 structures were prepared for simulations.

Then, to simulate both the turning on and turning off the rotaxane switch, we investigated the effect of oxidation of rotaxane molecule on the free energy profile, for three different oxidation states: the neutral state, the +1 oxidation state, and the +2 oxidation state.

The QM calculations of the charges for the nine different structures were repeated for each of the three oxidation states: 0, +1, and +2. The atomic partial charge distributions are tabulated in the Appendix E (Tables E.1, E.2, and E.3).

All quantum mechanical computations in this study were performed using Jaguar [53].



Figure 3.3: Charges for the initial nine structures obtained from QM with Mulliken analysis. In addition, we included two more structures beyond each station of the TTF and the DNP, using charges identical to those for the equilibrium $CBPQT^{4+}@TTF$ and $CBPQT^{4+}@DNP$ cases, respectively. Ten more structures were generated on the basis of these eleven structures. The position of the $CBPQT^{4+}$ ring for each additional structure was obtained using the arithmetic average of the two adjacent cases from the eleven structures. The charges were also averaged.

3.3.2 Constrained Molecular Dynamics Simulation

Next, we carried out a constrained NVT MD simulation at 300 K for 500 ps to equilibrate each system. This MD was then continued for an additional 3 ns at 300 K (constrained NVT MD) to compute the MF. The constraint was introduced using Gauss' principle of least constraints [54] to fix only the z-component of the center of mass (COM) of the CBPQT⁴⁺ ring parallel to the molecular axis direction (z-axis direction as in Figure 3.2b). To ensure that our constrained dynamics produces the correct equilibrium averages without bias due to ensemble sampling, we used Fixman's theorem [55] to evaluate the metric effect originating from the holonomic constraints. We determined that the metric effect only adds a constant scalar value to the absolute free energy values, which has no influence on the relative energetics. (Details are in the Appendix F.)

We also fixed the position of the last oxygen atom at each end of the backbone to retain the extended conformation. This restricts the conformational flexibility of the system, which suppresses conformational entropic contributions to the free energy. The mean force was sampled from such constrained MD simulations.

3.3.3 Force Field and MD Parameters

We used the generic DREIDING force field [56], which was found to lead to accurate results in our previous studies on rotaxane systems [43, 44, 45]. It was also successful in our studies on various other molecular systems, such as the hydrated polymer electrolyte membranes [57, 58, 59] and the surfactant-mediated air-water interface [60, 61].

The force field has the form

$$E_{\text{total}} = E_{\text{vdW}} + E_{\text{Q}} + E_{\text{bond}} + E_{\text{angle}} + E_{\text{torsion}} + E_{\text{inversion}}, \qquad (3.2)$$

where E_{total} , E_{vdW} , E_{Q} , E_{bond} , E_{angle} , E_{torsion} , and $E_{\text{inversion}}$ are the total energies, the van der Waals, electrostatic, bond stretching, angle bending, torsion, and inversion energy components, respectively, and the force field parameters are described in the original papers [56]. The atomic charges were obtained from a QM Mulliken population analysis as indicated above.

All MD simulations were performed using LAMMPS (large-scale atomic/molecular massively parallel simulator) MD code from Plimpton at Sandia [62, 63]. The equations of motion were integrated using the velocity-Verlet algorithm [64], with a time step of 0.01 fs. This unusually small time step was to ensure high quality sampling of phase space by avoiding abrupt changes in atomic positions.

The temperature was kept constant during the MD using the Berendsen thermostat with temperature damping time of 0.01 fs. To demonstrate that our MD leads to a proper canonical ensemble, the probability distribution function (PDF) of kinetic energy KE ($= mv^2/2$) is shown in Figure 3.4. The PDF is quite close to the Maxwell-Boltzmann distribution of energy at T = 300 K, indicating that the simulation describes a proper canonical ensemble. Furthermore, the PDF for each component of velocity is the same and the system obeys the equipartition theorem (Figure 3.5).

Figure 3.6 shows the typical behavior of the MF as a function of simulation time for two representative systems: one is the ground state, $CBPQT^{4+}@TTF$, green color, denoted as TTF and the other is the metastable state, the $CBPQT^{4+}$ ring on the DNP, red color, denoted as DNP. This shows that the mean force was well equilibrated for both cases.

The weakness of this blue moon sampling method is that the error in each MF measurement is integrated to obtain the PMF profile along the reaction coordinate. From block averages, we estimate the uncertainty of the MF values to be 0.04 kcal/mol/Å for CBPQT⁴⁺@TTF and 0.22 kcal/mol/Å for CBPQT⁴⁺@DNP. Assuming that these errors are random and that the average value is 0.13 kcal/mol/Å, we estimate that the error of the free energy difference between two stations is $38.8 \times 0.13/(20)^{1/2} = 1.13$ kcal/mol from integrating over the 38.8 Å distance. Similarly the error of the barrier from the DNP toward the TTF is $25.5 \times 0.13/(14)^{1/2} = 0.89$ kcal/mol from the integration over the 25.5 Å distance. Hence, the small errors in the MF values can lead to



Figure 3.4: Probability density function of kinetic energy KE $(=mv^2/2)$ is from the MD simulation of the CBPQT⁴⁺ ring@TTF (blue line) at 300 K. Here the time step was 0.01 fs and the total simulation time was 3 ns after 500 ps of equilibration. The black dashed line compares with the Maxwell-Boltzmann distribution of the energy, $2\left(\text{KE}/\pi (k_B T)^3\right)^{1/2} \exp(-\text{KE}/k_B T)$, for T = 300 K.



Figure 3.5: Probability density function of KE_x (= $mv_x^2/2$; blue line), KE_y (= $mv_y^2/2$; green line), and KE_z (= $mv_z^2/2$; red line) are cmputed from the MD simulation of the CBPQT⁴⁺ ring@TTF (blue line), which are identical to each other. These are compared with the Maxwell-Boltzmann distribution of KE_i , $\sqrt{1/(\pi \text{KE}_i k_B T)} \exp(-\text{KE}_i/k_B T)$ at 300 K. ($i \in \{x, y, z\}$; black dashed line)



Figure 3.6: Change of mean force as a function of simulation time. In each case this follows 500 ps of equilibration time. This plot shows two representative cases: the $CBPQT^{4+}$ ring@TTF (TTF) and the $CBPQT^{4+}$ ring@DNP (DNP).

substantial errors in the PMF value. However, previous studies that carefully compare various PMF calculation methods show that constraint-biased sampling to determine mean forces is one of the best methods to obtain reasonable PMF values, even though, statistically, they contain large error bars [52].

3.4 Results and Discussion

3.4.1 Charge Scheme: Adiabatic Approximation

We expected that no set of fixed charges scheme would be adequate enough to describe the electrostatic interactions as the highly charged ring is moved along the backbone. Thus, as described in Section 3.3.1, we obtained atomic charges from independent QM at each position as the ring is moved along the backbone.

This assumption of adiabatically adjusted charges assumes that charge re-distribution is much faster than the time for the ring to travel along the backbone. To test the effect of these charge

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Figure 3.7: Change of potential of mean force as a function of ring position along the backbone. The blue curve allows the charge to change adiabatically as the ring moves along the dumbbell, which is the reliable result. The other two curves show the error obtained when the charges are fixed: the green curve uses fixed charges from the ring@TTF; the red curve uses a fixed charge from the ring@DNP.

re-adjustments on the PMF, Figure 3.7 shows the PMF based on three different charge schemes for the neutral rotaxane system: the green curve was obtained using the fixed charges from the ring@TTF, the red curve was obtained using the fixed charges from the ring@DNP, and the blue curve was obtained using adiabatic charges.

Clearly, the green and red curves are biased to have a minimum PMF at the position for which the charge was calculated, leading to very bad estimates of the barrier. In contrast, the energy barrier between the TTF and the DNP sites, based on the adiabatic charges, is consistent with experimental observations. Thus, we used the adiabatic charges for all oxidation states from the neutral state to the +2 state.

3.4.2 Free Energy Profiles from PMF Calculations

Sampling the MFs from the constrained MD simulations (Figure 3.8a) and integrating them along the ring position, we calculated the profile of the PMF for the shuttling motion of the CBPQT⁴⁺ ring (Figure 3.8b). We found that each oxidation state (neutral state (0), oxidized states (+1 and +2)), leads to significantly different profiles.

3.4.2.1 ΔG_{T2D}

We calculated that the most stable complex for the neutral state (black) is CBPQT⁴⁺@TTF (ring at 8.9 Å) whereas the CBPQT⁴⁺@DNP state (ring at 47.7 Å) is less stable than the TTF by



Figure 3.8: (a) Change of the mean force as a function of ring position along the backbone. (b) Change of the potential of mean force as a function of ring position along the backbone. The green vertical lines denote the ring@TTF (8.90 Å) and ring@DNP (47.70 Å).

 $\Delta G_{\text{T2D}} = 1.0 \text{ kcal/mol.}$ This agrees with various experiments, which lead to $\Delta G_{\text{T2D}} = 1.4 - 1.6 \text{ kcal/mol} [15, 65, 66, 67, 68]$ on the basis of the difference in the binding free energies of the individual components of the rotaxane in the MeCN solvent. In addition, this calculation agrees with our previous computations from QM ($\Delta G_{\text{T2D}} = 2.0 \text{ kcal/mol}$) [43] and Hessian-based FF calculations ($\Delta G_{\text{T2D}} = 2.3 \text{ kcal/mol}$) [43]. We emphasize here that all previous experimental and theoretical studies studied ΔG_{T2D} by comparing the binding free energy of the TTF derivatives with the CBPQT⁴⁺ ring and the binding free energy of the DNP derivatives with the CBPQT⁴⁺ ring. Thus, our current calculation is the first direct measurement of the ΔG_{T2D} on a complete rotaxane.

3.4.2.2 $\Delta G_{\mathbf{T2D}}^{\ddagger}$ and $\Delta G_{\mathbf{D2T}}^{\ddagger}$ for Neutral Case

We calculate that the free energy barrier is $\Delta G_{\text{T2D}}^{\ddagger} = 19.03$ kcal/mol from the TTF toward the DNP, and $\Delta G_{\text{D2T}}^{\ddagger} = 18.03$ kcal/mol in the opposite direction. The relaxation barrier in the neutral state was measured for a similar bistable [2]rotaxane in which the triphenylene spacer was missing, leading to [15] (see Table 3.1)

- $\Delta G_{\rm D2T}^{\ddagger} = 16.2$ kcal/mol ($\tau \sim 0.095$ s) in MeCN solvent,
- $\Delta G_{\text{D2T}}^{\ddagger} = 18.1 \text{ kcal/mol} (\tau \sim 2.4 \text{ s})$ in a MeCN/polymethylmethacrylate/propylene carbonate/LiClO₄ polymer matrix containing weight ratios of 70:7:20:3, and
- $\Delta G_{\text{D2T}}^{\ddagger} = 22.21 \text{ kcal/mol} (\tau \sim 2.5 \times 10^3 \text{ s})$ in the molecular switch tunnel junction.

In addition, the devices fabricated with this derivative containing the triphenylene spacer exhibit a relaxation half-life of $\tau \sim 90 \text{ min } [2] (\Delta G_{\text{D2T}}^{\ddagger} = 22.66 \text{ kcal/mol}).$

In addition, our free energy barrier is quite comparable to the barriers to circumrotation of [2]catenanes. Leigh and co-workers used NMR to determine ΔG^{\ddagger} of interlocked catenane molecules as 11 - 20 kcal/mol for various solvents and calculated the free energy barrier as 10 - 20 kcal/mol using force-field based Hessians [69, 70, 71].

Although our simulations were performed in the gas phase, the $\Delta G_{\text{D2T}}^{\ddagger}$ of 18 kcal/mol agrees well with the experimental barriers (17 - 22 kcal/mol) [15, 34, 49] for a variety of environments. This suggests that the energy barrier does not depend strongly on environment.

We did not include the counterions in this study because preliminary calculations showed that the charges would sometimes change in erratic ways due to the floppy energy landscape for the countercharges. Indeed, the good agreement with experiment for the barriers suggests that the instantaneous changes in the potential due to counterions can be neglected.

3.4.2.3 $\Delta G_{\mathbf{T}2\mathbf{D}}^{\ddagger}$ and $\Delta G_{\mathbf{D}2\mathbf{T}}^{\ddagger}$ for Oxidized Cases

Although the neutral state prefers to have the CBPQT⁴⁺ ring at the TTF, we find that the +1 and +2 oxidized states lead to a completely different energy profile (Figure 3.8b). In both cases, the DNP becomes the global minimum with the TTF destabilized by $\Delta G = 25.75$ kcal/mol for the +1 oxidation state and $\Delta G = 47.78$ kcal/mol for the +2 oxidation state.

Starting with the ring at the TTF site and oxidizing, we find that the ring moves first by ~ 5 Å to a local minimum on the ethylene oxide linker (with an energy decrease by $\Delta G = 3.25$ kcal/mol for the +1 and $\Delta G = 5.49$ kcal/mol for the +2). Then, it has a free energy barrier of $\Delta G = 8.70$ kcal/mol (+1 state) or 8.02 kcal/mol (+2 state) to continue past the triphenylene spacer and toward the DNP for oxidation states.

Using the Eyring rate equation $[1/\tau = (k_B T/h) \exp(-\Delta G^{\ddagger}/RT)]$, the time required to overcome this barrier to move onto the DNP is 2.9×10^{-7} s for the +1 oxidation state and 9.0×10^{-8} s for the +2 oxidation state. It would be interesting to design an experiment to probe for this predicted barrier. It has been assumed that the huge Coulomb potential of the +4 ring with the +2 TTF would preclude a barrier. The origin of this barrier in the oxidized state is discussed below, which we find arises from the triphenylene spacer. We expect that there would be no barrier without this spacer.

Relative to the final state of the ring at the DNP site, the energy at the ethylene oxide linker (EO) near the TTF site is 22.52 kcal/mol higher (+1 oxidation), leading to a Boltzmann population of 10^{-17} . For the +2 oxidation state, the energy is 42.41 kcal/mol higher, leading to a population of 10^{-32} . Thus, for oxidation states +1 and +2, we expect the CBPQT⁴⁺ ring to stay on the DNP site until the system is reduced.

Indeed, there is an experimental estimate of this reverse barrier. Using a modified AFM with the ring attached, Brough *et al.* [72] measured the force exerted on the ring shuttling from the DNP to the TTF in the +2 oxidized system as 145 pN. Combining this experimental data with results from molecular mechanics simulations, they estimated the energy barrier to be 65 kcal/mol. This can be compared to our calculated barrier of 50.4 kcal/mol energy, validating the accuracy of the experiment. The maximum force measured in our simulation during the ring shuttling is 583 pN, which is similar to the experimental value of 145 pN.

3.4.2.4 Effect of Coulombic Energy and van der Waals Energy

To understand why the PMF profiles are so different between the neutral, +1, and +2 oxidation states, we calculated the change in the Coulombic interaction energy and the van der Waals (vdW) interaction energy as a function of ring position along the backbone, for these three oxidation states (Figures 3.9 and 3.10).

$\Delta G \; (\text{kcal/mol})$	${}^{a}k$ (s ⁻¹)	${}^{a}\tau_{1/2}$ (s)	condition
18.03 ± 1.5	0.33 ± 0.83	2.1 ± 5.4	gas phase
(simul.)			(neutral)
16.2 ± 0.3	7.3 ± 3.7	0.095 ± 0.048	(CH_3CN)
$(\exp[34])$			(neutral)
18.1 ± 0.2	0.3 ± 0.10	2.4 ± 0.082	^b polymer matrix
$(\exp[15, 34, 71])$			(neutral)
22.21 ± 0.04	$(2.7 \pm 0.19) \times 10^{-4}$	$(2.5 \pm 0.18) \times 10^3$	molecular-switch junction
$(\exp[15, 34, 71])$		· · · ·	(neutral)
31.22	6.3×10^{-11}	$1.1 imes 10^{10}$	gas phase
(simul.)			(oxidation +1)
50.43	4.5×10^{-25}	$1.5 imes 10^{24}$	gas phase
(simul.)			(oxidation $+2)$
65	_	_	c SAM on SiO ₂ wafers
$(\exp. + \operatorname{simul.}[72])$			(oxidation +2)

Table 3.1: Free Energy Barriers, Rate Constants, and Relaxation Half-Lives from DNP toward TTF (DNP \rightarrow TTF) at 298 K (All Simulation Results from this Work)

^aValues are calculated using the Eyring equation, $1/\tau = (k_B T/h) \exp(-\Delta G^{\ddagger}/RT)$. ^bWeight ratio 70:7:20:3 for CH₃CN/poly(methylmethacrylate)/propylene carbonate/LiClO₄. ^cThe modified AFM tip is attached to the CBPQT⁴⁺ ring.

For the neutral state, we find that the Coulombic energy increases by 60 kcal/mol as the ring moves from the TTF to the triphenylene spacer (barrier) and then drops by 45 kcal/mol as it moves to the DNP. On the other hand, the vdW energy changes, within a range of ± 4 kcal/mol, while the ring travels from the TTF to the DNP.

This indicates that the barrier is dominated by the differential Coulombic interactions with a peak of 443 kcal/mol at z = 28 Å (over the spacer). We were quite surprised because we expected the barrier to be dominated by vdW repulsions due to the bulky size of the triphenylene. To understand why Coulombic interactions are so important, we plot in Figure 3.11 the total charge on the ring along the pathway, in the neutral case. We see that at the TTF or the DNP positions there is strong delocalization from the ring onto the backbone, but as the ring passes over the triphenylene spacer (at z = 28 Å), this charge localizes back onto the ring. Thus, we conclude that localization of the ring charge increases the Coulombic repulsion and dominates the free energy barrier. This suggests that the barrier can be modified dramatically by changing the polarity of the spacer.

We also found that as the system is oxidized, the magnitude of Coulombic repulsion increases from 380 - 445 kcal/mol for the neutral state, to 520 - 545 kcal/mol for the +1 oxidation state, and finally, to 670 - 700 kcal/mol for the +2 oxidation state. In contrast, the vdW energy changes from 165 - 173 to 165 - 172 to 164 - 171 kcal/mol as the system is oxidized. This implies that the driving force inducing the mechanical movement of the ring is the increased Coulombic repulsion due to oxidization of the rotaxane. This confirms our view since the beginning of our experiments.

However, the PMF profile (Figure 3.7b) still differs substantially from the Coulombic energy



Figure 3.9: Change of Coulombic interaction energy as a function of the ring position: (a) neutral state; (b) oxidation state +1; (c) oxidation state +2.



Figure 3.10: Change of van der Waals interaction energy as a function of the ring position: (a) neutral state; (b) oxidation state +1; (c) oxidation state +2.

profile (Figure 3.9). For instance, in the neutral case, the Coulombic energy difference between two stations is 12.03 kcal/mol, which is ~ 12 times larger than $\Delta G_{\text{T2D}} = 1.0$ kcal/mol, and the Coulombic energy barrier for the shuttling from the DNP to the TTF is 46.75 kcal/mol, which is ~ 2.6 times larger than $\Delta G_{\text{D2T}}^{\ddagger} = 18.03$ kcal/mol. Thus, the key features of the PMF profile are not fully explained in terms of the Coulombic energy alone. Another possible contributor to the free energy is vibrational entropy, which can be investigated directly from the MD simulation trajectory [73, 74].

3.5 Conclusions

We used constrained MD simulations to calculate the free energy profile at 300 K for the shuttling of the $CBPQT^{4+}$ ring between the TTF and the DNP in the rotaxane molecule. This free energy profile was derived by calculating and integrating the MF acting on the ring as it is moved from one position to another position along the backbone. We found that it is particularly important to allow the charges to adjust adiabatically as the ring moves. Indeed, we find that the Coulomb interactions dominate the barriers for these systems.

We found that the free energy barrier from the DNP to the TTF is 18.03 kcal/mol for the neutral



Figure 3.11: Variations in the total charge on the ring as a function of the ring position for the neutral case.

system, which agrees well with experimental values of 17 - 22 kcal/mol for various environments. We calculate that the ΔG between the TTF and the DNP positions is 1.0 kcal/mol, which compares well with experimental results of 1.4 - 1.6 kcal/mol obtained from binding energies of separate DNP and TTF systems with the CBPQT⁴⁺ ring.

These results validate the accuracy of our computational procedure. Thus, we can now use this validated technique for estimating the switching kinetics for new designs of molecular architectures.

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Chapter 4

Sodium Diffusion through Aluminum-Doped Zeolite BEA System: Effect of Water Solvation

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4.1 Abstract

To investigate the effect of hydration on the diffusion of sodium ions through the aluminum-doped zeolite BEA system (Si/Al = 30), we used the grand canonical Monte Carlo (GCMC) method to predict the water absorption into aluminosilicate zeolite structure under various conditions of vapor pressure and temperature, followed by molecular dynamics (MD) simulations to investigate how the sodium diffusion depends on the concentration of water molecules. The predicted absorption isotherm shows first-order-like transition, which is commonly observed in hydrophobic porous systems. The MD trajectories indicate that the sodium ions diffuse through zeolite porous structures via hopping mechanism, as previously discussed for similar solid electrolyte systems. These results show that above 15 wt % hydration (good solvation regime) the formation of the solvation cage dramatically increases sodium diffusion by reducing the hopping energy barrier by 25 % from the value of 3.8 kcal/mol observed in the poor solvation regime.

4.2 Introduction

Zeolites constitute a unique class of the porous materials widely used in ion exchange, selective catalysis, and molecular sieve applications [1, 2]. An important property for many of these applications is migration of the absorbed water molecules. It has been observed that water migration in such porous materials proceeds differently than in the bulk water phase under the same temperature and chemical potential conditions [3, 4, 5, 6]; hence, we undertook a study of how nanoscale confinement in zeolites affects such of properties as structure, dynamics, and thermodynamics with absorbed molecules [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18].

In aluminosilicate zeolites the aluminum is generally incorporated in the three-dimensional framework in the form of AlO_4^- surrounded by neighboring SiO₄ while alkali metals such as Na⁺ or K⁺ are in the pores, interacting electrostatically with the zeolite framework. These positively charged and Movable cations in various zeolite systems have been studied intensively [7, 8, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29] since they impart many interesting properties to the zeolite systems. In particular, the ionic conductivity of zeolites can be controlled by the level of nonframework ions and their hydration (undoped zeolites are insulators with an electronic band gap of ~ 7 eV) [9]. The chemical nature, hydrophilicity, and selectivity for binding guest molecules in zeolites can be manipulated as appropriate for many practical applications [10, 11].

One recent interesting application of zeolites is as proton exchange membranes for fuel cells (PEMFC) [12, 13, 14, 15, 16, 17]. Here the molecular sieving capability and tunable acidity/hydro-philicity of zeolites can be incorporated to form a polyelectrolyte-based membrane that could improve the high temperature/low humidity performance of fuel cells [18].

We report here studies of the aluminosilicate zeolite BEA (Si/Al = 30). A distinct structural feature of interest for BEA is its three-dimensional channel structure which is characterized by ~ 1 nm diameter channels (Figure 4.1) in which water molecules may form a continuous phase, thereby facilitate ionic transport which makes membranes based on such materials useful as a replacement for polymer electrolyte membranes (PEM) for fuel cell applications. In PEM fuel cell membrane such at Nafion, the protons are transported through two mechanisms: vehicular diffusion of protonated waters and Grotthuss diffusion in which protons hop from water to water, with the relative contributions depending on the water content, counterions, porosity, temperature etc. Of course, diffusion of sodium or potassium cations occurs only through hopping. In this study, we determine how the nanometer scale confinement in the aluminosilicate zeolite BEA (Si/Al = 30) affects sodium diffusion.

First, we used grand canonical Monte Carlo (GCMC) simulations to predict the water absorption of aluminosilicate zeolite BEA system at various conditions, and then we applied the equilibrium molecular dynamics (MD) simulations on the diffusion starting with the hydrated systems obtained from the GCMC simulations. During such MD simulations, we sampled the time evolution of both the sodium diffusion and the water structure associated with the sodium ions.



Figure 4.1: Atomistic structure for the primitive periodic cell with composition of $Na_8Al_8Si_{248}O_{512}$. This shows green balls are aluminum and magenta balls are sodium. (a) Minimized aluminosilicate zeolite BEA structures without H_2O , (b) snapshot of zeolite BEA structures after the GCMC simulation for 298.15 K and 101.3250 kPa, and (c) snapshot of zeolite BEA structures after 4 ns NPT MD simulation at 298.15 K and 101.3250 kPa.

4.3 Simulation Details

4.3.1 Force Field

To calculate the energy and geometry of the zeolite framework, we employed Burchart force field (FF) [19] developed to describe aluminosilicate structures and the van der Waals interactions with the Na. This FF uses the Lennard-Jones 12 - 6 form for the van der Waals interactions between all atoms of the framework. To describe the interactions between water molecules, we used the F3C water FF [20]. For the off-diagonal van der Waals interactions between different types of atoms, we used the geometric-mean combination rule. The Lennard-Jones interactions were terminated beyond 18.0 Å, using a cubic spline function starting at 15.0 Å.

The atomic charges of the individual atoms of the zeolite frame were determined using the charge equilibration (QEq) method [21]. Since our simulation cell contains eight AlO_4^- sites, the total charge of the framework is set by -8. The eight sodium ions each were taken to have +1 charge, leading to charge neutrality of the simulation cell. The atomic charge of the water is from the F3C model [20]. The particle-particle particle-mesh (PPPM) method [22] was employed to compute the electrostatic using an accuracy criterion of 10^{-5} .

4.3.2 Grand Canonical Monte Carlo (GCMC) method and Molecular Dynamics (MD) Simulation

To predict the water absorption in aluminosilicate zeolite BEA framework as a function of partial pressure and temperature, we carried out grand canonical Monte Carlo (GCMC) simulations [23, 24] using the Sorption module of Cerius2 [25]. Since the chemical potential of the adsorbed phase equals the chemical potential of the bulk gas at equilibrium condition, the GCMC simulation makes multiple attempts to add one water molecule according to the probability

$$P_{add} = \min\left[1, \frac{V}{(N+1)\Lambda^3} \exp\left(-\frac{\Delta U}{k_B T}\right)\right],\tag{4.1}$$

or subtract one with the following probability

$$P_{sub} = \min\left[1, \frac{N\Lambda^3}{V} \exp\left(-\frac{\Delta U}{k_B T}\right)\right],\tag{4.2}$$

where V is the pore volume, N is the number of water molecules in the simulated system, Λ is the thermal de Broglie wavelength, and ΔU is the change in potential energy. For each GCMC simulation, we ran 2×10^8 Monte Carlo steps (MCS), during which the zeolite framework including sodium ions were fixed and water molecules were moved by the Metropolis sampling rule [26, 27]. Each Monte Carlo step is allowed four different types of operations-translation, rotation, creation, and destructions-of the water molecule with equal probabilities.

All molecular dynamics (MD) simulations were performed using the LAMMPS (large-scale atomic/molecular massively parallel simulator) MD code developed by Plimpton at Sandia [28, 29]. The velocity Verlet algorithm[30] was used to solve the equations of motion with a time step of 1.0 fs. The isobaric-isothermal ensembles (NPT) were generated using Nosé-Hoover thermostat with a temperature damping relaxation time of 0.1 ps and the Andersen-Hoover barostat with a dimension-less cell mass factor of 1.0. A series of MD simulations were conducted at constant temperature of 298.15 K with various pressure conditions from 0.1013 to 101.3250 kPa. To understand the effect of temperature, another set of simulations were performed at constant pressure of 101.3250 kPa with various temperature conditions from 298.15 K.

4.3.3 Construction of Models and Calculation of Properties

We used the $2 \times 2 \times 1$ superstructure of zeolite BEA (based on the X-ray crystallography database [31]) as the periodic simulation cell for the MD. Then, eight silicon atoms in the channels were randomly chosen and replaced with aluminum atoms to have the lowest energy using substitutional disorder option of Cerius2 [25]. This leads to a Si/Al ratio of 30, with a simulation cell consisting of 8 AlO₄⁻ and 248 SiO₄ tetrahedral sites with an overall composition of Na₈Al₈Si₂₄₈O₅₁₂.

The eight sodium ions were initially placed near the aluminum-doped sites, and the full structure of zeolite frame including the sodium ions were energy minimized. Then the water contents were determined from GCMC simulations at various pressure and temperature conditions.

Then we carried out 8 - 12 ns NPT MD simulations and evaluated such properties as density, pair correlation function, and diffusion coefficients using the full trajectory files.

4.4 **Results and Discussion**

4.4.1 Water Absorption

Using GCMC, the chemical potential of water in zeolite frame was equilibrated with that of the external reservoir at various vapor pressure conditions ranging from 0.1013 to 101.3250 kPa. The water absorption isotherm at 298.15 K and the temperature dependence of water adsorption at 101.3250 kPa are shown at Figures 4.2 and 4.3, respectively.

We were unable to locate published water adsorption isotherms for zeolite BEA with Si/Al of 30. Thus the data shown in Figures 4.2 and 4.3 are from simulation only. We observe a stepwise condensation at 3.5 kPa. The amount of water uptake increases abruptly and then shows fast saturation up to ~ 50 molecules per crystallographic unit cell, which can be regarded as a maximum loading number at 298.15 K. Previous studies discovered that a spontaneous condensation of water



Figure 4.2: Dashed line is the least-squares fitted to $f(x) = a \tanh(bx)$, where a = 46.19 molecules/ unit cell and b = 0.753 (1/kPa). We obtain a vapor pressure of 3.578 kPa for the point at which the water uptake reaches to 99 % of the maximum loading uptake.

occurs in hydrophobic porous materials such as sodium faujasites of NaY and NaX [32], silicate-1 zeolites [33, 34] and carbon nanotubes [35]. Here, the term "hydrophobic" is used because of the spontaneous condensation behavior: if the surface of the nanopore were hydrophilic, then water absorption would proceed gradually over wide range of pressure through wetting the surface of the nanopore instead of increasing abruptly at a certain narrow pressure range. We expect that the capillary condensation would follow a first-order-like transition since the nonwetting character of the pore prohibits the intrusion of liquid water until a certain hydraulic pressure. This suggests that the aluminosilicate BEA zeolite system may sustain some extent of hydrophobicity even after some of the hydrophobic SiO₄ sites are replaced by hydrophilic AlO₄⁻ sites.

The temperature dependence of water absorption is plotted at Figure 4.3 at 101.3250 kPa. As the temperature increases, the amount of water uptake in zeolite frame decreases. This type of temperature dependency of water uptake has been observed in the experiments on the zeolite-4A structure [36] and in other simulation studies [32]. Of particular interest is that at 423 K, this BEA aluminosilicate zeolite frame still holds 20 % of water absorbed at 300 K. We expect that this capability to retain significant amount of water at high temperature could make these materials useful as a replacement for performance of the PEM for fuel cell operation under high temperature/low humidity condition.



Figure 4.3: Predicted temperature-dependence of water uptake at 101.3250 kPa when the zeolite BEA has no aluminum doping (red curve) and Si/Al = 30 (blue curve). The presence of aluminum-doped sites as well as sodium ions enhance the water uptake amount especially in the high temperature.

4.4.2 Structure of Water in Zeolite

To characterize the water structure we calculated the density-normalized O(water)-O(water) pair correlation function, $4\pi r^2 \rho g_{O(water)-O(water)}$ where r is the distance and ρ is the number density of water. Figure 4.4a shows $4\pi r^2 \rho g_{O(water)-O(water)}$ plots for water absorbed in various vapor pressure conditions and compares to the values for bulk water. Integrating the first peak in Figure 4.4a leads to the coordination number CN. For bulk water we obtain CN = 4.59, in good agreement with CN = 4.5, from neutron diffraction experiment [37]. Figure 4.4b summarizes the change of the coordination numbers as a function of pressure, showing a behavior identical with the absorption isotherm in Figure 4.2. This provides clear evidence for the spontaneous condensation in which all the water molecules absorbed into the system participate in water clusters. Figure 4.4 shows that the structure of the water absorbed in the zeolite framework approaches to that of bulk phase water as the water uptake/pressure is increased to 101.3250 kPa. However, the saturated value of CN of the absorbed phase (~ 3.8) is smaller than the CN of the bulk phase (4.5). This is reasonable because of the huge surface area of 1362.99 m²/g of the nanopores of the zeolite (cf. activated carbon has 500 - 1500 m²/g). We observed similar behavior for water in Nafion and Dendrion polymer membranes [38, 39, 40].

In order to investigate the effect of the sodium ion on the water structure, we analyzed the density-normalized Na-O(water) pair correlation function, $4\pi r^2 \rho g_{Na-O(water)}$ and the water coordination number of sodium ion as shown in Figure 4.5, parts a and b, respectively. Similar to $4\pi r^2 \rho g_{O(water)-O(water)}$ in Figure 4.4 we see that $4\pi r^2 \rho g_{Na-O(water)}$ increases with increasing pressure with a first peak position that does not change with pressure. However, the increase of the



Figure 4.4: (a) Probability of finding additional water molecules at a specific distance from each water molecule. This is obtained as the product of pair correlation functions of water oxygens, $g_{O(water)-O(water)}$ with water density ρ and $4\pi r^2$. (b) Water coordination number (CN) of water molecule as a function of pressure. The CN of water molecule is obtained from the integration of curve a up to first minimum, which is at 3.7 Å. The saturated value of CN of the absorbed phase (~ 3.8) is smaller than the CN of the bulk phase (4.5).

first peak intensity of $4\pi r^2 \rho g_{Na-O(water)}$ up to ~ 3.5 Å was not significant compared to that of $4\pi r^2 \rho g_{O(water)-O(water)}$. This indicates that the first water solvation shell for the sodium ion saturates rapidly toward CN = ~ 5.0 (see Figure 5b inset), which is consistent with the previous indication that water molecules cluster with sodium rather than interact with the surface of the nanopore, (indicating a hydrophobic nature of the nanopore surface). We believe that this is because the strong interaction of the net charge in the sodium ion enhances the development of its solvation structure. This value shows excellent agreement with the experiment which finds 4.82 [41].

4.4.3 Effect of Water Contents on Sodium Diffusion

The diffusion coefficient of the sodium ion was calculated at pressures ranging from 0.1013 to 101.3250 kPa, as summarized at Table 4.1. To characterize the nature of the diffusion, Figure 4.6 shows the log-log plot of the mean square displacements (MSD) versus time. For times up to ~ 20 ps, the MSD increases as a function of $t^{1/2}$ indicating single file diffusion (SFD) behavior. For simulation times longer than 20 ps, the MSD shows a normal Fickian behavior (MSD $\propto t$). This transition of MSD from SFD to normal Fickian diffusion occurs when the pore confines the particles but still allows the particles to pass by each other [42]. In the long time Fickian regime, we obtained the diffusion coefficient D from the mean square displacements of the sodium ions using Equation 4.3,

$$D = \left\langle (r(t) - r(0))^2 \right\rangle / 6t.$$
(4.3)

In order to examine how the dynamics of sodium ion is influenced by its water solvation shell, we analyzed the diffusion coefficient of sodium ion versus water coordination number at 298.15 K. From Figure 4.7, we observed a dramatic jump at about CN = 4.5 that corresponds to the point of the water uptake saturation in the absorption isotherm (Figure 4.2). Indeed, Faux and his coworkers [43, 44, 45] reported theoretical studies that the diffusion coefficient of sodium in zeolite-4A system increases from 1×10^{-7} cm²/s to 10×10^{-7} cm²/s as the number of water molecules per unit cell increases from 0 to 224 in agreement with the trend and order of magnitude of the diffusion coefficient in our simulations. Furthermore, Faux et al. also observed a sudden jump of the sodium diffusion coefficient between 112 and 168 water molecules per unit cell, but did not explain the origin. We believe that this results directly from the degree of solvation. This spontaneous condensation of water (discussed in Section 4.4.1), leads to two regimes for the ionic diffusion in the presence of water. Detailed analysis of sodium ion trajectories allows us to enunciate why a threshold amount of water uptake is critical to enhance the diffusion of the ion from the microscopic point of view. The doped AlO_4^- sites are Brönsted acid sites [46] that bound the nonframework cations via strong Coulomb interaction. Parts a and b of Figure 4.8 show the time profile of the Al-Na distances for the good solvation regime (vapor pressure = 101.3250 kPa) and the poor solvation regime (vapor



Figure 4.5: (a) Probability of finding sodium ions at a specific distance from each water molecule. This is obtained as the product of pair correlation functions of sodium atoms and water oxygen, $g_{Na-O(water)}$ with water density ρ and $4\pi r^2$. (b) Water coordination number (CN) of sodium ions as a function of pressure. The CN of water molecule is obtained from the integration of curve a up to first minimum, which is at 3.5 Å. The saturated value of CN of the absorbed phase (~ 5.0) is same to the CN of the bulk phase.



Figure 4.6: Log-log plot of mean square displacements (MSD) vs time at 298.15 K and 101.3250 kPa based on a trajectory of 12 ns. Initially the MSD shows MSD $\propto t^{1/2}$ up to $t = \sim 20$ ps, but the times $> \sim 2$ ns, we see normal 3D Fickian behavior (MSD $\propto t$). The Fickian regime leads to a diffusion coefficient of $D = 1.233 \times 10^{-7}$ cm²/s.

Table 4.1: Vapor Pressures, Water Uptake/Cell, Water Coordination Numbers of the Water Molecule (up to 3.7 Å Cutoff), Water Coordination Numbers of the Sodium Ion (up to 3.5 Å Cutoff), and Diffusion Coefficients from NPT MD at Temperature of 298.15 K

vapor pressure	water uptake/cell	CN	CN	diffusion coefficient
(kPa)		(water)	(sodium)	$(\mathrm{cm}^2/\mathrm{s})$
0.1013	10.15	1.55	3.51	$(0.338 \pm 0.033) \times 10^{-7}$
0.5066	16.57	2.22	3.94	$(0.382 \pm 0.048) \times 10^{-7}$
1.0133	30.08	3.01	4.39	$(0.642 \pm 0.219) \times 10^{-7}$
1.9006	40.10	3.16	4.29	$(1.431 \pm 0.041) \times 10^{-7}$
3.1677	41.86	3.29	4.67	$(1.170 \pm 0.035) \times 10^{-7}$
10.1325	46.18	3.54	4.68	$(1.478 \pm 0.368) \times 10^{-7}$
101.3250	50.00	3.77	5.04	$(1.466 \pm 0.601) \times 10^{-7}$

pressure = 0.1013 kPa), respectively. This shows clearly that each sodium ion localizes within ~ 5 Å of one of the aluminum-doped sites and diffuses by hopping from one site to a nearest neighbor aluminum site. Thus, the diffusion of sodium ion occurs through the hopping mechanism between AlO_4^- sites (the Brönsted acid sites) with the energy barrier of 3.5 - 4.0 kcal/mol caused by the electrostatic interaction. Figure 4.8a indicates that the hopping events occur every 2 ns on average in the good solvation regime, whereas Figure 4.8b shows just 1 hop within 12 ns in the poor solvation regime. This explains why the diffusion coefficient of sodium ion is ~ 10 times larger in the good solvation regime than in the poor solvation regime as in Table 4.1. Sufficient numbers of water molecules are the most critical in creating solvation cage and helping the ionic hopping.

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Figure 4.7: Dependence of diffusion coefficient of sodium ion on water coordination number (CN) of sodium ion. The diffusion coefficients were calculated from three partitioned trajectories of 12 ns NPT simulations (each partition has 4 ns length), and the error bars were evaluated from the diffusion coefficients obtained from the three partitioned trajectories. This represents pressures from 0.1013 to 101.3250 kPa at 298.15 K. At a pressure of ~ 2.0 kPa, we find an abrupt change in the water CN. When the sodium ion is solvated by > 4.5 water molecules, its diffusion coefficient increases abruptly by a factor of 3.5. The dashed line is to guide the eye.

4.4.4 Effect of Temperature on Sodium Diffusion

We calculated the diffusion coefficients of the sodium ions confined in the aluminosilicate zeolite BEA membrane are obtained for various temperatures ranging 298.15 K to 453.15 K. For each temperature, the amount of water uptake was determined using GCMC simulation (Figure 4.3). The temperature effect on the sodium diffusion was taken from MD simulations based on the hydrated zeolite. These diffusion coefficients are presented in Table 4.2 and Figure 4.9. Up to 373.15 K, the diffusion coefficient of sodium ion increases with increasing temperature, as expected for a normal activated process. However, we observe from Figure 4.9 that the diffusion coefficient decreases with increasing temperature from 373.15 K to 453.15 K. This anomaly is a consequence of the less hydration of the zeolite at high temperature as previously discussed in Section 4.4.2. Here, the insufficient water absorption results in a less developed solvation shell, which cannot facilitate the sodium ion hopping events. Thus, the diffusion coefficient decreases at high temperature range with less number of water molecules. Therefore, just as in the discussion about good solvation and poor solvation regimes that depend on the vapor pressure, we consider that the good solvation regime applies up to 373.15 K, while the poor solvation regime applies beyond 400 K (the 393.15 K point lies within the transition regime.)

Normally, the temperature dependence for diffusion coefficient is written in terms of a standard Arrhenius equation, Equation 4.4.



Figure 4.8: Time dependence of the distances of one sodium ion to all 8 aluminum atoms of the zeolite membrane. The distance to each aluminum atom is shown with a different color. (a) Vapor pressure is 101.3250 kPa (good solvation regime) at 298.15 K. This shows that it took 2 ns for the Na to hop from a position 4.8 Å from the purple Al to a position 7.5 Å from the black Al. Here a distance of 4.8 Å indicates one water shell between the Na and the Al, while 7.5 Å indicates separate water shells around each; (b) vapor pressure is 0.1013 kPa (poor solvation regime) at 298.15 K. In this case the Na remains at 4 Å from the Al which indicates that the Na remains coordinated to the O of the Al.

$$D = A_{diff} \exp\left(-\frac{\Delta E}{k_B T}\right),\tag{4.4}$$

where the ΔE implies the energy barrier for the hopping from one site to another site. $A_{diff} = L^2 k_B T/h \exp(ns/R)$ is the prefactor, a product of frequency factor (activation entropy term) with a hopping-related length (L). k_B is the Boltzmann constant and T is the absolute temperature. In order to include the solvation effect, we define the stabilization energy ΔE_{solv} due to the solvation. This leads to a modified Equation 4.4 where $A_{diff-solve}$ now includes a correction for solvation.

$$D = A_{diff-solve} \exp\left(-\frac{\Delta E - \Delta E_{solv}}{k_B T}\right).$$
(4.5)

We assume that the ΔE_{solv} is a step function which is zero for the poor solvation regime and nonzero for the good solvation regime, which implies that the incomplete solvation shell of sodium ion has no effect to stabilization. The Arrhenius plot for each regime is shown in Figure 4.10 and the curve for each regime is fitted with a linear equation using least-squares fitting method. From the slope of the fitted line, we estimate the $\Delta E = 3.810$ kcal/mol for the poor solvation regime and the $\Delta E - \Delta E_{solv} = 3.540$ kcal/mol for the good solvation regime. Thus, the stabilization energy by solvation (ΔE_{solv}) becomes 0.270 kcal/mol. The *y*-intercepts lead to $A_{diff} = -10.70 \text{ cm}^2/\text{s}$ and $A_{diff-solve} = -9.76 \text{ cm}^2/\text{s}$. The nearly unit value for A suggests that the diffusion mechanism for both regimes is basically identical, supporting the Equation 4.5. Although no experimental data has been reported for the energy barrier of the diffusion of sodium ion, the energy barrier for the diffusion of sodium ion in the β alumina (known as a good ionic conductor) has been measured experimentally [47, 48]. Since the sodium ion in the β alumina is also believed to jump around aluminum oxide sites, these values should be comparable with ours. Kim et al. [47] reported that the barrier as 3.275 kcal/mol from the measurement of ionic conductivity and 3.897 kcal/mol from the measurement of sodium tracer diffusion. Also the values from Whittingham and Huggins [48] obtained values of 3.81 kcal/mol from the tracer diffusion measurement and 3.95 kcal/mol from the dielectric loss measurement. All these values are very comparable to our ΔE value of 3.540 kcal/mol, supporting the accuracy of our simulations. On the basis of these comparable values of the energy barrier, we expect that the stabilization energy for the hydrated system would also be reasonable although the effect of hydration in such aluminosilicate system has yet been reported.

4.5 Conclusions

Combining GCMC and MD simulations, we studied the effect of hydration on the sodium dynamics. From the absorption isotherm, we observed that the water absorption in BEA zeolites proceeds with a spontaneous condensation at a pressure of 3.5 kPa and a temperature of 298.15 K even though

temperature	water uptake/cell	CN	CN	diffusion coefficient		
(K)		(water)	(sodium)	$(\mathrm{cm}^2/\mathrm{s})$		
298.15	50.00	3.77	5.04	$(1.466 \pm 0.601) \times 10^{-7}$		
325.15	46.25	3.73	4.71	$(2.372 \pm 0.024) \times 10^{-7}$		
353.15	42.12	3.72	4.24	$(3.762 \pm 0.822) \times 10^{-7}$		
373.15	36.50	3.46	4.39	$(4.806 \pm 0.226) \times 10^{-7}$		
393.15	26.17	3.27	4.08	$(3.725 \pm 0.188) \times 10^{-7}$		
423.15	13.73	2.45	3.63	$(2.630 \pm 0.459) \times 10^{-7}$		
453.15	9.75	1.74	3.42	$(3.042 \pm 0.301) \times 10^{-7}$		

Table 4.2: Temperature, Water Uptake/Cell, and Diffusion Coefficients at Constant Pressure Condition of 101.3250 kPa



Figure 4.9: Dependence of the sodium diffusion coefficient on the temperature for a vapor pressure of 101.3250 kPa. The diffusion coefficients were calculated from three partitioned trajectories of 12 ns NPT simulations (each partition has 4 ns length), and the error bars were evaluated from the diffusion coefficients obtained from the three partitioned trajectories. Up to 373.15 K, the diffusion coefficient increases with increasing temperature, whereas it decreases beyond 373.15 K due to the depletion of the water solvation.



Figure 4.10: Arrhenius plots of diffusion coefficient from each solvation regime: the red squares are for the poor solvation regime and the blue diamond is for the good solvation regime. The solid black line is a linear fitting of each regime. This leads to $D_{300K} = 3.762 \times 10^{-8} \text{ cm}^2/\text{s}$ and $E_{act} = 3.810 \text{ kcal/mol}$ for the poor solvation regime and $D_{300K} = 1.512 \times 10^{-7} \text{ cm}^2/\text{s}$ and $E_{act} = 3.540 \text{ kcal/mol}$ for the good solvation regime, and the equation of each fitted line and R2 value are inset in the figure.

the internal space of zeolite remains hydrophobic. Below the pressure of 101.3250 kPa, the water uptake of the zeolite decreases monotonically with increasing temperature. From the pair correlation functions, we found that the tetrahedral water solvation structure for water molecule is suppressed by the hydrophobic pore surfaces. In contrast, the water solvation structure surrounding the sodium ion remains ~ 5.0 . This difference is a direct consequence of the strong electrostatic interaction of the positively charged sodium ion with water molecules.

The MD trajectories indicate that the sodium ions are electrostatically bound to the aluminumdoped sites and the diffusion of the sodium ions proceeds via hopping mechanism among these aluminum-doped sites (Figure 4.8).

On the basis of the spontaneous water condensation process, we found the two regimes: a good solvation regime below 373.15 K and a poor solvation regime above 400 K. The Arrhenius plot of each regime leads to an energy barrier of 3.540 kcal/mol for the diffusion of sodium ion for the good solvation regime and of 3.810 kcal/mol for the poor solvation regime. This leads to an estimate of 0.270 kcal/mol for the stabilization energy due to the solvation of sodium ion.

This study of the sodium diffusion through BEA zeolite shows that the ionic diffusion in the confined geometry depends on the degree of solvation by water which distinguishes it from bulk diffusion. As a next step, we are planning to directly investigate the proton diffusion through the aluminum-doped zeolite BEA system based on results of the current study.

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Chapter 5

Experimental and Theoretical Investigation into the Correlation between Mass and Ion Mobility for Choline and Other Ammonium Cations in N_2

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5.1 Abstract

A number of tertiary amine and quaternary ammonium cations spanning a mass range of 60–146 amu (trimethylamine, tetramethylammonium, trimethylethylammonium, N, N-dimethylaminoethanol, choline, N, N-dimethylglycine, betaine, acetylcholine, (3-carboxypropyl)trimethylammonium) were investigated using electrospray ionization ion mobility spectrometry. Measured ion mobilities demonstrate a high correlation between mass and mobility in N₂. In addition, identical mobilities within experimental uncertainties are observed for structurally dissimilar ions with similar ion masses. For example, dimethylethylammonium (88 amu) cations and protonated N, N-dimethylaminoethanol cations (90 amu) show identical mobilities (1.93 cm² V⁻¹ s⁻¹) though N, N-dimethylaminoethanol contains a hydroxyl functional group while dimethylethylammonium only contains alkyl groups. Computational analysis was performed using the modified trajectory (TJ) method with nonspherical N₂ molecules as the drift gas. The sensitivity of the ammonium cation collision cross-sections to the details of the ion-neutral interactions was investigated and compared to other classes of organic molecules (carboxylic acids and abiotic amino acids). The specific charge distribution of the molecular ions in the investigated mass range has an insignificant affect on the collision cross-section.

5.2 Introduction

The development of soft ionization methods such as electrospray ionization (ESI) [1] have expanded the application of ion mobility spectrometry (IMS) [2, 3] to structural investigations of nonvolatile biomolecules in the gas phase [4]. ESI allows soft sampling by transferring intact ions directly from the solution phase to the gas phase. Using this distinctive advantage of ESI, the shapes and sizes of various biomolecular ions from monomeric molecules to macrosize protein complexes have been investigated. The combination of ESI and IMS has facilitated conformational studies of macroions including clusters (oligomers) [5, 6, 7], peptides [8, 9], and proteins [10, 11, 12]. In addition, ion mobilities of organic molecules such as amino acids [13, 14], carboxylic acids [15], and dinucleotides [16], as well as other organic molecules [17, 18], have been reported.

To provide a firm foundation for studies of the shapes of complex organic molecular ions using IMS, many research groups have endeavored to develop theoretical models to predict ion mobilities and related cross-sections of gas-phase molecular ions. Griffin *et al.* [19] have shown that mass and mobility are only correlated on the order of 20 % within a collection of structurally unrelated compounds spanning a mass range of ~ 70 – 500 amu. The correlations are improved up to 2 % when only structurally related compounds are considered. Karpas and co-workers have established models to predict the mobility for a number of compound classifications including acetyls, aromatic amines, and aliphatic amines drifting in He, N₂, air, Ar, CO₂, and SF₆ [20, 21]. Our laboratory has applied a 12 – 4 potential model in studies of amino acids and carboxylic acids drifting in N₂ and CO₂ [14, 15]. Recently, Steiner *et al.* have reported predictions of mobilities for a series of different classes of amines (primary, secondary, tertiary) in various drift gases, such as He, Ne, Ar, N₂, and CO₂, using several theoretical models (rigid-sphere, polarization-limit, 12-6-4, and 12-4 potential model [22].

Computational modeling related to interpretation of IMS data has been developed by several groups. Efforts toward theoretical ion mobility predictions using computational methods face difficulties associated with complicated collision integrals and the design of functions to accurately describe the ion-neutral interaction potential. Bowers and co-workers have proposed a project approximation method, which is based on a hard-sphere description of the interaction potential [23]. The trajectory (TJ) method, which has been proposed by Jarrold and co-workers, adopts more realistic soft-core interactions [24].

Ion mobility constants (K) can be derived from the collision cross-section using the equation [25]

$$K = \frac{(18\pi)^{1/2}}{16} \frac{1}{\mu^{1/2}} \frac{ze}{(k_B T)^{1/2} \Omega_D} \frac{1}{N},$$
(5.1)

where μ is reduced mass, N is the number density of the neutral gas molecule, and z is the charge of the ion. The collision cross-section, Ω_D , is given by [24]

$$\Omega_D = \frac{1}{8\pi^2} \int_0^{2\pi} d\theta \int_0^{\pi} d\phi \int_0^{2\pi} d\gamma \frac{\pi}{8} \left(\frac{\mu}{k_B T}\right)^3 \int_0^{\infty} dg e^{-\mu/2k_B T} g^5 \int_0^{\infty} db 2b \left(1 - \cos\chi\left(\theta, \phi, \gamma, g, b\right)\right)$$
(5.2)

and θ , ϕ , and γ are the three-dimensional collision angles, g is the relative velocity, and b is the impact parameter. Because the scattering angle $\chi(\theta, \phi, \gamma, g, b)$ depends on the pairwise potential between the ion and neutral gas molecules, the accuracy of computed cross-section values is determined by the quality of the interaction potential model. The potential employed in the TJ method [24] for a He drift gas is given by

$$\Phi\left(\theta,\phi,\gamma,b,r\right) = 4\epsilon \sum_{i}^{n} \left[\left(\frac{\sigma}{r_{i}}\right)^{12} - \left(\frac{\sigma}{r_{i}}\right)^{6} \right] - \frac{\alpha}{2} \left(\frac{ze}{n}\right)^{2} \left[\left(\sum_{i}^{n} \frac{x_{i}}{r_{i}^{3}}\right)^{2} + \left(\sum_{i}^{n} \frac{y_{i}}{r_{i}^{3}}\right)^{2} + \left(\sum_{i}^{n} \frac{z_{i}}{r_{i}^{3}}\right)^{2} \right].$$

$$(5.3)$$

The first term is a sum over short-range van der Waals interactions, and the second term represents long-range ion-induced dipole interactions. In the expression, ϵ is the depth of the potential well, σ is the value of distance (r) between the centers of mass of the each atom in the ion and neutral gas molecule at the potential minimum, and R is the neutral polarizability. The coordinates, r_i, x_i , y_i , and z_i , are defined by the relative positions of the atoms with respect to the neutral. Utilizing the given ion-neutral interaction potential functions, the integrals in Equation 5.2 can be processed numerically. Monte Carlo integration schemes are used for the integration over θ , ϕ , γ , and b. The numerical integration over g is performed using a combination of the Runge-Kutta-Gill integration method and the Adams-Moulton predictor corrector integration method.

Choline is a precursor for phosphatidylcholine, sphingomyelin, and other important biological molecules [26]. Further, it is a component of cell membrane lipids in biological systems, and it plays an important role in their repair. Choline can be oxidized to betaine, which is readily demethylated to yield N, N-dimethylglycine [26]. Decomposition of choline yields trimethylamine and dimethylamine [27]. Searching for lipids and their components (i.e., choline) may be a valuable strategy in the search for evidence of extinct or extant life elsewhere in the cosmos. Under the high oxidizing conditions and significant ultraviolet flux found on the surface of Mars, one would expect decomposition products of lipids to include various alkylamines [28].

In the present study, mobilities have been measured for a number of quaternary and tertiary ammonium cations related to choline and its derivates drifting in N₂. Of particular interest was the possible dependence of mass-mobility correlations with the heavy atom (C, N, O) complements present in the molecular ion, comparing, for example, alkylated ammonium ions to abiotic amino acids (betaine and N, N-dimethylglycine). A modified TJ method for the ion-neutral interaction, to account for the potential associated with the nonspherical drift gas N_2 , has been applied to predict cross-sections of these polyatomic ammonium cations and to test the sensitivity of collision cross-section to details of the ion-neutral interaction. Comparisons of the results from the ammonium cations to other classes of organic molecules (carboxylic acids and abiotic amino acids) are presented. The origin of the observed correlation between mass and mobility of ammonium cations is discussed.

5.3 Experimental Section

5.3.1 Chemicals and Reagents

All the compounds studied in this work were purchased from Sigma Aldrich (St. Louis, MO) and were used without further purification. All solvents (water, methanol, acetic acid) were HPLC grade and were purchased from EMD Chemicals Inc. (Gibbstown, NJ). Quaternary ammonium samples were prepared by dissolving known quantities of ammonium ions in a solvent consisting of 50 % water and 50 % methanol by volume to give sample concentrations in the range of 100 μ M. Tertiary amine samples were prepared as 300 μ M in a solvent of 50:50 water and methanol with 1 % acetic acid by volume.

5.3.2 Electrospray Ionization Ion Mobility Spectrometer

The ESI-IMS instrument and the data acquisition system used in this investigation were based on designs previously described by Hill and co-workers [17, 29] and have been described in detail by Johnson *et al.* [14]. The drift length of the ion mobility spectrometer was 13.65 cm and was operated in the positive mode. A drift voltage of 3988 V, corresponding to electric field strength of 292 V/cm, was employed. All measurements were made at local atmospheric pressure (~ 730 Torr) while a counterflow of the preheated drift gas was introduced at the detection end of the drift region at a flow rate of ~ 800 mL/min. The sample solution was delivered by an Eldex Micropro liquid chromatography pump at a flow rate of 3 μ L/min into a stainless steel electrospray needle, which was held at a potential 3 – 4 kV above the entrance to the desolvation region of the spectrometer. The gap between the electrospray needle and the entrance electrode was ~ 2 cm.

Ions were introduced into the drift region through the ion gate in 0.2-ms pulses. Signals collected at the Faraday cup were amplified by a factor of 10^9 (Stanford Research Systems model SR570 low-noise current preamplifier) and recorded as a function of drift time in 0.02-ms-wide channels. Typically, 1000 individual 0 – 25-ms scans were averaged to produce the final spectra used in the analysis. Resolution of the instrument was found to be ~ 0.43 ms full width at half-maximum (FWHM) with drift times in the range 12 - 17 ms for the ions studied and the parameters employed in these experiments. Throughout this work, it was assumed that ESI of the prepared samples resulted in singly charged ammonium cations. The assumption was confirmed by ESI mass spectrometric analysis using a Finnigan LCQ Deca XP ion trap mass spectrometer. The mass spectra of all nine samples in the present study show singly charged monomeric molecular cations as the major ionic species. Since the experiments were conducted with the drift cell at 473 K, it was further assumed that there was no significant water cluster formation based on previous IMS-MS studies [18, 30].

Reduced ion mobilities, K_0 , were determined from the recorded spectra and the experimental parameters according to the usual relation,

$$K_0 = \left(\frac{273 \text{ K}}{T}\right) \left(\frac{P}{760 \text{ Torr}}\right) \frac{D^2}{Vt},\tag{5.4}$$

where V is the voltage drop across the drift region, D is the drift length, t is the drift time, P is the pressure, and T is the temperature. With the above parameters expressed in units of V, cm, s, Torr, and K, respectively, Equation 5.4 gave the reduced mobility in the typical units of cm² V⁻¹ s⁻¹. The experimental uncertainties of the determined K_0 values are estimated to be ~ 3 % based on the half width at half-maximum (HWHM) of each drift time peak in the averaged ion mobility spectra.

5.3.3 Computational Modeling

More than 500 possible molecular conformations were investigated through dihedral angles of -180° to 180° at the PM5 level using CAChe 6.1.12 (Fujitsu, Beaverton, OR). Then, the lowest-energy structures were determined using density functional theory (DFT) with a number of candidate low-energy structures from the previous PM5 calculations. DFT calculations were performed using Jaguar 6.0 (Schrödinger, Inc., Portland, OR) utilizing the Becke three-parameter functional (B3) [31] combined with the correlation functional of Lee, Yang, and Parr (LYP) [32], using the 6-31G** basis set [33]. The optimized structures of ammonium cations investigated in the present study are shown in Figure 5.2.

The TJ method [24], originally developed by Jarrold and coworkers, was modified to describe the interaction between ions and an N₂ drift gas and expand the applicability of the TJ method beyond cases of ions drifting in He. As shown in Equation 5.3, the potential used in the original TJ method consists of two terms representing van der Waals and ion-induced dipole interactions, which are characterized by the Lennard-Jones parameters (ϵ, σ) and the neutral polarizability (α), respectively. We set the polarizability of N₂ at the experimentally determined value [34] of 1.710 × 10⁻²⁴ cm² and took the Lennard-Jones parameters described in the universal force field [35], which is a general purpose force field optimized for all the elements in the periodic table. Due to the linear geometry of N₂, two more consequences should be additionally taken into account; the ion-quadrupole interaction

and the orientation of the molecule. We mimic the quadrupole moment of N₂, $(-4.65 \pm 0.08) \times 10^{-40}$ C cm² [36], by displacing charges by negative q (0.4825e) to each nitrogen atom and one positive 2q at the center of the nitrogen molecule. Hence, the ion-quadrupole potential can be expressed with simple summations of partial charges as follows:

$$\Phi_{IQ} = \sum_{j=1}^{3} \sum_{i}^{n} \frac{z_i z_j e^2}{r_{ij}},$$
(5.5)

where indexes i and j denote the atoms of the ion, three points of N₂. j = 1 and 3 indicate the two nitrogen atoms, and j = 2 indicates the center of mass position of N₂.

To consider the orientation of the nitrogen molecule rigorously, all possible trajectories with varying molecular orientations were taken into account. It has been widely accepted that the ion field does not exclusively quench the rotational angular momentum of the neutral molecule and only partial locking occurs during the collision process [37, 38]. Thus, we assumed that the interaction potential averaged over the rotational degree of freedom generates an appropriated average impact parameter [39]. The calculated rotation time of a N₂ molecule (~ 620 ns) implies that approximately three molecular rotations occur during a collision between an ion and N₂ taking place (~ 2 ps). The orientations of N₂ are sampled along with x, y, and z axes to represent all the three-dimensional rotational space. Then the orientation averaged interaction potential is evaluated, and this potential is used to compute the collision cross-section.

For the calculations of collision cross-section of ions, it is assumed that the DFT optimized structures are rigid. To ensure that the assumption is valid for the ammonium cations investigated in the present study, the collision cross-sections of two extreme conformations for the largest two ionic molecules, acetylcholine and (3-carboxypropyl)trimethylammonium, are estimated. The DFT calculated electronic energies reveal that the extended structures of both acetylcholine and (3-carboxypropyl)trimethylammonium are unstable by 4.24 and 0.547 kcal/mol, respectively, compared to cyclic structures shown in Figure 5.2. The maximum difference between two conformations of (3-carboxypropyl)-trimethylammonium is calculated as ~ 7 Å², which we can set as a maximum error bound originating from the structural uncertainty.

5.4 Results

5.4.1 Mass-Mobility Correlation of Ammonium Cations

IMS spectra were obtained as described above. The drift times of the ammonium cations were determined from the location of the peak maximums. Figure 5.1 shows example spectra taken with pure



Figure 5.1: Examples of the ion mobility spectra taken in this study. Shown are two spectra taken in 730 Torr N₂. The electric field strength and the temperature of the drift tube were 292 V/cm and 473 K, respectively. The dash curve is a spectrum taken with pure solvent being introduced to the electrospray needle while the solid curve is a spectrum of solvent and 300 μ M N, N-dimethylammoniumethanol. The two spectra were smoothed (10 point adjacent averaging) and shifted in intensity by an additive constant to avoid overlap. The N, N-dimethylammoniumethanol feature is indicated in the figure. The unlabeled features correspond to ionized solvent (water, methanol, acetic acid) and atmospheric constituents ionized through proton transfer (due to the open nature of the ESI-IMS instrument).

solvent being introduced to the electrospray needle and with 300 μ M N, N-dimethylammoniumethanol dissolved in the solvent. These spectra are characteristic of those considered in this work. Measured drift times, reduced ion mobilities (in N₂ drift gas), and determined Ω_D for the nine ammonium cations chosen for this study are listed in Table 5.1 along with their respective molecular weights. The 12-4 potential model, which has proven satisfactory to model experimental data [14, 15, 20, 21, 22] has been used for the analysis of the experimentally determined mobilities of ammonium cations. The potential is expressed as

$$\Phi(r) = \frac{\epsilon}{2} \left\{ \left(\frac{\sigma - a}{r - a} \right)^{12} - 3 \left(\frac{\sigma - a}{r - a} \right)^4 \right\},\tag{5.6}$$

where ϵ , r, and σ are defined above and the parameter a is the location of center charge from the center of mass in the ion. Rearrangement of Equation 5.6, along with the substitution of the appropriate constants, yields

$$K_0^{-1} = (1.697 \times 10^{-4}) (\mu T)^{1/2} \sigma^2 \Omega^{(1,1)*},$$
(5.7)

which gives the reduced ion mobility in terms units of cm² V⁻¹ s⁻¹. $\Omega^{(1,1)*}$ is the dimensionless collision integral, where $\Omega_D = \pi \sigma^2 \Omega^{(1,1)*}$. Derivation of Equation 5.7 from Equation 5.6 is well described by Johnson *et al.* [14]. Equation 5.7 was fit to the data set of ammonium ion mobilities in N₂ using a nonlinear least-squares fitting procedure [14]. The plot of K_0^{-1} versus ion mass for ammonium cations drifting in N₂ is shown in Figure 5.2 along with the best fit to the data. As seen in Figure 5.2, all nine ammonium cations investigated in the present study exhibit a good correlation ($R^2 = 0.99$) between mass and mobility of ion. In particular, the two different classes of ammonium cations (tertiary and quaternary) investigated in this study exhibit a common massmobility correlation. Further, the heteroatomic complements of the molecular ions do not impact the mass-mobility correlation.

5.4.2 Tertiary and Quaternary Ammonium Cations with Similar Molecular Weights

Two sets of cations, which have similar molecular weights but different structures, were chosen to investigate the influence of the composition and structural details of the ion on the mobility. The molecular weights of trimethylethylammonium and N, N-dimethylammoniumethanol are 88 and 90 amu, respectively. There is a significant structural difference between these two ions in addition to variation in the degree of alkylation to the ammonium groups. Protonated N, Ndimethylammoniumethanol possesses a hydroxyl group at the ethyl group while trimethylethylammonium possesses only alkyl groups. The molecular weights of choline and N, N-dimethylglycine



Figure 5.2: Plot of K_0^{-1} for 3° and 4° ammonium cations drifting in N₂ versus ion mass. Experimentally determined data for 3° ammonium and 4° ammonium cations are shown as asterisks and solid squares, respectively. The solid line is the fit of the 12 – 4 potential model to the ammonium cation data set. DFT optimized structure of each numerically or alphabetically labeled ion is shown above. Optimized geometries are obtained at B3LYP/6-31G** level. The hydrogen bonds are indicated with dashed lines.

mass (amu)

ammonium cation	^a MW	$^{b}\mathrm{DT}$	$^{c}K_{0}$	$^{d}\Omega_{D}$
trimethylammonium	60	12.1	2.15	91.2
tetramethylammonium	74	12.7	2.04	95.3
${\it trimethylethylammonium}$	88	13.4	1.93	102.2
N, N-dimethylammoniumethanol	90	13.4	1.93	100.9
choline	104	14.1	1.84	104.5
N, N-dimethylglycine	104	14.1	1.84	102.3
betaine	118	14.7	1.76	105.3
acetylcholine	146	16.3	1.59	118.5
(3- carboxy propyl)trimethylammonium	146	16.4	1.58	115.9

Table 5.1: Drift Times, Reduced Mobilities, and Collision Cross-Sections of Ammonium Cations in N_2 Drift Gas

^{*a*}Molecular weight (amu). ^{*b*}Drift time (ms). ^{*c*}Reduced mobility (cm² V⁻¹ s⁻¹). ^{*d*}Collision cross-section (Å²).

cation are both 104 amu. Protonated N, N-dimethylglycine cations contain a carboxyl group while choline possesses a hydroxyl group. Experimentally determined mobility values of trimethylethylammonium and N, N-dimethylammoniumethanol are identical at 1.93 cm² V⁻¹ s⁻¹. Mobilities of both choline and N, N-dimethylglycine cation are measured as 1.84 cm² V⁻¹ s⁻¹. It is inferred that the contribution of the oxygen atom to the mobility (ion-neutral ion-neutral interaction) is not significantly different from that of a methylene group in the investigated ammonium cations.

5.4.3 Functional Group Isomers of Ammonium Cations

Two functional group isomers, acetylcholine and (3-carboxypropyl)-trimethylammonium cation, were examined to study the influence of the location of oxygen atoms on the molecular ion's mobility. As seen in Figure 5.2, acetylcholine and (3-carboxypropyl)trimethylammonium are not distinguishable based on their mobilities.

5.4.4 Collision Cross-Sections of Ions in N₂ via the Trajectory Method

Theoretical Ω_D of the ammonium cations investigated in this study were evaluated using the modified TJ method. Prior to application of the modified TJ method to the ammonium cations, we tested the model on previously published experimental data. Figure 5.3a shows the plot of experimentally determined Ω_D of carboxylic acid anions [15] and abiotic amino acid cations [14] in N₂ versus those determined theoretically using the modified TJ method following the procedure described in the Experimental Section. Theoretical Ω_D of both carboxylic acid anions and abiotic amino acid cations and abiotic amino acid cations exhibit good agreement with experimental values. The agreement is within 5 % in the worst-case deviation with less than 2 % deviation on average. Figure 5.3b shows the plot of Ω_D of ammonium cations obtained experimentally versus theoretical collision cross-sections calculated



Figure 5.3: (a) Plot of experimentally determined collision cross-sections (Ω_D) of abiotic amino acid cations [14] and carboxylic acid anions [15] in N₂ versus theoretically determined Ω_D using the modified TJ method for N₂ drift gas. Abiotic amino acid cation data are shown as solid squares and carboxylic acid anion data are shown as empty circles. The solid line is y = x. (b) Plot of experimentally determined collision cross-sections (Ω_D) of 3° and 4° ammonium cations in N₂ versus theoretically determined Ω_D using the modified TJ method for N₂ drift gas. 3° ammonium cation data are shown as asterisks and 4° ammonium cation data are shown as solid squares. Each ion is labeled with the appropriate identifying number and alphabet shown in Figure 5.1. The solid line is y = x.
using the modified TJ method. The worst observed deviation of the model from the experimental cross-sections is 5 % with an average deviation of 2.5 %.

5.5 Discussion

5.5.1 Classical Ion-Neutral Collision Model

The cross-section includes the information regarding the ion-neutral interaction. An ion and a neutral interact through the long-range ion-induced dipole potential, which is given by

$$\Phi_{IID} = -\frac{(ze)^2\alpha}{2r^4},\tag{5.8}$$

where z, R, and r are defined above. The effective potential, $\Phi_{eff}(r)$, is expressed as $\Phi_{IID} + L^2/2\mu r^2$, where L is angular momentum of the collision partners about the center of mass of the combined system. The critical impact parameter $b^* = (2\alpha e^2/\text{KE})^{1/4}$ is derived by setting KE equal to the maximum effective potential, $\Phi_{eff}^*(r)$, which is given by $1/2(\text{KE})^2 b^4/\alpha e^2$, where KE is the relative kinetic energy. Then the Langevin capture cross-section is

$$\Omega_L = \pi \left(b^*\right)^2 = \pi \sqrt{\frac{2\alpha e^2}{\mathrm{KE}}}.$$
(5.9)

When the hard-sphere collision radius, R_c , is greater than b^* , the Langevin model is no longer appropriate and collisions are dominated by large angle deflections appropriate for a hard-sphere model. In this case, momentum transfer is no longer dominated by long-range interactions. In order to assess the ion-neutral collision under our experimental conditions, b^* and Ω_L are evaluated from the mean relative kinetic energies. The evaluated Ω_L and b^* are then compared to the experimental Ω_D and R_c (Table 5.2). The hard-sphere collision radius R_c is determined from the experimental Ω_D by equating it to πR_c^2 . Experimental mean relative kinetic energies can be determined from the Wannier energy formula,

$$KE = \frac{1}{2}\mu g^2 = \frac{3}{2}k_B T + \frac{1}{2}Mv_d^2,$$
(5.10)

where M is mass of drift gas molecule and v_d is drift velocity of ion [40]. Under the current experimental conditions described in the Experimental Section, b^* is calculated on the order of 5 Å. Comparison with R_c shows that b^* in our system is on the same order, i.e., less than 1 Å smaller (Table 5.2). It is therefore inferred that the group of molecules studied here are on the borderline between being dominated by long-range versus short-range interactions, favoring some orbiting at lower collision energies, which would then determine the cross-section for momentum transfer and hence the mobility.

5.5.2 Computational Trajectory Method

Ammonium cations investigated in this study exhibit a correlation between mass and mobility (Figure 5.2). In order to understand and estimate the effect of the each component of the ion-neutral interaction potential in terms of the observed mass-mobility correlation in our experimental system, theoretical calculations were performed using the modified TJ method. The collision cross-sections (Ω_D) were evaluated using molecular ions with restricted interaction potentials and artificial charge distributions. Comparisons of the Ω_D of tertiary (3°) and quaternary (4°) ammonium cations, abiotic amino acid cations, and carboxylic acid anions, which are calculated with different interaction potentials, are shown in Figures 5.4 and 5.5.

5.5.3 Ion-Quadrupole Potential

In order to understand the role of the ion-quadrupole interaction in ion-neutral interactions, the Ω_D are computed without ion-quadrupole interactions. The presence of the quadrupole moment elevates the Ω_D by 2.8 % for the ammonium cations, 2.7 % for the abiotic amino acid cations, and 4.2 % for carboxylic acid anions (Figure 5.4a). Overall, it is observed that the addition of the ion-quadrupole potential to the model for ion-N₂ interaction improves the agreement between experimental and theoretical Ω_D values. Previously, Su and Bowers reported quadrupole effects for molecules with high quadrupole moments using the average quadrupole orientation theory [41]. They demonstrated the significance of quadrupole effects, especially in the case when the ionic charge and quadrupole moment have the same polarity [41]. In analogy, a larger quadrupole effect is observed in carboxylic acid anions versus ammonium and abiotic amino acid cations, since nitrogen has a negative quadrupole moment. During the collision process, therefore, the change of a favorable orientation. This causes the observed difference of the N₂ drift gas in ion-neutral interactions compared to spherical drift gas (i.e., He).

5.5.4 Ion-Induced Dipole Potential

In order to understand the effect of the long-range ion-induced dipole interactions between ions and neutral N₂ molecules, theoretical collision cross-section with the van der Waals and ion-induced dipole potential ($\Omega_{D,VDW+IID}$) of molecular ions are compared to collision cross-sections computed after assigning the total charge of the ionic molecule as neutral ($\Omega_{D,VDW}$). The calculated $\Omega_{D,VDW}$ with the van der Waals-only potential are ~ 8–23 % smaller than the calculated $\Omega_{D,VDW+IID}$. The observed difference is attributed mainly to the lack of long-range interactions. Figure 5.4b shows plots of theoretically determined $\Omega_{D,VDW}$ over the theoretical $\Omega_{D,VDW+IID}$ of 3° and 4° ammonium cations, abiotic amino acid cations, and carboxylic acid anions in N₂ versus ion mass. The agreement



Figure 5.4: Plots of theoretically determined collision cross-sections (Ω_D) (a) with potential from van der Waals and ion-induced dipole (VDW + IID) interactions over the theoretical Ω_D with original pairwise potential, van der Waals + ion-induced dipole + ion-quadrupole (VDW + IID + IQ)interactions, and (b) with potential from van der Waals potential (VDW) over the theoretical Ω_D with potential from van der Waals and ion-induced dipole (VDW + IID) interactions of 3° and 4° ammonium cations, abiotic amino acid cations, and carboxylic acid anions in N₂ versus ion mass. The ammonium cation data, the abiotic amino acid cation, and carboxylic acid anion data are shown as solid squares, empty circles, and asterisks, respectively.

ammonium cation	KE	b^*	Ω_L	R_c
	$(\rm kcal/mol)$	(Å)	(\AA^2)	(Å)
trimethylammonium	1.70	5.08	81.0	5.41
tetramethylammonium	1.69	5.09	81.3	5.48
${\it trimethylethylammonium}$	1.67	5.10	81.7	5.57
N, N-dimethylammoniumethanol	1.67	5.10	81.7	5.55
choline	1.65	5.11	82.1	5.66
N, N-dimethylglycine	1.65	5.11	82.1	5.67
betaine	1.64	5.12	82.5	5.75
acetylcholine	1.60	5.15	83.4	6.01
(3-carboxy propyl)trimethylammonium	1.60	5.15	83.5	6.01

Table 5.2: Critical Impact Parameter, b^* , Langevin Capture Cross-Section, Ω_L , and Mean Relative Kinetic Energies, KE, during the Experiments with Experimentally Determined Hard-Sphere Collision Radius, R_c for Each Ammonium Cation

between the $\Omega_{D,VDW}$ of ions and the $\Omega_{D,VDW+IID}$ increases from 75 to 92 % along with the mass of the molecular ion increases (Figure 5.4b). This is easy to rationalize since the contribution of the van der Waals interaction increases as the size (i.e., number of atoms) of the molecular ion increases. As a result, it can be concluded that the contribution of long-range ion-induced dipole interaction is important for the Ω_D of small size molecular ions, while the van der Waals interaction prominently affects to the Ω_D in large size molecular ions in this study.

5.5.5 Van der Waals Potential

The plots of the Ω_D of 3° and 4° ammonium cations, abiotic amino acid cations, and carboxylic acid anions determined only with the van der Waals potential versus ion mass are shown in Figure 5.5, providing the comparison with the corresponding Ω_D from original pairwise potential, which is the combined potential of van der Waals, ion-induced dipole, and ion-quadrupole interactions. It is notable that the characteristic relative $\Omega_{D,VDW}$ show high similarity to the relative Ω_D from the original theoretical calculations. It is inferred that the distinction between the Ω_D for each ion is largely due to the short-range van der Waals interaction between ion and neutral N₂ molecule. The molecular weight and specific geometry of the ions is considered to dominate the short-range van der Waals interaction, which affect the collision cross-section of the ion.

5.5.6 Mass-Mobility Correlation

It has been suggested from the classical ion-neutral collision calculation that our ion-neutral collision occurs at the borderline between systems dominated by either long-range or short-range interactions. This is well supported from the theoretical investigation using the TJ method. The contribution of long-range interaction to the Ω_D of ammonium cations is large (~ 30 %) for small ions and decreases



Figure 5.5: Plots of theoretically determined collision cross-sections (Ω_D) of 3° and 4° ammonium cations, abiotic amino acid cations, and carboxylic acid anions in N₂ versus ion mass. The calculated Ω_D of the molecular ions only with van der Waals (VDW) interaction with N₂ are shown as empty squares (left y-axis). The calculated Ω_D of the molecular ions with original pairwise potential, van der Waals + ion-induced dipole + ion-quadrupole (VDW + IID + IQ) interactions, with N₂ are shown as solid circles (right y-axis).

Table 5.3: Theoretically Determined Collision Cross-Sections of 3° and 4° Ammonium Cations

ammonium cation	$^{a}\Omega_{D}$	$^{a}\Omega_{D}$	$^{a}\Omega_{D}$	$^{a}\Omega_{D}$
	$(^{b}VDW +$	$(^{b}VDW +$	(^{b}VDW)	$(^{e} \text{center})$
	c IID $+^{d}$ IQ)	c IID)		charge)
trimethylammonium	91.2	86.9	69.3	91.3
tetramethylammonium	95.3	91.6	75.6	95.1
${\it trimethylethylammonium}$	102.2	99.2	83.7	101.0
N, N-dimethylammoniumethanol	100.9	97.7	81.9	100
choline	104.5	101.5	87.0	104
N, N-dimethylglycine	102.3	99.2	83.0	101.7
betaine	105.3	102.4	87.7	105.3
acetylcholine	126.3	123.7	110.3	120.2
(3-carboxypropyl)trimethylammonium	121.1	119.0	105.4	117.8

^{*a*}Collision cross-section (Å²). ^{*b*}Van der Waals potential. ^{*c*}Ion-induced dipole interaction. ^{*d*}Ion-quadrupole interaction. ^{*e*}Ionic charge at center of mass.

to less than 10 % as the size of the ion increases.

Previous studies have suggested that charge localization on certain functional groups and the specific structure of the ion play major roles in the interaction between ions and neutral gas molecules in IMS [7, 8, 9]. In order to assess the effect of specific charge distribution in the molecular ion on Ω_D , the ionic Ω_D were evaluated after assigning the charge of the molecular ion at the center of mass. In general, Ω_D of ions, in which a total charge +1 has been assigned at the center of mass in the molecule exhibit insignificant deviations from the Ω_D of the ions determined with DFT calculated Mulliken charge distributions. The Ω_D of the ammonium cations with the charge at the center of mass show an average deviation of 0.7 % from the Ω_D of ions with Mulliken charge distributions (Table 5.3). The Ω_D of the carboxylic acid anions and abiotic amino acid cations exhibit 0.64 and 2.7 % deviations, respectively, between the two models. This implies that the influence of the ion charge distribution on Ω_D is minimal. The distance of the center of charge from the center of mass was calculated to investigate the specific charge distribution of the molecular ion in the present study. The average distance between the centers of charge from the centers of mass in the molecular ions is 0.7 Å for ammonium cations, and 0.9 Å for abiotic amino acid cations and carboxylic acid anions. It is inferred that the sizes of the molecular ions investigated in this study are too small to expect localization of the charge to a specific site.

In the previous section, we discussed that all potential terms, ion-quadrupole, ion-induced dipole, and van der Waals potential, are important considerations in determining the collision cross-section of the ions. Especially 75–95 % of collision cross-section is contributed by van der Waals interactions, which implies that strong mass-mobility correlations are highly affected by the geometries of the ions. This can explain the correlation observed in previous studies such as carboxylic acids and amino acids in terms of their structural similarity [14, 15]. However, it is not able to explain the strong correlation among the ammonium cations. Localization of the charge in molecular ions induces specific gas-phase intramolecular cyclic structures of deprotonated carboxylate anions [15, 42] and protonated abiotic amino acid cations [14]. However, DFT optimized structures of highly alkylated ammonium cations show no significant influence of the localization of the charge on the structures (Figure 5.2).

To evaluate the pure geometrical effect on the Ω_D , we calculated the molecular volume and surface area of ions in N₂, which are also known as solvent-excluded volume and area [43], using the Maximal Speed Molecular Surface (MSMS) program [44]. The volume and surface area of ion are traced by the inward-facing part of the probe sphere as it rolls over the ion [43]. The radius of the probe sphere is set to be the hard-sphere diameter of N₂ molecule, 3.70 Å. A distinct mass-volume correlation among the ammonium cations with different numbers of oxygen atoms is found. However, the surface area demonstrates a higher correlation with ion mass for the overall mass range. For example, the volume increases 7.6 and 5.6 % from trimethylethylammonium (88 amu) to choline



Figure 5.6: Plot of the total shape asymmetry (AS) of the ammonium cations versus ion mass. The ammonium cations with no oxygen atom are shown as solid squares. The ions containing one oxygen atom and two oxygen atoms are shown as empty triangles and empty circles, respectively. The DFT optimized structure of each numerically or alphabetically labeled ion is shown in Figure 5.2.

(104 amu) and betaine (118 amu) while the surface area increases 6.1 and 6.8 %, respectively. Using the obtained molecular volume and surface area, the molecular ion's asymmetry of the total shape is determined (Figure 5.6). The asymmetry of the total shape (AS) is expressed as

$$AS = \left(\frac{S}{4\pi}\right) \left(\frac{3V}{4\pi}\right)^{-2/3} = \frac{1}{4.836} \left(\frac{S}{V^{2/3}}\right),$$
(5.11)

where S and V are molecular surface area and volume, respectively. When the molecular ion is symmetrical (i.e., spherical) AS becomes unity, with AS increasing from unity as the asymmetry in shape increases. As seen in Figure 5.6, higher asymmetry is observed as the number of oxygen atoms and the size of the ion increase. Although the larger content of oxygen atom makes for smaller molecular volumes, it increases the asymmetry of the total shape, which increases the surface area of the ion. It is therefore inferred that our observed strong mass-mobility correlation is largely due to geometrical factors. This allows us to comprehend the observed mass-mobility correlation among two different classes of ammonium cations with the heteroatom complements in the present study.

5.6 Conclusions

A high correlation between mass and mobility in N_2 is observed from a number of tertiary and quaternary ammonium cations. The classical ion-neutral collision calculation implies that the group of molecules studied here are on the borderline between being dominated by long-range versus shortrange interactions, favoring some orbiting at lower collision energies, which would then determine the cross-section. Theoretical investigation using a modified trajectory (TJ) method also indicates that all potential terms, ion-quadrupole, ion-induced dipole, and van der Waals potential, are important considerations in determining the collision cross-section of the ions. For the smaller molecular ions, the importance of long-range interaction is emphasized, while short-range interactions dominate the collision cross-sections of the larger molecular ions. The evaluated volume and surface area suggest that shape asymmetry of the ammonium cations plays a small but significant role in determining the observed correlation between mass and mobility. The increase of the asymmetry in the shape of an ion compensates the reduction of the ion's volume, which finally yields similar mobilities of the ammonium cations with similar molecular weight investigated in this study, independent of their heteroatom complement.

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Chapter 6

Structural Characterization of Unsaturated Phospholipids Using Traveling Wave Ion Mobility Spectrometry

6.1 Abstract

A number of phosphatidylcholine (PC) cations spanning a mass range of 400 to 1000 Da are investigated using electrospray ionization mass spectrometry coupled with traveling wave ion mobility spectrometry (TWIMS). A high correlation between mass and mobility is demonstrated with saturated phosphatidylcholine cations in N_2 . A significant deviation from this mass-mobility correlation line is observed for the unsaturated PC cation. We found that the double bond in the acyl chain causes a 5 % reduction in drift time. The drift time is reduced at a rate of ~ 1 % for each additional double bond. Theoretical collision cross-sections of PC cations exhibit good agreement with experimentally evaluated values. Collision cross-sections are determined using the recently derived relationship between mobility and drift time in TWIMS stacked ring ion guide (SRIG) and compared to estimate collision cross-sections using empiric calibration method. Computational analysis was performed using the modified trajectory (TJ) method with nonspherical N₂ molecules as the drift gas. The difference between estimated collision cross-sections and theoretical collision cross-sections of PC cations is related to the sensitivity of the PC cation collision cross-sections to the details of the ion-neutral interactions. The origin of the observed correlation and deviation between mass and mobility of PC cations is discussed in terms of the structural rigidity of these molecules using molecular dynamics simulations.

6.2 Introduction

Lipids are essential biological components and have critical roles for cell structure, energy storage, and metabolic control [1]. Characterizing their structures is an essential part of lipid analysis. In addition, searching for lipid molecules is a valuable strategy for finding traces of extinct or extant life elsewhere in outer space. Lipids and biomembranes can be preserved for a long period; thus, detailed characterization of these biomarker compositions allows for the assessment of major contributing species [2]. Lipids offer records of modern and ancient life, environmental conditions, and changes in history. However, the variety and *in situ* alteration of lipids also increases complexity, making them difficult to characterize fully [3].

The separation and characterization of phospholipids using tandem ion mobility mass spectrometry (IM-MS) has been investigated by several research groups [4, 5, 6, 7]. Utilizing matrix-assisted laser desorption ionization (MALDI) with IM-MS, phospholipid ions have been separated from other biomolecule ions [4, 8]. Separation can be achieved based on the correlation between mass and ion mobility. Phospholipids in tissue samples have been directly analyzed using MALDI-IM-MS [4, 5]. These studies have reported that phospholipid ions have slower mobility than peptide, carbohydrate, and nucleotide ions with similar masses [4, 7, 8, 9]. In general, peptides, nucleotides, and carbohydrates form globular conformations in the gas phase due to intramolecular Coulombic interactions [10, 11, 12]. However, such interactions are difficult to achieve for phospholipid molecules because their major components are aliphatic acyl chains. Recently, Jackson *et al.* reported the effects of various head and tail groups of phospholipids on mass-mobility correlations using MALDI-IM-MS [6]. They report a slight increase in the mobility of phospholipids as the degree of unsaturation on the acyl chain increases.

The correlation between the mass and mobility of molecular ions has been used to separate and characterize ions related to the mobility of gas phase ion molecules. In the early 1970s, Griffin *et al.* [13] showed that mass and mobility are strongly correlated for structurally related compounds. In the late 1980s, Karpas and Berant demonstrated distinct mass-mobility correlations of acetyls, aromatic amines, and aliphatic amines drifting in various drift gases including He, N₂, CO₂, and air [14, 15]. Clemmer and co-workers have demonstrated distinct mass-mobility correlations for peptides with molecular weights of 500 to 2500 Da [16]. Recently, Thalassinos *et al.* characterized phosphorylated peptides as having higher mobilities than their non-phosphorylated counterparts [17].

Our laboratory has investigated the distinct mass-mobility correlations of amino acids and carboxylic acids drifting in N_2 and CO_2 [18, 19]. Recently, we experimentally observed a high correlation between mass and mobility of tertiary and quaternary ammonium cations in N_2 [20]. This observed correlation was investigated using classical ion-neutral collision dynamic theories and computational calculation using a modified trajectory (TJ) method. From these theoretical investigations, the ammonium cations in the mass range from 60 Da to 150 Da are on the borderline between being dominated by long range versus short range interactions with N_2 . In addition, all potential terms, ion-quadrupole, ion-induced dipole, and van der Waals potential are important considerations for determining the collision cross-sections of the ions in N_2 .

In this paper, we measure drift times for a number of phosphatidylcholines (PC) spanning a mass range of 400 to 1000 Da in N₂ using a commercial traveling wave ion mobility spectrometry (TWIMS) coupled with orthogonal acceleration time-of-flight (oa-TOF) mass spectrometry (Waters Synapt HDMS). Of particular interest is the possible dependence of mass-mobility correlations on the symmetry, length, and degree of saturation of the acyl chains. Despite a wide range of TWIMS applications in various chemistry fields [17, 21, 22, 23, 24, 25], studies have only begun to understand the principal physics behind the TWIMS drift time and ion mobility. A number of studies have employed the empiric calibration method to estimate mobilities and collision cross-sections of analyte ions from the drift times in TWIMS [17, 21, 22, 25, 26]. Recently, Shvartsburg and Smith quantitatively revealed the relationship between drift time and ion mobility in TWIMS [27].

Jarrold and co-workers have proposed a TJ method based on a soft-core ion-neutral interaction potential to interpret collision cross-sections of ion molecules [28]. A modified TJ method for the ion-neutral interaction to account for the potential associated with the non-spherical drift gas N_2 has been applied to predict collision cross-sections of PC cations and to test the sensitivity of these cross-sections in order to detail the structural rigidity of these molecules [20]. Results from the estimated collision-cross sections using empiric calibration are compared with the evaluated relationship between TWIMS drift time and mobility by Shvartsburg and Smith [27]. The origin of the observed correlation and deviation between PC mass and mobility is discussed.

6.3 Experimental Section

6.3.1 Chemicals and Reagents

All phosphatidylcholines studied in this work were purchased from Avanti Polar Lipids (Alabaster, AL) and were used without further purification. All solvents (water, methanol, and formic acid) were HPLC grade and were purchased from EMD Chemicals Inc. (Gibbstown, NJ). Calibrant peptides (GGGGGG and AAAAAA), cytochrome C, and trypsin from porcine pancreas were purchased from Sigma-Aldrich (St. Louis, MO). Samples were prepared by dissolving known quantities of molecules in a solvent consisting of 1 : 1 water and methanol with 0.1 % formic acid by volume to yield sample concentrations in the range of 50 μ M. Trypsin digest of cytochrome C was prepared by incubating 200 μ M of cytochrome C with 6 μ g of trypsin from porcine pancreas in 1 mL of water containing 25 mM ammonium bicarbonate (NH₄HCO₃) at 37°C for 4 hours. The trypsin was then removed

using a Millipore Microcon centrifugal filter fitted with an Ultracel YM-10 membrane. The sample solution was diluted to an appropriate concentration for ESI with 1:1 water/methanol and 0.1 % formic acid by volume. Phospholipid and peptide ions examined in this study are listed in Table 6.1 along with their respective molecular weights.

Phosphatidylcholines examined in this study are named by their acyl chain length and number of double bonds. For example, 1-steroyl-2-oleoyl-*sn*-phosphatidylcholine (SOPC), which comprises two 18 carbon acyl chains and one double bond, is referred to as 18:0-18:1 PC.

6.3.2 Electrospray Ionization Traveling Wave Ion Mobility Mass Spectrometer

Experiments were performed on a Synapt HDMS traveling wave ion mobility orthogonal acceleration time-of-flight (TW-IM-oa-TOF, Waters, Manchester, U.K.) in positive ion mode. The details of the instrument have been described elsewhere [29, 30]. Source temperature of 100°C, capillary voltage of 3 kV, desolvation temperature of 250°C, and cone voltage of 30 V were set as parameters for ESI. Other parameters of the instrument were optimized to achieve the best separation of phospholipids without the roll-over effect [29]. Nitrogen drift gas was introduced to the TWIMS stacked ring ion guide (SRIG) at a 25 mL/min flow rate, which corresponds to 0.39 Torr. The traveling wave (T-wave) height and velocity were optimized as 8 V and 300 m/s, respectively. For each sample, 150 spectra were obtained and averaged for analysis. The drift times of the singly charged phospholipid cations and peptides were determined from the location of the ion mobility peak maxima extracted manually using MassLynx (v 4.1) software (Waters corp. Milford, MA). Resolution of the instrument was found to be ~ 0.8 ms in full width at half maximum (FWHM) with drift times for the ions studied and the parameters employed in this study.

6.3.3 Collision Cross-Section Calibration

Previously published collision cross-sections of singly charged peptide hexaglycine, hexaalanine, and tryptic digest of cytochrome C in helium drift gas were used to create a calibration curve [16]. Recently published PC collision cross-sections determined in helium drift gas were also used for the calibration [9]. The calibration procedure was adopted from Thalassinos *et al.* [17]. The effective drift time (t''_{a}) of the calibrant was corrected for mass independent and mass dependent time. The published collision cross-section of the calibrant was scaled by reduced mass in N₂. The effected drift time was plotted against the corrected published collision cross-section (Ω'_D) . The plot was used to fit a linear and power trend. The equation from the fitting result was used to estimate collision cross-sections of phospholipids with reduced mass.

Name	cationization	c mass	$t_d (\mathrm{ms})$	$^{d}t_{d}^{\prime}$ (ms)
^a 5:0-5:0 PC	H^+	426	3.58	3.39
	Na^+	448	3.97	3.77
^{<i>a</i>} 8:0-8:0 PC	H^+	510	4.99	4.78
	Na^+	532	5.50	5.29
^{<i>a</i>} 11:0-11:0 PC	H^+	595	6.40	6.18
	Na^+	617	6.85	6.62
^{<i>a</i>} 14:0-16:0 PC	H^+	707	8.06	7.82
	Na^+	729	8.32	8.07
a 16:0-16:0 PC	H^+	735	8.64	8.39
	Na^+	757	8.77	8.51
^{<i>a</i>} 18:0-14:0 PC	H^+	735	8.58	8.33
	Na^+	757	8.77	8.51
a,b 16:0-18:2 PC	H^+	759	8.51	8.26
^{<i>a</i>} 18:0-16:0 PC	H^+	763	8.96	8.71
	Na^+	785	9.15	8.89
^{<i>a</i>} 16:0-20:4 PC	H^+	783	8.58	8.32
a,b 18:0-18:2 PC	H^+	787	8.90	8.64
^{<i>a</i>} 18:0-18:1 PC	H^+	789	8.96	8.70
^{<i>a</i>} 18:0-18:0 PC	H^+	791	9.41	9.15
a 16:0-22:6 PC	H^+	807	8.83	8.57
^{<i>a</i>} 24:0-24:0 PC	H^+	959	12.2	11.9
b KK (cytC)	H^+	275	1.86	1.70
b HK (cytC)	H^+	284	1.86	1.70
b GKK (cytC)	H^+	332	2.37	2.20
b GGGGGG	H^+	362	2.18	2.00
^{b} ATNE (cytC)	H^+	434	3.20	3.01
^b AAAAAA	H^+	446	3.14	2.94
^{b} KATNE (cytC)	H^+	563	4.29	4.07
^{b} Ac-GDVEK (cytC)	H^+	590	4.80	4.58
b GITWK (cytC)	H^+	605	5.12	4.89
^{b} IFVQK (cytC)	H^+	635	5.70	5.46
^{b} YIPGTK (cytC)	H^+	679	6.02	5.78
^{b} MIFAGIK (cytC)	H^+	780	7.36	7.10
^b Bradykinin	H^+	1061	10.2	9.94
^b TGPNLHGLFGR (cytC)	H^+	1169	11.8	11.5

Table 6.1: Mass, Drift time, and Corrected Drift Time of Ion Molecule Used in This Study

 a Molecules examined in this study. b Molecules used as calibrant. c All ions are singly charged. d Mass dependent corrected drift time.

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6.3.4 Computational Modeling

Collision cross-sections of ions were calculated using the modified TJ method [20], which consists of two potential terms representing van der Waals and ion-induced dipole interactions characterized by Lennard-Jones parameters and neutral polarizability, respectively [28]. The modified TJ method describes the interaction between ions and an N₂ drift gas that expands applicability beyond cases of ions drifting in He (details of this modification can be found elsewhere) [20]. In brief, we set the polarizability of neutral gas for N₂ ($1.710 \times 10^{-24} \text{ cm}^2$). Due to the linear geometry of N₂, two more consequences were taken into account: ion-quadrupole interaction and molecule orientation. The ion-quadrupole interaction is expressed in simple summations of partial charges of negative q(0.4825e) to each nitrogen atom and one positive 2q at the center of the nitrogen molecule. The orientations of N₂ are sampled along the x-, y-, and z-axis; the averaged interaction potential is evaluated using Boltzmann weighting.

In order to consider the effect of structural fluctuation on the collision cross-section at room temperature, we performed NVT molecular dynamics (MD) simulations using a Nosé-Hoover thermostat at 300 K. The inter-atom interactions are described with the all-atom CHARMM PARAM27 force field [31] using the LAMMPS (large-scale atomic/molecular massively parallel simulator) code [32]. We adopted the "sp₂ C-sp₃ C-sp₂ C" angle parameter and the "sp₂ C-sp₂ C-sp₃ C-sp₂ C" dihedral parameters from reference [33], which were optimized using 1, 4-pentadiene. The partial charge distribution of protonated phosphate (O₃P-O-H) was optimized using Mulliken charge distributions from density functional theory (DFT) calculations (Table 6.2), since the common CHARMM force field only has a partial charge distribution of negatively charged phophate (O₃P-O⁻). The systems are pre-equilibrated for 100 ps, and the conformations are sampled every one ps from the 200 ps simulations. We note that such a procedure allows for canonical sampling of the conformations at 300 K. We analyzed the collision cross-sections and potential energies of all sampled conformations of PC.

6.4 Results

6.4.1 Saturated Phosphatidylcholine Cations

The drift times, t_d , of the PC cations were determined as described above. The drift times were then corrected with the mass dependent flight time, defined as the time that an ion spent in the TOF [17, 26]. Measured and corrected drift times for the PC cations chosen for this study are found in Table 6.1. The corrected drift time from TWIMS was plotted against the mass to charge (m/z) of the ion, and the plot was used to fit a linear trend. The plot of drift time versus mass for singly protonated PC cations is shown in Figure 6.1 along with the linear fit to the data. As seen

Table 6.2: Optimized Partial Charge Distribution of Protonated Phosphate from the DFT Calculation of Protonated Dimethyl Phosphate (The Partial Charges with Atom Types for CHARMM Force Field are Tabulated.)



 $^a{\rm Computed}$ from density functional theory (DFT) calculation using Jaguar 6.0 of Schrödinger company with B3LYP functional and 6-31G** basis set.

in Figure 6.1a, all saturated PC cations investigated in this study (400 - 1000 Da) exhibit a good correlation $(R^2 > 0.999)$ between mass and drift time (i.e., ion mobility). In particular, symmetry of the two acyl chains in the phospholipid does not affect the common mass-mobility correlation of a saturated PC cation.

6.4.2 Unsaturated Phosphatidylcholine Cations

The usual acyl chain length of membrane phospholipids vary from 18 to 20 carbon atoms [34]. Most unsaturated phospholipids contain one acyl chain with one or more *cis*-double bonds and a saturated one as a second acyl chain [34]. We have selected unsaturated PC cations with these characteristics to investigate the dependence of mass-mobility correlations on the presence of double bonds in the acyl chains of membrane phospholipids (Table 6.1).

Figure 6.1b shows a plot of corrected drift time versus mass for PC cations from 700 Da to 810 Da along with the linear fit to the data. A good correlation $(R^2 = 0.984)$ is still observed for the saturated PC cations within the mass range. However, a poor correlation between mass and mobility from unsaturated and saturated PC cations is also observed $(R^2 = 0.487)$. Unsaturated PC cations show higher mobilities (i.e., faster drift time) compared to saturated PC cations. Corrected drift times of 16:0-18:2 PC (MW 759) and 16:0-20:4 PC (MW 783) are measured as 8.26 ms and 8.32 ms, respectively. They traveled in the SRIG faster than smaller saturated PC cations such as 16:0-16:0 and 18:0-14:0 (MW 735), which have 8.39 ms and 8.33 ms drift times, respectively. The corrected drift time of 16:0-22:6 PC (MW 807) is measured as 8.57 ms. Compared to the 8.71 ms and 9.15 ms, which are corrected drift times of two smaller saturated PC cations, 18:0-16:0 PC (MW 763) and 18:0-18:0 PC (MW 791), respectively, 16:0-22:6 PC travels across the SRIG faster.

The presence of a *cis*-double bond causes the acyl chain to bend. In addition, a double bond causes a relatively rigid acyl chain structure compared to that of the saturated acyl chain. It is inferred that these two factors cause smaller collision cross-sections and thus faster mobility than unsaturated PC cations.

6.4.3 Sodiated Phosphatidylcholine Cations

Figure 6.1c shows the plot of drift time versus mass for protonated and sodiated PC cations. The sodiated PC cations investigated in this study exhibit a good mass-mobility correlation ($R^2 = 0.996$) with protonated PC ions. A recent investigation by Kim *et al.* reported that short range interactions are most important for the collision cross-sections of molecular ions larger than 150 Da [20]. The PC cations (400 - 1000 Da) investigated in this study are larger than ions that Kim *et al.* [20] investigated (60 - 250 Da). Thus, the importance of short range interactions is emphasized for collision cross-sections of PC cations. In numerous cases, metal cations have been shown to cause



Figure 6.1: (a) Plot of drift time of saturated phosphatidylcholine (PC) cations in traveling wave ion mobility spectrometer versus ion mass. Experimentally determined data for symmetric PC and asymmetric PC cations are shown as solid squares and empty circles, respectively. The black dash and red solid lines are the linear fit to the symmetric PC cation data set and to both symmetric and asymmetric PC cation data set, respectively. (b) Plot of drift time of PC cations spanning mass range 700 – 800 Da in traveling wave ion mobility spectrometer versus ion mass. Experimentally determined data for saturated PC and unsaturated PC cations are shown as solid squares and empty circles, respectively. The black dash and red solid lines are the linear fit to the saturated PC cation data set and to both saturated and unsaturated PC cation data set, respectively. (c) Plot of drift time of protonated and sodiated PC cations in traveling wave ion mobility spectrometer versus ion mass. Experimentally determined data for protonated PC and sodiated PC cations are shown as solid squares and empty circles, respectively. The black dash and red solid lines are the linear fit to the protonated PC cation data set and to both protonated PC cations are shown as solid squares and empty circles, respectively. The black dash and red solid lines are the linear fit to the protonated PC cation data set and to both protonated PC cation data set, respectively.

Table 6.3: Collision Cross-Sections of Phosphatidylcholine Cations in N_2 Drift Gas Estimated and	nd
Evaluated using Empiric Calibration Method and Equations from Shavartsburg and Smith [2	7],
respectively. Theoretically Determined Collision Cross-Sections in N ₂ and He are also Listed.	

				$\Omega_D (\text{\AA}^2)$		
\mathbf{PC}	mass	Estimated	Estimated	Evaluated	a Theoretical	^a Theoretical
		(linear fit $)$	(power fit)		$(in N_2)$	(in He)
5:0-5:0	426	143.4	136.1	244.8	255.3	162.5
8:0-8:0	510	171.0	159.5	289.2	301.3	197.3
11:0-11:0	594	193.1	183.0	327.3	335.0	223.8
14:0-16:0	706	214.9	210.7	367.0	361.1	248.2
16:0-16:0	734	221.9	220.4	379.9	400.7	277.1
18:0-14:0	734	221.1	219.3	378.4	363.7	254.4
16:0-18:2	758	220.1	218.0	376.7	388.2	265.8
18:0-16:0	762	225.5	225.7	386.7	364.1	254.2
16:0-20:4	782	220.7	218.9	377.8	357.0	250.6
18:0-18:2	786	224.5	224.4	385.0	387.1	270.3
18:0-18:1	788	225.3	225.5	386.4	396.2	274.4
18:0-18:0	790	230.5	233.2	396.2	395.3	275.3
16:0-22:6	806	223.6	223.2	383.3	366.8	258.0
24:0-24:0	958	258.7	280.4	451.2	423.4	305.1

^aAveraged over 200 conformations.

specific peptide structures in the gas phase through Columbic interactions with backbone amide, carboxyl, amine, and functional groups [35, 36]. In contrast, PC is composed of two esterified acyl chains and one phosphorylcholine attached to glycerol [1]. In the sodiated PC cations, sodium cation interacts solely with the phosphate group without inducing a noticeable conformation change of PC. Thus, a good correlation between mass and mobility is observed from PC cations regardless of whether they are protonated or sodiated.

6.4.4 Estimated Collision Cross-Sections of Ions Using T-Wave Calibration

A number of studies have employed empiric calibration methods to estimate collision cross-sections of ions using a set of calibrant ions [17, 21, 22, 25, 26]. To understand the structural characteristics related to collision cross-sections of PC cations, the calibration method was applied to estimate collision cross-sections. Figure 6.2a shows the calibration plots of Ω'_D versus t''_d for 14 singly charged peptides and 6 PC cations (Table 6.1). Due to the different natures of peptide and PC ions in the gas phase, we fit only the peptide calibrants first. Then we compared the fit of peptide calibrants to the fit result from the combined peptide and PC calibrants. Both linear fit and power fit to the calibrants were performed, and both fittings exhibit a high correlation coefficient ($R^2 = 0.98$ and 0.99, respectively). Thalassinos *et al.* reported that linear fit is appropriate for calibration with small peptides. However, a slightly higher correlation was observed for power fitting in the present study. Nearly identical calibration curves were obtained from both fits for peptide and combined peptide and PC calibrants. The nature of ions in the gas phase influenced the different mass-mobility correlations. However, the empiric calibration considered only the relationship between Ω'_D and t''_d . Thus, utilizing appropriate Ω_D for calibration is more important than the chemical category of the calibrant. Figure 6.2b summarizes the estimated collision cross-sections of protonated PC cations. The estimated collision cross-section values of PC cations are found in Table 6.3.

6.4.5 Determination of Collision Cross-Sections of Ions

Shavartsburg and Smith derived equations to describe the quantitative relationship between drift time and ion mobility in TWIMS [27]. Under the condition that $KE_{\text{max}} < s$, where K is ion mobility, E_{max} is maximum electric field (E), and s is wave velocity, the mobility of an ion is related to the average ion velocity in TWIMS as [27]

$$\bar{v} = \frac{K^2}{bs} \int_0^b E^2(x) \, ds,$$
(6.1)

where E(x) is a half-sinusoidal traveling wave function and b is the waveform baseline width. Note that the equation ignores the focusing field and restricts the dynamics to axial coordinates of the SRIG. The rearrangement of Equation 6.1 with drift length L and the corrected drift time t'_d yields

$$K = \sqrt{\frac{Lbs}{t'_d \int_0^b E^2(x) \, dx}}.$$
(6.2)

Once K is determined, the reduced mobility K_0 can be determined according to

$$K_0 = \left(\frac{273 \text{ K}}{T}\right) \left(\frac{P}{760 \text{ Torr}}\right) K,\tag{6.3}$$

where P and T are the experimental pressure and temperature, respectively. Finally, the collision cross-section of an ion is evaluated by the relation [37, 38]

$$\Omega_D = \frac{3q}{16N_0} \left(\frac{2\pi}{\mu_{N_2}k_BT}\right)^{1/2} \frac{1}{K_0},\tag{6.4}$$

where N_0 is the number density at standard state (273 K and 760 Torr), q is the charge on the ion, μ is the reduced mass of ion and N₂, k_B is the Boltzmann constant, T is the temperature in the drift region, and Ω_D is the collision cross-section. The evaluated collision cross-sections of the examined PC cations are listed in Table 6.3. Note that a significant difference is found between the estimated Ω_D and the evaluated Ω_D . The evaluated Ω_D values are on average ~ 42 % larger than the estimated Ω_D values from both power and linear fit. It is of note that the collision cross-sections of calibrants



Figure 6.2: (a) Plot of corrected empiric cross-sections versus effective drift times for 14 peptides and 4 phosphatidylcholines (PC). For each peptide and PC the singly charged cation is used. Linear trend and power trend lines are shown as solid and dash lines, respectively. (b) A plot of the estimated cross-sections versus the ion mass for PC cations investigated in this study. The estimated collision cross-sections from linear trend and power trend are shown as solid squares and empty circles, respectively.

are determined in He [9, 16] while the drift gas used in TWIMS is N₂. A strong contribution of short range interaction between ion and neutral is expected for Ω_D of an ion at the mass range of PC [20]. Yet, a considerable contribution is still considered from long range interactions of ion-neutral, linear shape, and larger mass in N₂ for the determination of Ω_D of an ion. It is inferred that the observed difference of Ω_D values are caused by lack of these terms in the calibration procedure.

6.4.6 Calculated Collision Cross-Sections of Ions Using the Trajectory Method

The Ω_D of the PC cations investigated in this study were calculated using the TJ method in N₂ [20] and He (Table 6.3) [28]. The MD simulation trajectories of the PC cation for 200 ps reveal that the two acyl chains undergo large structural fluctuation due to the thermal energy at 300 K. Figure 6.3a shows the time profile of the C-C distance between the carbon atoms at the end of each chain of the 18:0-18:0 PC during 200 ps of dynamics. The distance between two carbon atoms fluctuates in the range of 5 to 25 Å within a 5 to 20 ps time period. In order to account for the sufficient amount of conformational change required for Ω_D calculation, we need to sample the conformations at every 1 ps. Then, the average Ω_D can be determined using the TJ method in N₂ and He for the 200 structures on the MD simulation trajectories [20, 28].

Figure 6.3b shows the plot of Ω_D for PC cations evaluated using the Shavartsburg and Smith [27] equations versus the theoretical Ω_D in N₂ calculated using the modified TJ method. The theoretical Ω_D values of PC cations exhibit good agreement with the experimentally evaluated values. The agreement is within 6.2 % in the worst-case deviation with 3.2 % deviation on average. This shows that the experimental collision cross-sections of analyte ions can be determined using Synapt HDMS and the relationship between SRIG drift time and mobility derived by Shavartsburg and Smith [27]. In contrast, poor agreement was observed from the estimated Ω_D of PC cations from the linear fit and power fit calibration curves with deviations of 71.2 % and 73 % on average, respectively.

6.5 Discussion

6.5.1 Effect of Drift Gas on Ion Mobility

The difference between the estimated Ω_D of the PC cation using empiric calibration and the evaluated Ω_D using Equations 6.2 to 6.4 can be explained by the different polarizabilities, sizes, and shapes of He and N₂ molecules. In drift tube ion mobility spectrometry (DTIMS), the drift time, which corresponds to the effective drift time in TWIMS, t''_d , is inversely proportional to the ion mobility, K:



Figure 6.3: (a) Time profile of the distance between the carbon atoms at the end of each acyl chain of 18:0-18:0 phophatidylcholine during 200 ps of the molecular dynamics simulation. The fluctuation is ranging from ~ 5 Å to ~ 25 Å with the time period of 5 – 20 ps. Approximately 17 times of fluctuation is observed from this trajectory. (b) Plot of experimentally determined collision crosssections (Ω_D) of phosphatidylcholine (PC) cations in N₂ against theoretically determined Ω_D using the modified TJ method for N₂ drift gas. The theoretical Ω_D is obtained by averaging Ω_D for 200 structures from MD simulations. The solid line is y = x. (c) Plot of theoretical Ω_D in He over theoretical Ω_D in N₂ versus mass of PC cations.

$$K = L^2 / V t_d'', \tag{6.5}$$

where V is voltage across the drift tube. The relationship between K and Ω_D is described as [39]

$$K = \frac{3q}{16N} \left(\frac{2\pi}{\mu k_B T}\right)^{1/2} \frac{1}{\Omega_D}.$$
(6.6)

The corrected collision cross-section, Ω'_D , for the empiric calibration is defined as [17, 26]

$$\Omega_D' = \frac{\Omega_D \mu^{1/2}}{q}.$$
(6.7)

From Equations 6.5 through 6.7, we obtain the proportional relationship between t''_d and Ω'_D . As discussed earlier, the default drift gas of TWIMS of Synapt HDMS is N₂ [17, 30, 40]. Calibration methods commonly employ the empirical Ω_D determined in He [16]. Thus, the corrected collision cross-section, Ω'_{D,N_2} , using the reduced mass in N₂, μ_{N_2} , is related to the Ω_D in He as

$$\Omega_{D,N_2}' = \frac{\Omega_{D,N_2} \mu_{N_2}^{1/2}}{q} = \frac{\Omega_{D,He} \mu_{N_2}^{1/2}}{q}.$$
(6.8)

This relationship works if $\Omega_{D,He} \approx \Omega_{D,N_2}$. Hill and co-workers have demonstrated the high dependence of Ω_D of ions on drift gas [41, 42]. Beegle *et al.* demonstrated the different polarizability effects of the drift gas molecule on the Ω_D of the ion molecule using a series of homologous Gly peptides [41]. As the size of the Gly peptide increases, the difference between Ω_D in N₂ and in He decreases. The short range interaction for Ω_D becomes more important as the ion size increases [20]. Thus, the pre-assumption for the empiric calibration is valid when the size of the ion is very large; geometric factors of neutral and long range ion-neutral interactions are completely negligible for the determination of Ω_D [26]. Theoretically calculated Ω_D in N₂ and He further support this argument. Figure 6.3c shows the plot of the theoretical Ω_D in He divided by Ω_D in N₂ versus the mass of PC cations. As the size of the cation increases from 426 Da to 959 Da, the agreement between the two theoretical Ω_D values increases from 64 % to 72 %. As a result, for the mass range of the PC cations (400 - 1000 Da), estimating Ω_D using the empiric calibration method is not valid.

6.5.2 Geometrical Effect on the Collision Cross-Sections of Phosphatidylcholine Cations

Figure 6.4a shows the plot of theoretical characteristic Ω_D of PC cations versus ion mass compared with the corresponding surface area of PC cations in N₂ at 300 K using the Maximal Speed Molecular Surface (MSMS) program [43, 44]. Note that high similarity is observed from the characteristics of relative Ω_D from theoretical calculation and the relative surface areas of PC cations. This implies that the Ω_D for each PC cation is largely influenced by the short range van der Waals interaction between the ion and the neutral N₂ molecule. The molecular weight and specific geometry of the ions dominate the short range van der Waals interaction, which affects the collision cross-section of the ion [20].

The mobility of ion K becomes field-dependent at a high electric field [45]. The field dependence of K depends on the nature properties of ion-neutral interactions. In general, high field behavior of an ion is observed when the ion acquires enough energy from E to change the nature of the ion-neutral collisions [45]. The total average energy of the ions can be determined from the Wannier energy formula as follows:

$$\frac{3}{2}k_B T_{eff} = \frac{3}{2}k_B T + \frac{1}{2}Mv_d^2,$$
(6.9)

where T_{eff} is an effective temperature of ion, M is the mass of a drift gas molecule, and v_d is the drift velocity of an ion [46]. The thermal kinetic energy is $3/2k_BT$, and the field energy is $1/2Mv_d^2$. The low field behavior of an ion is achieved when

$$\frac{3}{2}k_BT \gg \frac{1}{2}Mv_d^2.$$
 (6.10)

Ion mobility spectrometers typically operate at low electric fields. The typical E/N range for the low field is a few Townsend (Td = 10^{-17} Vcm²) [18, 45]. Although the applied voltage in the TWIMS is as low as 8 V in this study, due to the low pressure of the SRIG (0.39 Torr in this study), the average E/N is ~ 80 Td. This is an order of magnitude larger than common IMS operating field. In addition, E/N increases to as much as ~ 230 Td at E_{max} of traveling wave.

The primary effect of a high electric field is to heat the ions [45], which increases their internal energy through ion-neutral collisions. This collisional activation can result in conformation changes of the ions. Figure 6.4b shows the plots of the Ω_D of PC cations evaluated using the Shavartsburg and Smith [27] equations versus ion mass compared with the corresponding surface area of PC cations in N₂ at 300 K and 400 K. Greater similarity is observed from the characteristic relative Ω_D and the relative surface areas of PC cations at 400 K compared to the relative surface areas at 300 K. Although the experiment was performed at ~ 300 K, field heating induced a shift in ion conformation distribution to slightly higher energy state. This results in a greater similarity of the characteristic between relative Ω_D at 300 K and relative surface area at higher temperature, 400 K.

6.5.3 Mass-Mobility Correlations of Phophatidylcholine Cations

Saturated PC cations investigated in this study exhibit a good correlation between mass and mobility (Figure 6.1a). However, deviations from the correlation are observed in unsaturated PC cations (Figure 6.1b). In the previous study, we discussed the importance of van der Waals potential for



Figure 6.4: (a) Plots of theoretically determined collision cross-sections (Ω_D) and surface areas of phosphatidylcholine (PC) cations in N₂ versus ion mass. The calculated average Ω_D of the 200 ion conformations are shown as solid squares (left *y*-axis). The calculated surface areas of PC cations in N₂ at 300 K are shown as empty circles (right *y*-axis). (b) Plots of experimentally evaluated Ω_D and surface areas of phosphatidylcholine (PC) cations in N₂ versus ion mass. The Ω_D of PC cations are shown as solid squares (left *y*-axis). The calculated surface areas of PC cations are shown as solid squares (left *y*-axis). The calculated surface areas of PC cations are shown as solid squares (left *y*-axis). The calculated surface areas of PC cations in N₂ at 300 K are shown as empty circles and empty triangle, respectively (right *y*-axis).

determining the collision cross-section of an ion as the ion size increases [20]. This implies that strong mass-mobility correlation is highly affected by the geometry of the ion. In order to understand the mass-mobility correlation of saturated PC cations and deviations of unsaturated PC cations from the correlation plot, we investigate structures of PC cations with corresponding Ω_D .

The minimum energy (E_0) structures of some of the saturated PC cations examined in this study are shown in Figure 6.5a. The structures with the closest Ω_D to the experimental values are also shown along with their corresponding relative energy values (E^*) . The plot of Ω_D for the PC cations experimentally evaluated using the Shavartsburg and Smith [27] equations versus the theoretical Ω_D values of E_0 and E^* is shown in Figure 6.5b. Slightly larger Ω_D values are observed from PC cations with longer acyl chains (≥ 18 carbon) compared to the Ω_D values calculated from minimum energy structures. In contrast, smaller Ω_D values are observed from PC cations with short acyl chains (≤ 16 carbon). Note that PC cations with an acyl chain longer than 16 carbons form globular structures that are energetically favored. It is inferred that intramolecular van der Walls interactions of acyl chains drives the globular conformation to be preferred for large PC cations. However, extended structures are energetically favored for those with a shorter acyl chain (fewer than 16 carbons), whose steric effects prevent them from forming globular conformations in the gas phase. In contrast to peptide or protein ions, PC cations do not have strong intramolecular interactions to stabilize certain conformations. The energy difference between the E_0 structure and the E^* structure is only 19 kcal/mol on average. Thus, the conformations of these ions may fluctuate while traveling in the SRIG. As discussed earlier, the internal energy of an ion increases with collisional activations from the traveling wave electric field, which results in continual excitation of the ion [27]. The shift in ion conformations occurs toward slightly excited (E^*) state. Especially for larger molecules (18 or more carbon acyl chains), a significant increase in Ω_D occurs, since the increase in internal energy of these large molecules increases the importance of the entropy. As a result, the structural similarity of the saturated PC cations is maintained with moderately extended structures regardless of the length and symmetry of the PC acyl chains (Figure 6.5a); this promotes a good correlation between mass and mobility.

6.5.4 Characterizing Unsaturated Phosphatidylcholines from Mass-Mobility Correlation

Unsaturated PC cations exhibit significantly deviated mobility values from the mass-mobility correlation plot of saturated PC cations (Figure 6.1b). The drift time is reduced by ~ 5 % for the unsaturated PC cation with one double bond; the drift time reduces further at a rate of ~ 1 % for the additional double bond. Jackson *et al.* recently reported a ~ 0.5 % reduction in drift time for each additional double bond of phospholipids in DTIMS. In the present study, the larger difference in



Figure 6.5: (a) MD simulated structures of saturated phosphatidylcholine cations at minimum energy state (E_0) are shown. The structures of the closest Ω_D to the experimental values are also shown along with corresponding relative energy values (E^*) . (b) Plot of experimentally determined collision cross-sections (Ω_D) of phosphatidylcholine (PC) cations in N₂ against theoretically determined Ω_D at E_0 and E^* using the modified TJ method for N₂ drift gas. The solid line is y = x.

PC	Ω_{D,E_0} (Å ²)	$\Delta\Omega_D$ (%)	$\Delta E \; (\text{kcal/mol})$
5:0-5:0	267.08	9.1	15.2
8:0-8:0	295.44	2.1	10.6
11:0-11:0	311.24	-4.9	34.7
14:0-16:0	369.21	0.6	10.3
16:0-16:0	390.55	2.8	15.9
18:0-14:0	343.25	-9.3	11.4
16:0-18:2	382.85	1.6	10.4
18:0-16:0	343.38	-11.2	28.7
16:0-20:4	333.7	-11.7	26.8
18:0-18:2	362.37	-5.9	10.6
18:0-18:1	380.32	-1.6	2.21
18:0-18:0	368.93	-6.9	31.5
16:0-22:6	358.53	-6.5	30.2
24:0-24:0	388.94	-13.8	30.4

Table 6.4: Theoretically Determined Collision Cross-Sections (Ω_D) of Phosphatidylcholine Cations at Minimum Energy State (E_0) . The Differences of Ω_D $(\Delta\Omega_D)$ and Potential Energy (ΔE) from the PC Structure at E_0 to Experimentally Determined Ω_D .

the mobility of unsaturated PC cations compared to saturated PC cations results from the different rate of conformation changes in TWIMS. Figure 6.6 shows structures of selected unsaturated PC cations at E_0 along with the conformations at E^* . For unsaturated PC cations, a smaller shift in Ω_D is observed from the Ω_D of the most stable conformation compared to saturated PCs of similar mass. For those PC cations with more than 16 carbon acyl chains, saturated PC cations exhibit a ~ 10 % difference in Ω_D on average, while unsaturated PC cations show only ~ 5 % difference on average (Table 6.4). As observed in Figure 6.6, the major change in conformation occurs at the saturated acyl chain, while the conformation of the unsaturated acyl chain (yellow) maintains a bent structure. The presence of *cis*-double bonds in an acyl chain prevents the unsaturated acyl chain from extending by activation. As a result, less fluctuation in the ion structure occurred among unsaturated PC cations in the TWIMS. Unsaturated PC cations show smaller Ω_D values than saturated PC cations, which can form more extended conformations. This is logical given that globular structures of unsaturated PC cations are more compact and therefore have smaller collision crosssections. This allows us to characterize unsaturated PC cations based on their mobility, and thus collision cross-sections, using TWIMS.

6.6 Conclusions

A high correlation between mass and mobility in N_2 is observed from a number of saturated PC cations in TWIMS. A significant deviation from this mass-mobility correlation is observed with unsaturated PC cations. Theoretical investigation using a modified TJ method indicates that the



Figure 6.6: MD simulated structures of unsaturated phosphatidylcholine cations at minimum energy state (E_0) are shown. The structures of the closest Ω_D to the experimental values are also shown along with corresponding relative energy values (E^*) . Unsaturated acyl chain is colored in yellow.

empiric calibration method is not suitable to estimate collision cross-sections for PC cations. Instead, we evaluate collision cross-sections using a quantitative relationship between drift time and mobility derived by Shavartsburg and Smith [27]. In addition to the lack of intramolecular interactions among PC cations, collisional excitation of the ions in the SRIG induces a shift in ion conformational distribution. The unsaturated acyl chain remains bent, while the saturated acyl chain extends under the electric field, which causes larger collision cross-sections for saturated PCs and smaller ones for unsaturated PCs. The initial double bond in the acyl chain yields an approximately 5 % reduction in drift time, with further drift time reduction at the rate of ~ 1 % for each additional double bond. As a result, greater separation and characterization of unsaturated PC cations can be achieved using TWIMS.

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Chapter 7

Interfacial Reactions of Ozone with Lipids and Proteins in a Model Lung Surfactant System

7.1 Abstract

Oxidative stresses from irritants such as hydrogen peroxide and ozone (O_3) can cause dysfunction of the pulmonary surfactant (PS) in the human lung, resulting in chronic diseases of the respiratory tract. For identification of structural changes of major components of PS due to the heterogeneous reaction with O_3 , field induced droplet ionization (FIDI) mass spectrometry is utilized to probe the surfactant layer system. FIDI is a soft ionization method in which ions are extracted from the surface of micro liter volume droplets. We report the structurally specific oxidative changes of $SP-B_{1-25}$ (a shortened version of human surfactant protein B) and 1-palmitoyl-2-oleoyl-sn-phosphatidylglycerol (POPG) due to reaction with O_3 at the air-liquid interface. We also present studies of the interfacial oxidation of $SP-B_{1-25}$ in a non-ionizable 1-palmitoyl-2-oleoyl-sn-glycerol monolayer as a model lung surfactant system, where the competitive oxidation of the two components is observed. Our results indicate that the heterogeneous reaction at the interface is different from that in the bulk phase. For example, we observe the hydroxyhydroperoxide and the secondary ozonide as major products of the heterogeneous ozonolysis of POPG. These products are metastable and difficult to observe in the bulk-phase. In addition, compared to the nearly complete homogeneous oxidation of $SP-B_{1-25}$, only a subset of the amino acids known to react with ozone is oxidized in the hydrophobic interfacial environment. Combining these experimental observations with the results of molecular dynamics simulations provides an improved understanding of the interfacial structure and chemistry of a model lung surfactant system when subject to oxidative stress.

7.2 Introduction

The human lung is constantly exposed to airborne environmental insults. Long-term and immediate exposure of lungs to pathogens, air pollutants, and other irritants can be a major cause of acute and chronic injuries such as cardiopulmonary mortality and lung cancer [1, 2, 3]. Lung disease is the third leading cause of death in the United States and \sim \$154 billion is spent for direct and indirect lung disease-related health care every year [3]. Lung disease death rates are still increasing and more efforts to understand the chemical as well as the physical characteristics of lung system are required.

Pulmonary surfactant (PS) is a complex mixture of lipids and proteins [4] found in the lungs that reduces the surface tension of the alveolar sacs during the breath cycle. Phospholipids form oriented monolayers at the air-liquid interface. The principal phospholipid component of the layer, 1, 2dipalmitoyl-sn-phosphatidylcholine (DPPC), can achieve a very low surface tension ($\sim 0 \text{ mN/m}$) [5, 6] while the higher fluidity of unsaturated phospholipids such as 1-palmitoyl-2-oleoyl-sn-phosphatidylglycerol (POPG) improves the adsorption and spreading properties of surfactant at the air-liquid interface [6]. Surfactant protein B (SP-B) enhances phospholipid adsorption and spreading from the sub-phase to the interface [7], and inherited deficiencies in SP-B are lethal at birth [8]. Despite its vital importance, little is known about the interactions of the protein with phospholipids to form final lipid-protein complexes in the PS [9] as well as the manner in which this complex environment modifies the interaction of reative oxygen species (ROS) with individual components.

A number of studies have reported the chemical changes of major components of PS under various oxidative stresses [10, 11, 12], as well as changes in physical properties, which cause acute lung injury and respiratory failure [1, 13, 14]. For example, Uppu *et al.* used human red-blood cell membranes as a model lung system and demonstrated their oxidation via a bulk-phase O_3 application [11]. The alteration of structure and physical properties of SP-B by ROS has been reported by Possmayer and co-workers [12, 14]. Yet, understanding detailed mechanisms of chemical and physical changes in the complex PS system is still an active and challenging field of research. In particular, the oxidative change of major PS components by a heterogeneous air-liquid reaction with an external oxidative source (i.e. O_3) has not been studied thoroughly at the molecular level. An increasing number of studies have focused on the heterogeneous chemistry of small molecules at the air-liquid interface, mainly using mass spectrometric [15] and spectroscopic [16] techniques, as well as theoretical methods [17]. Fewer studies have considered the air-liquid interfacial chemistry of biologically relevant systems. Exemplifying the latter, Colussi and co-workers recently reported heterogeneous reactions with O_3 of ascorbic acid [18] and uric acid [19], which are components of the pulmonary epithelial lining fluid, using mass spectrometry.

Field induced droplet ionization mass spectrometry (FIDI-MS) comprises a soft ionization method to sample ions from the surface of microliter droplets [15, 20, 21]. It is ideally suited to monitor time dependent heterogeneous reactions at the air-liquid interface. A pulsed electric field stretches neutral droplets until they develop dual Taylor cones, emitting streams of positively and negatively charged submicron droplets in opposite directions. In practice, a quiescent hanging droplet is formed on the end of a capillary and then exposed to gas-phase reactants for a variable period of time, followed by FIDI-MS sampling of molecular species present in the interfacial layer (Figure 7.1).

In this study, we utilize FIDI-MS for probing air-liquid interfacial oxidation of POPG, representative of the major unsaturated anionic lipids in lung surfactant, and SP-B₁₋₂₅ (FPIPLPY-CWLCRALIKRIQAMIPKG) by O₃. Synthetic α -helical SP-B₁₋₂₅ is reported to produce the same effect as the entire 79 amino acid SP-B [22, 23, 24]. Sampling droplets with an interfacial layer of POPG or SP-B₁₋₂₅ exposed to O₃ gas over a range of reaction times reveals distinct air-liquid interfacial chemistry. In addition, we examine the heterogeneous reaction of a model PS system comprising SP-B₁₋₂₅ and 1-palmitoyl-2-oleoyl-*sn*-glycerol (POG) with O₃. POG is non-ionizable lipid with properties at the air-liquid interface similar to POPG. It is employed to avoid undesired competition of ionization with SP-B₁₋₂₅ at the surface of the droplet during the FIDI experiment. For comparison to the observed heterogeneous chemistry, we also report homogeneous reactions of SP-B₁₋₂₅ with dissolved ozone. Structures of POPG, POG, and SP-B₁₋₂₅ are shown in Figure 7.2. The observed interfacial reactions are correlated with positioning of SP-B₁₋₂₅ in a lipid monolayer as determined by means of molecular dynamic (MD) simulations.

7.3 Methods

7.3.1 Chemicals and Reagents

Sodium salts of POPG and POG were purchased from Avanti Polar Lipid (Alabaster, AL). SP- B_{1-25} was purchased from Biomer Technology (Hayward, CA). All solvents were purchased from EMD Chemicals Inc. (Gibbstown, NJ).

7.3.2 Online FIDI-MS Technique and Heterogeneous Oxidation by O₃

The FIDI-MS instrument used in this investigation were based on designs previously described by Grimm *et al.* [15]. A ~ 2 mm o.d. droplet of analyte solution is suspended from the end of a 28-gauge stainless steel capillary (Small Parts Inc.). The droplet is located on center in the region between the plate electrode and the MS inlet; the plate and inlet were separated by 6 mm. A high-voltage pulse ($\pm 7 \times 10^5$ V m⁻¹, 20 ms) is applied on the parallel plate electrode and sampling capillary to achieve FIDI. Ozonolysis reactions occur between 0 and 30 s after a quiescent droplet is achieved (~ 1 - 2 s). A pencil-style UV calibration lamp (model 6035, Oriel) generates ~ 20 ppm O₃. 100 μ M POPG, 50 μ M SP-B₁₋₂₅, or mixtures of 100 μ M POG and 50 μ M SP-B₁₋₂₅ in 1:1



Figure 7.1: Illustration of FIDI-MS methodology for studies of interfacial reactions. (a) A quiescent hanging droplet of analyte-containing solution is formed on the end of a capillary. All electrical components remain at ground as the droplet is formed and reacts in a field-free environment. (b) The droplet is exposed to gas-phase reactants for a variable period of time to allow for heterogeneous reactions between gas-phase and solution-phase species. (c) After a reaciton period, a pulsed electric field stretches the neutral droplet until it emits stream of positively and negatively charged submicron droplets in opposite directions. Ionized reactants and products from heterogeneous reactions enter the capillary inlet of the mass analyzer. Either positive or negative ions can be sampled.



 $\begin{array}{l} {\sf Phe_1-Pro_2-lle_{3^*}Pro_4-Leu_5-Pro_6-Tyr_7-Cys_8-Trp_9-Leu_{10}-Cys_{11}-Arg_{12}-Ala_{13}-Leu_{14}}\\ {\sf Gly_{25}-Lys_{24}-Pro_{23}-lleu_{22}-Met_{21}-Ala_{20}-Gln_{19}-lle_{18}-Arg_{17}-Lys_{16}-lle_{15}}\\ \end{array}$

SP-B₁₋₂₅

Figure 7.2: Structures of POPG, POG, and $SP-B_{1-25}$ investigated in this study.

(by volume) water and methanol feed the droplet source. The FIDI-MS spectra reported in this study were obtained by averaging five to ten individually acquired spectra from separately prepared droplets. The m/z of each ion was determined from the locations of the peak maxima identified in the mass spectra. The experimental details for the bulk-phase O_3 application and the Fenton reaction of SP-B₁₋₂₅ are described in Appendix H.

7.3.3 Molecular Dynamic Simulations

The MD simulations were performed with the all-atom CHARMM PARAM27 [25] force field using the LAMMPS (large-scale atomic/molecular massively parallel simulator) code [26]. To describe the water, we used a flexible TIP3P potential, which needs additional Hooke's constants, K of 900 kcal/mol/Å² for OH bond and K of 110 kcal/mol/rad² for HOH angle to the 3-site-rigid TIP3P model [25]. The initial conformation of SP-B₁₋₂₅ was taken from the Protein Data Bank structure (1DFW). The particle-particle particle-mesh (PPPM) method [27] was employed to compute the electrostatic using an accuracy criterion of 10^{-5} .

The initial structures for the lipid monolayer-water systems were prepared with 48 hexagonallypacked lipids on the 3168, 3264, 3744, and 4464 water molecules for the 55, 60, 65, and 70 Å²/lipid surface densities, respectively. A pure-repulsive wall potential, $E = \epsilon \left[2/15 \left(\sigma/r \right)^9 - \left(\sigma/r \right)^3 \right]$, where $\epsilon = 0.1521$ kcal/mol and $\sigma = 3.1538$ Å with cut-off distance of 2.7071 Å, was applied at z = 0 to

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Figure 7.3: (a) Heterogeneous reaction of POPG with O_3 as a function of time. In the absence of ozone, the negative ion FIDI-MS spectrum of POPG is dominated by the singly deprotonated POPG peak at m/z 748. POPG is depleted after 15 s of the exposure and oxidation products are dominated by deprotonated hydroxyhydroperoxide (HHP) at m/z 672. The aldehyde, carboxylic acid, and methoxyhydroperoxide products are observed at m/z 638, m/z 654, and m/z 686, respectively. The secondary ozonide (SOZ) and sodiated alcohol products show up in the spectra at m/z 796 and m/z 662, respectively. (b) Summary of heterogeneous oxidation of POPG with O_3 at the air-liquid interface. R' is H for water and CH₃ for methanol.

prevent the water from diffusing in the negative z-direction. The dimensions of the simulation cells used were (55.21 Å × 47.82 Å × 200.0 Å) for the 55 Å²/lipid, (57.67 Å × 49.94 Å × 200.0 Å) for the 60 Å²/lipid, (60.02 Å × 51.98 Å × 200.0 Å), for the 65 Å²/lipid, and (62.28 Å × 53.94 Å × 200.0 Å) for the 70 Å²/lipid surface densities. The systems were equilibrated for 0.5 ns using 300 K NVT MD simulations by applying Nosé-Hoover thermostat with a temperature damping relaxation time of 0.1 ps. Then, 2.0 ns NVT MD simulations were performed, and these trajectories are employed for the analysis of the atomic profiles.

The initial structure for the SP-B₁₋₂₅ in the POG or POPG monolayer was constructed using the final structure after the simulation of the lipid monolayer-water system with the surface density of 60 Å². After removing six neighboring lipids, the SP-B₁₋₂₅ is inserted into the resultant cavity with an α -helical axis orientation angle of 34° to the interfacial plane. Then the dimensions of the simulation cells were slightly adjusted to (57.88 Å × 50.12 Å × 200.0 Å). Similar to the lipid monolayer simulations, 0.5 ns equilibration followed by 2.0 ns NVT MD simulation was performed at 300 K. To analyze the trajectories, we averaged the population over the last 0.5 ns of the 2.0 ns trajectories.

7.4 Results and Discussion

7.4.1 Interfacial Reaction of POPG with O₃

The *cis*-double bond of an unsaturated phospholipid reacts with O₃ yielding aldehyde and carboxylic acid products directly from primary ozonide (POZ) or through energetic Crigee intermediates (CI), while saturated phospholipids such as DPPC remain intact. In this study we have investigated the heterogeneous reaction of O₃ with POPG as a representative unsaturated phospholipid in PS system. The negative ion FIDI-MS spectra for ozonolysis of POPG in a water/methanol (1:1 by volume) droplet are shown in Figure 7.3a along with the proposed reaction mechanisms (Figure 7.3b). Singly deprotonated POPG, observed at m/z 748, is seen as a dominant species in the FIDI-MS spectrum before O₃ application (Figure 7.3a). Products resulting from ozonolysis of POPG appear at least as early as 5 s after exposing the droplet to O₃. The relative abundance of the reactant POPG decreases dramatically after 15 s of exposure, and then the FIDI-MS spectrum is dominated by ozonolysis products after 30 s. The time for consuming 90 – 99 % of POPG to form the primary ozonide (POZ) at the air-liquid interface is calculated to be ~ 10 – 20 s (see Appendix G). This agrees well with the experimental observation of this study.

It is noteworthy that hydroxyhydroperoxide (HHP), methoxyhydroperoxide (MHP), and the SOZ, which are known to be metastable species in the bulk-phase, are observed as major products of POPG ozonolysis in the FIDI-MS spectra (Figure 7.3a) [28]. In order to yield HHP, a Criegee intermediate (CI) or a POZ is required to react with a water molecule [28, 29]. Rapid decomposition of HHP through proton transfers from water molecules yields ROS [29], which makes it difficult to observe HHP directly in the bulk-phase. The water density at the air-liquid interfacial region is significantly lower than in the bulk-phase [30]. In addition, water molecules in a lipid monolayer are observed to be localized within the lipid head group region due to the strong interactions with polar head groups [31]. These conditions allow HHP to be abundant in the lipid monolayer at the air-liquid interface, which is a characteristic of the heterogeneous reaction of POPG compared to the homogeneous reaction [29]. The observed MHP originates from the reaction of a CI or POZ with a methanol molecule in the droplet.

A significant abundance of SOZ is observed in the FIDI-MS spectra after exposing the droplet to O_3 for 15 s. The structure of SOZ (m/z 796) is confirmed by low energy collision induced dissociation (CID), which yields the aldehyde (m/z 638) and carboxylic acid (m/z 654) fragments. The peak corresponding to SOZ continues to build up in the spectrum as the POPG lipid is depleted. We infer that the observed SOZ is not formed by direct rearrangement of POZ but rather by recombination of the CI with aldehydes (Figure 7.3b) [28, 32]. In the bulk-phase, however, faster reaction with water molecules prevents the CI from reacting with aldehyde to form SOZ [33]. A significant amount of the sodiated alcohol product (m/z 662) is observed after exposing the droplet to O_3 for 30 s. This



Figure 7.4: (a) Air-liquid interfacial oxidation of SP-B₁₋₂₅ by O₃ as a function of time. In the absence of ozone, the positive ion FIDI-MS spectrum of SP-B₁₋₂₅ is dominated by the doubly protonated SP-B₁₋₂₅ peak at m/z 1465. The products at m/z 1481 and m/z 1489 correspond to doubly protonated SP-B₁₋₂₅ with two oxygen atoms and with three oxygen atoms, respectively, appear after the droplet is exposed to O₃ for 5 s. The triply oxygenated product at m/z 1489 dominates the FIDI-MS spectrum after exposing the droplet to O₃ for 10 s. No further oxidation of the peptide is observed up to 30 s of exposure. (b) FIDI-MS² of doubly charged triply oxygenated SP-B₁₋₂₅ product from heterogeneous oxidation yields an exclusive fragment at m/z 1457 resulting from the elimination of hydrosulfinylmethane (CH₄SO). (c) The oxidation mechanisms of Trp by ozonolysis and hydrolysis with hydrolysis mechanism of Met in peptide. (d) Air-liquid interfacial oxidation of SP-B₁₋₂₅ products with two oxygen atoms and with three oxygen atoms appear after the droplet is exposed to O₃ for 10 s. The triply oxygenated product at m/z 1457 resulting form the elimination of hydrosulfinylmethane (CH₄SO). (c) The oxidation mechanisms of Trp by ozonolysis and hydrolysis with hydrolysis mechanism of Met in peptide. (d) Air-liquid interfacial oxidation of SP-B₁₋₂₅ by O₃ in the POG monolayer as a function of time. Doubly protonated SP-B₁₋₂₅ products with two oxygen atoms and with three oxygen atoms appear after the droplet is exposed to O₃ for 10 s. The triply oxygenated product dominates the FIDI-MS spectrum after exposing the droplet to O₃ for 15 s and no further oxidation of the peptide is observed up to 30 s of exposure.

product is due to the dissociation of SOZ followed by the association with sodium cation. This suggests that after SOZ is produced under an anhydrous environment, the newly formed hydrophilic molecule interacts with sodium cation in the liquid-phase to yield the sodiated alcohol product. These SOZ and sodiated alcohol products are characteristic of specific air-liquid interface chemistry during POPG ozonolysis.

7.4.2 Interfacial Oxidation of SP-B₁₋₂₅

The positive ion FIDI-MS spectra for the oxidation of SP-B_{1-25} by O_3 are shown in Figure 7.4a. The doubly protonated SP-B_{1-25} is observed as the dominant species in the FIDI-MS spectrum before O_3 application. Products resulting from the oxidation of SP-B_{1-25} by O_3 appear after the droplet is exposed to O_3 for 5 s. The products at m/z 1481 and m/z 1489 correspond to doubly protonated SP-B_{1-25} with two oxygen atoms and with three oxygen atoms, respectively. The FIDI-MS spectrum of the droplet with SP-B_{1-25} is dominated by the triply oxygenated product at m/z

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1489 after exposing the droplet to O_3 for 10 s. No further oxidation of the peptide is observed up to 30 s of exposure. The FIDI-MS spectra show that the doubly oxygenated product immediately undergoes further oxidation to form the stable product with three oxygen atoms.

The FIDI collision induced dissociation (CID) spectrum (FIDI-MS²) of the product at m/z 1489 is shown in Figure 7.4b. The CID of triply oxygenated SP-B₁₋₂₅ from heterogeneous oxidation yields an exclusive fragment at m/z 1457 resulting from the elimination of hydrosulfinylmethane (CH₄SO), which is the characteristic CID fragment of methionine sulfoxide (MetSO) [34]. This indicates that the oxidation of the methionine residue (Met₂₁) in SP-B₁₋₂₅ results from the heterogeneous ozonolysis. The other two oxygen atoms are added to the tryptophan residue (Trp₉) forming Nformylkynrenine (NFKyn) (see Appendix H).

In order to investigate the difference between the interfacial and bulk-phase reactions of O_3 with SP-B₁₋₂₅, O_3 was bubbled into a solution containing SP-B₁₋₂₅. Oxidation using the Fenton reaction is also performed to compare the bulk-phase ozonolysis to bulk-phase oxidation by OH radical (see Appendix H for detailed analysis). The Fenton reaction yields a series of oxidized SP-B₁₋₂₅ products with up to 10 oxygen atoms while the bulk-phase O_3 reaction yields dominating products of 3- and 9-oxygenated SP-B₁₋₂₅. For the comparison to heterogeneous ozonolysis of SP-B₁₋₂₅, the products with three additional oxygen atoms from both reactions are analyzed. Bulk-phase O_3 application yields two triply oxygenated SP-B₁₋₂₅ products, one with NFKyn (+ 2O) and MetSO (+ 1O), and the other with hydroxy-N-formylkynrenine (HNFKyn, + 3O). The Fenton reaction yields only the product with HNFKyn.

Ozone has limited solubility in water. For a gas-phase concentration of 20 ppm O_3 , the equilibrium concentration of O_3 dissolved in aqueous solution is calculated as 22.6 nM by Henry's law [35]. In addition, O_3 is unstable in water, and rapidly forms secondary oxidants [36]. The major secondary oxidant formed by O_3 in water is OH radical [37]. This implies that two major O_3 oxidation pathways, ozonolysis and hydroxylation, can be observed at the air-liquid interface. The triply oxygenated $SP-B_{1-25}$ is formed concomitantly with the formation of the doubly oxygenated SP-B₁₋₂₅ after exposing the droplet to O_3 for 5 – 10 s (Figure 7.4a). The oxidation mechanisms of Trp and Met in peptide are shown in Figure 7.4c. The NFKyn can be formed via direct ozonolysis of Trp [38] or hydrolysis of hydroxytryptophan (HTrp) [12]. However, the formation of MetSO from Met occurs primarily by secondary oxidants [39]. The NFKyn of the heterogeneous reaction results from the direct ozonolysis of Trp_9 , which is located at the hydrophobic N-terminal side of $SP-B_{1-25}$. Met₂₁, which likely forms MetSO, is located at the hydrophilic C-terminal site. Intact Cys₈ and Cys_{11} support this observed O_3 oxidation of SP-B₁₋₂₅. The rate constant for reaction of Cys with ozone is three orders of magnitude larger than that of Trp and Met [40]. However, the oxidation of Cys to yield sulfonic acid occurs primarily by reactions with secondary oxidants [41], which are not present in significant concentration in the vicinity of the hydrophobic segment of the peptide where Cys₈ and Cys₁₁ are located. The formation of HNFKyn requires at least one secondary oxidation step (Figure 7.4c). After NFKyn is formed by either direct ozonolysis or reaction with secondary oxidants, the Met and NFKyn undergo competitive oxidation to yield MetSO ($k = 1.4 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹) and HNFKyn ($k = 1.3 \times 10^{-11}$ cm³ molecule⁻¹ s⁻¹) by ROS in the bulk-phase [42]. The heterogeneous ozonolysis of Trp₉ induces a change in peptide orientation at the interface. This results in Cys₈ and Cys₁₁ being exposed to ROS for oxidation in the bulk phase, which yields total 9-oxygenated SP-B₁₋₂₅.

7.4.3 Oxidation of SP- B_{1-25} in POG Monolayer by O_3

The interfacial reaction of SP-B₁₋₂₅ with ozone was also examined in a monolayer of the nonionizable lipid POG. Almost identical FIDI-MS spectra are observed compared to the spectra obtained for ozonolysis of SP-B₁₋₂₅ without POG except for an ~ 5 s time delay for initiation of the reaction (Figure 7.4d). The FIDI-MS spectrum of the SP-B₁₋₂₅/POG droplet is dominated by the triply oxygenated product after 15 s of exposure. No further oxidation of the peptide is observed up to 30 s exposure.

The observed time delay of the reaction provides a critical clue regarding the location of SP-B₁₋₂₅ in the monolayer. From the FIDI-MS spectra, it takes ~ 10 – 20 s for POPG at the air-liquid interface to be consumed by O₃ (Figure 7.3a). Both POG and POPG possess a palmitic acid chain and an oleic acid chain, the latter of which reacts with O₃. Under the assumption that the reactivity of POG is similar to that of POPG, the initiation of the SP-B₁₋₂₅ ozonolysis is expected after the droplet is exposed to O₃ for 10 – 20 s, if the peptide is completely shielded by lipid acyl chains. However, the observed short time delay of the initiation of SP-B₁₋₂₅ ozonolysis suggests that the peptide competes directly with POG for reaction with O₃. This is consistent with a picture in which the peptide is colocated at the air-liquid interface with POG at the surface of the droplet.

7.4.4 Interactions of SP-B₁₋₂₅ in a Lipid Monolayer

We carried out MD simulations for the POPG monolayer and POG monolayer in a water box for 2.0 ns with four different surface densities (55, 60, 65, and 70 Å²/lipid), which are reported as a proper density range for pulmonary surfactant function from previous theoretical studies [43, 44, 45]. Figure 7.5 shows the atomic density profiles of oxygen atoms of water molecules, saturated carbon atoms, and unsaturated carbon atoms of lipid acyl chains along $\pm \Delta z$, which is z-direction relative to the averaged phosphorous atom of POPG or hydroxyl hydrogen of POG. The POPG monolayer and POG monolayer exhibit almost identical atomic density profiles. Slightly stronger interaction between POPG and water is observed from their larger area of overlapping density (~ 1.6 times). This is due to the strong ion-dipole interactions between POPG phosphate group



Figure 7.5: Atomic density profiles of POPG monolayer systems (solid lines) and POG monolayer systems (dotted lines) as a function of Δz , where the air/liquid interface is 0, and proceeding left to right from the water to the lipid layer. The lipid surface densities are (a) 55 Å²/lipid, (b) 60 Å²/lipid, (c) 65 Å²/lipid, and (d) 70 Å²/lipid. Blue lines denote the density profiles of oxygen atoms of water molecules, black lines denote that of saturated carbons of lipid acyl chains, and red lines denote that of unsaturated carbons of lipid acyl chains.



Figure 7.6: (a) Final snapshot after 2.0 ns of MD simulation of SP-B₁₋₂₅ in a POG monolayer at 60 Å²/lipid. The peptide is shown in rainbow color (C-terminal: red, N-terminal: blue). Lipids, water molecules, and chloride are shown in purple, cyan, and red, respectively. (b) AA hydrophobicities [46] (top) and Δz of C_{α} of each residue averaged during the last 0.5 ns of a 2.0 ns duration MD simulation (bottom) are plotted as a function of amino acid residue number. The air/water interface is located near $\Delta z = 0$. (c) Atomic density profiles of SP-B₁₋₂₅ in POG monolayer at 60 Å²/lipid as a function of Δz during the last 0.5 ns of the 2.0 ns MD simulation. Blue dash line denotes the density profiles of oxygen atoms of water molecules. Black and red dash lines denote those of separately summed saturated and unsaturated carbons of lipid acyl chains, respectively. Wine, magenta, cyan, and olive solid lines denote the 100 times scaled density profiles of the C_{α} carbon of Cys₈, Trp₉, Cys₁₁, Met₂₁ residues, respectively.

and water molecules, which is absent from the POG monolayer. The water density at the double bond of POPG (5 – 20 Å) is ~ 0.0005 atom/Å³, which is ~ 70 times less dense than in the bulk-phase (~ 0.035 atom/Å³). The low water concentrations around the double bond explains the experimental observation of the intermediates and metastable products from heterogeneous ozonolysis, including SOZ, HHP, and MHP (Figure 7.3a), which are difficult to observe in water-rich environments [28, 29, 33].

We performed 2.0 ns duration MD simulations of the POG/SP-B₁₋₂₅/water monolayer with 60 Å²/lipid surface density as a representative case. The final snapshot in Figure 7.6a shows that the SP-B₁₋₂₅ is located at the air-liquid interface. The hydrophobicity index of each amino acid (AA) residue in the peptide is shown in Figure 7.6b (top) [46]. Relatively strong hydrophobicity is found for the N-terminal side of the peptide with Leu, Ile, and Pro residues. In contrast, hydrophilicity is expected from C-terminal side due to Arg, Lys, and Gln residues. The MD simulated Δz of C_{α} of each residue exhibits a good correlation with the hydrophobicity index. The hydrophobic N-terminal side of the peptide is located above the air-liquid interface, while the hydrophilic C-terminal side is



Figure 7.7: (a) The xy-projected density profiles of saturated carbon atoms of lipid acyl chains from MD simulations is shown with colors and the averaged positions of C_{α} carbons of SP-B₁₋₂₅ in the POG monolayer is shown with a black line (each residue is shown with cross). (b) Top view of final snapshot after 2.0 ns of MD simulation of SP-B₁₋₂₅ in a POG monolayer at 60 Å²/lipid. The peptide is shown in rainbow color (C-terminal: red, N-terminal: blue). Lipids and water molecules are shown in gray and cyan, respectively. Black spheres denote unsaturated carbon atoms of lipid acyl chains, and orange spheres denote hydroxyl oxygen atoms.

located under the interface (Figure 7.6b bottom). Figure 7.6c shows the atomic density profiles of oxygen atoms of water molecules as well as saturated and unsaturated carbon atoms of POG acyl chains along Δz . The 100 times scaled atomic density profiles of the C_{α} carbon of Cys₈, Trp₉, Cys₁₁, and Met₂₁ residues are also shown in Figure 7.6c. The density profiles show a good agreement with the hydrophobicity index. In practice, a low water density is found around Trp₉, which leads to the formation of NFKyn via direct ozonolysis. The water density around Met₂₁ is observed to be sufficiently high to expect ROS formation and subsequent reaction to yield MetSO. In contrast, the low water density near Cys₈ and Cys₁₁ inhibits their oxidation by ROS.

Based on the competitive reactivity of POG and SP-B₁₋₂₅ with O₃ we suggest above that they are colocated at the interface. The MD simulations of SP-B₁₋₂₅ in a lipid monolayer support our interpretation. Trp₉ and Met₂₁ of SP-B₁₋₂₅ lie below (in the z-direction) the location of the lipid double bonds (Figure 7.6c). Figure 7.7a shows the xy-projected density profiles of saturated carbon atoms of lipid acyl chains with the averaged positions of C_{α} of AA residues of SP-B₁₋₂₅. It is noteworthy that lipid acyl chains do not shelter the peptide at the air-liquid interface. The top view of the MD simulation final snapshot in Figure 7.7b illustrates that SP-B₁₋₂₅ is not shielded by unsaturated carbons (black spheres) of lipids. The strong amphiphilic characteristic and the large surface area of SP-B₁₋₂₅ cause the peptide to position itself at the air-liquid interface where it displaces lipids. As a result, SP-B₁₋₂₅ forms an island in a lipid monolayer that causes the hydrophobic portion of the peptide to be exposed to O₃ despite its location below the position of lipid double bonds. We also simulated SP-B₁₋₂₅ in the POPG monolayer. The peptide penetrates deeper into the POPG monolayer due to the strong electrostatic interaction between the cationic AA residues (Arg₁₂, Arg₁₇, and Lys₁₆) and the anionic phosphate group of POPG (Figures 7.8a and 7.8b), which agrees with previous simulations in anionic lipid monolayers [43, 47]. SP-B₁₋₂₅ forms an island in the POPG monolayer and the anhydrous environments in the lipid monolayer may lead SP-B₁₋₂₅ to be more susceptible to direct ozonolysis than to modification by ROS (Figures 7.8c and 7.9).

7.5 Conclusions

Summarizing, to understand the unique chemistry at a model lung surfactant/air interface under O_3 exposure, we utilized the FIDI-MS technique to analyze chemical reactions at this interface. In the FIDI-MS spectra, oxidized products distinct from those formed in the bulk-phase were observed from SP-B₁₋₂₅ alone and imbedded in the POG monolayer. We also carried out MD simulations that provide additional insights into the interactions between lipids, SP-B₁₋₂₅, and water molecules in the interfacial region. In these simulations the location of SP-B₁₋₂₅ relative to the lipids provides a rationalization for the experimental observation that the peptides compete with the lipids for reaction with O_3 .

The oxidation of PS causes surface dysfunction in adsorption, respreading, and reduction of surface tension [14, 48]. Once the O_3 traverses the air-liquid interface, it decays rapidly concomitant with the formation of ROS in regions with high water densities [36]. However, due to the high reactivity with PS at the interface, it has been thought that little or none of the O_3 can penetrate the PS monolayer to attack the epithelium cells below [49]. Instead of direct attack by O_3 and its ROS derivates, secondary oxidized products of PS, such as HHP, have been expected to yield cellular damage [49]. We have found that more than 60 % of the heterogeneous oxidation products of POPG by O_3 are peroxides. These products, which are more water soluble than others, eventually dissolve into the water droplet. Then, rapid decomposition of products yields reactive oxygen species (ROS) [29] which causes cellular damage below the monolayer.

Possible protection of SP-B from homogeneous oxidation by PS lipids has been suggested in an earlier study [12]. However, we have shown that SP-B₁₋₂₅ is oxidized directly by heterogeneous reaction with O_3 since it is located at the air-liquid interface with significant exposure to O_3 . The homogeneous oxidation of SP-B by ROS is known to reduce its surface activity and function [12, 14]. We have observed fast formation of NFKyn from the direct ozonolysis of Trp₉ at the hydrophobic N-terminal side of SP-B₁₋₂₅. The oxidized residue reduces the hydrophobicity of the N-terminal side of the peptide. This induces a change in peptide orientation in the monolayer that results in NFKyn, Cys₈, and Cys₁₁ being exposed to ROS for further oxidation. As a result, further oxidation of SP-B₁₋₂₅ by a heterogeneous reaction with O_3 produces effects similar to those seen in homogeneous



Figure 7.8: (a) Final snapshot after 2.0 ns MD simulation of SP-B₁₋₂₅ in POPG monolayer at 60 Å²/lipid is shown at top panel. The peptide is shown in rainbow color (C-terminal: red, N-terminal: blue), lipids in gray, water molecules in cyan, and chloride ions in red. Lower left and right show that Arg residues and Lys residues (displayed with sticks) are interacting with phosphate groups of lipids, respectively. (Phosphorous atoms are in magenta.) (b) AA index for hydrophobicity scale [46] (top) and Δz of C α of each residue averaged during the last 0.5 ns trajectory of 2.0 ns duration MD simulations (bottom) are plotted as a function of amino acid residue number. The air/water interface is located near $\Delta z = 0$. (c) Atomic density profiles of SP-B₁₋₂₅ in POG monolayer at 60 Å²/lipid as a function of Δz during the last 0.5 ns of the 2.0 ns MD simulation. Blue dash line denotes the density profiles of oxygen atoms of water molecules. Black and red dash lines denote those of saturated and unsaturated carbons of lipid acyl chains, respectively. Wine, magenta, cyan, and olive solid lines denote the 100 times scaled density profiles of the C_{α} carbon of Cys₈, Trp₉, Cys₁₁, and Met₂₁ residues, respectively.



Figure 7.9: The *xy*-projected density profiles of saturated carbon atoms of lipid acyl chains is shown with colors and the averaged positions of C_{α} carbons of SP-B₁₋₂₅ in the POPG monolayer is shown with a black line (each residue is shown with cross).

oxidation.

Our findings present a detailed explanation for the mechanisms of the possible damage to the pulmonary system by ROS or direct ozone exposure. Further studies with a more elaborate model system comprising SP-B, SP-C, and various lipids could further clarify the effect of other environmental exposures, such as smoking and airborne particles, on the lung surfactant system.

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Appendix A

Discussions on Coarse-Graining of Time- and Length-Scale in Monte Carlo Simulations for AN-OPE SAM

In order to connect from the atomistic quantum level to macroscopic level, it is necessary to coarse grain the system. We discuss below some of the consequences of the coarse graining on time- and length-scale.

A.1 Time-Scale

From the NN model, the energies required to initiate the P-to-T transition under 1.2 V/Å and T-to-P transition without external field are $\Delta E^{\ddagger} = 11.58 \text{ kcal/mol}$ and $\Delta E^{\ddagger} = 12.52 \text{ kcal/mol}$, respectively. Assuming $\Delta S^{\ddagger} = k_B \ln(2500)$, from Eyring equation, $k = k_B T/h \exp(\Delta S^{\ddagger}/k_B) \exp(-\Delta E^{\ddagger}/k_B T)$, we obtain $\tau_0 = 1/k = 1.9 \times 10^{-8}$ s and $\tau_0 = 9.3 \times 10^{-8}$ s for P-to-T case and T-to-P case, respectively. By comparing these values with MC results of $\tau_0 = 274, 193 \text{ MCS}$ and $\tau_0 = 357, 135 \text{ MCS}$, we can estimate 1 MCS as an order of $\sim 10^{-13}$ s. Thus, in actual unit, the sweep rates of $1 \times 10^{-8} \text{ V/MCS}$, $4 \times 10^{-8} \text{ V/MCS}$, and $2 \times 10^{-7} \text{ V/MCS}$ are around $1 \times 10^5 \text{ V/s}$, $4 \times 10^5 \text{ V/s}$, and $2 \times 10^6 \text{ V/s}$, which are $\sim 10^6$ times faster than the experimental conditions.

A.2 Length-Scale

We found that in our simulations, the total time taken for the complete P-to-T transition under the constant external field of F, $t_{P-to-T}(F)$ is highly overestimated when F is near F_c due to the periodic boundary condition. It is a well known fact that the finite-size effect in simulations becomes serious near the critical point of phase transition [1]. This artifact makes the transition occur at once after



Figure A.1: Total time taken for the complete P-to-T transition, t_{P-to-T} by varying the area of the periodic simulation cell as $10 \times 10 = 100$, $30 \times 30 = 900$, $40 \times 40 = 1600$, $50 \times 50 = 2500$, and $60 \times 60 = 3600$. Black line denotes the change of t_{P-to-T} under the external field of F = 1.2 V/Å, red line denotes the change of t_{P-to-T} scaled by 10 under the external field of F = 1.0 V/Å, and blue line denotes the change of t_{P-to-T} scaled by 15 under the external field of F = 0.95 V/Å. The t_{P-to-T} value is converged at the area of 900–1600 and 2500–3600 when F = 1.2 V/Å and 1.0 V/Å, respectively. When F = 0.95 V/Å, the t_{P-to-T} value is not converged until the area of 3600. This infers that we need much larger simulation cell to get the right converged value of t_{P-to-T} as the F approaches to the critical field, $F_c = 0.56 \text{ V/Å}$. Otherwise, we will get the overestimated value of t_{P-to-T} near F_c .

the bias voltage is increased sufficiently, and finally yields a narrower range of NDR (Figure A.1).

Appendix B

Effect of Molecular Fluctuations on the Electrical Conductivity of AN-OPE SAM

Electrical conductivity through the AN-OPE is estimated using the fitting equation of Figure 2.8 based on the twisting angles, χ_1 and χ_2 , from MD simulations with (10×10) unit cell. We mimicked two sets of voltage sweep cycle by following MD procedures:

- (a) QM optimized P structure is employed for the initial structure, then, annealed in the absence of external field. The conformations are almost co-planar as predicted from QM calculation with a well-developed HB network. Estimated conductivity is large with the averaged value of 0.035.
- (b) External field of 1.2 V/Å is turned on to the final structure of (a). The SAM structure is partially disordered and χ_1 has largest probability at 90°. Estimated conductivity 3.21 times decreases to 0.011.
- (c) QM optimized T structure is employed for the initial structure, then, annealed under the external field of 1.2 V/Å. Structural fluctuation allows AN-OPEs to have ~ 90° twisted conformations, resulting the loss of HB network. SAM is well-ordered. Estimated conductivity remains same to (b) with the value of 0.011.
- (d) External field is turned down from the final structure of (a). SAM forms a pretty disordered structure and χ_1 has no strongly preferring angle. Estimated conductivity 1.23 times increases to 0.013.
- (e) The final structure from step (d) is annealed in the absence of external field. SAM still has disordered structure, however, probability at $\chi_1 = 90^{\circ}$ slightly decreases. Estimated conductivity is slightly increased to 0.014.

- (f) External field of 1.2 V/Å is re-turned on to the final structure of (e). Structure and twisting angle is similar to (b), however, it is a bit more disordered. Thus, estimated conductivity is a bit smaller than (b) with the value of 0.010.
- (g) The final structure from step (d) is annealed under the external field of 1.2 V/Å, and the SAM has still similar structure to (f). Estimated conductivity remains same to (f) with the value of 0.010.
- (h) External field is re-turned down from the final structure of (g). SAM forms a more disordered structure to (d). Thus, estimated conductivity is smaller than (d) with the value of 0.012.
- (i) The final structure from step (h) is annealed in the absence of external field. SAM still has a disordered structure, however, probability at $\chi_1 = 90^\circ$ slightly decreases. Estimated conductivity is 1.05 times increased to 0.013.

The conductivities during the second cycle (f,g,h,i) shows ~ 6 % smaller values compared to the conductivities during the first cycle (b,c,d,e). These results are shown at Figure B.1.



Figure B.1: (top panel) Electrical conductivity through the AN-OPE is estimated based on the twisting angles from MD simulations with (10×10) unit cell. (bottom panels) The final snapshot after each step is shown with the populations of χ_1 and χ_2 , which are averaged during the last 0.5 ns dynamics.

Appendix C NDR in Other OPE-derivative Systems

We investigated that how our mechanism predicts the possibility of NDR in other systems containing other OPE derivatives.

C.1 Bare OPE

For bare OPE (B-OPE) with no functional groups our mechanism would suggest that there is no NDR effect, since the lack of functional groups leads to only a small molecular dipole moment to interact with the external field and there is no mechanism for the increased applied field to convert from the high conductance P phase to the low conductance T phase. Reference [2] shows the experimental data on B-OPE, which shows no NDR effect.

C.2 Nitro OPE

We calculated that the SAM of 5-nitro monosubstituted OPE system (N-OPE) on Au (111) surface. We figured out that N-OPE also can have two conformations of P and T on the SAM by forming weak HB networks along [11 $\overline{2}0$] direction and [10 $\overline{1}0$] direction, respectively. The lack of amino group makes NO₂ form a weak HB with the positive aromatic H atoms of the adjacent molecules (Figure C.1).

The twist angles are $\chi = 4^{\circ}$ and $\chi = 163^{\circ}$ and the heights of the terminal ring are 8.73 Å and 7.63 Å for P and T, respectively. These are almost identical to the values in AN-OPE case. Therefore, we expect the conductance ratio for N-OPE to be very similar to AN-OPE.

From PBE DFT calculations, P is more stable than T by 6.57 kcal/mol when no external field is applied. The dipole moment components in the [0001] direction are 3.83 (2.01) debye for P and 6.61 (3.86) debye for T from the analysis of Mulliken charges, while the parenthetical values are from quantum mechanical wave-function. Thus, the favorable state is changed from P to T as the external field is applied (Figure C.2). This suggests that the N-OPE also undergoes conformational change from P to T as the bias voltage increases. The critical field F_c is calculated as 0.49 V/Å and 0.74 V/Å when using dipole moments from Mulliken charge and QM wave-function, respectively. Since these are in the range of the F_c in AN-OPE system (0.56 V/Å), the critical bias voltage where NDR occurs is similar to the critical bias voltage of AN-OPE system of ~ 0.6 V. Reference [2] also shows the experimental data on N-OPE, which shows a well-defined hysteretic NDR at ~ 0.6 V as predicted from our calculations.



Figure C.1: (a) Optimized geometry for the low field structure (P) of N-OPE SAM. Here [0001] is the surface normal and the views are along z-axis (upper middle), y-axis (lower middle), and x-axis (lower right). The left picture is a perspective along the axis of one plane of molecules. The weak hydrogen bonding network is aligned along the [11 $\overline{2}0$] direction. (b) Optimized geometry for the high field structure (T) of N-OPE SAM. Here [0001] is the surface normal and the views are along z-axis (upper middle), y-axis (lower middle), and x-axis (lower right). The left picture is a perspective along the axis of one plane of molecules. The weak hydrogen bonding network is aligned along the [10 $\overline{1}0$] direction.



Figure C.2: (a) Energies of various conformations of N-OPE relative to the AP conformation computed with a 0.6 V/Å external field from FF calculations (black histograms). (b) Energies of various conformations of N-OPE relative to the AP conformation computed with no external field from FF calculations (black histograms), and QM calculations (green histograms).

Appendix D

Conversion Factor between External Electric Field and Bias Voltage

To connect the NEGF results and MC simulations, we need to convert the magnitude of external field, F, into the bias voltage, V. Since the critical bias voltage V_c is observed as ~ 0.6 V from the experiment and the critical field F_c is 0.56 V/Å in our NN model, we set the linear coefficient c as 0.93 Å⁻¹, which is defined by F/V.

Appendix E

Mulliken Charge Distributions of Bistable [2]Rotaxane Molecular Switch Depending on CBPQT⁴⁺ Ring's Position

The shuttling motion of charge accepting cyclobis-(paraquat-*p*-phenylene) (CBPQT⁴⁺) between the charge donating stations such as tetrathiafulvalene (TTF) and 1,5-dioxynaphthalene (DNP) moieties is governed by the charge transfer amount between the ring and the backbone. Since the potential energy surface that the CBPQT⁴⁺ ring suffers while traveling along the backbone has a large dependency on the local charge distribution of the rotaxane molecule, we performed DFT calculations for 9 different rings' positions by varying the oxidation states, 0, +1, and +2. Computed Mulliken charge distributions are tabulated in this section.





Figure E.1: Structures of a) backbone part and b) $CBPQT^{4+}$ ring part with numbered atoms. The assigned numbers on the atoms are associated with the partial charge distribution data shown in Tables E.1, E.2, and E.3.

Table E.1: Partial Charge Distribution of Neutral Rotaxane when the Center of Mass of the CBPQT⁴⁺ Ring Moves from z = 10.92 Å (TTF side) to z = 44.83 Å (DNP side)

z =	10.92 Å														
01	-0.5382	C25	-0.3287	C49	-0.1555	H73	0.1454	C97	-0.1001	C121	-0.1305	H145	0.1753	C169	-0.0964
C2	0.0386	S26	0.2392	C50	-0.0636	H74	0.1450	Н98	0.1234	C122	0.1089	H146	0.1392	C170	-0.0997
C3	0.0644	C27	-0.2631	C51	-0.0545	H75	0.1133	C99	0.0338	C123	-0.1530	H147	0.1390	H171	0.1167
n4	-0.5061	C28	-0 1531	C52	-0.0662	H76	0 1136	C100	0 0458	C124	0 1503	H148	0 1206	H172	0 1187
CS	0.0809	920	0 2279	C53	-0.0660	H77	0 1135	C101	=0 1075	N125	-0 4090	H149	0 1203	C173	=0 1699
00	0.0000	020	0.2275	000	0.0000	1170	0.1100	1100	0.1075	0100	0.4000	11140	0.1200	1174	0.1000
07	0.0400	021	0.0521	004	0.0041	1170	0.1102	0102	0.1201	0120	0.1034	11100	0.1747	0175	0.4121
07	-0.5102	031	-0.5111	000	-0.0041	11/5	0.1038	0103	-0.1094	0127	0.0515	1151	0.1/4/	0175	0.1042
68	0.0910	032	0.0469	056	-0.1512	H80	0.1037	H104	0.1219	C128	-0.1228	H152	0.1676	C176	-0.1350
C9	-0.1521	C33	0.0546	C57	0.4161	H81	0.3257	C105	0.0442	C129	-0.1221	H153	0.1396	C177	0.1107
C10	-0.2770	034	-0.5323	H58	0.1162	H82	0.1725	C106	-0.1097	C130	0.0930	H154	0.1467	C178	-0.1538
S11	0.2519	H35	0.1195	H59	0.1165	H83	0.1836	H107	0.1160	C131	-0.1025	H155	0.1713	C179	0.1485
C12	-0.3314	H36	0.0993	H60	0.1121	H84	0.1514	C108	-0.1073	C132	-0.0962	C156	0.1030	H180	0.1752
S13	0.2401	H37	0.1066	H61	0.1123	H85	0.1541	H109	0.1246	C133	-0.1670	C157	-0.1264	H181	0.1518
H14	0.3251	838	0 1120	862	0 1132	86	0 1684	C110	0.0278	N134	-0.4094	C158	0 1579	H182	0 1386
U1E	0.0201	1100	0.1120	102	0.1122	100	0.1615	C111	-0.1017	C125	0.1591	N1E0	-0.4001	1102	0.1500
115	0.0985	139	0.1190	103	0.1133	107	0.1615		-0.1017	0135	0.1561	N159	-0.4091	H103	0.1569
H16	0.1002	H40	0.1108	H64	0.1406	H88	0.1557	H112	0.1217	C136	-0.1275	C160	0.1412	H184	0.1691
H17	0.1048	041	-0.5246	H65	0.1408	H89	0.1626	C113	-0.1234	C137	0.1055	C161	-0.1499	H185	0.1802
H18	0.1024	C42	0.0409	066	-0.4800	C90	-0.1002	H114	0.1130	C138	-0.1411	H162	0.1514	H186	0.1291
H19	0.0961	C43	0.0594	C67	0.0066	H91	0.1229	C115	0.3105	C139	0.1509	H163	0.1743	H187	0.1321
H20	0.0861	044	-0.5104	C68	0.0661	C92	-0.1185	C116	-0.1241	H140	0.1670	C164	-0.1660	H188	0.1761
H21	0.1065	C45	0.0615	069	-0.4963	H93	0.1330	H117	0.1181	H141	0.1414	C165	0.0905	H189	0.1751
H22	0 1183	C46	0.0157	C70	0.0609	C94	0 3278	C118	-0 1012	H142	0 1502	C166	-0 1151	H190	0 1627
823	0.0908	047	-0 4889	071	0.0341	C05	=0.1183	H110	0 1243	H143	0 1742	C167	=0 1154	H101	0 1373
1120	0.1100	010	0.4100	070	0.0041	1000	0.1100	0100	0.1240	11140	0.1742	0107	0.0077	T-+-1	4.0000
n24	0.1100	646	0.4122	072	=0.5266	п96	0.1323	0120	0.1554	n144	0.1770	0100	0.0977	Iotai	4.0000
z =	15.66 A														
01	-0.5354	C25	-0.3661	C49	-0.1546	H73	0.1468	C97	-0.1017	C121	-0.1304	H145	0.1792	C169	-0.1051
C2	0.0359	S26	0.2715	C50	-0.0629	H74	0.1463	H98	0.1198	C122	0.0989	H146	0.1450	C170	-0.1064
C3	0.0682	C27	-0.2746	C51	-0.0530	H75	0.1147	C99	0.0329	C123	-0.1558	H147	0.1434	H171	0.1284
04	-0.5076	C28	-0.1462	C52	-0.0660	H76	0.1150	C100	0.0439	C124	0.1486	H148	0.1146	H172	0.1268
C5	0.0749	S29	0.2325	C53	-0,0659	H77	0,1150	C101	-0,1090	N125	-0,4095	H149	0.1142	C173	-0,1644
CG	0.0423	C30	0.0856	C54	-0.0525	H78	0.1147	H102	0.1232	C126	-0.1559	H150	0.1758	N174	-0.4130
07	-0 5122	021	-0 E196	001	-0.0624	170	0 1052	C102	-0 1117	C107	0.0860	U1E1	0.1745	0175	0.1411
07	-0.0133	031	-0.5180	000	-0.0034	11/5	0.1052	0103	-0.1117	0127	0.0000	1151	0.1745	0175	0.1411
68	0.0915	032	0.0514	000	-0.1501	160	0.1052	n104	0.1156	0128	-0.1116	n152	0.1/64	01/0	-0.1341
C9	-0.1370	C33	0.0644	C57	0.4175	H81	0.3271	C105	0.0401	C129	-0.1133	H153	0.1486	C177	0.1040
C10	-0.2477	034	-0.5377	H58	0.1154	H82	0.1991	C106	-0.1119	C130	0.0935	H154	0.1513	C178	-0.1543
S11	0.2436	H35	0.0999	H59	0.1155	H83	0.1581	H107	0.1071	C131	-0.1146	H155	0.1754	C179	0.1551
C12	-0.3058	H36	0.1066	H60	0.1123	H84	0.1531	C108	-0.1087	C132	-0.1144	C156	0.0879	H180	0.1804
S13	0.2640	H37	0.1000	H61	0.1123	H85	0.1562	H109	0.1218	C133	-0.1607	C157	-0.1168	H181	0.1553
H14	0.3230	H38	0.1023	H62	0.1136	H86	0.1702	C110	0.0280	N134	-0.4175	C158	0.1067	H182	0.1366
H15	0.0995	H39	0.0950	H63	0 1137	H87	0 1636	C111	-0 1035	C135	0 1631	N159	-0 4037	H183	0 1650
u16	0.0004	100	0.0070	100	0.1415	100	0.1600	u110	0.1017	C126	-0.1211	C160	0.1521	1100	0.1749
110	0.0994	n40	0.0979	104	0.1415	100	0.1562	n112	0.1217	0130	-0.1311	0160	0.1531	R104	0.1746
H17	0.1030	041	-0.5255	H65	0.1416	H89	0.1648	C113	-0.1255	C137	0.0930	C161	-0.1407	H185	0.1796
H18	0.1033	C42	0.0421	066	-0.4785	C90	-0.1019	H114	0.0988	C138	-0.1571	H162	0.1581	H186	0.1417
H19	0.0962	C43	0.0589	C67	0.0052	H91	0.1192	C115	0.3010	C139	0.1475	H163	0.1819	H187	0.1407
H20	0.0964	044	-0.5101	C68	0.0654	C92	-0.1191	C116	-0.1266	H140	0.1764	C164	-0.1597	H188	0.1802
H21	0.1134	C45	0.0616	069	-0.4937	H93	0.1309	H117	0.1045	H141	0.1533	C165	0.0778	H189	0.1741
H22	0.1142	C46	0.0145	C70	0.0596	C94	0.3255	C118	-0.1029	H142	0.1507	C166	-0.1225	H190	0.1709
H23	0 1231	047	-0 4874	C71	0.0336	C95	-0 1190	H119	0 1247	H143	0 1779	C167	-0 1207	H191	0 1437
1120	0.1201	010	0.4074	070	0.0000	1000	0.1100	0100	0.1247	11140	0.1764	0107	0.1207	T-+-1	4.0000
n24	0.1247	040	0.4130	012	-0.0207	1 130	V. 1.30Z	0120	0.1002	11144	0.1/04	0100	0.0021	IULAL	4.0000
	10 75 8														
z =	18.75 Å											1			
z = 01	18.75 Å -0.5336	C25	-0.3276	C49	-0.1537	H73	0.1479	C97	-0.1044	C121	-0.1257	H145	0.1794	C169	-0.1082
2 = 01 C2	18.75 Å -0.5336 0.0349	C25 S26	-0.3276 0.2626	C49 C50	-0.1537 -0.0622	Н73 Н74	0.1479	C97 H98	-0.1044 0.1124	C121 C122	-0.1257 0.0874	H145 H146	0.1794 0.1468	C169 C170	-0.1082 -0.1069
2 = 01 C2 C3	18.75 Å -0.5336 0.0349 0.0686	C25 S26 C27	-0.3276 0.2626 -0.2950	C49 C50 C51	-0.1537 -0.0622 -0.0510	H73 H74 H75	0.1479 0.1474 0.1102	C97 H98 C99	-0.1044 0.1124 0.0293	C121 C122 C123	-0.1257 0.0874 -0.1464	H145 H146 H147	0.1794 0.1468 0.1486	C169 C170 H171	-0.1082 -0.1069 0.1133
z = 01 C2 C3 04	18.75 Å -0.5336 0.0349 0.0686 -0.5057	C25 S26 C27 C28	-0.3276 0.2626 -0.2950 -0.1555	C49 C50 C51 C52	-0.1537 -0.0622 -0.0510 -0.0662	H73 H74 H75 H76	0.1479 0.1474 0.1102 0.1105	C97 H98 C99 C100	-0.1044 0.1124 0.0293 0.0429	C121 C122 C123 C124	-0.1257 0.0874 -0.1464 0.1496	H145 H146 H147 H148	0.1794 0.1468 0.1486 0.1172	C169 C170 H171 H172	-0.1082 -0.1069 0.1133 0.1131
z = 01 C2 C3 04 C5	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723	C25 S26 C27 C28 S29	-0.3276 0.2626 -0.2950 -0.1555 0.2815	C49 C50 C51 C52 C53	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659	H73 H74 H75 H76 H77	0.1479 0.1474 0.1102 0.1105 0.1105	C97 H98 C99 C100 C101	-0.1044 0.1124 0.0293 0.0429 -0.1114	C121 C122 C123 C124 N125	-0.1257 0.0874 -0.1464 0.1496 -0.4116	H145 H146 H147 H148 H149	0.1794 0.1468 0.1486 0.1172 0.1170	C169 C170 H171 H172 C173	-0.1082 -0.1069 0.1133 0.1131 -0.1727
z = 01 C2 C3 04 C5 C6	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434	C25 S26 C27 C28 S29 C30	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756	C49 C50 C51 C52 C53 C54	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507	H73 H74 H75 H76 H77 H78	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103	C97 H98 C99 C100 C101 H102	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216	C121 C122 C123 C124 N125 C126	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591	H145 H146 H147 H148 H149 H150	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800	C169 C170 H171 H172 C173	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059
z = 01 C2 C3 04 C5 C6 07	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5126	C25 S26 C27 C28 S29 C30	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5150	C49 C50 C51 C52 C53 C54	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507	H73 H74 H75 H76 H77 H78 H70	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001	C97 H98 C99 C100 C101 H102 C103	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216	C121 C122 C123 C124 N125 C126 C127	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591	H145 H146 H147 H148 H149 H150	0.1794 0.1468 0.1486 0.1172 0.1170 0.1170 0.1800	C169 C170 H171 H172 C173 N174 C175	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1510
z = 01 C2 C3 04 C5 C6 07	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136	C25 S26 C27 C28 S29 C30 O31	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159	C49 C50 C51 C52 C53 C54 C55	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625	H73 H74 H75 H76 H77 H78 H79	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001	C97 H98 C99 C100 C101 H102 C103	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140	C121 C122 C123 C124 N125 C126 C127 C120	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627	H145 H146 H147 H148 H149 H150 H151	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800	C169 C170 H171 H172 C173 N174 C175	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519
z = 01 C2 C3 04 C5 C6 07 C8	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891	C25 S26 C27 C28 S29 C30 O31 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604	C49 C50 C51 C52 C53 C54 C55 C56	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484	H73 H74 H75 H76 H77 H78 H79 H80	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1103 0.1001 0.1000	C97 H98 C99 C100 C101 H102 C103 H104	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048	C121 C122 C123 C124 N125 C126 C127 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156	H145 H146 H147 H148 H149 H150 H151 H152	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1734	C169 C170 H171 H172 C173 N174 C175 C176	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312
z = 01 C2 C3 04 C5 C6 07 C8 C9	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367	C25 S26 C27 C28 S29 C30 D31 C32 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561	C49 C50 C51 C52 C53 C54 C55 C56 C57	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201	H73 H74 H75 H76 H77 H78 H79 H80 H81	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.1000 0.3230	C97 H98 C99 C100 C101 H102 C103 H104 C105	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307	C121 C122 C123 C124 N125 C126 C127 C128 C129	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181	H145 H146 H147 H148 H149 H150 H151 H152 H153	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1379	C169 C170 H171 H172 C173 N174 C175 C176 C177	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871
z = 01 C2 C3 04 C5 C6 07 C8 C9 C10	$\begin{array}{c} 18.75 \ \mbox{A} \\ \hline -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \end{array}$	C25 S26 C27 C28 S29 C30 D31 C32 C33 D34	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201 0.1132	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.1000 0.3230 0.2039	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1734 0.1379 0.1528	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492
$\begin{array}{c}z=\\01\\C2\\C3\\04\\C5\\C6\\07\\C8\\C9\\C10\\S11\end{array}$	$\begin{array}{c} 18.75 \ \mbox{A} \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \end{array}$	C25 S26 C27 C28 S29 C30 031 C32 C33 034 H35	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201 0.1132 0.1134	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.1000 0.3230 0.2039 0.1603	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1379 0.1528 0.1830	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455
$\begin{array}{c} z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \end{array}$	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367 -0.2433 0.3179 -0.2980	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088 0.1023	C49 C50 C51 C52 C53 C54 C55 C56 C55 C56 C57 H58 H59 H60	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0659 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1103 0.1001 0.3230 0.2039 0.1603 0.1541	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939 -0.1110	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1034	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1734 0.1379 0.1528 0.1830 0.0841	C169 C170 H171 C173 N174 C175 C176 C177 C178 C179 H180	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841
$\begin{array}{c}z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \end{array}$	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367 -0.2433 0.3179 -0.2980 0.3122	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088 0.1023 0.0927	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1121	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.1000 0.3230 0.2039 0.1603 0.1541 0.1579	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939 -0.1110 0.1198	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566
$\begin{array}{c}z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \end{array}$	$\begin{array}{c} 18.75 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088 0.1023 0.0927 0.0929	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1120 0.1138	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.1000 0.3230 0.3230 0.2039 0.1603 0.1541 0.1579 0.1736	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939 -0.1110 0.1198 0.0338	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607 -0.4152	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349
$\begin{array}{c}z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \\ H15 \end{array}$	$\begin{array}{c} 18.75 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.0999 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H36 H37 H38 H39	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088 0.1023 0.0927 0.0929	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63	-0.1537 -0.0622 -0.0510 -0.0659 -0.05507 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1120 0.1138	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H84 H85 H87	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.3230 0.2039 0.1603 0.1541 0.1579 0.1736	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939 -0.1110 0.1198 0.0338	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607 -0.4152 0.1586	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777
z = 01 C2 C3 04 C5 C6 07 C8 C9 C10 S11 C12 S13 H14 H15 H16	$\begin{array}{c} 18.75 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0691 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1000 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40	-0.3276 0.2626 -0.2950 0.1555 0.2815 0.0756 0.65159 0.0604 0.0561 0.5499 0.1088 0.1023 0.0927 0.0929 0.0951	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64	-0.1537 -0.0622 -0.0510 -0.0669 -0.0659 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1120 0.1138 0.1138 0.1138	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H82 H83 H84 H85 H86 H87 H88	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.1001 0.1000 0.3230 0.2039 0.1603 0.1541 0.1579 0.1736 0.1652 0.1605	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0393 -0.1110 0.1198 0.0338 -0.1041 0.1252	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607 -0.4152 0.1586 0.1586	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1734 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072 0.1460	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777 0.1777
$\begin{array}{c} z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \\ H15 \\ H16 \\ H17 \end{array}$	$\begin{array}{c} 18.75 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1030 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 Od 1	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1023 0.0927 0.0927 0.0929 0.0951 0.0956	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65	-0.1537 -0.0622 -0.0510 -0.06629 -0.06659 -0.06659 -0.1484 0.4201 0.1132 0.1132 0.1134 0.1121 0.1120 0.1138 0.1138 0.1418	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.3230 0.3230 0.2039 0.1603 0.1541 0.1579 0.1736 0.1652 0.1665	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0393 -0.1110 0.1198 0.0338 -0.1041 0.1252 -0.1320	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607 -0.4152 0.1586 -0.1229 0.0931	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1734 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072 0.1460	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777 0.1778
z = 01 C2 C3 04 C5 C6 07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18	$\begin{array}{c} 18.75 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2880 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1088 0.1023 0.0927 0.0929 0.0951 0.0956 -0.5280 0.02441	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65	-0.1537 -0.0622 -0.0510 -0.0662 -0.0659 -0.0507 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1120 0.1138 0.1138 0.1418 0.1421	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H87 H88 H89 C90	0.1479 0.1474 0.1102 0.1105 0.1105 0.1103 0.1001 0.2039 0.1603 0.1541 0.1579 0.1736 0.1652 0.1605 0.1681 -0.1047	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.0939 -0.1110 0.1198 0.0338 -0.1041 0.1252 -0.1390	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 0.1607 -0.4152 0.1586 -0.1229 0.0931 -0.1515	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C156 C157 C158 N159 C160 C161 H162	0.1794 0.1468 0.1486 0.1172 0.1170 0.1800 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072 0.1460 -0.1474 0.1563	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H184	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1445 0.1445 0.1349 0.1777 0.1777 0.1777 0.1778
z = 01 C2 C3 C4 C5 C6 07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19	$\begin{array}{c} 18.75 \ A \\ \hline 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.3999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \\ 0.0087 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43	-0.3276 0.2626 -0.2550 0.2155 0.2815 0.0756 -0.5159 0.0604 0.0561 -0.5499 0.1023 0.0927 0.0927 0.0929 0.0951 0.0956	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0669\\ -0.0659\\ -0.0625\\ -0.1484\\ 0.4201\\ 0.1132\\ 0.1134\\ 0.1121\\ 0.1120\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1418\\ 0.1421\\ -0.4753\\ 0.014\end{array}$	H73 H74 H76 H776 H777 H78 H779 H80 H81 H82 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91	0.1479 0.1479 0.1102 0.1105 0.1105 0.1105 0.1105 0.1103 0.1001 0.3230 0.1603 0.1641 0.1579 0.1652 0.1652 0.1652 0.1661 -0.1047	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 C110 C111 H112 C113 H114 C115	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0939 -0.1110 0.1198 0.0338 -0.1041 0.1252 -0.1390 0.0777 0.3001	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139	-0.1257 0.0874 -0.1464 -0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1181 0.0637 -0.1034 -0.1026 -0.1607 -0.4152 0.1586 -0.1229 0.0931 -0.1515 0.1520	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162	0.1794 0.1488 0.1486 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072 0.1460 -0.1474 0.1563	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H185 H186	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777 0.1777 0.1778 0.1818 0.1399 0.1401
$\begin{array}{c}z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \\ H15 \\ H16 \\ H17 \\ H18 \\ H19 \\ H20 \\ \end{array}$	$\begin{array}{c} 18.75 \\ -0.5336 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1667 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\$	C25 S26 C27 C28 S29 C30 C31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0604 0.06561 -0.5499 0.1088 0.1028 0.0927 0.0929 0.0956 -0.5280 0.0946 0.0441 0.0554 -0.5280	C49 C50 C51 C52 C53 C54 C56 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 O66 C67 C68	-0.1537 -0.0622 -0.0510 -0.0662 -0.0507 -0.0625 -0.1484 0.4201 0.1132 0.1134 0.1121 0.1138 0.1138 0.1138 0.1418 0.1418 0.1418	H73 H74 H75 H76 H77 H78 H77 H78 H79 H80 H81 H82 H83 H84 H83 H84 H85 H86 H87 H88 H89 C90 H91 H29 C92	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.1001 0.2039 0.1603 0.1579 0.1736 0.1652 0.1605 0.1665 0.1665 0.1665	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.1048 0.0307 -0.1140 0.10939 -0.1100 0.10939 -0.1110 0.1198 0.0338 -0.1252 -0.1390 0.0777 0.3001 -0.1390	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C135 C136 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C124 C122 C122 C123 C124 C125 C125 C125 C125 C126 C125 C126 C126 C126 C126 C126 C126 C126 C126	-0.1257 0.0874 -0.1464 -0.1464 -0.1591 0.0627 -0.1156 -0.1181 0.0627 -0.1034 -0.1034 -0.1034 -0.1034 -0.1607 -0.1452 0.0531 -0.1520 0.0531 -0.520	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C156 C156 C156 C156 C156 N159 C160 H162 H162 H162 H163 C164	0.1794 0.1488 0.1486 0.1170 0.1800 0.1770 0.1800 0.1734 0.1800 0.1734 0.1820 0.1830 0.0831 0.1830 0.0831 0.1851 0.1851 0.1460 -0.1474 0.1563 0.1841 -0.171841	C169 C170 H171 H172 C173 C175 C176 C177 C178 C177 H180 H181 H181 H181 H183 H184 H185 H186 H187 H188	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1492 0.1456 0.1349 0.1777 0.1777 0.1777 0.1778 0.1818 0.1399 0.1401
$\begin{array}{c}z=\\ 01\\ C2\\ C3\\ 04\\ C5\\ C6\\ 07\\ C8\\ C9\\ C10\\ S11\\ C12\\ S13\\ H14\\ H15\\ H16\\ H17\\ H18\\ H19\\ H20\\ V21\\ \end{array}$	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367 -0.2433 0.3179 -0.2433 0.3179 0.3122 0.3227 0.0999 0.1000 0.1039 0.1041 0.0987 0.0988 0.1047 0.00987 0.00987 0.0988 0.1047 0.00987 0.1047 0.1047 0.00987 0.1047 0.0988 0.1047 0.0988 0.1047 0.1047 0.0988 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.1047 0.0088 0.0	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C42 C43	-0.3276 0.2626 -0.2950 -0.2815 0.2815 0.075159 0.0664 0.0561 -0.5159 0.0664 0.1023 0.0927 0.0929 0.0921 0.0929 0.0951 0.0925 0.0951 0.0951 0.0554 -0.5104 -0.5104	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 C67 C68 C67 C68	-0.1537 -0.0622 -0.0510 -0.0663 -0.06659 -0.0659 -0.1484 0.1132 0.1134 0.1120 0.1138 0.1138 0.1138 0.1418 0.1421 0.1421 0.1425	H73 H74 H75 H76 H77 H78 H79 H80 H81 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C30 H91 C32 C30 H91	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.1543 0.1579 0.1652 0.1652 0.1661 0.1681 -0.1047 0.1124 -0.1206	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 C116 C116	-0.1044 -0.1124 0.0223 -0.1114 0.1114 0.1216 -0.1140 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.1048 -0.11198 0.0338 -0.1041 0.12390 -0.1390 0.0777	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140	-0.1257 0.0874 -0.1464 0.1496 -0.1496 -0.1591 0.0627 -0.1156 -0.1034 -0.1034 -0.1034 -0.1034 -0.1036 -0.1560 -0.1560 -0.1550 0.0931 -0.1515 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 0.0931 -0.15151 -0.1555 -0.1555 -0	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H163 C164 H163 C164	0.1794 0.1468 0.1468 0.1172 0.1170 0.1800 0.1774 0.1800 0.1734 0.1830 0.16841 -0.1294 0.1661 -0.4072 0.1464 0.1563 0.1641 -0.1474 0.1563	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C177 C178 C177 H180 H181 H182 H181 H182 H183 H184 H185 H186 H187 H188	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1845 0.1845 0.1349 0.1777 0.1778 0.1818 0.1339 0.1401 0.1838
z = 01 C2 C3 04 C5 C6 07 C8 C9 C10 S111 C12 S13 H14 H15 H16 H17 H18 H19 H20 H21	$\begin{array}{c} 18.75 \\ -0.5336 \\ -0.5346 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2433 \\ 0.3179 \\ -0.2860 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1000 \\ 0.1039 \\ 0.10041 \\ 0.0987 \\ 0.0987 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.09889 \\ 0.1137 \\ 0.00889 \\ 0.00$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C42	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0661 0.0661 0.1023 0.0927 0.0929 0.0955 -0.5280 0.0945 0.0956	C49 C50 C51 C52 C53 C54 C55 C56 C56 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68 D69 C72	-0.1537 -0.0622 -0.0510 -0.0669 -0.0659 -0.0657 -0.0625 -0.1484 0.1212 0.1134 0.1121 0.1122 0.1138 0.1121 0.1128 0.1138 0.1418 0.1418 0.1418 0.1418 0.1418 0.1418 0.1418	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91 C92 H93 C92 H93 C92	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.1001 0.1001 0.2039 0.1603 0.1541 0.1579 0.1762 0.1665 0.1652 0.1665 0.1661 0.1682 0.16047 0.1272 0.2721	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C116	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.0337 -0.1140 0.0337 -0.1140 0.0338 -0.1018 0.0338 -0.1018 0.1252 -0.1390 0.1252 -0.1390 0.0777 0.3001 -0.1390 0.0777 0.3001 -0.1252 0.0777 0.3001 -0.1252 0.0777 0.3001 -0.1252 0.0777 0.3001 -0.1252 0.0777 0.3001 -0.1252 0.0777 0.3001 0.077 0.0777 0.0015 0.0777 0.0777 0.0015 0.0777 0.0777 0.0015 0.0777 0.0777 0.0015 0.0777 0.0015 0.0777 0.0015 0.0777 0.0015	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C137 H140 H141 H+40	-0.1257 0.0874 -0.1464 -0.1464 -0.1416 -0.15191 0.0627 -0.1156 -0.1156 -0.1034 -0.1034 -0.1034 -0.1034 -0.1520 0.0515 0.1520 0.1761 0.1399 0.4752 0.4752 0.1761 0.1399 0.4752 0	H145 H146 H147 H148 H150 H151 H151 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C154 C164	0.1794 0.1468 0.1468 0.1172 0.1172 0.1170 0.1800 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1661 0.1661 0.1661 0.1661 0.1661 0.1661 0.1664	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H185 H186 H187 H188 H189 H187	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1455 0.1841 0.1566 0.1349 0.1777 0.1778 0.1399 0.1401 0.1339 0.1339
$\begin{array}{c}z = \\ \hline 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \\ H15 \\ H16 \\ H17 \\ H18 \\ H19 \\ H20 \\ H21 \\ H22 \\ \end{array}$	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367 -0.2433 0.3179 -0.2980 0.3122 0.32227 0.9989 0.1000 0.1034 0.0987 0.09887 0.09887 0.09887 0.1137 0.1146	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H35 H36 H37 H38 H39 H40 O41 C42 C43 O41 C42 C43 O41 C45 C45 C45	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0604 0.0561 -0.5499 0.1023 0.0927 0.0927 0.0929 0.0951 0.0929 0.0951 0.0951 0.05280 -0.5280 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5540 -0.5559 -0.5550 -0.5559 -0.5550 -0.5550 -0.5559 -0.55500 -0.55500 -0.55500 -0.55500 -0.55500 -0.55500 -0.55500 -0.55500 -0	C49 C50 C51 C52 C53 C54 C55 C56 C56 C56 C56 H59 H60 H61 H62 H63 H64 H65 D66 C67 C67 C68 D69 C70	-0.1537 -0.0622 -0.0510 -0.0665 -0.06659 -0.0650 -0.1484 0.1132 0.1134 0.1132 0.1138 0.1138 0.1138 0.1421 -0.4753 0.0699 -0.5035 0.0620	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H86 H81 H82 H86 H87 H88 H89 C90 H91 C92 H93 C94	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1652 0.1661 -0.1047 0.1206 0.1220 0.222	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 H109 C110 C111 H112 C113 H114 C115 C116 C116 C116 C116 C117 C118 C110 C101 C101 C101 C101 C101 C101	-0.1044 -0.1124 0.0223 -0.1114 0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0307 -0.1110 0.1198 0.0338 -0.1041 0.1252 -0.1390 0.0777 0.3001 -0.1395 -0.0780 -0.1031	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H1412	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1026 -0.1026 -0.1026 -0.1026 -0.1607 -0.1586 -0.1586 -0.1586 0.0931 -0.1515 0.0931 -0.1515 0.0939 -0.1515 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0931 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.1555 0.0935 -0.155 -0.1555 -0.155	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C165 C165 C165 C165 C165	0.1794 0.1488 0.1486 0.1472 0.1172 0.1170 0.1800 0.1734 0.1800 0.1734 0.1528 0.0841 -0.1294 0.1561 -0.4072 0.1460 0.1563 0.1563 0.1841 -0.1474 0.1563 0.1841 -0.1474 0.1563 0.1841 -0.1716 0.0753 -0.1068	C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 H180 H181 H181 H181 H184 H185 H186 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H187	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1452 0.1454 0.1546 0.1349 0.1777 0.1778 0.1818 0.1339 0.1401 0.1838 0.1401 0.1339
$\begin{array}{c}z=\\ 01\\ C2\\ C3\\ 04\\ C5\\ C6\\ 07\\ C8\\ C9\\ C10\\ S111\\ C12\\ S13\\ H14\\ H15\\ H16\\ H17\\ H18\\ H19\\ H20\\ H21\\ H22\\ H23\\ H22\\ H23\\ H23\\ H23\\ H23\\ H23$	$\begin{array}{c} 18.75 \\ -0.5336 \\ -0.5346 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2830 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ 0.0987 \\ 0.1137 \\ 0.1146 \\ 0.1281 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C43 O44 C43 C46 C46 C47	$\begin{array}{c} -0.3276\\ 0.2626\\ -0.2950\\ -0.1555\\ 0.2815\\ 0.0756\\ -0.5159\\ 0.6661\\ 0.0661\\ 0.1023\\ 0.0927\\ 0.0927\\ 0.0929\\ 0.0951\\ 0.0956\\ -0.5280\\ 0.0951\\ 0.0956\\ -0.5280\\ 0.0864\\ -0.5104\\ 0.0619\\ 0.0186\\ 0.0086\\ 0.008\\ 0.0086\\ 0.0086\\ 0.0086\\ 0$	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68 069 C70 C71	-0.1537 -0.0622 -0.0510 -0.0659 -0.0659 -0.0655 -0.1484 0.1132 0.1134 0.1121 0.1121 0.1121 0.1121 0.1121 0.1121 0.1128 0.1128 0.1128 0.1421 0.04753 0.0629 -0.6035 0.0620 0.0629	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H85 H86 H85 H86 H85 H86 H87 H88 H89 C90 H91 C92 H93 C94 C94 C95	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.1000 0.2039 0.1603 0.1541 0.1541 0.1579 0.1754 0.1652 0.1651 0.1652 0.1665 0.1665 0.1665 0.1665 0.1620 0.1272 0.3214 0.3214 0.3214	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119	-0.1044 0.1124 0.0293 0.0429 0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0399 -0.1140 0.0399 -0.1118 0.0399 -0.1118 0.0399 -0.1118 0.0399 -0.1140 0.0777 0.3001 0.0777 0.3001 0.0770 -0.1395 0.0780 -0.1031	C121 C122 C123 C124 C126 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C135 C136 C137 C138 C139 C139 H140 H141 H142 H143	-0.1257 0.0874 -0.1464 -0.1464 -0.1591 0.0627 -0.1156 -0.1591 0.0627 -0.1156 -0.1637 -0.1034 -0.1034 -0.1034 -0.1229 0.0931 -0.1515 0.1520 0.1761 0.1399 0.1530 0.1822	H145 H146 H147 H148 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C166 C167	$\begin{array}{c} 0.1794\\ 0.1488\\ 0.1486\\ 0.147\\ 0.1486\\ 0.1170\\ 0.1800\\ 0.1774\\ 0.1800\\ 0.1734\\ 0.1528\\ 0.1830\\ 0.0841\\ -0.1294\\ 0.1563\\ 0.0841\\ -0.4072\\ 0.1460\\ -0.4072\\ 0.1460\\ -0.4774\\ 0.1563\\ 0.1841\\ -0.1763\\ -0.1753\\ -0.1067\\ \end{array}$	C169 C170 H171 H172 C173 N174 C175 C176 C176 C177 C178 C177 C178 H181 H182 H183 H184 H185 H186 H187 H188 H189 H191	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 0.1841 0.1841 0.1845 0.1841 0.1566 0.1349 0.1777 0.1778 0.1399 0.1401 0.1389 0.1774 0.1354
$\begin{array}{c}z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ S11 \\ C12 \\ S13 \\ H14 \\ H15 \\ H16 \\ H17 \\ H18 \\ H19 \\ H20 \\ H21 \\ H22 \\ H23 \\ H24 \end{array}$	$\begin{array}{c} 18.75 & A \\ \hline 0.0349 \\ 0.0686 \\ 0.0723 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ 0.0988 \\ 0.1137 \\ 0.1146 \\ 0.1281 \\ 0.1291 \end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.6604 0.1083 0.1023 0.0951 0.0955 0.0957 0.0955 0.0957 0.0955 0.0957 0.0957 0.0955 0.0957 0.0955 0.00550 0.00550 0.00550 0.00550 0.005500000000	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H64 H65 C67 C68 C67 C68 C69 C70 C71 C72	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0652\\ -0.0659\\ -0.0659\\ -0.0659\\ -0.1132\\ 0.1132\\ 0.1132\\ 0.1132\\ 0.1132\\ 0.1132\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1421\\ -0.4753\\ 0.0619\\ -0.6039\\ -0.6375\\ \end{array}$	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H84 H85 H84 H85 H86 H87 H88 H87 H88 H87 H88 H89 C90 H91 C92 H93 C94 C95 H96	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1000 0.3230 0.2039 0.1603 0.1641 0.1579 0.1652 0.1652 0.1661 -0.1047 0.1124 0.3214 -0.1206 0.1221 0.3214	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 C110 C111 H112 C113 H114 C115 C116 H117 C118 H117 C120	$\begin{array}{c} -0.1044\\ -0.1124\\ 0.0293\\ 0.0429\\ -0.1114\\ 0.1214\\ 0.1114\\ 0.1214\\ 0.0307\\ -0.1140\\ 0.0307\\ -0.1140\\ 0.0308\\ -0.0141\\ 0.0338\\ -0.1041\\ 0.1252\\ -0.1390\\ 0.0770\\ 0.3001\\ -0.1395\\ 0.0780\\ -0.1031\\ 0.1252\\ \end{array}$	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1026 -0.1026 -0.1026 -0.1607 -0.1656 0.0931 -0.1550 0.0931 0.1550 0.1550 0.1550 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1550 0.1551 0.0931 0.1551 0.0931 0.1551 0.0931 0.1555 0.0931 0.1555 0.0931 0.1550 0.0931 0.1550 0.1550 0.0931 0.1550 0.1550 0.0931 0.1550 0.0931 0.1550 0.0931 0.1550 0.0931 0.1550 0.1550 0.0931 0.1550 0.0931 0.1550 0.0931 0.1550 0.0931 0.1550 0.0931 0.1550 0.1550 0.0931 0.1550 0.1550 0.0931 0.1550 0.1550 0.1550 0.0931 0.1550 0.1	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C166 C167 C168	$\begin{array}{c} 0.1794\\ 0.1468\\ 0.1486\\ 0.1472\\ 0.1172\\ 0.1170\\ 0.1800\\ 0.1774\\ 0.1580\\ 0.1379\\ 0.1528\\ 0.0841\\ -0.1294\\ 0.0841\\ -0.1294\\ 0.1561\\ -0.460\\ -0.1474\\ 0.1563\\ -0.1463\\ 0.1841\\ -0.1716\\ 0.0753\\ -0.1068\\ -0.1068\\ -0.1068\\ -0.0754\\ \end{array}$	C169 C170 Hi71 Hi72 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H184 H185 H186 H187 H188 H189 H190 Total	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1445 0.1492 0.1455 0.1481 0.1546 0.1349 0.1777 0.11818 0.1399 0.1401 0.1383 0.1777 0.11838 0.1772
z = 01 C2 C3 04 C5 C6 07 C8 C9 07 C10 S111 C12 S133 H14 H15 H16 H17 H18 H19 H21 H22 H24 H22 H24 H22 H24 H22 H24 H22 H24 H25 H24 H25 H24 H25 H26 H26 H26 H26 H26 H26 H26 H26	$\begin{array}{c} 18.75 \ \ A\\ \hline\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1009\\ 0.1039\\ 0.1009\\ 0.1039\\ 0.10041\\ 0.0987\\ 0.0987\\ 0.1137\\ 0.09889\\ 0.1137\\ 0.1146\\ 0.1281\\ 0.1291\\ 23.27 \ \ A\end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48	-0.3276 0.2626 0.2626 0.2815 0.2815 0.07559 -0.5559 -0.5649 0.1023 0.0927 0.0927 0.0927 0.0927 0.0927 0.09251 0.09551 0.09551 0.0586 -0.5286 -0.5104 0.0586 -0.5104 0.0136 -0.5104 0.0136 -0.5104 0.0136 -0.5104 0.0136 -0.5104 0.0136 -0.5104 0.0135 -0.5104 0.0135 -0.5104 0.0135 -0.5104 0.0135 -0.5104 0.0155 -0.5105 -0.5159 -0.559 -0	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H69 H60 H61 H62 H63 H64 H65 O66 C67 C68 O69 C70 C71 O72	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0659\\ -0.0507\\ -0.0659\\ -0.1484\\ 0.1132\\ 0.1132\\ 0.1134\\ 0.1120\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1418\\ 0.04753\\ 0.0019\\ -0.5035\\ 0.0620\\ 0.0369\\ -0.5375\end{array}$	H73 H74 H75 H76 H77 H78 H77 H80 H81 H83 H84 H83 H84 H85 H86 H85 H86 H87 H88 H89 C90 H91 C92 H93 C94 C95 H96	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1641 0.1579 0.1736 0.1652 0.1652 0.1661 0.1672 0.1661 0.1206 0.21272 0.3214 -0.1206 0.1261	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H109 C110 C111 H112 C113 H114 C115 C116 H117 C120	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0309 -0.1140 0.0399 -0.1110 0.1188 0.0338 -0.1041 0.1252 -0.1395 0.0777 0.3001 0.30000000000	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144	-0.1257 0.0874 -0.1464 -0.1496 -0.1416 -0.1591 0.0627 -0.1156 -0.1156 -0.1156 -0.1229 0.1586 -0.1229 0.0331 -0.1515 0.1520 0.0331 -0.1515 0.1520 0.0331 -0.1515 0.1520 0.0331 -0.1515 0.1520 0.0331 -0.1515 0.0331 -0.1515 0.0331 -0.1515 0.0331 -0.1515 0.0331 -0.1515 0.0331 -0.1515 0.1522 0.1551 0.1522 0.1551 0.1522 0.1551 0.1522 0.1551 0.1522 0.1551 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1555 0.1552 0.1555 0.1552 0.	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C166 C167 C168	$\begin{array}{c} 0.1794\\ 0.1486\\ 0.1486\\ 0.1172\\ 0.1170\\ 0.1800\\ 0.1734\\ 0.1528\\ 0.1528\\ 0.1634\\ -0.1294\\ 0.563\\ 0.0841\\ -0.294\\ 0.1563\\ 0.1847\\ -0.472\\ 0.1563\\ 0.1841\\ -0.1716\\ 0.0753\\ -0.1067\\ -0.1067\\ 0.0784\\ \end{array}$	C169 C170 H171 H172 C173 N174 C175 C176 C176 C177 C178 H180 H181 H182 H183 H184 H185 H186 H187 H188 H189 H191 Total	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0811 0.1546 0.1345 0.1345 0.1345 0.1345 0.1346 0.1356 0.1777 0.1778 0.1359 0.1401 0.1388 0.1774 0.1354 4.0000
z = 01 C2 C3 04 C5 C6 07 C10 S11 C12 C3 C6 07 C10 S11 C12 C12 C3 C4 C5 C6 C9 C10 C12 C12 C12 C12 C12 C12 C12 C12	$\begin{array}{c} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 C32 C33 C32 C33 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 C45 C48	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5159 0.0664 0.1023 0.0561 0.1023 0.0956 -0.5280 0.0951 0.0951 0.0951 0.0951 0.0584 -0.5280 0.0584 -0.5104 0.0584 -0.5104 0.0136 -0.4860 0.4151	C49 C50 C51 C52 C53 C54 C56 C56 C57 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68 D66 C67 C68 D66 C71 C71 C72	-0.1537 -0.0622 -0.0510 -0.0662 -0.0662 -0.0659 -0.1484 0.1121 0.1132 0.1134 0.1121 0.1138 0.1138 0.1138 0.1421 -0.4763 0.0019 0.0693 -0.5035 -0.0620 0.0369 -0.5375	H73 H74 H75 H76 H77 H78 H77 H78 H77 H80 H81 H82 H83 H84 H85 H85 H85 H85 H85 H87 H88 H89 C30 H91 C32 C94 C35 H96 H73	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.000 0.3230 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1661 -0.1044 0.1124 -0.1206 0.1221 0.3214 -0.1261	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 H119 C120 C97	-0.1044 -0.1124 0.0293 -0.1124 0.0429 -0.1114 0.1140 0.1048 0.0307 -0.1140 0.1048 0.0393 -0.1140 0.10939 -0.1110 0.1198 0.0393 -0.1041 0.1252 -0.1395 0.3001 -0.1395 0.3001 -0.1283 0.3001 -0.1285 0.3035 0.0789 0.0789 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0785 0.0778 0.0778 0.0778 0.0778 0.0777 0.0778 0.00780 0.00780 0.00780 0.00780 0.00780 0.00780000000000	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C136 C137 H140 H141 H142 H143 H144 C121	-0.1257 0.0874 -0.1464 0.1496 -0.416 -0.416 -0.627 -0.1156 -0.1026 -0.1026 -0.1026 -0.1026 -0.10586 -0.4152 0.0931 -0.1580 0.1520 0.1520 0.1520 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1556 0.1550 0.1556 0.1550 0.1556 0.1556 0.1556 0.1550 0.1556 0.1556 0.1550 0.1556 0.1550 0.1550 0.1556 0.1550 0.1550 0.1556 0.1550 0.1556 0.1550 0.1550 0.1556 0.1550 0.1550 0.1556 0.1550 0.1	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145	0.1794 0.1488 0.1486 0.1472 0.1172 0.1170 0.1800 0.1800 0.1379 0.1528 0.0841 -0.1294 0.0841 -0.1294 0.1561 -0.4472 0.1460 -0.1474 0.1684 -0.1716 0.0753 -0.1068 -0.1068 -0.0784	C169 C170 H171 C173 N174 C175 C176 C176 C177 C178 C179 H180 H181 H182 H183 H183 H183 H185 H186 H187 H188 H187 H189 H190 H190 H190 H190 H190 H190 H190 H19	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1482 0.1485 0.1481 0.1566 0.1349 0.1777 0.1482 0.1384 0.1374 0.1374 0.1374 0.14010000000000
$\begin{array}{c} z = \\ 01 \\ 12 \\ C3 \\ 04 \\ C5 \\ 07 \\ C6 \\ 07 \\ C9 \\ 010 \\ 011 \\ 11$	$\begin{array}{c} 18.75 \ \mbox{A} \\ \hline -0.5336 \\ 0.0349 \\ 0.0686 \\ 0.0349 \\ 0.0686 \\ 0.0517 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2433 \\ 0.3179 \\ -0.2433 \\ 0.3179 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ 0.0989 \\ 0.1137 \\ 0.1041 \\ 0.0987 \\ 0.0989 \\ 0.1137 \\ 0.1146 \\ 0.1281 \\ 0.1291 \\ 23.27 \ \mbox{A} \\ \hline -0.5279 \\ 0.0329 \\ \end{array}$	C25 S26 C27 C28 S29 C30 C32 C32 C32 C32 C33 C32 C33 C34 H35 H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.07559 -0.5159 0.0664 0.1023 0.0927 0.0927 0.09251 0.0927 0.09251 0.09251 0.09254 -0.5280 -0.5280 -0.5584 -0.5104 0.0136 -0.4860 0.4150 0.0136	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H62 H63 H64 H65 O66 C67 C68 O67 C70 C71 C49 C50	-0.1537 -0.0622 -0.0510 -0.0663 -0.06659 -0.0659 -0.1484 0.4201 0.1132 0.1134 0.1120 0.1138 0.1138 0.1138 0.1138 0.1138 0.1421 0.0699 -0.6055 0.0620 0.0629 -0.5375	H73 H74 H75 H76 H77 H78 H77 H78 H77 H78 H80 H81 H82 H83 H84 H85 H85 H86 H85 H86 H85 H86 H87 H91 C92 H91 C92 H93 C94 C95 H96 H73 H74	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1663 0.1541 0.1579 0.1562 0.1652 0.1652 0.1652 0.1652 0.1652 0.1652 0.1652 0.1206 0.1272 0.3214 -0.1206 0.3214 -0.1206 0.1221	C97 H98 C99 C100 C101 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0399 -0.1140 0.0399 -0.1110 0.1198 0.0338 -0.1041 0.1252 -0.1395 0.0777 0.3001 -0.1263 0.126	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C137 C138 C139 C139 C134 C141 C122 C121 C122	-0.1257 0.0874 -0.1464 -0.1464 -0.1464 -0.1591 0.0627 -0.1156 -0.1156 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1586 -0.1586 0.0931 0.1510 0.1522 0.1819 -0.1836 0.0917	H145 H146 H147 H147 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 C164 C166 C167 C168 H145 H145 H146	0.1794 0.1488 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.1330 0.1379 0.1528 0.13830 0.0841 -0.1294 0.1561 0.0841 -0.1294 0.1563 0.1563 0.1741 -0.1758 -0.1067 0.0758 -0.1067 0.0754	C169 C170 H171 H172 C173 C176 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184 H183 H184 H185 H186 H187 H188 H189 H190 H191 Total Total C169 C170	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1485 0.1841 0.1566 0.1349 0.1777 0.1777 0.1777 0.1399 0.1401 0.1838 0.1792 0.1354 4.0072 0.1354
$\begin{array}{c} z = \\ 01 \\ 1 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ 07 \\ C12 \\ S13 \\ H14 \\ H15 \\ H16 \\ H17 \\ H14 \\ H19 \\ H20 \\ H21 \\ H22 \\ H23 \\ H22 \\ H22 \\ H22 \\ H22 \\ H22 \\ C1 \\ C2 \\ C3 \\ C3 \\ C3 \\ C3 \\ C3 \\ C3 \\ C3$	$\begin{array}{c} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 031 C32 C32 C33 N34 H35 H35 H36 H37 H37 H37 H37 H40 041 C42 C43 044 C45 C46 047 C48	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5499 0.0661 0.1023 0.0929 0.0951 0.0956 -0.5280 0.0951 0.0584 -0.5104 0.0584 -0.4860 0.4151	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68 C68 C69 C70 C71 D72	-0.1537 -0.0622 -0.0510 -0.0662 -0.0662 -0.0659 -0.1484 0.1221 0.1132 0.1134 0.1121 0.1138 0.1138 0.1138 0.1421 -0.4753 0.0639 -0.5035 -0.0620 0.0369 -0.5375	H73 H74 H75 H76 H77 H78 H77 H78 H80 H81 H82 H83 H82 H83 H84 H85 H85 H86 H87 H88 H87 H87 H88 H87 H87 H91 C90 H91 C90 H91 C92 H93 C95 H96 H73 H75	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.3230 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1661 -0.1047 0.1124 -0.1206 0.1221 0.1224 -0.1206 0.1261	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1044 0.1124 0.0223 0.0429 -0.1140 0.1216 0.1140 0.1048 0.0307 -0.1140 0.0307 -0.1140 0.0398 -0.1041 0.0388 -0.1041 0.0388 -0.1041 0.0328 -0.1390 0.0780 0.3001 -0.1395 0.0780 0.0782 -0.1031 0.1253 0.1532 -0.1072 0.0129	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H142 C121 C122 C123 C121 C121 C122 C123 C124 C124 C124 C127 C128 C126 C126 C126 C126 C126 C126 C126 C126	-0.1257 0.0874 -0.1464 0.1496 -0.416 -0.416 -0.416 -0.627 -0.1166 -0.1026 -0.1026 -0.1026 -0.1026 -0.1026 -0.1026 0.0931 -0.1520 0.1520 0.1520 0.1520 0.1520 0.1520 0.1520 0.1530 0.1520 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1530 0.1550 0.15	H145 H146 H147 H148 H149 H151 H155 H155 H155 C156 C156 C156 C166 C167 C168 H165 C166 C166 C167 C168 H145 H145 H145 H145 H147	0.1794 0.1488 0.1486 0.1472 0.1172 0.1170 0.1800 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1683 0.1460 -0.1474 0.1668 -0.14716 0.0753 0.1068 -0.1076 0.0784	C169 C170 H171 H172 C173 N174 C175 C176 C176 C177 C178 H180 H180 H180 H182 H183 H183 H183 H185 H185 H185 H185 H185 H187 H189 H190 H190 H190 H191 Total	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1485 0.14841 0.1566 0.1349 0.1777 0.11818 0.1374 0.1401 0.1374 0.1401 0.1434 0.1772 0.1167 -0.1121 0.1121
$\begin{array}{c} z = \\ 01 \\ 12 \\ C3 \\ 04 \\ c5 \\ c6 \\ 07 \\ c8 \\ c9 \\ c10 \\ c12 \\ c12 \\ c13 \\ c12 \\ c13 \\ c14 \\ c1$	$\begin{array}{c} 18.75 \ \ A\\ \hline 0.0339\\ 0.0686\\ 0.0349\\ 0.0686\\ 0.0507\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2433\\ 0.3179\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1000\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.0988\\ 0.1137\\ 0.1146\\ 0.1281\\ 0.0987\\ 0.0988\\ 0.1137\\ 0.1146\\ 0.1281\\ 0.0987\\ 0.0329\\ 0.0686\\ 0.5799\\ 0.0686\\ -0.5649\end{array}$	C25 S26 C27 C28 S29 C30 031 C32 C32 C33 034 H35 H36 H37 H38 H39 H40 041 H37 H38 H39 C42 C43 C42 C43 C44 C42 C43 C44 C42 C43 C44 C42 C44 C44 C44 C44 C44 C44 C44 C44	-0.3276 0.2626 -0.2950 -0.2815 0.2815 0.2815 0.0561 -0.5159 0.0664 0.1023 0.0927 0.0927 0.0927 0.0927 0.0927 0.0921 0.0927 0.0924 -0.5280 0.0441 0.0584 -0.5104 0.0136 -0.5104 0.0136 -0.3543 -0.3086 0.3543 -0.3086	C49 C50 C51 C52 C53 C54 C56 C57 C56 C56 C57 H59 H60 H61 H62 H63 H64 H64 H65 C67 C70 C71 C72 C49 C50 C50 C51 C52 C52 C54 C54 C54 C55 C54 C55 C55 C55 C55 C55	-0.1537 -0.0622 -0.0510 -0.0663 -0.06659 -0.0659 -0.1484 0.1132 0.1134 0.1120 0.1134 0.1120 0.1138 0.1418 0.1138 0.1418 0.1418 0.1421 0.0699 -0.5375 -0.5375 -0.5582 -0.5575	H73 H74 H75 H76 H77 H79 H80 H81 H82 H83 H84 H85 H84 H85 H86 H87 H88 H87 H88 H87 H89 C90 H91 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76 H77	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.2039 0.1663 0.1579 0.1579 0.1652 0.1655 0.1655 0.1655 0.1655 0.1655 0.1655 0.1274 0.1206 0.21206 0.21206 0.21206 0.21216 0.22120000000000	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C197 H98 C97 H98 C97	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0399 -0.1140 0.0399 -0.1140 0.1988 -0.1041 0.1522 -0.1395 0.0777 0.3001 -0.1395 0.0701 0.1263 0.1523 -0.1012 0.0102	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C137 C138 H140 H141 H142 H143 H144 H144 H144 H144 H144 H144 H144	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1591 0.0627 -0.1156 -0.1156 0.0637 -0.1034 -0.1024 -0.1024 -0.1024 -0.1229 0.1586 -0.1520 0.1586 0.0931 -0.1515 0.1520 0.1522 0.1589 0.1522 0.1535 0.1522 0.1546 0.0931 0.1522 0.1546 0.0931 0.1522 0.1546 0.0917 0.1526 0.0917 0.0917 0.1546 0.0917 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0917 0.1546 0.0157 0	H145 H146 H147 H147 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C166 C167 C168 H145 H145 H145 H145 H145 H145	0.1794 0.1488 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.1330 0.1379 0.1528 0.1331 0.0841 -0.1294 0.1561 0.1563 0.1563 0.1563 0.1716 0.072 0.1474 0.1563 0.1741 0.1716	C169 C170 H171 C173 C173 C173 C176 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H185 H186 H187 H187 H190 H191 Total C169 C170 H171	-0.1082 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777 0.1778 0.1399 0.1777 0.1778 0.1339 0.1401 0.1838 0.1701 0.1838 0.1792 0.1354 4.0000 -0.1167 -0.1121 0.1147
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 04 \\ 07 \\ 07 \\ 08 \\ 07 \\ 08 \\ 07 \\ 08 \\ 07 \\ 08 \\ 07 \\ 08 \\ 07 \\ 08 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 331 C32 C33 C33 C33 C33 C33 C33 C33 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5499 0.0661 0.1023 0.0929 0.0951 0.0956 -0.5280 0.0951 0.0584 -0.5404 0.0584 -0.5404 0.0584 -0.4860 0.4151	C49 C50 C51 C52 C53 C54 C55 C56 C56 C56 C56 C56 H59 H61 H62 H64 H64 H64 H64 C67 C70 C58 O69 C70 C71 D72 C51 C72 C72	-0.1537 -0.0622 -0.0510 -0.0662 -0.0662 -0.0659 -0.1484 0.1121 0.1132 0.1134 0.1121 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.0019 0.0699 -0.5375 -0.0550 -0.0550 -0.0551 -0.0554 -0.0555 -0.1124 -0.0555 -0.0555 -0.0555 -0.0555 -0.1124 -0.01124 -0.01124 -0.0055 -0.0555 -0.0555 -0.1124 -0.01128 -0.01128 -0.0019 -0.0555 -0.055	H73 H74 H75 H776 H777 H779 H81 H81 H82 H83 H84 H85 H86 H85 H86 H87 H88 H87 H87 H87 H87 H87 H89 C30 H91 H87 H89 C30 H91 H87 H87 H73 H74 H75 H76 H77 H77 H77 H77 H77 H77 H779 H779 H	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.02039 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1661 -0.1074 0.1124 -0.1206 0.1124 0.1226 0.1261 0.1261	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H107 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100	-0.1044 0.1124 0.0223 0.0429 -0.1140 0.1216 0.0307 -0.1140 0.0307 -0.1140 0.0393 -0.1255 -0.1390 0.0719 -0.1255 -0.1390 0.07195 -0.1255 -0.1255 -0.1390 0.07195 -0.1255 -0.1255 -0.1390 0.0725 -0.1252 -0.1255 -0.1255 -0.1255 -0.1390 0.0725 -0.1252 -0.1252 -0.1255 -0.1	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C129 C130 C131 C132 C133 C133 C134 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 C124 C127 C128 C126 C126 C126 C126 C127 C128 C126 C126 C127 C128 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C130 C130 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C131 C132 C133 C134 C135 C136 C137 C136 C137 C138 C136 C137 C138 C137 C138 C139 C130 C131 C132 C138 C139 C136 C137 C138 C137 C138 C139 C136 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	-0.1257 0.0874 -0.1464 0.1496 -0.416 -0.416 -0.416 -0.627 -0.1166 -0.1026 -0.1026 -0.1026 -0.1026 -0.1026 -0.1026 -0.1026 0.0331 -0.1520 0.1	H145 H146 H147 H148 H149 H151 H155 H155 H155 C156 C156 C156 C156 C166 C161 H163 C164 H163 C166 C166 C166 C166 C166 C166 H145 H145 H145 H145 H145 H145 H145 H145	0.1794 0.1488 0.1486 0.1470 0.1170 0.1170 0.1800 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 0.1460 -0.1474 0.1563 0.14716 0.0753 0.1474 0.1563 0.1841 -0.0754	C169 C170 H171 C173 N174 C175 C176 C176 C177 C178 H180 H180 H180 H182 H183 H183 H183 H185 H185 H185 H185 H187 H188 H189 H190 H191 Total	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1485 0.1484 0.1549 0.1777 0.1188 0.1388 0.1777 0.1188 0.1401 0.1388 0.1777 0.1167 -0.1167 -0.1121 0.1171 -0.1171
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 04 \\ 05 \\ 05 \\ 05 \\ 05 \\ 05 \\ 05 \\ 05$	$\begin{array}{c} 18.75 \ \mbox{A} \\ \hline -0.536 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ 0.0989 \\ 0.1041 \\ 0.0987 \\ 0.0989 \\ 0.1041 \\ 0.0987 \\ 0.1041 \\ 0.0987 \\ 0.11281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.329 \\ 0.0686 \\ -0.5049 \\ 0.0712 \\ 0.0727 \\ 0.0712 \\ 0.0727 \\ 0.0722 \\ 0.0628 \\ -0.5049 \\ 0.0712 \\ 0.0722 \\ 0$	C25 S26 C27 C28 S29 C30 C31 C32 C33 C32 C33 C33 H36 H36 H37 H38 H39 H40 O41 H40 O41 C42 C43 C44 C45 C46 C48 C48 C27 C28 C32 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	-0.3276 0.2626 -0.2950 -0.2815 0.2815 0.2815 0.0664 0.5651 -0.5159 0.0664 0.1023 0.1023 0.1023 0.1023 0.0927 0.0951 0.0929 0.0951 0.0929 0.0951 0.0929 0.0951 0.0925 0.0441 0.0136 -0.5104 0.0136 -0.4860 0.0136 -0.4853 -0.2483 -0.24	C49 C50 C51 C52 C53 C54 C55 C55 C55 C55 C57 H58 H59 H60 H61 H62 H63 H64 H65 H65 D66 C67 C70 C71 2 C49 C50 C52 C52 C53 C74 C74 C74 C75 C75 C75 C75 C75 C75 C75 C75 C75 C75	-0.1537 -0.0622 -0.0510 -0.0663 -0.06659 -0.0650 -0.1484 0.1132 0.1134 0.1120 0.1138 0.11138 0.1413 0.1128 0.1138 0.1413 0.1421 0.0699 -0.5620 0.0669 -0.5574 -0.0574 -0.0574 -0.0574 -0.0574 -0.0574 -0.0650	H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H81 H82 H81 H84 H85 H86 H87 H88 H88 H89 H88 H89 H89 H89 H89 H89 H89	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.2039 0.1653 0.2039 0.1654 0.1579 0.1652 0.1652 0.1655 0.1655 0.1655 0.1651 0.1206 0.3214 -0.1206 0.3214 -0.1206 0.3214 0.1443 0.1443 0.1106 0.1106 0.1106 0.1106	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H109 C111 H112 C115 C116 H117 C118 H119 C118 H119 C197 H98 C97 H98 C100 C100 C100 C100	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1240 -0.1140 0.1048 0.0307 -0.1140 0.1048 -0.1140 0.0307 -0.1140 0.10198 -0.11198 0.0338 -0.1041 0.1390 0.0338 -0.1395 0.3000 -0.1395 0.3001 -0.1395 0.3001 -0.1395 0.3001 -0.1263 0.1523 -0.1072 0.0448 -0.1121 0.0222 0.0448 -0.1121 -0.1283 -0.1123 -0.1121 -0.1283 -0.1123 -0.1121 -0.1283 -0.1123 -0.1123 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1121 -0.1283 -0.1128 -0.1283 -0.1128 -0.1285 -0.	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C137 C138 C139 H140 H141 H142 H143 H143 H142 H143 H143 H143 H143 H143 H143 H143 H143	-0.1257 0.0874 -0.1464 0.1464 -0.1591 0.0627 -0.1156 -0.1156 -0.1156 -0.1156 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1024 -0.1550 0.1550 0.1550 0.1550 0.1550 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.1522 0.1550 0.0917 0.1550 0.0917 0.1550 0.0917 0.1550 0.0917 0.1550 0.0917 0.1550 0.0917 0.1462 0.146	H145 H146 H147 H147 H149 H150 H151 H152 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C167 C168 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	0.1794 0.1488 0.1486 0.1172 0.1170 0.1800 0.1774 0.1800 0.1734 0.1583 0.0841 -0.1294 0.1561 -0.4072 0.1464 0.1561 -0.4072 0.1563 0.01563 0.01741 0.1563 0.01741 0.1684 0.01741 0.1714 0.1741 0.1741	C169 C170 H171 C173 C173 C173 C176 C176 C177 C178 C177 H180 H181 H182 H183 H184 H185 H185 H185 H186 H187 H187 H187 H187 H190 H191 Total C169 C170 H171 C169 C170 H171 Total	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1841 0.1566 0.1349 0.1777 0.1778 0.1788 0.1339 0.1777 0.1778 0.1339 0.1401 0.1339 0.1401 0.1334 4.0000 4.0001 0.1167 -0.1121 0.1147 0.1171 -0.1104
z = 01 C2 C3 C5 C6 C7 C3 C9 01 C12 C3 C12 C3 C12 C3 C12	$\begin{array}{c} 18.75 \ \ A\\ \hline \\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1667\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.0989\\ 0.1136\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.5279\\ 0.0329\\ 0.0329\\ 0.5549\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.042\\ 0.042\\ 0.042\\ 0.0422\\ 0.042\\ 0.$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H36 H37 H38 H36 H37 H38 H36 H37 C43 C43 O41 C43 C43 O44 C45 S26 C27 C27 C28 S26 C27 C28 C30 C30 C30 C30 C30 C30 C30 C30 C30 C30	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0551 -0.5159 0.0664 0.1023 0.0661 0.1023 0.0956 0.1023 0.0951 0.0956 -0.5280 0.0951 0.0951 0.0951 0.0951 0.0951 0.0951 0.0644 0.0649 0.04151 -0.4854 -0.4853 -0.4425	C49 C50 C51 C52 C52 C55 C56 C56 C56 C57 H59 H60 H61 H62 H63 H64 H65 C67 C70 C68 C71 072 C71 072 C51 C51 C52 C53 C71 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	-0.1537 -0.0622 -0.0651 -0.0662 -0.0662 -0.0665 -0.1484 0.1121 0.1132 0.1134 0.1121 0.1120 0.1138 0.1138 0.1138 0.1138 0.1418 0.4421 -0.4753 0.0019 0.0639 -0.5375 -0.0654 -0.0654 -0.0654	H73 H74 H75 H76 H77 H78 H81 H81 H81 H83 H84 H85 H83 H84 H85 H86 H87 H88 H89 H83 C30 H93 C34 C39 H93 H74 H75 H75 H77 H77 H77 H77 H77 H77 H77 H77	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.1001 0.3230 0.2039 0.1603 0.1603 0.1603 0.1661 0.1652 0.1661 0.1736 0.1661 0.1272 0.3214 -0.1206 0.1261 0.1261	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C100 C1010 C101 H119 C120	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0308 -0.1400 0.0398 -0.1140 0.0398 -0.1140 0.0398 -0.1041 0.1252 -0.1390 0.0777 0.3001 -0.1532 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 0.1252 -0.1031 -0.1252 -0.1552 -0.1552	C121 C122 C123 C124 N125 C126 C127 C128 C127 C129 C130 C131 C132 C133 C133 C133 C133 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C124 C124 C125 C126 C126 C126 C126 C126 C127 C128 C126 C126 C127 C128 C126 C126 C127 C128 C126 C126 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C130 C130 C130 C131 C132 C133 C132 C133 C132 C133 C132 C136 C137 C138 C136 C137 C138 C136 C137 C138 C137 C138 C139 C130 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C139 H140 H141 H142 H142 C126 C127 C128 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C128 C137 C128 C128 C128 C128 C127 C128 C128 C128 C128 C127 C128 C128 C128 C128 C128 C128 C128 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4161 -0.627 -0.1156 -0.1021 0.0627 -0.1156 -0.1021 0.0637 -0.1026 -0.1021 0.026 -0.1607 -0.1617 -0.1515 0.1520 0.1520 0.1520 0.1520 0.1520 0.1520 0.1520 0.1539 -0.1627 -0.1647 -0.1541 -0.1520 0.15200 0.15200 0.15200 0.15	H145 H146 H147 H148 H149 H150 H151 H155 C156 C157 C158 N159 C160 C161 H163 C166 H163 C166 H163 C166 H145 H145 H145 H145 H148 H149 H150 H145 H148 H149 H150 H145 H148 H149 H150 H145 H146 H147 H148 H149 H150 H150 H146 H147 H148 H149 H150 H150 H165 H146 H147 H148 H147 H148 H147 H148 H147 H148 H147 H148 H149 H150 H151 H152 H165 H165 H165 H165 H165 H165 H165 H165	0.1794 0.1468 0.1468 0.1475 0.1170 0.1800 0.1800 0.1734 0.1528 0.0841 -0.1294 0.1551 0.1830 0.0841 -0.1561 0.1651 0.1460 0.1561 0.1461 0.0753 -0.1068 -0.1068 -0.1073 0.0784 0.1741 0.1418 0.0753 0.1741 0.1741 0.1741 0.1767	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H180 H180 H182 H183 H183 H183 H185 H185 H185 H187 H188 H187 H188 H189 H190 C169 C170 C169 C170 H171 Total	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1485 0.1484 0.1549 0.1487 0.1349 0.1777 0.1349 0.1777 0.1349 0.1777 0.1349 0.1774 0.1774 0.1782 0.1354 4.0000
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 04 \\ 05 \\ 05 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07$	$\begin{array}{c} 18.75 \ \mbox{A} \\ \hline 0.6349 \\ 0.06349 \\ 0.0686 \\ 0.0349 \\ 0.0686 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ -0.2980 \\ 0.3179 \\ 0.3227 \\ 0.0999 \\ 0.1000 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ 0.0987 \\ 0.0988 \\ 0.1137 \\ 0.1146 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.1281 \\ 0.0686 \\ -0.5049 \\ 0.0712 \\ 0.0632 \\ -0.5141 \\ \end{array}$	C25 C25 C27 C28 C28 C28 C28 C28 C28 C28 C28 C28 C30 C31 C32 C33 C33 C34 H35 H36 H37 H40 O41 C42 C43 C43 C44 C45 C48 C48 C25 C28 C30 C31 C32 C32 C32 C33 C33 C33 C33 C33 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0604 0.0561 -0.5159 0.0661 0.1023 0.1023 0.0927 0.0927 0.0929 0.0951 0.0929 0.0951 0.0951 0.0951 0.0584 -0.5104 0.0136 -0.4450 0.0136 -0.3433 -0.2433 -0.1425 0.3447 0.06853	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H65 H66 C67 C70 C77 C68 C57 C70 C71 C49 C50 C52 C55 C56 C56 C57 C77 C72 C56 C57 C77 C77 C77 C77 C77 C77 C77 C77 C77	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0652\\ -0.0659\\ -0.0507\\ -0.0659\\ -0.1484\\ 0.1122\\ 0.1134\\ 0.1120\\ 0.1120\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1138\\ 0.1418\\ 0.0119\\ 0.0699\\ -0.5075\\ -0.0659\\ -0.0574\\ -0.0650\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0661\\ -0.06652\\ \end{array}$	H73 H74 H75 H76 H77 H78 H81 H81 H82 H83 H84 H85 H87 H88 H84 H85 H86 H87 H88 H89 H89 H89 H89 H89 H89 H89 H89 H89	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.2039 0.1603 0.2039 0.1653 0.1652 0.1652 0.1652 0.1652 0.1652 0.1652 0.1206 0.1221 0.3214 -0.1206 0.1221 0.1443 0.1261 0.1443 0.1106 0.1112 0.1106 0.1106	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H109 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C120 C100 C101 H102 C103	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.124 0.0429 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.1110 0.1198 0.0338 -0.1041 0.1038 -0.1041 0.0339 -0.1395 0.0777 0.0777 0.0131 0.1522 -0.1019 0.0222 0.0446 0.1131 0.0222	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C136 C137 C138 C137 C138 C137 C124 C121 C122 C123 C124 C121 C122 C122 C123 C124 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C126 C127 C128 C127 C128 C130 C130 C131 C132 C133 C132 C133 C133 C134 C135 C136 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C137 C138 C122 C127 C128 C127 C128 C127 C128 C127 C128 C127 C127 C128 C127 C128 C127 C127 C127 C127 C127 C127 C127 C127	-0.1257 0.0874 -0.1464 0.1496 -0.1591 0.0627 -0.1156 -0.1156 -0.1156 -0.1034 -0.1034 -0.1024 -0.1024 0.1586 -0.1229 0.1586 -0.1515 0.0931 -0.1550 0.1520 0.1530 0.1520 0.1530 0.1522 0.1819 -0.1336 -0.1336 -0.1336 -0.13462 0.0947 -0.1462 0.0463 -0.1462 0.0648 -0.1462	H145 H146 H147 H147 H149 H150 H151 H153 H154 H155 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C166 C166 C166 C166 C166 H145 H145 H145 H145 H145 H145 H145 H145	$\begin{array}{c} 0.1794\\ 0.1486\\ 0.1486\\ 0.1486\\ 0.147\\ 0.1172\\ 0.1170\\ 0.1800\\ 0.1774\\ 0.1580\\ 0.1379\\ 0.1528\\ 0.0841\\ -0.1294\\ 0.0841\\ -0.1294\\ 0.1561\\ -0.4072\\ 0.1461\\ -0.4474\\ 0.1563\\ 0.0753\\ -0.1067\\ 0.0784\\ -0.1067\\ 0.0784\\ -0.1067\\ 0.0784\\ -0.1067\\ 0.0784\\ -0.1067\\ 0.0784\\ -0.1067\\ 0.0784\\ -0.1078\\ -0.1078\\ -0.1078\\ -0.1078\\ -0.1078\\ -0.1780\\ -0.$	C169 C170 H171 C173 C173 C176 C176 C176 C177 C178 C177 H180 H181 H182 H183 H184 H185 H185 H185 H186 H187 H187 H188 H187 H190 H191 Total C169 C170 H171 C173 N174 C175	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1451 0.1841 0.1566 0.1349 0.1777 0.1778 0.1349 0.1777 0.1778 0.1339 0.1401 0.1838 0.1401 0.1838 0.1401 0.1514 -0.1121 0.1147 0.1171 -0.1104 -0.1157
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \ A\\ \hline \\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1667\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1039\\ 0.0987\\ 0.0329\\ 0.0527\\ 0.0529\\ 0.0512\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0422\\ -0.5141\\ 0.0877\\ \end{array}$	C25 S26 C27 C28 S29 C30 C31 C32 C33 C33 H36 H37 H37 H38 H39 H40 Q41 H37 H38 H39 Q44 C42 C43 C44 C44 C44 C44 C44 C44 C44 C44 C44	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0551 -0.5159 0.0664 0.1023 0.0654 0.1023 0.0956 0.1023 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0951 0.0956 0.04151 0.0956 0.04151 -0.3086 0.3543 -0.2433 -0.1425 0.3447 0.0665 -0.5163 0.0676	C49 C50 C51 C52 C52 C53 C54 C55 C56 C56 H59 H60 H61 H59 H60 H61 H64 H65 C67 C70 C68 C71 D72 C51 C51 C52 C53 C54 C51 C51 C52 C55 C55 C55 C55 C55 C55 C55 C55 C55	-0.1537 -0.0622 -0.0652 -0.0662 -0.0662 -0.0665 -0.1484 0.1121 0.1120 0.1124 0.1121 0.1120 0.1128 0.1138 0.1138 0.1138 0.1418 0.1411 0.1421 -0.6035 0.0620 -0.5375 -0.1582 -0.0654 -0.0654 -0.0654	H73 H74 H75 H76 H77 H78 H81 H81 H81 H83 H84 H85 H83 H84 H85 H86 H87 H88 H88 H89 H93 C34 C30 H91 H73 H74 H75 H77 H77 H77 H80	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1001 0.1001 0.3230 0.2039 0.1603 0.1603 0.1661 0.1652 0.1661 0.1736 0.1661 0.1272 0.3214 -0.1206 0.1261 0.1261 0.1261 0.1261	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0308 -0.1400 0.0393 -0.1140 0.0393 -0.1140 0.0393 -0.1140 0.0393 -0.1041 0.1252 -0.1390 0.0770 -0.1721 -0.1252 -0.1051 0.0222 0.0446 -0.1251 -0.1251 0.0222 0.0446 -0.1251 0.0222 0.0446 -0.1251 0.1251 -0.1251 0.0222 0.0446 -0.1251 0.0222 0.0446 -0.1251 0.0222 0.0446 -0.1251 0.0222 0.0446 -0.1251 0.0222 0.0456 -0.1251 0.0222 0.0456 -0.1251 0.0222 0.0456 -0.1251 0.0252 -0.1251 -0.1252 -0.1253 -0.1255 -0.1255 -0.1255 -0.1255 -0.1255 -0.1555 -0.1555 -	C121 C122 C123 C124 N125 C126 C127 C128 C127 C129 C130 C131 C132 C133 C133 C133 C133 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C126 C127 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4169 -0.4169 -0.4161 0.0627 -0.1156 -0.1021 -0.028 -0.1024 -0.1026 -0.1026 -0.1657 -0.1026 -0.1657 -0.1269 0.0931 -0.1520 0.1520 0.1520 0.1520 0.1520 0.1529 -0.1336 0.0122 0.1819 -0.1336 0.0124 -0.1201	H145 H146 H147 H148 H149 H150 H151 H155 C156 C156 C156 C156 C156 C156 C156 C	0.1794 0.1488 0.1486 0.1486 0.1170 0.1170 0.1800 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 0.1651 0.1460 0.1561 0.1653 0.1841 -0.1068 -0.1068 -0.1073 0.0784 0.1741 0.1741 0.1741 0.1741 0.1767 0.1767 0.1767	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H180 H180 H182 H183 H182 H183 H183 H185 H185 H185 H187 H188 H187 H185 H189 H190 C170 C170 C173 N174 C175 C176 C176 C176 C176 C177 C178 C177 C178 C179 C177 C178 C179 C177 C178 C177 C178 C177 C178 C177 C178 C179 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C178 C177 C177	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1484 0.1549 0.1485 0.1349 0.1777 0.1349 0.1777 0.1349 0.1777 0.1539 -0.121 -0.167 -0.1121 0.1171 -0.1667 -0.1121 0.1171 -0.1667 -0.1241
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 04 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07$	$\begin{array}{c} 18.75 \ \ A\\ \hline 0.6336\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1041\\ 0.0987\\ 0.1041\\ 0.0987\\ 0.1041\\ 0.0987\\ 0.1041\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.0686\\ -0.5049\\ 0.0677\\ -0.5141\\ 0.0877\\ -0.5141\\ 0.0877\\ -0.5146\end{array}$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 C43 C43 C44 C45 C46 C43 C45 C48 C27 C28 S29 C30 O31 C32 C33 C33 C33 C33 C33 C33 C33 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.07559 -0.5159 0.0664 0.0561 -0.5499 0.00561 0.0227 0.0927 0.0951 0.0927 0.0951 0.0959 0.0951 0.0959 0.0951 0.0959 0.0951 0.0951 0.0584 -0.5104 0.0136 -0.4125 -0.3066 0.3543 -0.2483 -0.2483 -0.2483 -0.5163 0.0676 0.0676	C49 C50 C51 C52 C53 C54 C55 C56 C57 C57 H58 H60 H61 H62 H63 H64 H65 D66 C70 C71 C50 C71 C50 C71 C50 C72 C53 C54 C55 C55 C55 C55 C55 C55 C55 C55 C57 C57	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0652\\ -0.0659\\ -0.0659\\ -0.0659\\ -0.1484\\ 0.1122\\ 0.1132\\ 0.1132\\ 0.1132\\ 0.1132\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1421\\ -0.4753\\ 0.0609\\ -0.5375\\ -0.0650\\ -0.0574\\ -0.0650\\ -0.0674\\ -0.0660\\ -0.0674\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0652\\ -0.1524\\ 0.0552\\ -0.1524\\ 0.0552\\ -0.1524\\ 0.0512\\ -0.1524\\ -0.0652\\ -0.1524\\ -0.0552\\ -0.1524\\ -0.0552\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.1524\\ -0.052\\ -0.$	H73 H74 H75 H76 H77 H78 H81 H81 H81 H84 H85 H83 H84 H85 H84 H85 H84 H85 H84 H85 H87 H88 H89 C30 C34 C34 C34 C34 C34 C34 H74 H77 H78 H77 H78 H81 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H79 H80 H81 H84 H85 H78 H84 H85 H78 H84 H85 H78 H84 H85 H86 H87 H78 H84 H85 H86 H87 H78 H84 H85 H86 H87 H78 H84 H85 H86 H87 H78 H84 H85 H87 H78 H84 H85 H86 H87 H78 H84 H85 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H87 H86 H87 H87 H86 H87 H86 H87 H87 H86 H87 H86 H87 H86 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H87 H87 H87 H87 H87 H87 H87 H87	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.1603 0.2039 0.1603 0.2039 0.1631 0.1579 0.1652 0.1652 0.1652 0.1661 0.1272 0.3214 -0.1206 0.1221 0.3214 -0.1206 0.1439 0.1106 0.1439 0.1106 0.1112 0.1106 0.1112 0.1106	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H109 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C100 C101 H102 C103 H102 C103 H104	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.124 0.0429 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.1041 0.0328 -0.1041 0.1252 -0.1395 0.0777 0.0777 0.1031 0.1253 -0.1031 0.1253 -0.1019 0.0222 0.0446 -0.1131 0.1253 -0.1019 0.0222	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C136 C137 C136 C137 C138 C139 H140 H141 H142 H143 H144 H143 H144 C121 C122 C123 C124 C127 C128 C129 C120 C127 C128 C129 C120 C127 C128 C129 C120 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C130 C130 C130 C131 C132 C130 C131 C132 C132 C132 C132 C132 C132 C132	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1591 0.0627 -0.1591 0.0637 -0.1034 -0.1034 -0.1022 0.1586 -0.1229 0.0931 -0.1550 0.1520 0.1530 0.1520 0.1530 0.1520 0.1530 0.1522 0.1336 -0.1336 -0.1336 -0.1462 0.0941 -0.1462 0.0941 -0.1462 0.0941 -0.1462 0.0947 -0.1462 0.0948 -0.1209 -0.1462 0.0948 -0.1209 -0.1462 0.0948 -0.1209 -0.1462 0.0948 -0.1201 -0.1209 -0.1209 -0.1462 0.0948 -0.1201 -0.1201 -0.1209 -0.1201 -0.1202 -0	H145 H146 H147 H148 H149 H150 H151 H153 H154 H153 C156 C157 C158 C157 C158 C160 C161 H163 C164 C165 C166 C167 C168 H146 H147 H148 H149 H151 H151 H151 H153	$\begin{array}{c} 0.1794\\ 0.1486\\ 0.1486\\ 0.1486\\ 0.147\\ 0.1172\\ 0.1170\\ 0.1800\\ 0.1774\\ 0.1580\\ 0.1379\\ 0.1528\\ 0.0841\\ -0.1294\\ 0.0841\\ -0.1294\\ 0.1561\\ -0.4072\\ 0.1461\\ -0.4072\\ 0.1563\\ -0.1067\\ 0.1563\\ -0.1067\\ 0.0783\\ -0.1067\\ 0.0784\\ -0.1716\\ 0.0783\\ -0.1067\\ 0.1741\\ 0.1176\\ 0.1741\\ 0.1248\\ 0.1776\\ 0.1780\\ 0.1770\\ 0.1780\\ 0.167\\ 0.1607\\ 0.1607\\ 0.1780\\ 0.167\\ 0.1607\\ 0.1607\\ 0.1607\\ 0.1607\\ 0.1607\\ 0.1608\\ 0.1760\\ 0.1760\\ 0.161\\ 0.1248\\ 0.1760\\ 0.1607\\ 0.$	C169 C170 H171 C173 C173 C173 C176 C176 C177 C178 C177 H180 H181 H182 H183 H184 H185 H186 H185 H186 H185 H186 H187 H189 H190 H191 Total C169 C170 H171 C173 H172 C173 H172 C173 H175 C176 C177 C177 C177 C177 C177 C177 C177	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1455 0.1455 0.1455 0.1455 0.1455 0.1456 0.1339 0.1777 0.1778 0.1818 0.1339 0.1471 0.1818 0.1344 0.1777 -0.1121 0.1167 -0.1121 0.1167 -0.11537 -0.1537 -0.1537 -0.1537 -0.1544
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \ A\\ \hline \\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1281\\ 0.0987\\ 0.0329\\ 0.3227\\ A\\ \hline \\ -0.5279\\ 0.0329\\ 0.5527\\ 0.0329\\ 0.5527\\ 0.0329\\ 0.5527\\ 0.0329\\ 0.5549\\ 0.0712\\ 0.0422\\ -0.5141\\ 0.0877\\ -0.1360\\ \hline \\ 0.1261\\ \hline \\ 0.0422\\ -0.5141\\ 0.0877\\ -0.1360\\ \hline \\ 0.2406\\ \hline \end{array}$	C25 S26 C27 C28 S29 C30 C31 C32 C33 C33 C33 H35 H35 H37 H38 H39 C43 C45 C45 C45 C45 C45 C45 C27 C28 S29 C30 O31 C32 C32 C33 C34 C32 C33 C34 C32 C32 C33 C32 C33 C32 C33 C33 C34 C32 C33 C34 C32 C33 C34 C32 C33 C34 C32 C33 C34 C35 C35 C35 C35 C35 C35 C35 C35 C35 C35	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0551 -0.5159 0.0664 0.1023 0.0956 0.1023 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0956 0.0951 0.0956 0.0951 0.0956 0.04151 -0.5280 0.04151 -0.3864 -0.4151 -0.3863 -0.4151 -0.3863 -0.44151	C49 C50 C51 C52 C52 C53 C54 C55 C56 C57 H59 H60 H61 H61 H64 H65 C67 C71 D72 C49 C50 C71 D72 C51 C52 C53 C54 C55 C55 C55 C55 C55 C55 C55 C55 C55	-0.1537 -0.0622 -0.0652 -0.0662 -0.0662 -0.0665 -0.1484 0.1121 0.1121 0.1121 0.1121 0.1128 0.1138 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.0603 -0.6505 -0.5375 -0.0654 -0.0571 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0571 -0.0654 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0554 -0.0571 -0.0554 -0.0571 -0.0554 -0.0571 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0555 -0.1554 -0.0554 -0.0554 -0.0554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.1554 -0.0555 -0.	H73 H74 H75 H76 H77 H78 H87 H81 H81 H81 H83 H84 H85 H83 H84 H85 H86 H87 H88 H88 H89 H81 C30 C34 H93 C34 C30 H91 H73 H74 H75 H76 H77 H78 H77 H78 H80 H77 H77 H78 H77 H77 H77 H78 H80 H77 H77 H77 H77 H77 H77 H77 H77 H77 H7	0.1479 0.1474 0.102 0.1474 0.1105 0.1105 0.1105 0.1001 0.1001 0.3230 0.2039 0.2039 0.1603 0.1603 0.1661 0.1652 0.1661 0.1726 0.1661 0.1124 -0.1206 0.1221 0.1221	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C108 H107 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0308 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.0328 -0.1390 0.0370 -0.1390 0.0770 -0.1532 -0.1051 0.0229 0.0229 -0.1051 0.0229 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1552 -0.1552	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C126 C126 C126 C127 C128 C126 C127 C128 C129 C130 C121 C121 C122 C123 C124 C129 C130 C130 C130 C130 C130 C130 C130 C130	-0.1257 0.0874 -0.1464 0.1496 -0.4161 -0.1691 0.0627 -0.1156 -0.1131 0.0627 -0.1156 -0.1021 -0.1026 -0.1026 -0.1026 -0.1652 0.0391 -0.1520 0.0570 0	H145 H146 H147 H148 H149 H151 H155 C156 C156 C156 C156 C156 C156 C156 C	$\begin{array}{c} 0.1794\\ 0.1468\\ 0.1468\\ 0.1468\\ 0.1472\\ 0.1172\\ 0.1170\\ 0.1800\\ 0.1800\\ 0.1734\\ 0.1800\\ 0.1734\\ 0.1800\\ 0.0841\\ -0.1294\\ 0.1631\\ 0.1641\\ -0.4772\\ 0.1683\\ 0.1641\\ -0.1763\\ 0.1841\\ -0.1763\\ 0.0784\\ \hline 0.1741\\ 0.1418\\ 0.0773\\ 0.0784\\ \hline 0.1741\\ 0.1418\\ 0.1767\\ 0.1767\\ 0.1767\\ 0.1617\\ 0.1617\\ 0.1647\\ \hline 0$	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H180 H182 H183 H183 H183 H183 H184 H185 H185 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1619 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1485 0.1484 0.1549 0.1777 0.1349 0.1777 0.1349 0.1777 0.1349 0.1777 0.1349 0.1774 0.1774 0.1774 0.1774 0.1167 -0.1121 0.1167 -0.1121 0.1171 0.1171 -0.1604
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07$	$\begin{array}{r} 18.75 \ \ A\\ \hline 0.6336\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1000\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.1041\\ 0.0987\\ 0.1041\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.0686\\ -0.5049\\ 0.0712\\ 23.27 \ \ A\\ \hline -0.5279\\ 0.0329\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0877\\ -0.1360\\ -0.2406\\ 0.3762\\ \end{array}$	C25 S26 C27 C28 S29 C30 C30 C32 C32 C33 C32 C33 C34 H35 H39 H36 H37 H36 H37 C41 C42 C43 C45 C45 C48 C45 C48 C27 C28 C30 C32 C33 C32 C33 C32 C33 C32 C33 C32 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0604 0.0561 -0.5159 0.0664 0.1023 0.0927 0.0951 0.0927 0.0951 0.0927 0.0951 0.0959 0.0951 0.0959 0.0951 0.0959 0.0951 0.0951 0.0951 0.0951 0.0136 -0.5104 0.0136 -0.4125 -0.4125 -0.4283 -0.4125 -0.4283 -0.4255 -0.5163 0.0676 -0.5518 0.0476 -0.5518	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C77 C70 C71 C72 C50 C71 C50 C71 C52 C52 C52 C55 C56 C65 C65 C65 C65 C65 C65 C57 C57 C57 C57 C57 C57 C57 C57 C57 C5	$\begin{array}{c} -0.1537\\ -0.0622\\ -0.0510\\ -0.0652\\ -0.0659\\ -0.0659\\ -0.0659\\ -0.1484\\ 0.1132\\ 0.1132\\ 0.1134\\ 0.1132\\ 0.1134\\ 0.1132\\ 0.1138\\ 0.1138\\ 0.1138\\ 0.1418\\ 0.1421\\ -0.4753\\ 0.0699\\ -0.5075\\ -0.0659\\ -0.0574\\ -0.0660\\ -0.0574\\ -0.0652\\ -0.1582\\ -0.0652\\ -0.1582\\ -0.0652\\ -0.1582\\ -0.0652\\ -0.1582\\ -0.0652\\ -0.1582\\ -0.0652\\ -0.0574\\ -0.0652\\ -0.0574\\ -0.0652\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.0552\\ -0.1582\\ -0.055\\ -0.055\\ -0.05$	H73 H74 H75 H76 H77 H78 H81 H81 H81 H84 H85 H83 H84 H85 H83 H84 H85 H83 H84 H85 H83 H84 H85 H83 C34 C34 C34 C34 C34 C34 H81 H91 H74 H75 H76 H77 H78 H81 H83 H77 H78 H81 H82 H78 H81 H83 H78 H81 H81 H81 H81 H81 H81 H81 H81 H81 H8	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2039 0.2039 0.1603 0.2039 0.1631 0.1579 0.1652 0.1652 0.1652 0.1661 0.1206 0.1206 0.1206 0.1221 0.1206 0.1221 0.1206 0.1221 0.1261 0.1273 0.1261 0.1273 0.1261 0.1273 0.1261 0.1273 0.1261 0.1273 0.1261 0.1273 0.1261 0.1274 0.1274 0.1261 0.1274 0.1261 0.1261 0.1274 0.1261 0.1272 0.1261 0.1261 0.1272 0.1261 0.1261 0.1272 0.1261 0.1261 0.1261 0.1262 0.1261 0.1261 0.1262 0.1261 0.1261 0.1261 0.1261 0.1261 0.1261 0.1262 0.1261 0.	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C106 H107 C108 H109 C106 H107 C108 H117 C118 H119 C120 C97 H98 C99 C100 C100 C101 H102 C103 H104 C105 C106 H107 C105 C106 H107	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.124 0.0429 -0.1140 0.0429 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.1041 0.0328 -0.1041 0.0328 -0.1041 0.1252 -0.1395 0.0777 0.0777 0.1031 0.1552 -0.1072 0.0119 0.0222 0.0416 -0.1131 0.1252 -0.1072 0.0416 0.0417 -0.1230 0.0417 -0.1230 0.0437 -0.1282 0.0307 -0.1282 0.0307 -0.1282	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H143 H144 H144 H144 H144 H144 H144 H144	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1034 -0.0637 -0.1034 -0.0637 -0.1034 -0.1607 -0.4152 0.1586 -0.1515 0.0931 -0.1550 0.1520 0.1530 0.1520 0.1530 0.1522 0.1612 -0.11336 0.0917 -0.1462 0.0917 -0.1462 0.0948 -0.1462 0.0648 -0.1295 0.0648 -0.1295 0.0648 -0.1295 0.0648 -0.1295 0.06670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.0670 -0.1295 0.06670 -0.1295 0.0670 -0.1295 0.06670 -0.1295 0.06670 -0.1295 -0.1	H145 H146 H147 H147 H147 H151 H155 H155 H155 C156 C157 C158 C166 C167 C168 H163 C164 C166 C166 C166 C166 C166 C166 H145 H145 H145 H145 H145 H151 H155	0.1794 0.1486 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 -0.4072 0.1460 0.1563 0.1460 0.0753 -0.1464 0.0753 -0.1068 -0.1716 0.0784 0.1741 0.1741 0.1780 0.1770 0.1780	C169 C170 H171 C173 C173 C173 C176 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H185 H186 H187 H189 H190 H191 Total C169 C170 H171 Total C173 H172 C173 H172 C173 H172 C173 H172 C175 C176 C177 C178 C177 C178 C177 C178 C177 C178 C170 H171 H172 C173 H172 H180 H190 H171 H172 H180 H190 H171 H180 H181 H182 H182 H182 H182 H183 H182 H183 H182 H183 H182 H183 H182 H183 H182 H183 H184 H185 H186 H187 H187 H187 H187 H187 H187 H187 H187	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1445 0.1445 0.1445 0.1445 0.1349 0.1777 0.1778 0.1818 0.1339 0.1477 0.1818 0.1339 0.1471 0.1554 4.0000 -0.1167 -0.1121 0.1167 -0.1121 0.1167 -0.11537 0.1537 -0.1423 0.0941 0.0941 -0.1423
$\begin{array}{c} z = \\ 01 \\ 02 \\ 03 \\ 04 \\ 05 \\ 07 \\ 07 \\ 08 \\ 07 \\ 07 \\ 08 \\ 07 \\ 07$	$\begin{array}{c} 18.75 \ \ A\\ \hline\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1039\\ 0.0987\\ 0.0987\\ 0.09889\\ 0.1137\\ 0.1146\\ 0.1281\\ 0.0987\\ 0.0329\\ 0.0329\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0422\\ -0.5141\\ 0.0877\\ -0.1360\\ 0.3762\\ -0.3078\\ \end{array}$	C25 S26 C27 C28 S29 C30 C31 C32 C33 C31 C32 C33 C33 H35 H36 H37 H38 H39 O41 H38 H39 O44 C42 C45 C45 C46 C45 C27 C28 S29 C30 O31 C32 C32 C32 C33 C33 C32 C33 C33 C32 C33 C32 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0551 -0.5159 0.0664 0.1023 0.0956 0.1023 0.0929 0.0951 0.0956 0.0299 0.0951 0.0956 0.0299 0.0951 0.0956 0.0414 0.0669 0.04151 -0.5280 0.0619 0.01366 -0.4151 -0.3086 0.3543 -0.1425 0.3447 0.0685 -0.5438 -0.5425 -0.5455 -0.5425 -0.5455 -0.55555 -0.55555 -0.55555 -0.55555 -0.55555 -0.55555	C49 C50 C52 C52 C53 C54 C55 C56 C56 H59 H60 H61 H64 H65 H64 H64 H65 C67 C71 C72 C71 C72 C51 C51 C52 C53 C54 C55 C56 C55 C56 C57 C71 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	-0.1537 -0.0622 -0.0652 -0.0662 -0.0662 -0.0665 -0.1484 0.1121 0.1121 0.1121 0.1121 0.1128 0.1138 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.1421 -0.4753 0.0620 -0.6505 -0.5375 -0.0654 -0.0571 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0571 -0.0654 -0.0654 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0555 -0.0	H73 H74 H75 H76 H77 H78 H87 H81 H81 H81 H83 H84 H85 H83 H84 H85 H86 H87 H88 H88 H89 H81 C30 C34 H93 C34 C30 H91 H73 H74 H75 H76 H77 H78 H80 H77 H79 H80 H81 H77 H79 H80 H81 H79 H81 H79 H81 H79 H81 H77 H78 H77 H78 H81 H79 H81 H83 H84 H77 H78 H83 H79 H81 H83 H84 H77 H78 H83 H84 H77 H78 H81 H83 H84 H85 H84 H85 H84 H85 H85 H84 H85 H84 H85 H85 H85 H84 H85 H85 H84 H85 H85 H85 H85 H84 H85 H85 H84 H85 H85 H85 H85 H85 H85 H85 H85 H85 H85	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1001 0.1001 0.3230 0.2039 0.1603 0.1603 0.1661 0.1652 0.1661 0.1776 0.1124 -0.1206 0.1221 0.1221 0.1221 0.1439 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H101 C110 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C102 C103 C104 C105 C106 H104 C105 C106 H104	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0308 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.1252 -0.1390 0.0770 0.0770 -0.11532 -0.1051 0.0223 0.0252 -0.1251 0.0229 0.0229 -0.1251 0.0229 0.0229 -0.1251 0.0229 -0.1251 0.0229 -0.1251 0.0229 -0.1251 0.0229 -0.1251 0.0229 -0.1251 -0.1252 -0.1251 -0.1251 -0.1251 -0.1251 -0.1252 -0.1251 -0.1252 -0.1253 -0.1252 -0.1251 -0.1253 -0.1253 -0.1252 -0.1251 -0.1253 -0.1253 -0.1252 -0.1251 -0.1253 -0.1253 -0.1252 -0.1251 -0.1253 -0.1253 -0.1252 -0.1253 -0.1255 -0.1555	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C135 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C126 C126 C126 C127 C128 C126 C127 C128 C129 C130 C131 C132 C124 C135 C126 C127 C128 C135 C135 C136 C135 C136 C137 C138 C136 C137 C138 C137 C138 C139 C130 C131 C132 C137 C138 C136 C137 C138 C139 C130 C131 C132 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C137 C138 C139 C130 C131 C132 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C139 H140 C136 C137 C138 C139 H141 H142 H142 C126 C127 C128 C139 H141 C126 C127 C128 C139 H141 C126 C137 C138 C139 H141 C126 C127 C128 C139 H141 C126 C127 C128 C129 C128 C139 H141 C126 C127 C128 C128 C129 C128 C129 C128 C129 C128 C129 C128 C129 C128 C128 C128 C129 C128 C128 C128 C128 C128 C128 C128 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4161 -0.1691 0.0627 -0.1156 -0.1181 0.0627 -0.1185 -0.1026 -0.1026 -0.1026 -0.1621 0.1526 -0.1520 0.0391 -0.1520 0.0570 0	H145 H146 H147 H148 H149 H150 H151 H155 C156 C157 C158 N159 C160 C161 H163 C166 H163 C166 C166 C166 C166 C166 C166 H145 H145 H145 H145 H145 H145 H153 H154 H155 C156	0.1794 0.1488 0.1468 0.1468 0.1472 0.1172 0.1170 0.1800 0.1800 0.1800 0.1734 0.1528 0.1830 0.0841 -0.1293 0.1561 0.1661 0.1561 0.1561 0.1561 0.1561 0.0753 -0.1068 -0.1075 0.0784 0.1741 0.1741 0.1767 0.1767 0.1767 0.1617 0.1617 0.1617 0.1617	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H181 H182 H183 H183 H183 H183 H185 H185 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 N174 C176 C177 C178 C179 H180 H191 H191 H191 H191 H191 H191 H191 H19	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1619 -0.1312 0.0871 -0.1492 0.1485 0.1485 0.1485 0.1482 0.1482 0.1777 0.1818 0.1774 0.1399 0.1401 0.1838 0.1774 0.1782 0.1354 -0.167 -0.1121 0.1171 -0.1604 -0.1187 -0.1241 0.0941 -0.1488 0.17488 0.17488
z = 01 02 02 03 04 05 07 07 08 07 07 08 07 010 011 012 012 013 014 015 014 015 016 017 019 010 011 012 014 015 016 017 019 010 011 012 014 015 016 017 019 010 011 011 012 014 015 016 017 019 010 011 012 016 017 019 010 011 012 016 017 019 010 011 012 016 017 017 017 017 017 017 017 017	$\begin{array}{c} 18.75 \ \ A\\ \hline 0.5336\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1667\\ -0.2433\\ 0.3179\\ -0.2800\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1000\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.0987\\ 0.0988\\ 0.1137\\ 0.1146\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.327\\ A\\ -0.5279\\ 0.0329\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0686\\ -0.5049\\ 0.0712\\ 0.0329\\ -0.5279\\ 0.0329\\ -0.5279\\ 0.0329\\ -0.5279\\ 0.0329\\ -0.5279\\ 0.0329\\ -0.5279\\ 0.0329\\ -0.5279\\ -0.3762\\ -0.5141\\ 0.0877\\ -0.1360\\ -0.2406\\ 0.3762\\ -0.3078\\ -0.30762\\ -0.3078\\ -0.30762\\ -0.3078\\ -0.3078\\ -0.30762\\ -0.3078\\ -0.30762\\ -0.3078\\ -0.3078\\ -0.3076\\ -0.3078\\ -0.307$	C25 S26 C27 C28 S29 C30 C31 C32 C32 C33 C34 H35 H37 H36 H37 C42 C43 C43 C43 C43 C44 C43 C44 C45 C45 C46 C43 C45 C27 C27 C28 S29 C30 C33 C32 C33 C32 C33 C32 C33 C32 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.07816 -0.5159 0.0664 0.1023 0.0951 0.0956 -0.5280 0.0951 0.0955 -0.5280 0.0411 0.0581 0.0581 0.0581 0.0136 -0.4165 0.3843 -0.4125 -0.1428 0.3843 -0.1428 -0.5183 0.0647 6 0.3543 -0.4283 -0.1425 -0.15518 0.0476 -0.5518 0.0476 -0.5518 0.0476	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H65 D66 C67 C70 C70 C71 C72 C50 C70 C71 C72 C53 C54 C55 C55 C55 C56 C57 C57 C57 C57 C57 C57 C57 C57 C57 C57	-0.1537 -0.0622 -0.0510 -0.0652 -0.0659 -0.0659 -0.1484 0.1132 0.1132 0.1132 0.1132 0.1132 0.1138 0.1138 0.1138 0.1421 -0.4753 0.0629 -0.5035 0.0620 0.0650 -0.5650 -0.5650 -0.0552 -0.0654 -0.0655 -0.0654 -0.0655 -0.0655 -0.0659 -0.0559 -0	H73 H74 H75 H76 H77 H78 H81 H81 H82 H83 H84 H85 H83 H84 H85 H83 H84 H85 H83 H84 H85 H83 H84 H85 H87 H74 H75 H77 H76 H77 H77 H80 H81 H81 H81 H81 H81 H81 H81 H81 H81 H81	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1005 0.2039 0.2039 0.1603 0.2039 0.1603 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1661 0.1681 0.1206 0.1220 0.1221 0.1221 0.1221 0.1221 0.1221 0.1433 0.1108 0.1108 0.1108 0.1108 0.1108 0.1221 0.1221	C97 H98 C99 C100 C101 H104 C105 C106 C107 C108 H109 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C97 H98 C100 C100 C100 C100 C100 C100 C100 C103 H102 C105 C106 C107 C108	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.124 0.0429 -0.1140 0.0429 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.0418 0.0338 -0.1041 0.0328 -0.1041 0.1252 -0.1395 0.0770 0.0770 0.0780 -0.1395 0.0783 -0.1019 0.0252 -0.1019 0.0466 -0.1131 -0.1230 0.0466 -0.1231 -0.1230 0.0466 -0.1231 -0.1242 0.0466 -0.1231 -0.1242 0.0467 -0.1223 0.0307 -0.1282 0.0307 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 -0.1282 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307 0.0307	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C135 C136 C137 C138 C136 C137 C138 H140 H142 H143 H144 H142 C121 C122 C123 C124 N126 C126 C127 C128 C129 C130 C121 C122 C123 C124 C121 C122 C123 C133 C134 C135 C136 C137 C138 C136 C137 C138 C137 C138 C139 C130 C130 C137 C138 C139 C130 C130 C130 C137 C138 C139 C130 C130 C131 C132 C130 C137 C138 C139 C130 C130 C131 C132 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C137 C138 C139 C130 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C139 C137 C138 C129 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C127 C128 C129 C130 C131 C137 C138 C129 C130 C131 C137 C138 C137 C128 C129 C130 C131 C137 C138 C137 C138 C129 C130 C131 C137 C137 C138 C137 C137 C138 C129 C130 C137 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1026 -0.1026 -0.1027 -0.1026 -0.1657 -0.1026 -0.1550 0.0931 -0.1550 0.1520 0.1550 0.1550 0.1520 0.1530 0.1546 0.0947 -0.1546 0.0947 -0.1546 0.0947 -0.1546 0.0947 -0.1546 0.0648 -0.1250 0.0570 -0.1250 0.1550 0.1550 0.1540 0.1550 0.1	H145 H146 H147 H148 H149 H150 H151 H152 C156 C157 C158 C156 C161 H163 C164 C165 C166 C166 C166 C166 C166 H145 H146 H147 H148 H149 H149 H151 H155 C156 C156 C155	0.1794 0.1486 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.0841 -0.1294 0.1561 -0.4072 0.1460 0.1561 0.1460 0.1563 0.1460 0.0753 -0.1668 -0.1068 -0.10741 0.1780 0.1741 0.1780 0.1741 0.1780 0.1781 0.1780	C169 C170 H171 C173 C173 C173 C176 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H187 H188 H185 H186 H187 H189 H190 H191 Total C169 C170 H171 C173 N174 C175 C176 C177 C178 C177 C178 C177 C178 C177 H180 H191 H172 C177 C177 C178 C176 C177 C178 C176 C177 C178 C177 C178 H180 H191 H172 C176 C177 C178 H180 H171 H172 C177 C178 H180 H171 H182 H183 H182 H183 H184 H185 H185 H186 H187 H187 H187 H187 H187 H187 H187 H187	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1455 0.1455 0.1455 0.1451 0.1549 0.1777 0.1778 0.1818 0.1399 0.1477 0.15139 0.1477 0.1554 -0.1167 -0.1167 -0.1167 -0.1167 0.1537 -0.1231 0.0941 -0.1423 0.0941 -0.1423 0.1423
$\begin{array}{c} z = \\ 0 \\ 1 \\ 0 \\ 2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0$	$\begin{array}{c} 18.75 \ \ A\\ \hline \\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1367\\ -0.2433\\ 0.3179\\ -0.2800\\ 0.1367\\ -0.2433\\ 0.3179\\ -0.2800\\ 0.1322\\ 0.3227\\ 0.0999\\ 0.1000\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.1039\\ 0.1041\\ 0.0987\\ 0.11291\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.0329\\ 0.0329\\ 0.6686\\ -0.5049\\ 0.0712\\ 0.0422\\ -0.5141\\ 0.0877\\ -0.1360\\ -0.2406\\ 0.3762\\ -0.3078\\ 0.3603\\ 0.3942\\ \end{array}$	C25 S26 C27 C28 S29 C30 C32 C30 C32 C33 C32 C33 C32 C43 C43 C45 C46 C46 C46 C46 C46 C46 C46 C46 C46 C47 C48 C46 C47 C32 C30 C37 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0664 0.0664 0.1023 0.0929 0.0951 0.0929 0.0951 0.0929 0.0951 0.0929 0.0951 0.0929 0.0951 0.0951 0.0929 0.0551 0.0619 0.01366 -0.4151 -0.4151 -0.3086 0.3543 -0.4151 -0.3086 0.3543 -0.4151 -0.3086 0.3543 -0.4151 -0.3086 0.0676 0.0476 -0.51321 0.0676	C49 C50 C52 C52 C53 C54 C55 C56 C57 H59 H60 C67 H59 H60 H61 H64 H64 H65 C67 C71 C72 C59 C70 C71 C72 C51 C55 C56 C55 C56 C55 C56 C55 C55 C55 C55	-0.1537 -0.0622 -0.0510 -0.0662 -0.0669 -0.0665 -0.1484 0.1121 0.1132 0.1121 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.1421 -0.4753 0.0019 0.0669 -0.5375 -0.0550 -0.0571 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0574 -0.0554 -0.0571 -0.0554 -0.0571 -0.0554 -0.1524 -0.1100	H73 H74 H75 H76 H77 H78 H87 H81 H81 H81 H83 H84 H85 H84 H85 H84 H85 H86 H87 H88 H89 H81 H88 H89 H81 H88 H89 H93 C34 C34 H93 C34 C35 H96 H73 H74 H75 H76 H77 H78 H80 H77 H78 H80 H77 H78 H77 H78 H80 H77 H78 H77 H78 H80 H77 H78 H80 H77 H78 H77 H78 H80 H77 H78 H80 H77 H78 H80 H77 H78 H80 H77 H78 H80 H81 H83 H84 H85 H84 H85 H84 H85 H84 H85 H84 H85 H84 H85 H84 H85 H84 H85 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H78 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H78 H86 H87 H86 H87 H78 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H86 H87 H87 H86 H87 H86 H87 H86 H87 H86 H87 H87 H86 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H86 H87 H87 H87 H87 H86 H87 H87 H87 H87 H87 H87 H87 H87 H87 H87	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1001 0.1001 0.3230 0.2039 0.1603 0.1603 0.1603 0.1661 0.1736 0.1661 0.1736 0.1124 -0.1205 0.1221 0.1221 0.1221 0.1221 0.1109 0.1008 0.1008 0.1212 0.1439	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H101 C110 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H104 C105 H106	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 0.0337 -0.1140 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.1252 -0.1390 0.0777 0.3001 -0.1252 -0.1251 0.0229 0.0426 -0.1251 0.0229 0.0426 -0.1251 0.0229 0.0338 -0.1251 0.0229 -0.1251 0.0339 -0.1251 0.0329 -0.1251 0.0339 -0.1251 0.0329 -0.1251 0.0339 -0.1251 0.0359 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1251 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1252 -0.1551 -0.1	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C133 C133	-0.1257 0.0874 -0.1464 0.1496 -0.416 -0.1691 0.0627 -0.1156 -0.1627 -0.1156 -0.1627 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1316 0.1520 0.1520 0.1520 0.1520 -0.1531 -0.1336 -0.1621 -0.1336 -0.1621 -0.1336 -0.1621 -0.1622 -0.1633 -0.1622 -0.1622 -0.1632 -0.1625 -0.1625 -0	H145 H146 H147 H148 H149 H151 H155 C156 C157 C158 N159 C160 C161 H162 C166 H163 C164 H163 C164 H163 C164 H145 H145 H145 H145 H145 H145 H155 C156 C157 C157 C157	0.1794 0.1468 0.1462 0.1476 0.1170 0.1170 0.1800 0.1800 0.1739 0.1528 0.1830 0.0841 -0.1280 0.1651 0.1561 0.1561 0.1561 0.1561 0.1563 0.1563 0.0753 -0.1068 -0.1775 0.0784 0.1741 0.1784 0.17767 0.1784 0.1787 0.16177 0.1617 0.1617 0.1617	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H181 H182 H183 H184 H185 H189 H190 H191 Total C169 C170 C173 N174 C175 C176 C177 C178 C179 H191 H191 H191 H191 H191 H191 H191 H	-0.1082 -0.1089 -0.1069 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1451 0.1549 -0.1482 0.1485 0.1485 0.1482 0.1484 0.15349 0.1777 0.1818 0.1774 0.1399 0.1401 0.1818 0.1774 0.1537 -0.167 -0.167 -0.167 -0.167 -0.1637 -0.167 -0.1637 -0.167 -0.1637 -0.167 -0.16121 0.1648 -0.1637 -0.1488 0.1721 -0.1488 0.1488 0.1721 -0.1488 0.1480
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07$	18.75 Å -0.5336 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.5136 0.0891 -0.1367 -0.2433 0.3179 -0.2880 0.3122 0.3227 0.0999 0.1000 0.1039 0.1041 0.0987 0.0988 0.1137 0.1146 0.2281 0.1221 0.3227 0.0329 0.0329 0.0329 0.0329 0.0329 0.5279 0.3227 0.0329 0.0329 0.0329 0.5279 0.3227 0.0329 0.5279 0.3227 0.0329 0.5279 0.3227 0.0329 0.5279 0.3227 0.0329 0.5279 0.0329 0.05686 -0.5049 0.0712 0.5414 0.5279 0.0329 0.0587 -0.5441 0.5279 0.3276 0.5441 0.5279 0.3227 0.0329 0.0587 -0.5441 0.5442 -0.5441 0.5376 -0.5441 0.5422 -0.5441 0.5376 -0.5466 0.3762 -0.3078 0.3242 0.3242 0.3242 0.3242 0.3242 0.3376	C25 S26 C27 C28 S29 C30 C33 C32 C33 C32 C33 C33 C34 H35 H37 H38 H39 C42 C43 C43 C42 C43 C43 C42 C43 C42 C43 C42 C43 C42 C43 C42 C77 C43 C42 C77 C43 C42 C43 C43 C42 C43 C43 C42 C43 C43 C43 C43 C43 C43 C43 C43 C43 C43	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0756 0.0561 -0.5159 0.0664 0.1023 0.0956 0.1023 0.0927 0.0956 -0.5280 0.0411 0.0851 0.0956 -0.5280 0.0411 0.0584 -0.1125 0.0126 -0.4151	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H64 H65 D66 C67 C71 C72 C71 C72 C33 C54 C55 C57 C54 C52 C54 C52 C55 C54 C52 C55 C55 C57 C57 C57 C57 C57 C57 C57 C57	-0.1537 -0.0622 -0.0510 -0.0652 -0.0659 -0.0659 -0.1484 0.1132 0.1132 0.1132 0.1132 0.1132 0.1138 0.1138 0.1138 0.1421 -0.4201 0.1421 0.1421 0.0019 0.0699 -0.5035 0.0620 0.03699 -0.5375 -0.1582 -0.0650 -0.0574 -0.0650 -0.0574 -0.0652 -0.0554 -0.0650 -0.0574 -0.0652 -0.0554 -0.0652 -0.0554 -0.0650 -0.5574 -0.0652 -0.0557 -0.1582 -0.0650 -0.5574 -0.0652 -0.5574 -0.0652 -0.5574 -0.0652 -0.1522 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0557 -0.1552 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0554 -0.0555 -0.1552 -0.0559 -0.1552 -0.0559 -0.1552 -0.0559 -0.1552 -0.0559 -0.1552 -0.0559 -0.1552 -0.0559 -0.1552 -0.0559 -0.0557 -0.0559 -0.0557 -0.0577 -0.0557 -0.0557 -0.0557 -0.0577 -0.0557 -0.0557 -0.0557 -0.0577 -0.0557 -0.0577 -0.0557 -0.0577 -0.0557 -0.0557 -0.0557 -0.0557 -0.0557 -0.0557 -0.0557 -0.0	H73 H74 H76 H77 H78 H79 H80 H81 H81 H82 H83 H84 H85 H83 H84 H83 H84 H85 H86 H87 H78 H89 H74 H75 H86 H77 H76 H77 H76 H77 H77 H78 H77 H78 H78 H78 H78 H78 H78	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1000 0.2039 0.1603 0.2039 0.1603 0.1641 0.1579 0.1652 0.1652 0.1661 0.1661 0.1272 0.3214 -0.1206 0.1221 0.1221 0.1221 0.1433 0.1439 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1221 0.1439 0.1108 0.1221 0.1221 0.1221 0.1221 0.1221 0.1221 0.1221 0.1221 0.1433 0.1261 0.12210 0.12210 0.12210000000000	C97 H98 C99 C100 C101 H104 C105 C106 C107 C108 H104 C105 C106 C107 C108 H109 C111 H112 C113 H114 C115 C116 C117 C118 H117 C120 C97 H98 C97 H98 C100 C101 C102 C103 H104 C105 C108 H109 C110	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.124 0.0429 -0.1140 0.1047 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.041 0.0309 -0.1110 0.1252 -0.1395 0.0780 -0.1031 0.1252 -0.1031 0.0780 -0.1031 0.0780 -0.1031 0.0252 -0.1031 0.0252 -0.1031 0.0252 -0.1031 0.0252 -0.1031 0.0252 -0.1131 0.0252 -0.1282 0.0307 -0.1282 0.1295 0.1215 0	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C130 C131 C132 C133 C133 C133 C133 C136 C136 C137 C138 C139 H140 H141 H142 H144 H144 C121 C122 C123 C124 C126 C127 C128 C126 C127 C128 C131 C132 C133 H144 H144 H144 H144 H144 H144 H144 H	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1026 -0.1026 -0.1026 -0.1607 -0.1026 -0.1652 0.0931 -0.1550 0.0931 -0.1550 0.0931 -0.1550 0.1550 0.1550 0.1550 0.1550 0.1520 0.1530 0.1530 0.1493 -0.1463 -0.1463 0.0648 -0.1229 -0.1463 0.0648 -0.1257 0.06670 -0.1229 -0.1250 0.06670 -0.1250 0.0229 -0.1250 0.06670 -0.1250 0.0670 -0.1022 -0.1022 -0.1022 -0.1022 -0.1022 -0.1250 -0.1250 -0.1250 -0.1250 -0.1250 -0.1450 -0.1450 -0.1250 -0.1450 -0.1450 -0.1450 -0.1250 -0.1450 -0.1450 -0.1250 -0.1450 -0.	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 C160 C161 H163 C164 C165 C166 C166 C166 C166 C166 H145 H145 H145 H145 H145 H145 H145 H145	0.1794 0.1488 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.0841 -0.1294 0.1681 -0.460 -0.1460 -0.1461 0.0753 -0.1460 0.0754	C169 C170 H171 C170 H172 C173 N174 C175 C176 C177 C178 C177 C178 H180 H1812 H183 H184 H185 H186 H187 H188 H185 H186 H187 H189 H190 H190 H191 Total C169 C170 H171 C175 C176 C177 C178 C177 C177	-0.1082 -0.1089 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1455 0.1455 0.1451 0.1492 0.1451 0.1549 0.1777 0.1549 0.1339 0.1777 0.1519 0.1401 0.1339 0.1777 0.1167 0.1167 -0.1167 -0.1121 0.1171 0.1171 0.1171 0.1171 0.1171 0.1171 0.1171 0.1171 0.1164 -0.1121 0.0941 -0.1423 0.0941 -0.1423 0.1423 0.1423 0.1423
$\begin{array}{c} z = \\ 01 \\ 02 \\ 03 \\ 04 \\ 05 \\ 06 \\ 07 \\ 08 \\ 07 \\ 08 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 C32 C30 C32 C32 C33 C32 C33 C32 C43 C43 C44 C45 C44 C44 C45 C44 C44 C44 C44 C44	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0664 0.0561 -0.5499 0.0927 0.0929 0.0929 0.0929 0.0951 0.0926 -0.5280 0.023 0.0929 0.0951 0.0951 0.0564 -0.5280 0.0641 0.0641 0.0641 0.0543 -0.4851 0.0641 0.0543 -0.4851 0.3543 -0.1425 0.3543 -0.1425 0.3543 -0.1425 0.3543 -0.1425 0.3543 -0.1425 0.3543 -0.1425 0.0565 -0.5513 -0.5510 -0.5513 -0.5510 -0.5	C49 C50 C52 C52 C53 C54 C55 C56 C56 C57 H58 H60 H61 H62 H63 C70 C71 H72 C50 C68 C69 C70 C71 C72 C51 C51 C51 C55 C56 C56 C55 C66 H59 H60 C71 H72 C52 C55 C75 C75 C75 C75 C75 C75 C75 C75 C75	-0.1537 -0.0622 -0.0510 -0.0662 -0.0665 -0.0659 -0.1484 0.1132 0.1132 0.1132 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.1421 -0.4753 0.0019 0.0669 -0.5375 -0.1582 -0.0654 -0.0657 -0.0571 -0.0654 -0.0657 -0.0657 -0.0571 -0.0654 -0.0657 -0.0657 -0.0571 -0.0657 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0574 -0.0654 -0.0571 -0.0574 -0.0575 -0.0574 -0.0575 -0.057	H73 H74 H75 H76 H77 H78 H81 H81 H81 H84 H85 H84 H85 H84 H85 H84 H87 C30 H93 C34 C30 H93 C34 C30 H93 C34 C35 H96 H77 H75 H76 H77 H78 H77 H78 H83 H74 H78 H83 H78 H78 H78 H78 H78 H78 H78 H78 H78 H78	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1001 0.1001 0.2039 0.2039 0.1603 0.1603 0.1661 0.1662 0.1661 0.1736 0.1661 0.1736 0.1272 0.1205 0.1272 0.1205 0.1221 0.1443 0.1109 0.1108 0.1108 0.1109 0.1108 0.1109 0.1108 0.1109 0.1108 0.1109 0.1108 0.1109 0.1108 0.1109 0.1108 0.1108 0.1109 0.1108 0.1109 0.1108 0.1124 0.1208 0.	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C110 C111 C112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H104 C106 H107 C108 H104 C107 H108 H109 C100 C110 C106 H109 H109 C110 C110	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0307 -0.1140 0.0339 -0.1140 0.0339 -0.1140 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.1252 -0.1390 0.0777 0.3001 -0.1522 -0.1522 -0.1522 -0.1522 -0.1252 0.0839 0.0835 -0.1213 0.0835 -0.1213 0.0835 -0.1213 0.0835 -0.1213 0.0855 -0.1213 0.0855 -0.1213 0.0855 -0.1213 0.0855 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0355 -0.1213 0.0159 -0.1213 0.0355 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1213 0.0159 -0.1215 -0.1255 -0.1555 -0.15	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C136 C137 C138 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C124 C125 C126 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C133 C133	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1521 0.0627 -0.1156 -0.126 -0.1027 -0.1156 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1029 -0.1336 -0.1819 -0.1336 -0.1621 -0.1336 -0.1621 -0.1642 -0.1643 -0.1645 -0.1645 -0.1620 -0.1761 -0.1336 -0.1620 -0.1633 -0.1620 -0.1633 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1761 -0.1366 -0.1229 -0.1366 -0.1229 -0.1366 -0.1229 -0.1376 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1761 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1761 -0.1650 -0.1650 -0.1761 -0.1650	H145 H146 H147 H148 H149 H151 H155 C156 C156 C156 C162 H163 C164 H165 C166 H166 C166 H166 C167 C168 H146 H147 H148 H149 H150 H151 H152 H155 C156 C156 H151 H152 H155 C157 C158 N159 C157 C158 N159 C156 H153 H154 H155 C157 C158 N159 C157 C158 N159 N150	0.1794 0.1488 0.1488 0.1487 0.1172 0.1172 0.1170 0.1800 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 0.1561 0.1561 0.1561 0.1563 0.1563 0.0753 -0.1068 -0.4772 0.0753 -0.1068 -0.17741 0.1774 0.1774 0.1774 0.1774 0.1777 0.1643 0.1784 0.1787 0.1643 0.1787 0.1643 0.1797 0.1643 0.1797 0.1645 0.1797 0.1645 0.1787	C169 C170 H171 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H184 H185 H183 H184 H185 H187 H188 H189 H190 C170 C176 C177 C178 C179 C178 C179 C178 C179 H171 H172 C178 C176 C176 C177 C178 H181 H181 H181 H182 H183 H181 H181 H182 H183 H181 H182 H183 H182 H183 H182 H183 H182 H183 H183 H183 H183 H183 H183 H183 H183	-0.1082 -0.1082 -0.1069 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1485 0.1484 0.1584 0.1349 0.1777 0.1818 0.1349 0.1777 0.1818 0.1774 0.1349 0.1774 0.1774 0.1818 0.1774 0.1182 0.1537 -0.167 -0.167 -0.1121 0.1187 -0.1687 -0.1485 0.1731
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07 \\ 07$	$\begin{array}{c} 18.75 \ \dot{A} \\ \hline 0.5336 \\ 0.0349 \\ 0.0686 \\ 0.0349 \\ 0.0686 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2800 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1039 \\ 0.0329 \\ 0.0339 \\ 0.0329 \\ 0.0339 \\ 0.$	C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 C32 C43 C43 C43 C43 C44 C43 C44 C43 C44 C44	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5159 0.0664 0.0561 -0.5499 0.0661 0.1023 0.0927 0.0956 -0.5280 0.0499 0.0956 -0.5280 0.0415 0.0584 -0.5104 0.0584 -0.4860 0.4151 -0.3086 0.4151 -0.3086 0.4151 -0.3086 0.4475 0.06843 -0.1425 0.3447 0.06853 -0.5163 0.0676 0.0476 -0.5181 0.0746 -0.5181 0.1294 0.05818 -0.5181 0.05818 -0.5183 0.0676 0.0476 -0.5518 0.05181 0.1294 0.05818 -0.5518 0.05818 -0.5518 0.0576 0.05818 -0.5518 0.0576 0.0576 0.0576 0.0576 0.0576 0.0576 0.0576 0.0576 0.05750 0.05750 0.05750 0.05750 0.05750 0.05750000000000	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 C67 C70 C67 C70 C67 C71 C68 C67 C71 C72 C53 C54 C55 C54 C52 C54 C54 C54 C54 C54 C54 C54 C55 C55 C65 C65 C65 C65 C65 C65 C55 C55	-0.1537 -0.0622 -0.0510 -0.0652 -0.0659 -0.0659 -0.1484 0.1121 0.1121 0.1121 0.1121 0.1121 0.1121 0.1128 0.1138 0.1138 0.1418 0.1411 0.0019 0.0699 -0.5035 0.0620 0.03699 -0.5375 -0.1582 -0.0650 -0.0574 -0.0650 -0.0574 -0.0650 -0.0557 -0.1582 -0.0650 -0.0557 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.0559 -0.1582 -0.1	H73 H74 H76 H77 H78 H79 H80 H81 H81 H81 H84 H89 C30 H81 H88 H89 C30 C30 H81 H88 H89 H81 H83 H84 H81 H83 H74 H76 H77 H76 H81 H77 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H86 H87 H78 H81 H81 H81 H81 H81 H81 H81 H81 H81 H8	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1105 0.2039 0.2039 0.2039 0.1603 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1652 0.1661 0.1127 0.1124 0.1206 0.1221 0.1221 0.1261 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1224 0.1224 0.1251 0.1224 0.1251 0.1555	C97 H98 C99 C100 H104 C105 C106 H104 C105 C106 H104 C105 C106 H107 C118 H117 C118 H117 C118 H117 C120 C97 H98 C100 C101 H104 C105 C106 H107 C108 H107 C108 H107 C108 H107 C108 H109 C110 C111	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.1216 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0393 -0.1110 0.1198 0.0330 -0.1390 0.0330 -0.1395 0.3001 -0.1395 0.0780 0.1252 -0.1395 0.0780 0.1253 -0.1019 0.0780 0.01253 -0.1019 0.0222 0.0446 -0.11230 0.0426 -0.1230 0.0426 -0.1231 0.0428 -0.1231 0.0535 -0.1231 0.0455 -0.1659 -0.1150 0.0592 -0.1150 -0.1251 -0.1230 0.0307 -0.1231 -0.1231 -0.1231 -0.1231 -0.1231 -0.1251 -0.1551	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C136 C137 C136 C137 C136 C137 C136 C137 C122 C122 C122 C122 C122 C122 C122 C12	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1156 -0.1031 0.0637 -0.1036 -0.1032 -0.1607 -0.4152 0.0391 -0.4152 0.0391 -0.1550 0.0391 -0.1550 0.1520 0.1520 0.1530 0.1530 0.1530 0.1632 0.1632 0.1633 0.0463 -0.1463 0.0464 -0.1223 -0.1463 0.0464 -0.1233 0.0463 -0.1453 0.0464 -0.1233 0.0463 -0.1453 0.0464 -0.1233 0.1453 0.0464 -0.1233 0.1453 0.0464 -0.1233 0.0463 -0.1453 0.0464 -0.1233 0.1453 0.0464 -0.1233 0.1453 -0.1453 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 0.0464 -0.1233 -0.1463 -0.1455 0.0570 -0.1155 0.0464 -0.1233 -0.1463 -0.1233 -0.1463 -0.1232 -0.1155 -0.1232 -0.1453 -0.1455 -0.1555 -0.1455 -0.1555 -0.1455	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C166 C167 C168 C166 C166 C166 C166 C166 C166 C166	0.1794 0.1488 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.0841 -0.1294 0.0841 -0.1294 0.1561 -0.4072 0.1460 -0.1474 0.1561 -0.4072 0.1464 -0.1474 0.1684 -0.1684 -0.1684 -0.1716 0.0784 -0.1677 0.1780 0.1741 0.1770 0.1780 0.1741 0.1777 0.1780 0.1797 0.16177 0.1797 0.1797 0.1797 0.1798 -0.1265 0.1456 -0.1456 0.1430	C169 C170 H171 C170 H171 C173 C173 C176 C176 C177 C178 H180 H181 H182 H183 H183 H184 H185 H186 C177 C178 C169 C170 H171 H172 C175 C176 C177 H180 H190 H190 H171 H172 C175 C176 C177 H180 H191 H172 C175 C176 H180 H171 H172 H183 H184 H183 H184	-0.1082 -0.1089 -0.1089 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1482 0.1482 0.1484 0.1546 0.1349 0.1777 0.1482 0.1349 0.1777 0.1483 0.17782 0.1364 -0.1167 -0.1121 0.1177 0.1171 0.1171 0.1171 0.1171 0.1171 0.1173 0.1423 0.0941 -0.1423 0.1485 0.1497 0.1485 0.1477 0.1485 0.1477 0.1485 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1477 0.1487 0.1485 0.1477 0.1485 0.1477 0.1485 0.1477 0.1485 0.1485 0.1477 0.1485 0.14
$\begin{array}{c} z = \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\$	$\begin{array}{c} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 C32 C32 C33 C32 C32 C33 C32 C43 C43 C44 C45 C44 C44 C45 C44 C44 C45 C27 C28 C27 C28 C30 C44 C44 C45 C27 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0604 0.0561 -0.5499 0.0929 0.0929 0.0929 0.0929 0.0929 0.0929 0.0929 0.0951 0.0926 -0.5280 0.0041 0.00564 -0.5280 0.0641 0.0664 0.0641 0.0551 0.0554 0.0641 0.0654 0.0641 0.0554 0.0641 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0555 0.0554 0.0555 0.	C49 C50 C52 C52 C53 C54 C55 C56 C57 H59 H60 C67 H59 H60 C67 H59 H60 C67 C70 C51 C52 C51 C51 C52 C51 C51 C55 C56 C55 C56 C66 H59 H60 C71 D72 C52 C55 C75 C75 C75 C75 C75 C75 C75 C75 C75	-0.1537 -0.0622 -0.0510 -0.0662 -0.0665 -0.0659 -0.1484 0.1132 0.1132 0.1132 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1418 0.1411 0.1421 -0.4753 0.0019 0.0669 -0.5375 -0.1582 -0.0654 -0.0657 -0.0571 -0.0654 -0.0657 -0.0571 -0.0654 -0.0657 -0.0654 -0.0657 -0.0657 -0.0571 -0.0654 -0.0657 -0.0571 -0.0654 -0.0657 -0.0571 -0.0654 -0.0657 -0.0571 -0.0654 -0.0571 -0.0654 -0.0571 -0.0575 -0.05	H73 H74 H75 H76 H77 H78 H81 H81 H81 H84 H85 H84 H85 H84 H85 H86 H87 H93 C34 C30 H93 C34 C39 H93 C34 C39 H93 C39 H93 H74 H75 H76 H77 H78 H77 H78 H77 H78 H83 H79 H83 H74 H78 H84 H79 H78 H78 H77 H78 H78 H79 H83 H78 H78 H78 H78 H78 H78 H78 H78 H78 H78	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1001 0.1001 0.2039 0.2039 0.1603 0.1603 0.1661 0.1662 0.1662 0.1661 0.1736 0.1661 0.1776 0.1272 0.1205 0.1272 0.1221 0.1241 0.1124 0.1221 0.1109 0.1008 0.2212 0.1487 0.1487 0.1487 0.1487 0.1487 0.1568 0.1568 0.1568 0.1568	C97 H98 C99 C100 H102 C103 H104 C105 C106 C107 C108 H107 C108 H107 C110 C111 C112 C113 H114 C115 C116 C116 C117 C18 H119 C120 C97 H98 C99 C100 C101 C102 C103 H104 C106 H109 C110 C111 H112	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 0.0307 -0.1140 0.0307 -0.1140 0.0339 -0.1140 0.0339 -0.1140 0.0338 -0.1041 0.0338 -0.1041 0.1252 0.0777 0.3001 -0.1390 0.0777 0.1052 -0.1390 0.0222 0.0446 -0.1231 0.0222 0.0483 -0.1252 -0.1552 -0.1	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C136 C136 C137 C128 C126 C121 C122 C123 C124 N124 C121 C122 C123 C124 C124 C127 C128 C126 C127 C128 C127 C128 C126 C127 C128 C127 C128 C126 C127 C128 C127 C128 C129 C130 C131 C135 C126 C127 C128 C137 C138 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C137 C138 C139 C130 C137 C138 C136 C137 C138 C137 C138 C136 C137 C128 C128 C128 C128 C128 C128 C128 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.1501 0.0627 -0.1156 -0.126 -0.1027 -0.1156 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027 -0.1026 -0.1027	H145 H146 H147 H148 H149 H151 H155 C156 C156 C156 C156 C161 H162 H163 C164 H165 C166 H166 C167 C168 H146 H147 H148 H149 H150 H151 H152 H155 C156 C157 C158 N159 C161	0.1794 0.1488 0.1488 0.1487 0.1172 0.1172 0.1170 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 0.1561 0.1561 0.1561 0.1561 0.1563 0.1563 0.0753 -0.1068 -0.4772 0.0753 -0.1068 -0.17741 0.17767 0.17741 0.1403 0.17767 0.1767 0.1643 0.1784 0.1785 0.1785 0.1785 0.1785 0.1785 0.1785 0.1785 0.1787 0.1583 0.1787 0.1583 0.1787 0.1583 0.1787 0.1583 0.1787 0.1583 0.1787 0.1583 0.1488 0.1787 0.1583 0.1489 0.1583 0.1485 0.1485 0.1583 0.1485 0.1583 0.1583 0.1485 0.1583 0.1583 0.1485 0.1583 0.1485 0.1583 0.1585 0.1485 0.0784	C169 C170 H171 C173 N174 C175 C176 C177 C178 H180 H1812 H183 H184 H185 H189 H190 H191 Total C169 C170 H171 H172 C173 H171 C178 C176 C176 C177 C178 C176 C177 C178 C176 C177 H171 C178 C176 C176 C177 H171 H172 C178 C176 C176 C177 H181 H181 H181 H183 H183 H183 H185	-0.1082 -0.1089 -0.1089 0.1133 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1485 0.1484 0.1584 0.1349 0.1777 0.1818 0.1349 0.1777 0.1818 0.1774 0.1778 0.1399 0.1401 0.1818 0.1774 0.1167 -0.1167 -0.1167 -0.1167 -0.1167 -0.1167 -0.1167 -0.1487 0.1537 -0.1488 0.1770 0.1489 0.1489 0.1489 0.1489 0.1487 0.1587 0.1489
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \mbox{\dot{A}}\\ \hline -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2860 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ -0.5049 \\ 0.0527 \\ 0.0329 \\ 0.0586 \\ -0.5049 \\ 0.0712 \\ 0.0422 \\ -0.5141 \\ 0.0877 \\ -0.1360 \\ -0.2406 \\ 0.3762 \\ -0.3078 \\ 0.3603 \\ 0.3242 \\ 0.0266 \\ 0.3603 \\ 0.3242 \\ 0.1026 \\ 0.1025 \\ 0.1048 \\ 0.1053 \\ \end{array}$	C25 S26 C27 C28 S29 C30 D31 C32 C33 D34 H35 H36 H37 H38 H39 D41 C42 C43 C43 C44 C43 C44 C43 C44 C44 C45 S26 C47 C43 C27 C28 S29 C30 D4 H35 H36 H37 H38 H39 H39 H39 H30 Q41 C32 C32 C32 C32 C33 C32 C33 C32 C33 C32 C33 C33	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5159 0.0664 0.1023 0.0950 0.1028 0.0951 0.0956 -0.5280 0.0951 0.0956 -0.5280 0.0584 -0.5104 0.0584 -0.5104 0.0584 -0.4860 0.4151 -0.4860 0.44151 -0.3086 0.3433 -0.1425 0.3643 -0.5163 0.0647 0.0647 0.0645 0.3643 -0.5163 0.0647 0.0645 0.3643 -0.5163 0.0647 0.0645 0.3643 -0.5163 0.0647 0.0645 0.3643 -0.5163 0.0647 0.0645 0.3643 -0.5163 0.0647 0.1221 0.1224 0.1224 0.1224 0.1224 0.1224 0.1224 0.1224	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H65 C67 C70 C68 C67 C71 C72 C53 C54 C55 C54 C54 C54 C54 C54 C54 C54 C54	-0.1537 -0.0622 -0.0510 -0.0652 -0.0659 -0.0659 -0.1484 0.1121 0.1132 0.1132 0.1134 0.1121 0.1138 0.1138 0.1418 0.1421 -0.4753 0.0629 -0.5035 0.0620 0.0369 -0.5375 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0551 -0.0552 -0.0551 -0.0551 -0.0551 -0.0551 -0.0559 -0.5375 -0.0551 -0.0551 -0.0551 -0.0559 -0.0551 -0.0551 -0.0559 -0.0551 -0.0559 -0.0551 -0.0551 -0.0559 -0.0551 -0.0551 -0.0559 -0.0559 -0.0551 -0.0551 -0.0551 -0.0551 -0.0559 -0.0551 -0.0559 -0.0557 -0.0559 -0.0557 -0.0559 -0.0557 -0.0557 -0.0559 -0.0557 -0.05777 -0.05777 -0.0577777777777777777777777777777777777	H73 H74 H75 H76 H77 H78 H79 H80 H81 H81 H84 H85 H89 C30 H84 H85 H87 H73 H74 H75 H77 H76 H77 H77 H78 H77 H77 H78 H77 H78 H77 H78 H77 H78 H77 H78 H73 H74 H78 H78 H78 H78 H78 H78 H78 H78 H78 H78	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1105 0.1001 0.2029 0.2029 0.1603 0.2029 0.1603 0.1541 0.1579 0.1652 0.1651 0.1652 0.1661 -0.107 0.1124 -0.1206 0.1261 0	C97 H98 C99 C100 H104 C105 C106 H104 C105 C106 H104 H104 C105 C106 H107 C110 C111 H112 C113 H114 C115 C116 C116 C117 C118 H119 H119 H119 G120 C97 H98 C99 C100 C1010 C102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1204 0.0429 -0.1140 0.1048 0.0307 -0.1140 0.1048 0.0393 -0.1140 0.1198 0.0393 -0.1110 0.1198 0.0330 -0.1395 0.3001 -0.1395 0.3001 -0.1395 0.3001 -0.1395 0.3001 -0.1283 0.1532 -0.1019 0.0222 0.0446 -0.1150 0.0223 0.0423 0.0335 -0.1223 0.0335 -0.1223 0.0335 -0.1223 0.0355 -0.1253 0.0355 -0.1150 0.0355 -0.1150 0.0591 -0.1150 0.0392 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1234 -0.1234 -0.1231 -0.1231 0.0355 -0.1159 -0.1234 0.0392 -0.1346 0.0382 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0381 -0.1346 0.0385 -0.1365 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.1655 -0.	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C130 C131 C132 C133 C133 C133 C134 C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 N126 C127 C128 C129 C130 C131 C132 C123 C124 N126 C127 C128 C126 C127 C128 C126 C127 C128 C130 C131 C135 C136 C137 C138 C137 C128 C129 C123 C122 C123 C124 C122 C123 C124 C126 C127 C128 C129 C128 C129 C128 C129 C128 C129 C128 C129 C128 C129 C128 C129 C128 C129 C131 C132 C128 C128 C129 C131 C132 C128 C129 C131 C132 C128 C129 C131 C132 C128 C129 C131 C132 C128 C129 C133 C131 C132 C133 C133 C133 C133 C133	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.4165 -0.1591 0.0627 -0.1156 -0.1026 -0.1026 -0.1607 -0.1036 -0.1607 -0.10586 -0.1607 -0.4152 0.0931 -0.1550 0.1520 0.1525 -0.1627 -0.1530 0.1627 -0.1630 -0.1632 0.1632 0.1632 -0.1633 -0.4165 -0.1525 -0	H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C166 C167 C168 C161 C164 C165 C166 C166 C167 C168 H145 H145 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162	0.1794 0.1486 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.0841 -0.1294 0.0841 -0.1294 0.1681 -0.4072 0.1480 -0.1480 0.0783 -0.1460 -0.1474 0.1681 0.0784 -0.1294 0.1741 0.1418 0.0784 -0.1777 0.0784 -0.1777 0.1780 0.1741 0.1418 0.1777 0.1779 0.1780 0.1741 0.16177 0.1617 0.1780 0.1718 0.1797 0.1617 0.1780 0.1718 0.1780 0.16157 0.1465 0.1457 0.16173 0.16173	C169 C170 H171 C170 C173 N174 C175 C176 C177 C178 H180 H181 H182 H183 H183 H185 H186 C170 C177 H189 H190 H190 H190 H190 H190 H190 H190 H19	-0.1082 -0.1089 -0.1089 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1485 0.1485 0.1485 0.1485 0.1485 0.1586 0.1349 0.1777 0.1482 0.1374 0.1374 0.1374 0.1374 0.1374 0.1377 0.1167 -0.1121 0.1167 -0.1121 0.1177 0.1164 -0.4187 0.1237 0.1488 0.1737 0.1488 0.1737 0.1481 0.1481 0.1488 0.1737 0.1481 0.1177 0.1177 0.1411 0.1481 0.1177 0.1411 0.1177 0.1411 0.1481 0.11777 0.11777 0.11777 0.
$\begin{array}{c} z = \\ 01 \\ C2 \\ C3 \\ 04 \\ c5 \\ c6 \\ c7 \\ c8 \\ c9 \\ c10 \\ c12 \\ c1$	$\begin{array}{r} 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	C25 S26 C27 C28 S29 C30 C32 C30 C32 C32 C33 H35 H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 S26 C27 C28 S29 C30 O34 H35 H36 H37 C32 C33 C32 C32 C33 C44 C44 C45 C32 C32 C33 C44 C44 C45 C32 C32 C33 C44 C44 C45 C32 C32 C44 C45 C44 C43 C32 C32 C44 C44 C43 C32 C32 C44 C44 C44 C44 C43 C32 C32 C32 C44 C44 C44 C45 C32 C32 C32 C44 C44 C44 C45 C32 C32 C44 C44 C44 C45 C32 C32 C32 C44 C44 C44 C45 C32 C32 C32 C44 C44 C45 C32 C32 C32 C44 C44 C45 C32 C32 C32 C32 C33 C44 C44 C45 C32 C32 C32 C32 C33 C44 C44 C45 C32 C32 C32 C32 C32 C33 C44 C44 C45 C32 C32 C32 C32 C32 C32 C34 C44 C45 C32 C32 C32 C32 C32 C32 C32 C34 C44 C45 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 -0.5159 0.0661 -0.5499 0.0927 0.0927 0.0929 0.0956 -0.5280 0.0929 0.0956 -0.5280 0.0944 0.0564 -0.5280 0.0441 0.0564 -0.4860 -0.4451 -0.4860 0.3543 -0.3443 -0.1425 0.3443 0.0576 0.3443 0.0576 0.3443 0.0576 0.3443 0.0576 0.3443 0.0576 0.3443 0.0576 0.3243 0.0576 0.3443 0.05518 0.3245 0.3443 0.05518 0.3245 0.3443 0.05518 0.3245 0.3443 0.05518 0.3245 0.3245 0.3443 0.05518 0.3245 0.3443 0.05518 0.3245 0.3245 0.3245 0.3443 0.05518 0.3245 0.3245 0.3245 0.3245 0.3245 0.3443 0.05518 0.3245 0.32518 0.3255 0.34555 0.34555 0.34555 0.34555 0.34555 0.34555 0.345555 0.34555	C49 C50 C52 C52 C53 C54 C55 C56 C57 H59 H60 C57 H59 H60 C67 C71 H54 H64 H65 C67 C71 C52 C53 C54 C55 C56 C57 H59 H60 C51 C52 C53 C53 C51 C52 C53 C71 C52 C55 C55 C71 H59 H60 C55 C65 C55 C55 C55 C55 C55 C55 C55 C55	-0.1537 -0.0622 -0.0510 -0.0662 -0.0665 -0.0659 -0.1484 0.1132 0.1132 0.1132 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.1138 0.14142 0.4753 0.0019 -0.5035 0.0620 -0.0537 -0.1582 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0654 -0.0571 -0.0571 -0.0571 -0.0654 -0.0571 -0.0571 -0.0571 -0.0571 -0.0574 -0.0571 -0.0574 -0.	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C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 C107 C108 H107 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C102 C103 H104 C105 C106 H109 C111 H114	-0.1044 -0.1124 0.0293 0.0429 -0.1114 0.1216 -0.11140 0.13216 -0.1307 -0.1140 0.0339 -0.1140 0.0339 -0.1140 0.0338 -0.10140 0.0338 -0.10140 0.0338 -0.1390 0.0338 -0.1390 0.0777 0.3001 -0.1223 0.1532 -0.1532 -0.1532 -0.1231 0.0222 0.0446 -0.1231 0.0355 -0.1231 0.0355 -0.1213 0.0355 -0.1213 0.0355 -0.1167 0.0891 0.0129 -0.1346 0.0891 0.02971	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C133 C136 C137 C138 C136 C137 C128 C121 C122 C123 C124 N124 C121 C122 C123 C124 C126 C127 C128 C126 C127 C128 C126 C127 C128 C127 C128 C127 C128 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C137 C138 C137 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C138 C138 C137 C128 C127 C128 C127 C128 C127 C128 C127 C128 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	-0.1257 0.0874 -0.1464 0.1496 -0.1496 -0.1591 0.0627 -0.1156 -0.1156 -0.1156 -0.1024 -0.1024 -0.1024 -0.1026 -0.167 -0.1550 0.0931 -0.1550 0.1520 0.1520 0.1520 -0.1672 -0.1550 0.0931 -0.1520 0.1520 0.0917 -0.1462 0.0468 -0.1221 -0.1633 -0.1623 -0.1635 -0.163	H145 H146 H147 H148 H149 H151 H155 C156 C157 C168 H165 H165 H165 C156 C157 C168 H145 H145 H146 H147 H148 H147 H148 H149 H150 H145 H152 H153 H155 H156 C157 C158 N159 C161 H163	0.1794 0.1468 0.1468 0.1467 0.1172 0.1172 0.1170 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1561 0.1661 0.1661 0.1661 0.1663 0.1661 0.0753 -0.1067 0.0774 0.0774 0.1761 0.1761 0.1403 0.1170 0.1767 0.1767 0.17767 0.1767 0.1784 0.1783 0.1423 0.1783 0.1423 0.1563 0.1425 0.1573 0.1424 0.1573 0.1424 0.1573 0.1424	C169 C170 H171 C173 N174 C175 C176 C176 C177 C178 H180 H180 H182 H183 H184 H185 H189 H190 H191 Total C170 C170 C173 N174 C175 C176 C176 C177 C178 C177 C178 C179 H181 H181 H182 H183 H184 H185 H186 H187	-0.1082 -0.1089 -0.1089 0.1133 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1482 0.1485 0.1484 0.1586 0.1349 0.1777 0.1818 0.1349 0.1777 0.1818 0.1777 0.1818 0.1774 0.1772 -0.1667 -0.1121 0.1167 -0.1637 -0.1488 0.1737 -0.1488 0.1737 -0.1481 0.1488 0.1737 -0.1481 0.1488 0.1737 -0.1481 0.1737 -0.1481 0.1737 -0.1481 0.1737 -0.1481 0.1737 -0.1481 0.1737 0.1488 0.1737 0.1488 0.1737 0.1481 0.1777 0.1481 0.1777 0.1481 0.1777 0.1481 0.1777 0.1772 0.1777 0.1772 0.1777 0.1777 0.1772 0.17777 0.17777 0.17777 0.17777 0.1777
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \mbox{\dot{A}}\\ \hline -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2800 \\ 0.3122 \\ 0.3227 \\ 0.0999 \\ 0.1039 \\ 0.1026 \\ 0.3762 \\ -0.5049 \\ 0.3762 \\ -0.5049 \\ 0.0712 \\ 0.0422 \\ -0.5141 \\ 0.0877 \\ -0.1360 \\ -0.2406 \\ 0.3762 \\ -0.3078 \\ 0.3603 \\ 0.3242 \\ -0.5078 \\ 0.3603 \\ 0.3242 \\ 0.1026 \\ 0.1025 \\ 0.1048 \\ 0.1005 \\ 0.1007 \\ \end{array}$	C25 S26 C27 C28 S29 C30 C33 C32 C33 C32 C33 C33 C32 H35 H35 H36 C43 C45 C45 C44 C45 C44 C45 C44 C45 C27 C28 S29 C30 C31 C32 C32 C30 C32 C32 C32 C32 C32 C32 C32 C34 H35 H35 H36 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5499 0.0661 0.1028 0.0929 0.0951 0.0956 -0.5280 0.0411 0.0584 -0.5104 0.0584 -0.5104 0.0584 -0.4860 0.4151 -0.4865 -0.4865 -0.4855 -0.5163 0.0676 0.0476 -0.5163 0.0676 0.0476 0.0476 0.0476 0.1321 0.1294 0.0984	C49 C50 C51 C52 C52 C54 C55 C56 C56 C57 H59 H60 H61 H62 H63 H64 H65 C67 C70 C67 C70 C67 C71 C72 C53 C71 C72 C53 C71 C72 C53 C71 C72 C53 C74 H60 H61 H62 H63 H64 H65 C56 C56 C57 C72 C72 C73 C72 C73 C72 C73 C72 C73 C74 H59 H60 H61 H62 H63 C74 C77 C72 C73 C74 H59 H64 H65 C77 C74 C77 C77 C77 C77 C77 C77 C77 C77	-0.1537 -0.0622 -0.0510 -0.0662 -0.0662 -0.0662 -0.0662 -0.1124 0.1121 0.1120 0.1121 0.1120 0.1124 0.1121 0.1128 0.1121 0.1128 0.1121 0.019 0.0659 -0.5375 -0.0650 -0.0652 -0.0652 -0.0571 -0.0652 -0.0571 -0.0652 -0.0571 -0.0652 -0.1582 -0.0551 -0.0552 -0.0551 -0.	H73 H74 H75 H76 H77 H78 H81 H81 H81 H84 H85 H83 H84 H85 H86 H87 H96 H91 C32 C34 H93 C34 C34 H93 C34 H93 C35 H96 H73 H74 H77 H77 H77 H78 H77 H78 H96 H91 C35 H96 H97 H78 H78 H78 H78 H78 H78 H78 H78 H78 H7	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1001 0.2029 0.1603 0.2029 0.1603 0.2029 0.1603 0.1541 0.1579 0.1652 0.1651 0.1652 0.1661 -0.1074 0.1124 -0.1206 0.12610	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C111 H112 C113 H114 C115 C116 C117 C118 H114 C110 C101 C102 C103 H104 C105 C106 C100 C1010 C1010 C110 C111 H112 C110 C110 C111 H112 C111 H114 C115	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1214 0.0293 -0.1140 0.1048 0.0307 -0.1140 0.1088 -0.1041 0.0398 -0.1041 0.0398 -0.1390 0.0393 -0.1395 0.3001 -0.1395 0.3001 -0.1395 0.3001 -0.1395 0.3001 -0.1253 0.1252 -0.1395 0.3001 -0.1263 0.1253 0.1252 -0.1395 0.0376 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0395 -0.1263 0.0397 -0.1263 0.0385 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0375 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1263 0.0385 -0.1365 0.0385 -0.1365 0.0385 -0.1365 0.0385 -0.1365 0.0385 -0.1365 0.0385 -0.1365 0.0385 -0.1385 -0.	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C130 C131 C132 C133 C133 C133 C136 C137 C138 C129 C120 C122 C122 C122 C122 C122 C122 C123 C124 N124 C121 C122 C123 C124 N124 C121 C122 C123 C124 N124 C121 C122 C123 C124 C123 C124 C127 C138 C129 C130 C131 C132 C133 C134 C135 C136 C137 C138 C137 C137 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.151 0.0627 -0.1131 0.0627 -0.1131 0.0627 -0.1034 -0.1036 -0.1036 -0.1037 -0.1034 0.0931 -0.1520 0.1520 0.1520 0.1520 0.1632 0.1632 0.1632 0.1632 0.1633 -0.1463	H145 H146 H147 H147 H147 H151 H152 H153 H154 H155 C156 C167 C158 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H147 H148 H147 H148 H147 H151 H152 H153 H155 C156 C157 C158 H165 C157 C158 H165 C167 C168 H165 H165 H165 H155 H155 H155 H155 H155	0.1794 0.1486 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1528 0.1830 0.0841 -0.1294 0.1680 -0.1480 -0.1480 -0.1480 0.0783 0.1480 0.1481 0.1481 0.1716 0.0784 0.1684 0.1741 0.1418 0.1767 0.1780 0.1777 0.1780 0.1777 0.1780 0.16177 0.16177 0.161 0.16177 0.1780 0.1420 0.1440 0.1440 0.14411 0.14411 0.144110 0.144110000000000	C169 C170 H171 C173 N174 C175 C176 C176 C177 C178 H180 H181 H182 H183 H183 H185 H185 H185 H185 H185 H187 H190 H190 Total C169 C170 C177 C178 C179 H180 C177 C176 C177 C178 H181 H172 C176 C177 C177 H180 H191 H171 H172 C176 C177 C178 H180 H191 H171 H172 C176 C177 H180 H191 H171 H172 C176 C177 H180 H191 H172 H175 H175 H180 H171 H172 H175 H180 H181 H181 H182 H183 H184 H185 H186 H187	-0.1082 -0.1089 -0.1089 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1482 0.1485 0.1485 0.1484 0.1586 0.1349 0.1777 0.1482 0.1349 0.1777 0.1183 0.1401 0.1383 0.1774 0.1383 0.1772 0.1167 -0.1121 0.1167 -0.1121 0.1167 -0.1241 0.1167 -0.1241 0.1167 -0.1241 0.1177 0.1177 0.1177 0.1177 0.1177 0.1183 -0.11837 -0.1248 0.11737 0.1488 0.1773 0.1488 0.1775 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485 0.1777 0.1481 0.1485
$\begin{array}{c} z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ C7 \\ C8 \\ 07 \\ C10 \\ C12 \\ C1$	$\begin{array}{r} 18.75 \ \mbox{A} \\ \hline -0.5336 \\ -0.5336 \\ 0.0349 \\ 0.0686 \\ -0.5057 \\ 0.0723 \\ 0.0434 \\ -0.5136 \\ 0.0891 \\ -0.1367 \\ -0.2433 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.2830 \\ 0.3179 \\ -0.5279 \\ 0.0989 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1039 \\ 0.1041 \\ 0.0987 \\ 0.3227 \\ A \\ -0.5279 \\ 0.0329 \\ 0.0686 \\ -0.5049 \\ 0.0712 \\ 0.0422 \\ -0.5141 \\ 0.0877 \\ -0.5279 \\ 0.0329 \\ 0.0712 \\ 0.0422 \\ 0.1048 \\ 0.1053 \\ 0.3078 \\ 0.3078 \\ 0.3242 \\ 0.1025 \\ 0.1025 \\ 0.1048 \\ 0.1053 \\ 0.1001 \\ 0.1158 \\ \end{array}$	C25 S26 C27 C28 S29 C30 C30 C32 C32 C32 C33 H36 C42 C43 H37 H38 H39 H40 O41 C42 C43 C44 C45 S26 S26 S26 S26 S27 C28 S29 C30 O31 C32 C32 C44 H36 H37 H38 H39 H40 C42 C43 C33 C44 C45 C44 C45 C33 C34 C44 C45 C35 C35 C47 C44 C45 C35 C47 C44 C45 C35 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0661 -0.5499 0.0661 0.0927 0.0927 0.0927 0.0929 0.0956 -0.5280 0.0944 0.0564 -0.5280 0.0944 0.0564 -0.5280 0.0564 -0.5280 0.0564 -0.5280 0.06419 0.0665 -0.3643 -0.3643 -0.3643 -0.3643 -0.3645 0.3543 -0.3665 -0.3645 0.3447 0.0665 -0.5518 0.0476 0.0576 0.0476 0.0576 0.0476 0.0576 0.0476 0.0576 0.0476 0.05518 0.0476 0.1221 0.05518 0.1221 0.0476 0.1221 0.0444 0.0651 0.1224 0.0444 0.0611 0.1051 0.1051	C49 C50 C51 C52 C53 C54 C55 C56 C56 C57 H58 H60 H61 H64 H65 C67 C71 C52 C54 C68 C66 C67 C71 C72 C51 C52 C53 C54 C55 C56 C56 C56 C56 C56 C56 C57 C57 C57 C57 C57 C57 C57 C57 C57 C57	-0.1537 -0.0622 -0.0510 -0.0659 -0.0659 -0.0659 -0.1484 0.1132 0.1134 0.1132 0.1138 0.1138 0.1431 0.1421 -0.4753 0.0609 -0.5375 -0.0660 -0.0574 -0.6650 -0.0574 -0.6650 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.0660 -0.0574 -0.1132 0.1132 0.1132 0.1132 0.1132 -0.1132 0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.1132 -0.0057 -0.	H73 H74 H75 H76 H77 H78 H81 H81 H82 H83 H84 H85 H83 H84 H85 H87 H88 H89 C30 C34 C34 C34 C34 C34 C34 C34 C34 C34 C34	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1105 0.2039 0.1603 0.2039 0.1603 0.2039 0.1603 0.2039 0.1631 0.1579 0.1652 0.1652 0.1652 0.1652 0.1652 0.1651 0.1124 0.1206 0.1206 0.1206 0.1120 0.1106 0.1120 0.1106 0.1120 0.1008 0.1106 0.1120 0.1008 0.1108 0.1106 0.1105 0.1528 0.1521 0.1558 0.	C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 C107 C108 H104 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C102 C103 H104 C105 C106 H107 C118 H114 C113 H114 C113 H114 C115 C116 H117	-0.1044 0.1124 0.0293 0.0429 -0.1114 0.1216 -0.1140 0.13216 -0.1307 -0.1140 0.0339 -0.1140 0.0339 -0.1140 0.0338 -0.10110 0.1252 -0.1390 0.0777 0.3001 -0.1263 0.1532 -0.1532 -0.1532 -0.1532 -0.1532 -0.1213 0.0355 -0.1213 0.0355 -0.1167 0.0355 -0.1167 0.0355 -0.1167 0.0355 -0.1167 0.0355 -0.1167 0.0359 -0.1167 0.0359 -0.1167 0.0399 -0.1389 -0.1651 -0.1	C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C133 C133 C136 C136 C137 C138 C136 C137 C138 C139 H140 H141 C121 C122 C123 C124 C125 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C129 C130 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C128 C137 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C137 C138 C137 C128 C137 C138 C137 C128 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C137 C138 C137 C137 C138 C137 C137 C138 C137 C137 C138 C137 C138 C137 C138 C137 C138 C137 C137 C137 C138 C137 C137 C137 C137 C137 C138 C137 C137 C137 C138 C137 C137 C137 C137 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	-0.1257 0.0874 -0.1464 0.1464 0.1466 -0.1591 0.0627 -0.1156 -0.1156 -0.1156 -0.1024 -0.1024 -0.1024 0.1586 -0.1229 0.1586 -0.1229 0.1580 0.1520 0.1530 0.1520 0.1530 0.1520 0.1617 -0.1336 -0.1336 -0.1221 -0.1201 -0.1221 -0.1633 -0.1221 -0.1633 0.0648 -0.1221 -0.1633 0.0670 -0.1221 -0.1633 0.0670 -0.1221 -0.1633 0.0670 -0.1221 -0.1633 0.0961 -0.1221 0.1423 0.1423 0.0906 -0.1222 0.1423 0.1423 0.0906 -0.1221 0.1423 0.1423 0.0906 -0.1222 -0.1423 0.1443 0.1443 0.1443	H145 H146 H147 H148 H149 H151 H155 C156 C157 C160 C161 H162 H163 C164 H165 C166 C166 C166 H146 C167 C168 H145 H150 H151 H152 H153 H154 H155 N159 C160 C161 H162 H163 C164 H163 C164 H163 C164 H163 C164	0.1794 0.1468 0.1468 0.1468 0.1172 0.1172 0.1170 0.1800 0.1800 0.1379 0.1528 0.1830 0.0841 -0.1294 0.1661 0.1661 0.1661 0.1661 0.1661 0.1661 0.1663 0.16841 -0.4742 0.1765 0.0753 -0.1067 0.0753 -0.1067 0.1741 0.1403 0.1170 0.1767 0.1767 0.1767 0.1767 0.1767 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1617 0.1768 0.1617 0.1767 0.1467 0.14	C169 C170 H171 C173 N174 C175 C176 C176 C177 C178 H180 H180 H182 H183 H184 H185 H189 H190 H191 Total C170 C173 N174 C173 N174 C175 C176 C177 C178 C179 H180 H191 Total C177 C178 C179 H180 H181 H181 H182 H183 H184 H185 H186 H187 H188	-0.1082 -0.1089 -0.1069 0.1133 0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1455 0.1455 0.1455 0.1455 0.1455 0.1492 0.1455 0.1492 0.1492 0.1492 0.1492 0.1492 0.1339 0.1492 0.1339 0.1410 0.1339 0.1410 0.1537 -0.1121 0.1537 -0.1167 -0.11241 0.1537 -0.1423 0.1777 0.1447 0.1537 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1777 0.1447 0.1537 0.1423 0.1423 0.1423 0.1777 0.1447 0.1537 0.1423 0.1423 0.1423 0.1777 0.1778 0.1423 0.1423 0.1777 0.1778 0.1423 0.1423 0.1777 0.1778 0.1423 0.1423 0.1423 0.1421 0.1777 0.1778 0.1777 0.1778 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1421 0.1777 0.1778 0.1777 0.1777 0.1777 0.1778 0.1777 0.1775 0.17
$\begin{array}{c} z = \\ 01 \\ 01 \\ 02 \\ 03 \\ 03 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01 \\ 01$	$\begin{array}{c} 18.75 \ \mbox{A}\\ \hline -0.5336\\ -0.5336\\ 0.0349\\ 0.0686\\ -0.5057\\ 0.0723\\ 0.0434\\ -0.5136\\ 0.0891\\ -0.1667\\ -0.2433\\ 0.3179\\ -0.2980\\ 0.3122\\ 0.3227\\ 0.0999\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1039\\ 0.1146\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.3277\\ \mbox{A}\\ 0.5279\\ 0.0329\\ 0.$	C25 S26 C27 C28 S29 C30 C33 C32 C33 C33 C33 C33 C33 H36 H37 H38 H40 O41 C42 C43 C45 C46 C44 C45 C27 C28 S29 C30 O31 C44 C45 C32 C30 C32 C32 C30 C32 C32 C32 C32 C32 C32 C34 H36 H37 H38 H39 H30 C32 C27 C32 C32 C32 C32 C32 C33 C32 C32 C32 C32	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0756 0.0561 -0.5499 0.0661 0.1023 0.0929 0.0951 0.0956 -0.5280 0.0951 0.0956 -0.5280 0.0951 0.0956 -0.5280 0.0411 -0.6499 0.04151 -0.649 0.0551 0.0551 0.0553 -0.549 0.0551 0.0555 -0.549 0.0551 0.0555 -0.549 0.0551 0.0555 -0.549 0.0551 0.0555 -0.5153 0.0665 0.1321 0.1021 0.0565 -0.5163 0.0565 -0.5163 0.0565 0.1321 0.1021 0.0580 0.0565 0.1321 0.1021 0.0565 0.0566 0.0565 0.0566 0.0565 0.0566 0.0565 0.0566 0.0565 0.0566 0.0566 0.0565 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660 0.05660000000000	C49 C50 C51 C52 C52 C53 C54 C55 C56 C57 H59 H60 H61 H62 H63 H64 H65 D66 C67 C70 C71 C72 C55 C71 D72 C55 C56 C57 C71 C72 C53 C54 C55 C55 C56 C57 C72 C72 C72 C73 C72 C72 C73 C72 C73 C72 C72 C73 C72 C74 C73 C72 C74 C73 C72 C74 C75 C74 C75 C74 C72 C74 C75 C74 C72 C74 C75 C74 C75 C74 C75 C74 C75 C74 C75 C74 C75 C74 C75 C75 C74 C75 C75 C75 C75 C75 C75 C75 C75 C75 C75	-0.1537 -0.0622 -0.0510 -0.0652 -0.0659 -0.0659 -0.1484 0.1121 0.1132 0.1134 0.1121 0.1138 0.1138 0.1138 0.1418 0.1411 0.1411 0.0476 0.0699 -0.5375 -0.0654 -0.0654 -0.0654 -0.0654 -0.0554 -0	H73 H74 H75 H76 H77 H78 H81 H81 H81 H83 H84 H85 H86 H87 H88 H89 C30 H91 C32 C34 H84 H85 H93 C34 H93 H74 H75 H76 H77 H77 H77 H77 H77 H78 H93 H74 H77 H78 H93 H74 H77 H78 H79 H81 H85 H85 H86 H87 H77 H78 H79 H80 H77 H78 H79 H81 H78 H78 H78 H78 H78 H78 H78 H78 H78 H78	0.1479 0.1474 0.1102 0.1474 0.1105 0.1105 0.1105 0.1105 0.1001 0.1000 0.3230 0.2039 0.1603 0.1541 0.1579 0.1652 0.1652 0.1661 0.1736 0.1661 -0.107 0.1124 -0.1206 0.1261 0.1221 0.1212 0.12161 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1108 0.1109 0.1108 0.1108 0.1108 0.1108 0.1109 0.1108 0.1108 0.1108 0.1109 0.1108	C97 H98 C99 C100 H102 C103 H104 C105 C106 H107 C108 H107 C110 C111 H112 C113 H114 C115 C106 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 H107 C106 H107 C106 H107 C106 H107 C110 C111 H112 C111 H112 C111	-0.1044 0.1124 0.0293 0.0429 -0.1140 0.1216 0.0307 -0.1140 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1041 0.0338 -0.1390 0.0780 -0.1390 0.0780 -0.1390 0.0780 -0.1251	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C129 C130 C131 C132 C133 N134 C136 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C123 C124 N124 N124 C126 C127 C128 C126 C127 C128 C126 C127 C128 C126 C127 C128 C129 C130 C131 C135 C126 C127 C128 C129 C130 C137 C138 C129 C130 C137 C138 C129 C130 C137 C138 C129 C130 C137 C138 C129 C130 C137 C138 C129 C130 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C128 C129 C128 C129 C128 C128 C128 C128 C128 C128 C128 C128	-0.1257 0.0874 -0.1464 0.1496 -0.4116 -0.151 0.0627 -0.1166 -0.1607 -0.1026 -0.1607 -0.1026 -0.1607 -0.1026 -0.1607 -0.1229 0.0931 -0.1520 0.1520 0.1520 0.1520 0.1533 -0.1483 -0.1483 -0.1483 -0.1483 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1202 -0.1533 -0.1483 -0.1483 -0.1202 -0.1533 -0.1483 -0.	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$\begin{array}{c} z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ C7 \\ C8 \\ 07 \\ C10 \\ C11 \\ C12 \\ C1$	18.75 Å -0.5336 0.0349 0.0686 0.0349 0.0686 -0.5057 0.0723 0.0434 -0.1367 -0.2433 0.3179 -0.2433 0.3179 -0.2433 0.3179 -0.2433 0.3179 -0.2433 0.3179 -0.2430 0.3122 0.3227 0.0999 0.1000 0.1039 0.1041 0.0987 0.1137 0.1291 0.221 23.27 Å -0.5279 0.0329 0.0686 -0.5279 0.0329 0.0686 -0.5279 0.0329 0.0686 -0.5279 0.0329 0.0686 -0.5279 0.0529 0.0686 -0.5279 0.0529 0.0686 -0.5279 0.0529 0.0686 -0.5279 0.0529 0.0686 -0.5279 0.0529 0.0686 -0.5049 0.0712 0.0422 -0.5049 0.0762 -0.3078 0.3603 0.3242 0.1025 0.1048 0.1053 0.1001 0.1158 0.1164 0.1342	C25 S26 C27 C28 S29 C30 C30 C32 C33 C32 C33 C32 C42 C43 C43 C42 C43 C44 C45 C44 C45 C27 C28 S26 C27 C28 S29 C30 C31 C32 C32 C32 C33 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C45	-0.3276 0.2626 -0.2950 -0.1555 0.2815 0.0604 0.0561 -0.5159 0.0604 0.1023 0.0927 0.0951 0.0927 0.0951 0.0927 0.0951 0.0959 0.0951 0.0959 0.0951 0.0959 0.0951 0.0959 0.0951 0.0955 0.0951 0.0955 0.0955 0.0955 0.0927 0.0955 0.0955 0.0927 0.0955 0.0955 0.0955 0.0927 0.0955 0.0955 0.0955 0.0955 0.0955 0.0955 0.0955 0.0955 0.0955 0.0126 0.0126 -0.5280 0.4151 0.0485 0.0476 0.0476 0.0476 0.0976 0.0476 0.1224 0.0955 0.0111 0.1055 0.0111 0.1055 0.0044 0.0055 0.0111 0.1055 0.0046 0.0047 0.0955 0.00476 0.0476 0.0955 0.00476 0.00476 0.0055 0.00476 0.00476 0.0055 0.00476 0.0055 0.00476 0.0055 0.00476 0.0055 0.00476 0.0055 0.00476 0.0055 0.00476 0.0055 0.00476 0.00550 0.00550 0.00550 0.00550 0.00550 0	C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C70 C71 C50 C70 C71 C50 C70 C71 C50 C70 C71 H58 H60 H61 H62 H63 C54 C55 C55 C65 C65 C67 C77 C70 C71 C70 C71 C70 C71 C70 C70 C70 C70 C70 C70 C70 C70 C70 C70	-0.1537 -0.0622 -0.0510 -0.0662 -0.06659 -0.06659 -0.1484 0.1132 0.1134 0.1132 0.1134 0.1132 0.1134 0.1138 0.1138 0.1418 0.1421 -0.4753 0.0629 -0.5035 -0.0660 -0.0574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06650 -0.06574 -0.06574 -0.06574 -0.06574 -0.06574 -0.06550 -0.06574 -0.06574 -0.06574 -0.06550 -0.065744 -0.065744 -0.065744 -0.0657444	H73 H74 H75 H76 H77 H78 H81 H81 H81 H82 H83 H84 H85 H83 H84 H85 H83 H84 H85 H83 H84 H75 H74 H75 H74 H76 H77 H76 H77 H77 H81 H81 H81 H81 H81 H82 H84 H85 H81 H81 H81 H81 H81 H81 H81 H81 H81 H81	0.1479 0.1474 0.1102 0.1105 0.1105 0.1105 0.1105 0.1105 0.2039 0.2039 0.2039 0.1603 0.2039 0.1631 0.1579 0.1652 0.1652 0.1652 0.1652 0.1652 0.1661 0.1272 0.1206 0.1206 0.1221 0.1206 0.1221 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1208 0.1212 0.1221 0.1439 0.1662 0.3234 0.1588 0.1520 0.1521 0.1521 0.1521 0.1522 0.1521 0.1523 0.1521 0.1528 0.1528 0.1528 0.1528 0.1528 0.1528 0.1528 0.1528 0.1588 0.1528 0.1528 0.1528 0.1588 0.1528 0.1528 0.1528 0.1588 0.1528 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1588 0.1528 0.1528 0.1588 0.1528 0.	C97 H98 C99 C100 C101 H104 C105 C106 H107 C108 H109 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 C100 C101 H102 C103 H104 C105 C106 C106 C107 C108 H109 C111 H112 C113 H114 C115 C116 H117 C118	-0.1044 0.1124 0.0223 0.0429 -0.1114 0.0223 -0.1140 0.0429 -0.1140 0.0307 -0.1140 0.0307 -0.1140 0.0308 -0.1041 0.0328 -0.1041 0.0328 -0.1041 0.1252 -0.1395 0.0770 0.0777 0.0301 -0.1395 0.0777 0.1019 0.0222 -0.1031 -0.1252 -0.1167 0.0367 -0.1159 -0.1167 0.0387 -0.1282 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1167 0.0387 -0.1389 0.0159 -0.1346 0.2978 -0.1389 0.0384 -0.1389 0.1251 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0387 -0.1389 0.0386 -0.1389 0.0386 -0.1252 -0.1389 0.0387 -0.1252 -0.1389 0.0387 -0.1282 -0.1389 0.0387 -0.1282 -0.1389 0.0387 -0.1282 -0.1389 0.0387 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1389 -0.1282 -0.1285	C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C130 C131 C132 C133 N134 C136 C137 C138 C136 C137 C138 H140 H141 H142 C121 C122 C123 C124 C127 C128 C129 C120 C121 C122 C123 C124 C127 C128 C127 C128 C137 C138 H140 C121 C122 C123 C131 C132 C131 C132 C131 C132 C133 H141 C135 C126 C127 C128 C136 C137 C138 C139 H141 C135 C126 C137 C138 C136 C137 C138 C139 H141 H141 H141 H141 H141 H141 H141 H14	-0.1257 0.0874 -0.1464 0.1496 -0.4165 -0.1591 0.0627 -0.1591 0.0627 -0.1591 0.0637 -0.1034 -0.022 0.1566 -0.1229 0.0391 -0.1550 0.0931 -0.1550 0.0931 -0.1550 0.0931 -0.1550 0.0931 -0.1550 0.0917 -0.1622 0.1829 -0.1836 -0.2239 -0.1842 0.0947 -0.1868 -0.1201 -0.1850 0.0947 -0.1820 -0.1820 -0.1820 -0.1820 -0.1820 -0.1820 -0.1835 0.0967 -0.1920 -0	H145 H146 H147 H147 H147 H151 H152 C156 C157 C158 C160 C161 H163 C164 C165 C166 C167 H146 H147 H148 H149 H149 H149 H145 H145 H145 H145 H145 H145 H145 H151 H153 H154 H153 H154 H153 H154 C156 C156 C156 C156 C157 C158 H155 C156 C156 C156 C156 C157 C158 H155 C156 C156 C157 C158 H155 H155 H155 H155 H155 H155 H155 H	0.1794 0.1486 0.1486 0.1486 0.1172 0.1170 0.1800 0.1774 0.1580 0.1379 0.1528 0.0841 -0.1294 0.1561 -0.4072 0.1460 0.1561 0.1460 0.1563 0.1460 0.0753 -0.1464 0.0753 -0.1464 0.0753 -0.1668 -0.1716 0.0784 -0.1741 0.1741 0.1780 0.1770 0.1780 0.1780 0.1407 0.1407 0.1407 0.1407 0.1407 0.1407 0.1456 0.1456 0.1456 0.1456 0.1456 0.1456 0.1456 0.1456 0.1457 0.1456 0.1456 0.1456 0.1456 0.1457 0.1456 0.1456 0.1456 0.1457 0.1456 0.1457 0.1456 0.	C169 C170 H171 H172 C173 N174 C176 C176 C177 C178 H180 H180 H182 H183 H184 H185 H184 H185 H184 H185 H186 H187 H171 H172 C173 N174 C176 C176 C176 C177 C178 C179 H180 H191 Total	-0.1082 -0.1089 -0.1069 0.1133 -0.1131 -0.1727 -0.4059 0.1519 -0.1312 0.0871 -0.1492 0.1455 0.1445 0.1445 0.1445 0.1349 0.1777 0.1778 0.1818 0.1399 0.1401 0.1818 0.1399 0.1401 0.1818 0.1399 0.1401 0.1818 0.1399 0.1417 0.1554 4.0000 -0.1167 -0.1121 0.1537 -0.1423 0.1423 0.1423 0.1423 0.1424 0.1537 -0.1423 0.1457 0.1423 0.1457 0.1477 0.1777 0.1778 0.1537 0.1423 0.1423 0.1423 0.1423 0.1477 0.1537 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1477 0.1537 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1457 0.1423 0.1457 0.1423 0.1423 0.1457 0.1423 0.1457 0.1453 0.1457 0.1456 0.15

z = 1	28.17 Å		
01	-0.5279	C25	-0.3052
C2	0.0336	S26	0.4090
C3	0.0642	C27	-0.2440
04	=0 /1978	C28	=0 1406
CE	0.0609	920	0.4042
0.5	0.0098	323	0.4042
СБ	0.0368	030	0.0737
07	-0.5149	031	-0.5186
C8	0.0870	C32	0.0555
C9	-0.1348	C33	0.0403
C10	-0.2362	034	-0.5223
S11	0.4294	H35	0.1449
C10	-0.2105	100	0 1409
012	-0.3105	130	0.1426
513	0.4158	H37	0.1076
H14	0.3259	H38	0.1057
H15	0.1039	H39	0.1262
H16	0.1038	H40	0.1250
H17	0.1086	041	-0.5175
H18	0 1090	C42	0.0313
1110	0.1000	042	0.0315
H19	0.1038	043	0.0778
H20	0.1045	044	-0.5162
H21	0.1215	C45	0.0451
H22	0.1221	C46	0.0596
H23	0.1439	047	-0.5225
H24	0 1448	C48	0 3625
	20.00 Å	010	0.0020
	32.22 A		
01	-0.5161	C25	-0.3055
C2	0.0282	S26	0.4047
C3	0.0666	C27	-0.2433
04	-0.4995	C28	-0.1396
C5	0.0678	S29	0.3949
C6	0.0406	C30	0.0786
07	-0.5148	031	-0.5159
C 9	0.0960	(22)	0.0525
00	0.0002	032	0.0325
69	-0.1360	033	0.0441
C10	-0.2385	034	-0.5289
S11	0.4169	H35	0.1408
C12	-0.3088	H36	0.1388
S13	0.4024	H37	0.1123
H14	0.3290	H38	0,1120
H15	0 1095	H30	0.1213
110	0.1095	1139	0.1213
H16	0.1093	n40	0.1201
H17	0.1086	041	-0.5425
H18	0.1090	C42	0.0439
H19	0.1043	C43	0.0756
H20	0.1049	044	-0.5151
H21	0 1192	C45	0 0478
100	0 1102	C16	0.0116
122	0.1198	040	0.0440
H23	0.1404	047	-0.5135
H24	0.1412	C48	0.3821
z = z	36.84 A		
01	-0.5259	C25	-0.3059
C2	0.0323	S26	0.4327
C3	0.0659	C27	-0 2407
04	=0.5007	C28	=0 1385
CE	0.0700	920	0.4108
65	0.0700	529	0.4198
C6	0.0375	C30	0.0813
07	-0.5148	031	-0.5156
C8	0.0867	C32	0.0471
C9	-0.1354	C33	0.0490
C10	-0.2366	034	-0.5321
S11	0.4426	835	0 1446
011	0.4420	1100	0.1440
610	0 2000	1120	0 1404
C12	-0.3096	H36	0.1424
C12 S13	-0.3096 0.4262	H36 H37	0.1424 0.1114
C12 S13 H14	-0.3096 0.4262 0.3257	H36 H37 H38	0.1424 0.1114 0.1115
C12 S13 H14 H15	-0.3096 0.4262 0.3257 0.1046	H36 H37 H38 H39	0.1424 0.1114 0.1115 0.1225
C12 S13 H14 H15 H16	-0.3096 0.4262 0.3257 0.1046 0.1044	H36 H37 H38 H39 H40	0.1424 0.1114 0.1115 0.1225 0.1210
C12 S13 H14 H15 H16 H17	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074	H36 H37 H38 H39 H40 041	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477
C12 S13 H14 H15 H16 H17	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074	H36 H37 H38 H39 H40 041	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477
C12 S13 H14 H15 H16 H17 H18	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079	H36 H37 H38 H39 H40 041 C42	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541
C12 S13 H14 H15 H16 H17 H18 H19	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030	H36 H37 H38 H39 H40 041 C42 C43	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649
C12 S13 H14 H15 H16 H17 H18 H19 H20	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037	H36 H37 H38 H39 H40 041 C42 C43 044	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210	H36 H37 H38 H39 H40 041 C42 C43 044 C45	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210 0.1216	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210 0.1216 0.1443	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23 H24	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210 0.1216 0.1443 0.1451	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047 C48	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23 H23 H24	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1037 0.1210 0.1216 0.1443 0.1443	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047 C48	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469
C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23 H24 Z = -	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1037 0.1037 0.1210 0.1216 0.1443 0.1445 140.99 Å	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0640 -0.5284 0.3469
$\begin{array}{c} \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \hline \hline \\ z = - \\ 01 \end{array}$	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210 0.1216 0.1423 0.1451 40.99 Å	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C45 C46 047 C48	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067
$\begin{array}{c} \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H23} \\ \text{H24} \\ \hline \hline \\ \hline $	-0.3096 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1037 0.1210 0.1216 0.1443 0.1451 40.99 Å	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067 0.4372
$\begin{array}{c} \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \\ \textbf{C2} \\ \text{C3} \end{array}$	$\begin{array}{c} -0.3096\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1044\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1423\\ 0.1451\\ \hline 40.99\ \bar{A}\\ \hline -0.5159\\ 0.0293\\ 0.0656\\ \end{array}$	H36 H37 H38 H39 H40 D41 C42 C43 D44 C45 C46 D47 C48 C25 S26 C27	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067 0.4372 -0.2398
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \hline \begin{array}{c} z = - \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ \end{array} \right.$	$\begin{array}{c} -0.3096\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1044\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1443\\ 0.1451\\ -0.5159\\ 0.0293\\ 0.0656\\ -0.4982\end{array}$	H36 H37 H38 H39 H40 041 C42 C43 C43 C45 C46 047 C48 C46 047 C48 C25 S26 C27 C28	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067 0.4372 -0.2398 -0.1378
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ \end{array}$	$\begin{array}{c} -0.3096\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1044\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1210\\ 0.1212\\ 0.1443\\ 0.1451\\ \hline 40.99\ A\\ \hline -0.5159\\ 0.0293\\ 0.0656\\ -0.4982\\ 0.0661\end{array}$	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C25 S26 C27 C28 S29	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067 0.4372 -0.2398 -0.1378 0.4222
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \end{array}$	$\begin{array}{c} -0.3096\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1044\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0656\\ -0.4982\\ 0.0681\\ 0.0382\end{array}$	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C46 O47 C48 C25 S26 C27 C28 S29 C30	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3067 0.4372 -0.2398 -0.1378 0.4222 0.0830
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \end{array}$	-0.3096 -0.4262 0.3257 0.1046 0.1044 0.1074 0.1074 0.1030 0.1037 0.1210 0.1216 0.1443 0.1451 40.99 Å -0.5159 0.0656 -0.4982 0.0666	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31	0.1424 0.1114 0.1114 0.1210 -0.5477 0.0649 -0.5206 0.0625 0.0640 -0.5284 0.3469 -0.3284 0.3469 -0.3349 -0.3367 0.4372 -0.3398 -0.1372 0.4372 0.4322 0.6350 -0.5151
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ \end{array}$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1074 0.1079 0.1030 0.1070 0.1216 0.1245 0.1451 40.99 Å -0.5159 0.0283 0.0666 0.0382 -0.4982 0.0661 0.0382 -0.5149 0.08681	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C45 C46 O47 C45 S26 C27 C25 S26 C27 C28 S29 C30 O31 C32	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5225 0.0649 -0.5224 0.0525 0.0525 0.0524 0.0525 0.0524 0.0526 0.0528 0.0526 0.0549 -0.5284 0.3469 -0.5284 0.3469 -0.5372 -0.2398 -0.1378 0.4222 0.0830 0.0830 0.05150 0.0849
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ \end{array}$	$\begin{array}{c} -0.3096\\ -0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1070\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1451\\ 0.1451\\ 0.1451\\ 0.0293\\ 0.0656\\ -0.492\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0661\\ 0.0364\\ 0.0662\\ 0.0364\\ 0.0062\\ 0.006$	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031 C32 C33	0.1424 0.1114 0.1115 0.1225 0.1225 0.1225 0.0649 -0.5206 0.0625 0.0649 -0.5284 0.3649 -0.5284 0.3649 -0.5284 0.3649 -0.367 0.4372 -0.3388 -0.3372 0.43720 0.43720 0.43720 0.43720 0.43720000000000000000000000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C9} \\ {\rm C10} \\ \end{array}$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1074 0.1079 0.1030 0.1030 0.1030 0.1216 0.1240 0.1451 40.99 Å -0.5159 0.0283 0.0656 -0.4982 0.0382 -0.5149 0.0382 -0.3159 -0.3159	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 O34	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.526 0.0640 -0.525 0.0640 -0.525 0.0640 -0.526 0.3469 -0.3469 -0.3469 -0.3469 -0.3372 -0.3378 -0.3378 -0.3378 -0.3378 -0.3557 -0.6527 -0.527
$\begin{array}{c} C12\\ S13\\ H14\\ H15\\ H16\\ H17\\ H18\\ H19\\ H20\\ H21\\ H22\\ H23\\ H24\\ C2\\ C3\\ C3\\ C4\\ C5\\ C6\\ C7\\ C8\\ C9\\ C10\\ C8\\ C9\\ C8\\ C9\\ C10\\ C8\\ C9\\ C8\\ C9\\ C10\\ C8\\ C9\\ C8\\ C9\\ C10\\ C8\\ C9\\ C8\\ C9\\ C8\\ C9\\ C10\\ C8\\ C9\\ C8\\ C9\\ C10\\ C10\\ C8\\ C8\\ C9\\ C10\\ C10\\ C8\\ C8\\ C9\\ C10\\ C10\\ C8\\ C8\\ C9\\ C10\\ C8\\ C9\\ C10\\ C8\\ C8\\ C9\\ C10\\ C10\\ C8\\ C8\\ C9\\ C10\\ C8\\ C8\\ C8\\ C9\\ C10\\ C8\\ C8\\ C8\\ C9\\ C10\\ C8\\ C8\\ C8\\ C8\\ C9\\ C10\\ C8\\ C8\\ C8\\ C8\\ C8\\ C8\\ C8\\ C8\\ C8\\ C8$	$\begin{array}{c} -0.3066\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1073\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1245\\ 0.1445\\ 0.1451\\ 0.0293\\ 0.0656\\ 0.0293\\ 0.0656\\ 0.0382\\ 0.06661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.0661\\ 0.0382\\ 0.038$	H36 H37 H38 H39 H40 041 C42 C43 C44 C45 C46 C47 C48 C25 S26 C27 C28 S29 C30 D31 C32 C33 D34 H27	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0649 -0.5206 0.0649 -0.526 0.0649 -0.5284 0.3649 -0.5284 0.3649 -0.5284 0.3649 -0.367 0.4372 -0.3388 -0.1372 0.43720 0.43720 0.4372000000000000000000000000000000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H17} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C10} \\$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1074 0.1079 0.1030 0.1030 0.1210 0.1216 0.1245 0.14451 40.99 Å -0.5159 0.0263 0.0666 -0.4982 0.0682 -0.6159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 0.0382 -0.5159 -0.5159 0.0382 -0.5144 0.0382 -0.5159 0.0382 -0.5144 0.0382 -0.5144 0.0382 -0.5144 0.0382 -0.5144 0.0382 -0.5144 0.0382 -0.5144 0.0382 -0.3159 0.0444 0.0444 0.0444 0.04443 0.04444444444	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047 C48 C46 C47 C48 C25 S26 C27 C28 S29 C30 031 C32 C32 C33 034 H35 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0505 0.0649 -0.5206 0.0525 0.0649 -0.5206 0.0525 0.0649 -0.5264 0.3469 -0.3469 -0.3469 -0.3469 -0.3469 -0.3469 -0.5377 0.4222 0.0830 -0.5449 0.05477 0.0449 0.05477 0.0449 0.05477 0.0449 0.05477 0.0449 0.05477 0.0449 0.05477 0.0449 0.05477 0.0449 0.0557 0.0449 0.05477 0.0449 0.05477 0.0449 0.0557 0.0449 0.05477 0.0449 0.0557 0.0449 0.0557 0.0449 0.0557 0.0449 0.05570000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H14} \\ {\rm H15} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C1$	$\begin{array}{c} -0.3066\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1073\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1246\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0661\\ 0.0293\\ 0.0681\\ 0.0382\\ -0.4982\\ -0.6149\\ 0.0681\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3370\\ 0.6443\\ -0.3093\\ -0.443\\ -0.3093\\ -0.443\\ -0.3093\\ -0.5492\\ -0.5370\\ -0.4443\\ -0.3093\\ -0.5492\\ -0.5370\\ -0.4443\\ -0.3093\\ -0.5393\\ -0.5$	H36 H37 H38 H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031 C32 C33 034 H35 H35 H35 H35	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.12407 0.0641 0.0641 0.0649 -0.5206 0.0525 0.0640 0.0640 0.0525 0.0640 0.0640 0.06437 0.4372 -0.2388 0.4372 0.447 0.
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm S13} \\ {\rm S13} \\ \end{array}$	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.1262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1070\\ 0.1030\\ 0.1037\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0666\\ 0.0382\\ -0.5159\\ 0.0662\\ -0.3159\\ 0.0662\\ -0.3159\\ 0.0662\\ -0.3159\\ 0.0662\\ -0.3159\\ 0.0662\\ -0.3159\\ 0.0662\\ -0.327\\ 0.4443\\ 0.2266\\ 0.32$	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C46 O47 C48 C25 S26 C27 C28 S29 C33 C31 C32 C33 O34 H36 H37	0.1224 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5205 0.0609 -0.5205 0.0609 -0.5205 0.0624 0.3469 -0.3469 -0.3469 -0.3469 -0.3472 -0.3398 -0.3378 0.4222 0.0830 -0.5150 0.0449 0.5247 0.02449 0.5247 0.0249 0.0547 0.1443 0.0547 0.0249 0.05547 0.0249 0.05547 0.0249 0.05547 0.0249 0.05547 0.0249 0.0554 0.0255 0.0249 0.0555 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255 0.0249 0.0255
	$\begin{array}{c} -0.3066\\ 0.4262\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1073\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1243\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0233\\ 0.06661\\ 0.0233\\ 0.06661\\ 0.0382\\ -0.5149\\ 0.0681\\ 0.0382\\ -0.5149\\ 0.0862\\ -0.3270\\ 0.4443\\ -0.3033\\ 0.4266\\ \end{array}$	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C45 C26 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1115\\ 0.1125\\ 0.1225\\ 0.1225\\ 0.1210\\ -0.6541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3699\\ \hline 0.3672\\ -0.2384\\ -0.3137\\ 0.4372\\ -0.2384\\ -0.3137\\ 0.4322\\ 0.0830\\ -0.5150\\ 0.4422\\ 0.0830\\ -0.5150\\ 0.4422\\ 0.0830\\ -0.5150\\ 0.4422\\ 0.0330\\ -0.5150\\ 0.4422\\ 0.0330\\ -0.5150\\ 0.4422\\ 0.0330\\ -0.5150\\ 0.4422\\ 0.0527\\ -0.5347\\ 0.1422\\ 0.1100\\ 0.1100\\ \end{array}$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm S11} \\ {\rm H15} \\ \end{array}$	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.1262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1070\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1214\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0662\\ -0.4982\\ 0.0661\\ 0.0382\\ -0.5159\\ 0.0662\\ 0.3822\\ -0.51359\\ -0.2370\\ 0.6443\\ -0.3159\\ 0.0282\\ 0.0662\\ 0.3225\\ 0.4266\\ 0.3285\\ 0.4266\\ 0.3285\\ 0.1087\end{array}$	H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C32 S29 C30 O31 C32 C33 O34 H35 H35 H35 H37 H38 H39	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1210\\ -0.5477\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.3469\\ \hline 0.0525\\ 0.0649\\ -0.3398\\ -0.3372\\ -0.3398\\ -0.3372\\ 0.03472\\ -0.3398\\ -0.1378\\ 0.0422\\ 0.0830\\ -0.5150\\ 0.0449\\ 0.0527\\ -0.5347\\ 0.1443\\ 0.1215\\ \hline \end{array}$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ \hline \\ z = - \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ \end{array}$	$\begin{array}{c} -0.3066\\ -0.4262\\ 0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99 A\\ -0.5159\\ 0.0223\\ 0.0661\\ 0.0283\\ 0.0661\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3159\\ -0.2370\\ 0.0443\\ -0.3093\\ 0.4266\\ 0.3285\\ 0.1087\\ 0.3285\\ 0.1087\\ 0.1087\\ \end{array}$	H36 H37 H37 H38 H39 O41 C42 C43 C43 C44 C44 C44 C44 C46 C46 C46 C47 C46 C47 C46 C47 C46 C47 C46 C47 C48 C46 C47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	0.1424 0.1114 0.1114 0.1115 0.1220 0.1210 0.0541 0.05477 0.05641 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0547 0.3369 0.3369 0.3369 0.3369 0.0337 0.0330 0.0547 0.0337 0.0330 0.0547 0.0337 0.0547 0.0337 0.0547 0.0357 0.0357 0.0547 0.0357 0.0547 0.0555 0.0547 0.0357 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.0057 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.0577 0.0357 0.01100 0.0577 0.01100000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \end{array}$	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.4262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0666\\ 0.3822\\ -0.5492\\ 0.0662\\ 0.3622\\ -0.1359\\ -0.3622\\ 0.0662\\ 0.3622\\ 0.0662\\ 0.3622\\ 0.0662\\ 0.3622\\ 0.0662\\ 0.3622\\ 0.0662\\ 0.3622\\ 0.0662\\ 0.362\\ 0.0662\\ 0.325\\ 0.0662\\ 0.0$	H36 H37 H38 H39 H40 041 H40 041 H30 C42 C43 C45 C46 C43 C45 C46 C46 C46 C47 C48 C25 C27 C30 C30 C31 C32 C33 C34 H35 H36 H37 H38 H39 H40 041	$\begin{array}{c} 0.1424\\ 0.1124\\ 0.1115\\ 0.1255\\ 0.1210\\ -0.5477\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.3469\\ \hline 0.0525\\ 0.0649\\ -0.3469\\ \hline 0.0525\\ 0.0649\\ -0.3396\\ -0.3396\\ -0.1378\\ 0.0422\\ 0.0830\\ -0.5150\\ 0.0449\\ 0.0527\\ -0.539\\ 0.0449\\ 0.0527\\ -0.539\\ 0.0449\\ 0.0527\\ -0.539\\ 0.0449\\ 0.0527\\ -0.541\\ 0.1215\\ 0.1211\\ 0.1101\\ 0.1105\\ 0.1215\\ 0.2013\\ 0.0541\\ 0.$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ \end{array}$	$\begin{array}{c} -0.3066\\ -0.4262\\ 0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99 \mbox{ A} \\ -0.5159\\ 0.0293\\ 0.0661\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3370\\ 0.0862\\ -0.3370\\ 0.0382\\ -0.3370\\ 0.0382\\ -0.3393\\ 0.3285\\ 0.1087\\ 0.3285\\ 0.1087\\ 0.1087\\ 0.1082\\ 0.1092\\ 0.1092\\ \end{array}$	H36 H37 H38 H39 H40 O41 H40 C42 C43 C45 C46 C45 C46 C45 C46 C47 C48 C46 C47 C48 S29 C47 C28 S29 C37 C27 C28 S29 C37 C32 C33 C34 C45 S26 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5205 0.0649 -0.5205 0.0649 -0.525 0.0640 -0.525 0.0640 -0.524 0.3469 -0.3469 -0.3469 -0.3469 -0.3469 -0.3472 -0.3372 -0.3378 -0.1378 0.4222 0.0830 0.0543 -0.5150 0.0543 -0.1100 0.1100 0.1210 0.1100 0.1210 0.1100 0.1210 0.1115 0.1221 0.0251 0.1221 0.1221 0.1221 0.0251 0.1221 0.1221 0.1221 0.0251 0.1221 0.1221 0.0251 0.1221 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.1221 0.0251 0.0251 0.1221 0.0251 0.0
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} $	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.1262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1214\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0666\\ 0.0382\\ -0.5159\\ 0.0662\\ 0.0681\\ 0.0682\\ -0.3159\\ 0.0662\\ 0.322\\ -0.51359\\ -0.6322\\ 0.0662\\ 0.322\\ 0.0682\\$	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 C46 C46 C47 C48 C46 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 0.0541 0.0649 0.0525 0.06049 0.0525 0.06049 0.0525 0.06049 0.0525 0.0624 0.3469 -0.3369 -0.3372 -0.3398 -0.3372 -0.3398 -0.1378 0.0422 0.0830 -0.51378 0.0422 0.0830 -0.524 0.0449 0.0527 -0.5398 0.0449 0.0524 -0.5443 0.0649 0.0547 0.0449 0.0525 0.0449 0.0527 0.0449 0.0547 0.0547 0.0549 0.0547 0.0547 0.0552 0.0540 0.0547 0.0552 0.0540 0.0547 0.0552 0.0547 0.0552 0.0552 0.0552 0.0547 0.0552 0.0552 0.0552 0.0549 0.0552 0.0547 0.0552 0.0552 0.0552 0.0552 0.0552 0.0549 0.0552 0.0
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H19} \\ {\rm H19} \\ {\rm H19} \\ {\rm H10} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H10$	$\begin{array}{c} -0.3066\\ -0.4262\\ 0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1037\\ 0.1210\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99 \mbox{ A} \\ -0.5159\\ 0.0293\\ 0.0661\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3393\\ 0.0661\\ 0.3825\\ 0.1085\\ 0.4443\\ -0.3033\\ 0.4266\\ 0.1085\\ 0.1087\\ 0.10$	H36 H37 H38 H39 H40 O41 H40 C42 C43 C45 C46 C45 C46 C45 C46 C47 C48 S29 C47 C48 S29 C47 C28 S29 C30 C31 C32 C33 C32 C33 C34 H37 H38 H39 H37 H37 H38 H39 C42 C42 C43 C42 C43 C42 C43 C45 C42 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.5284 0.3649 -0.5284 0.3649 -0.4372 -0.2398 -0.4372 -0.3376 0.4372 -0.3367 0.4322 0.0630 0.4222 0.0630 0.4222 0.0630 0.4222 0.0527 -0.5347 0.1422 0.1444 0.1422 0.1444 0.1422 0.1444 0.1422 0.1444 0.1422 0.1444 0.1422 0.1444 0.1422 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444 0.1421 0.1444
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \end{array} $	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.4262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0666\\ 0.3822\\ -0.5149\\ 0.0662\\ 0.3622\\ -0.51359\\ -0.3622\\ 0.0662\\ 0.3625\\ 0.0662\\ 0.3625\\ 0.0662\\ 0.3625\\ 0.0662\\ 0.3625\\ 0.0662\\ 0.3625\\ 0.0662\\ 0.066\\ 0.0662\\ 0.066\\ $	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 C46 C46 C46 C47 C48 C77 C28 S26 C77 C28 S29 C30 O41 H36 H37 H38 H39 H40 O41 C42 C43 O44	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.06649 -0.5206 0.0525 0.06649 -0.5206 0.0525 0.06525 0.06525 0.06525 0.06525 0.06547 0.3367 -0.3378 0.0422 0.03830 -0.1378 0.0429 0.0524 0.0429 0.0547 0.1423 0.06547 0.1423 0.0544 0.1120 0.1215 0.1220 0.0547 0.0549 0.0555 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.0557 0.0557 0.0429 0.0557 0.0429 0.0557 0.0429 0.05570000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C13} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm C11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm C12} \\ {\rm C1$	$\begin{array}{c} -0.3066\\ -0.4262\\ 0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1070\\ 0.1030\\ 0.1030\\ 0.1030\\ 0.1216\\ 0.1441\\ 0.1451\\ 40.99 \mbox{ A} \\ -0.5159\\ 0.0293\\ 0.0666\\ 0.0293\\ 0.06661\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.3370\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.359\\ -0.3370\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3285\\ 0.1087\\ -0.3033\\ 0.4246\\ 0.3285\\ 0.1086\\ 0.1092\\ 0.1061\\ 0.1051\\ 0.1051\\ 0.1051\\ 0.1211\\ \end{array}$	H36 H37 H38 H39 H40 C42 C42 C43 C46 D47 C48 C47 C48 C27 S26 C27 S29 C30 D31 C32 C33 D34 H37 H38 H37 H38 H39 O44 C42 C43 O44 C42 C43 O44	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1115\\ 0.1125\\ 0.1225\\ 0.1225\\ 0.1220\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3699\\ \hline 0.3672\\ -0.5284\\ 0.34699\\ \hline 0.3672\\ -0.3672\\ 0.4372\\ -0.3386\\ 0.4322\\ 0.0830\\ -0.4372\\ 0.0437\\ -0.5160\\ 0.4492\\ 0.0422\\ 0.0330\\ -0.5160\\ 0.4422\\ 0.0330\\ -0.5160\\ 0.4222\\ 0.0330\\ -0.5160\\ 0.422\\ 0.1010\\ 0.1215\\ 0.1201\\ 0.1215\\ 0.1201\\ 0.0691\\ 0.0524\\ -0.5160\\ 0.0620\\ \hline \end{array}$
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ \end{array} $	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.4262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0662\\ -0.4982\\ 0.0661\\ 0.0382\\ -0.5159\\ 0.0662\\ 0.332\\ -0.5139\\ 0.0662\\ 0.332\\ -0.5139\\ 0.0662\\ 0.322\\ 0.1359\\ -0.323\\ 0.0662\\ 0.322\\ 0.1359\\ -0.325\\ 0.0662\\ 0.325\\ 0.065\\ 0.065\\ 0.065\\ 0.005\\ 0$	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 C46 C46 C27 C28 C27 C28 C27 C28 C30 O41 C48 C46 C32 C32 C32 C33 C34 H36 H37 H38 H39 H40 O41 C42 C43 C44 C42 C43 C44 C45 C44 C42 C43 C44 C44 C45 C44 C45 C46 C47 C47 C48 C47 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C47 C48 C47 C48 C47 C48 C47 C48 C47 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	$\begin{array}{c} 0.1424\\ 0.1124\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1210\\ -0.5477\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.3469\\ -0.3469\\ -0.3469\\ -0.3396\\ -0.3378\\ -0.3378\\ -0.3378\\ 0.0422\\ 0.0830\\ -0.5150\\ 0.0449\\ 0.0524\\ -0.5140\\ 0.1215\\ 0.1201\\ -0.5414\\ 0.0524\\ -0.5140\\ 0.0651\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0651\\ 0.0674\\ \end{array}$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S111} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \end{array}$	$\begin{array}{c} -0.3066\\ -0.4262\\ 0.3257\\ 0.1046\\ 0.3257\\ 0.1046\\ 0.1074\\ 0.1074\\ 0.1079\\ 0.1030\\ 0.1030\\ 0.1030\\ 0.1021\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99 \mbox{ A} \\ -0.5159\\ 0.0223\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0666\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.3159\\ -0.2370\\ 0.0866\\ 0.0382\\ -0.3033\\ 0.4246\\ 0.3285\\ 0.1087\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.5149\\ 0.0382\\ -0.1359\\ -0.2370\\ 0.0866\\ 0.1086\\ 0.1092\\ 0.1061\\ 0.1051\\ 0.1051\\ 0.1211\\ 0.1217\\ 0.1211\\ 0.1217\\ 0.1211\\ 0.1217\\ 0.1211\\ 0.1217\\ 0.1211\\ $	H36 H37 H38 H39 H40 O41 C42 C43 C44 C47 C48 C47 C48 C47 C48 C27 S26 C27 S29 C30 O31 C32 C33 O34 H37 H38 H39 H40 O41 C42 C43 O44 C42 C43 O44 C45 C46 O47	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1114\\ 0.1115\\ 0.1125\\ 0.1225\\ 0.1225\\ 0.1220\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3699\\ \hline 0.3672\\ -0.5284\\ 0.34699\\ \hline 0.3672\\ -0.3672\\ -0.3378\\ 0.4222\\ 0.0830\\ -0.4372\\ -0.3378\\ 0.4222\\ 0.0830\\ -0.4372\\ 0.1378\\ 0.4222\\ 0.0830\\ -0.4222\\ 0.0830\\ -0.4222\\ 0.0830\\ -0.4222\\ 0.0437\\ 0.1443\\ 0.4222\\ 0.0651\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.6140\\ 0.0524\\ -0.6140\\ 0.0621\\ \hline 0.0620\\ 0.0622\\ 0.$
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \end{array} $	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.4262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0666\\ 0.3322\\ -0.5149\\ 0.0662\\ 0.3322\\ -0.5149\\ 0.0662\\ 0.3322\\ -0.5149\\ 0.0662\\ 0.3257\\ 0.1087\\ 0.10862\\ 0.3257\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086\\ 0.1087\\ 0.1086$	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C46 O47 C46 O47 C48 C25 C27 C28 S26 C27 C28 S29 C30 O31 C32 C32 C32 C33 C32 C33 H36 H36 H37 H38 H39 H40 O41 C42 C43 C43 C44 C45 C44 C42 C43 C44 C45 C44 C45 C44 C45 C46 C47 C48 C47 C47 C48 C47 C48 C47 C48 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C48 C47 C47 C48 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1220\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5284\\ 0.3469\\ -0.5284\\ 0.3469\\ -0.3367\\ 0.4372\\ 0.0633\\ 0.0437\\ 0.1378\\ 0.0437\\ 0.1423\\ 0.06524\\ 0.0429\\ 0.0524\\ 0.0524\\ -0.5150\\ 0.1422\\ 0.1101\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.0651\\ 0.0624\\ -0.5140\\ 0.0627\\ -0.5140\\ 0.0627\\ 0.0478\\ -0.5280\\ 0.0528\\ 0.0678\\ 0.068$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H24} \\ {\rm H25} \\ {\rm H24} \\ {\rm H26} \\ {\rm H26} \\ {\rm H27} \\ {\rm H26} \\ {\rm H27} \\ $	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1074 0.1079 0.1030 0.1030 0.1030 0.1210 0.1216 0.1443 0.1451 40.99 Å -0.5159 0.0283 0.0685 -0.4982 -0.4982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3982 -0.3993 0.0882 -0.3285 0.0882 -0.3285 0.1086 0.1086 0.1092 0.1081 0.1092 0.1081 0.1081 0.1081 0.1081 0.1092 0.1081 0.1092 0.1091 0.1010 0.1011 0.1010 0.1011 0.1010 0.0010 0.000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.000000	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 C47 C48 C27 C28 S29 C30 O31 H35 H36 H37 H38 H39 H31 H32 H33 H34 H35 H36 H37 H38 H39 H39 H31 H33 H34 C45 C45 C46 C47 C48	$\begin{array}{c} 0.1424\\ 0.1124\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1210\\ -0.5477\\ 0.0541\\ 0.06541\\ 0.0652\\ 0.0649\\ -0.5264\\ 0.3469\\ -0.5264\\ 0.3469\\ -0.524\\ -0.3367\\ -0.3367\\ 0.4372\\ -0.3378\\ -0.3378\\ -0.3378\\ -0.3378\\ -0.3378\\ -0.3378\\ -0.3378\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.524\\ -0.520\\ 0.0478\\ -0.522\\ -0.5350\\ -0.520\\ -0.500\\ -$
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H22} \\ {\rm H22} \\ {\rm H22} \\ {\rm H24} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\$	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1079 0.1030 0.1030 0.1210 0.1216 0.1443 0.1451 40.99 Å -0.5159 0.0293 0.0656 0.0651 0.0652 0.0662 -0.4982 0.0662 -0.359 0.0662 -0.359 0.0662 -0.359 0.0662 0.0662 -0.359 0.0662 0.067 0.067 0.067 0.067 0.067 0.067 0.067 0.067 0.067 0.0662 0.0662 0.0662 0.067 0.070 0.067 0.0700000000	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 O47 C48 C46 C46 C46 C46 C47 C48 C27 C28 S26 C27 C28 S26 C27 C28 S26 C27 C30 O41 C32 C32 C32 C33 C32 C33 C34 H36 H37 H38 H37 H37 H37 H37 H38 H37 H37 H37 H37 H37 H37 H37 H37 H37 H37	0.1424 0.1114 0.1115 0.1225 0.1210 -0.5477 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3469 -0.3469 -0.3347 0.4322 0.0330 -0.3377 0.4322 0.0330 -0.5398 -0.1378 0.0449 0.0524 0.0449 0.0524 0.0449 0.0544 0.1101 0.1215 0.1225 0.1423 0.142 0.1423 0.1433 0.1433 0.1433 0.1433 0.1433 0.1433 0.1433 0.1433 0
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C1} \\ {\rm C12} \\ {\rm C12} \\ {\rm C11} \\ {\rm C11} \\ {\rm C12} \\ {\rm C11} \\ {\rm C11}$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1030 0.1030 0.1210 0.1210 0.1216 0.1443 0.1451 40.99 40.955 0.0656 -0.4982 -0.4982 -0.355 0.0685 -0.4982 -0.359 0.0882 -0.359 0.0443 -0.359 0.4443 0.1086 0.1086 0.1086 0.1086 0.1081 0.1091 0.1081 0.1091 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0081 0.0082 0.00810000000000	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 C47 C48 C27 C28 S29 C30 O31 H35 H36 H37 H38 H39 H40 O41 C42 C33 H37 H38 H39 H40 O41 C45 C46 O47 C48 C25	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 0.0541 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.0525 0.0649 0.03469 0.03469 0.0330 0.0330 0.0429 0.0527 0.1378 0.0443 0.0527 0.1443 0.1422 0.1100 0.1215 0.1201 0.1201 0.0541 0.0524 0.05413 0.0524 0.05413 0.0524 0.0552 0.05413 0.0524 0.0552 0.05413 0.0524 0.0554 0.0552 0.0554 0.0555 0.0554 0.0557 0.0557 0.0549 0.0557 0.0549 0.0557 0.0549 0.0557 0.0577 0.0573 0.0570 0.0577 0.0557 0.0552 0.0552 0.0552 0.0552 0.0552 0.0570 0.0552 0.0570 0.05520 0.05520 0.05520 0.05520 0.0550000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {$	$\begin{array}{c} -0.3066\\ -0.3267\\ 0.4262\\ 0.3257\\ 0.1044\\ 0.1074\\ 0.1074\\ 0.1074\\ 0.1030\\ 0.1030\\ 0.1210\\ 0.1210\\ 0.1216\\ 0.1216\\ 0.1443\\ 0.1451\\ 40.99\ A\\ -0.5159\\ 0.0293\\ 0.0656\\ 0.3822\\ -0.1359\\ 0.0662\\ -0.4982\\ 0.0682\\ -0.1359\\ 0.0682\\ -0.1359\\ 0.0682\\ -0.1359\\ 0.0682\\ -0.1359\\ 0.0682\\ 0.0682\\ -0.1359\\ 0.0682\\ 0.0$	H36 H37 H38 H39 H40 O41 C42 C43 C25 S26 C27 C28 C27 C28 C27 C33 C32 C33 C32 C33 C34 H37 H38 H37 H38 H39 H40 O41 C42 C43 D44 C45 C46 O47 C46 O47 C46 O47 C25 S26	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1220\\ 0.0547\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3469\\ -0.33067\\ -0.3307\\ 0.4372\\ -0.3398\\ -0.1378\\ 0.4372\\ -0.3398\\ -0.1378\\ 0.4322\\ 0.0830\\ -0.5150\\ 0.0449\\ 0.0524\\ 0.0524\\ 0.1101\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.0524\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5228\\ 0.3500\\ -0.3069\\ 0.0410\\ \end{array}$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C6} \\ {\rm O7} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H2} \\ {\rm H2} \\ {\rm C3} \\ {\rm C3} \\ \end{array}$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1037 0.1210 0.1216 0.1443 0.1451 40.99 40.955 0.0656 -0.4982 -0.4982 -0.4982 -0.355 0.0686 0.0382 -0.359 0.4443 0.4226 0.1087 0.1086 0.1086 0.1086 0.1086 0.1086 0.1081 0.1082 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1082 0.1081 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0082 0.0081 0.0082 0.0082 0.0081 0.0082	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C48 C27 S26 C27 S29 C30 O31 C32 C33 O34 H37 H38 H39 O44 C42 C33 O34 H37 H38 H39 O41 C42 C43 O44 C45 C46 C47 C48 C25 S26	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.6441 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2398 -0.1378 0.4222 0.0430 0.4372 -0.2394 -0.5100 0.4222 0.0430 0.4222 0.0430 0.4222 0.0429 0.422 0.0429 0.422 0.0534 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.0524 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.0524 0.1215 0.1215 0.0524 0.0524 0.0524 0.0524 0.0525 0.0525 0.0525 0.0525 0.0525 0.0547 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.1215 0.0525 0.0427 0.1215 0.0525 0.0427 0.0427 0.1215 0.0525 0.0427 0.0477 0.0477 0.0477000000000000000000
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ \end{array} $	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1074 0.1030 0.1030 0.1210 0.1210 0.1216 0.1216 0.1443 0.1451 40.99 Å -0.5159 0.0293 0.0656 -0.4982 0.0661 0.0382 -0.5139 0.0662 -0.31359 -0.31359 -0.31359 0.0682 0.1087 0.1097 0.1098 0.1098 0.1098 0.1099 0.1099 0.0082 0.008	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 O47 C48 C27 C28 C27 C33 C27 C30 C32 C33 C32 C33 C34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47 C43 O44 C46 C47 C25 C26 C27 C28	$\begin{array}{c} 0.1424\\ 0.1124\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1220\\ 0.0547\\ 0.0547\\ 0.0547\\ 0.0547\\ 0.0547\\ 0.0542\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3469\\ -0.3367\\ -0.3367\\ -0.3398\\ -0.1378\\ 0.0422\\ 0.0330\\ -0.5150\\ 0.0449\\ 0.0524\\ 0.0524\\ 0.0524\\ 0.1422\\ 0.1101\\ 0.1215\\ 0.1215\\ 0.1215\\ 0.15213\\ 0.0691\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5228\\ 0.3300\\ -0.3306\\ -0.3396\\ -0.3394\\ -0.3394\\ -0.5394\\ -0.5394\\ -0.5394\\ -0.3394\\ -0.$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C11} \\ {\rm C12} \\ {\rm C10} \\ {\rm C11} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H190} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H25} \\ {\rm H23} \\ {\rm H24} \\ {\rm H24} \\ {\rm H24} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H10} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ $	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1030 0.1210 0.1210 0.1210 0.1210 0.1210 0.1241 0.1443 0.4451 40.99 40.95 0.0656 0.0382 -0.4982 -0.4982 -0.4982 -0.4982 -0.4982 -0.4982 -0.359 0.0686 0.3582 -0.443 0.4266 0.3285 0.1087 0.1086 0.1087 0.1086 0.1087 0.1086 0.1087 0.1081 0.0081 0.0082 0.0081 0.0081 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.0081 0.0082 0.00	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C48 C25 S26 C27 S28 S29 C30 O31 C32 C33 O34 H37 H38 H39 O44 C33 O34 H37 C33 O34 H37 H38 H39 O41 C42 C43 O44 C45 C46 C47 C48 C25 S26 S26 S26	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0640 -0.6206 0.0525 0.0640 -0.5284 0.3649 -0.5284 0.3649 -0.5284 0.3649 -0.5284 0.3378 0.4222 0.0330 -0.4372 -0.3378 0.4222 0.0330 -0.4373 0.4222 0.0330 0.4222 0.0350 0.4422 0.1443 0.1421 0.1443 0.1422 0.1443 0.1443 0.1422 0.1443 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0.1444 0
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} \equiv = \\ \hline \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C9} \\ {\rm O1} \\ {\rm O1} \\ {\rm O2} \\ {\rm O2} \\ {\rm O1} \\ {\rm O2} \\ {\rm O1} \\ {\rm O2} \\ {\rm O1} \\ {\rm O2} \\ {\rm O2} \\ {\rm O1} \\ {\rm O2} \\ {\rm O2} \\ {\rm O2} \\ {\rm O2} \\ {\rm O1} \\ {\rm O2} \\ {\rm O2} \\ {\rm O3} \\ {\rm O4} \\ {\rm C5} \\ {\rm O4} \\ {\rm O4} \\ {\rm C5} \\ {\rm O4} \\ {\rm O4} \\ {\rm C5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O5} \\ {\rm O4} \\ {\rm O4} \\ {\rm O1} \\ {\rm O4} \\ {\rm O4} \\ {\rm O1} \\ {\rm O4} \\ {\rm O1} \\ {\rm O4} \\ {\rm O1} \\ {\rm O1} \\ {\rm O1} \\ {\rm O1} \\ {\rm O2} \\ {\rm O1} \\ {\rm O1} \\ {\rm O1} \\ {\rm O1} \\ {\rm O2} \\ {\rm O1} \\ {\rm O1} \\ {\rm O2} \\ {\rm O1} \\$	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1074 0.1030 0.1030 0.1210 0.1216 0.1037 0.1210 0.1216 0.1443 0.1451 40.99 Å -0.5159 0.0265 -0.4982 0.0666 0.3822 -0.5149 0.0682 -0.3159 0.0682 -0.3159 0.0682 -0.3159 0.0682 -0.3159 0.0682 0.0682 -0.3159 0.0682 -0.3159 0.0682 -0.3159 0.0682 -0.3159 0.0682 -0.3159 0.0682 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1057 0.0057 0.	H36 H37 H38 H39 H40 O41 C42 C43 C45 C46 O47 C48 C27 C28 C27 C30 C32 C32 C33 C34 H36 H37 H38 H36 H37 H38 O44 C45 C32 C33 O41 C42 C44 O41 C45 C46 O47 C46 C47 C28 S29 C27 C30 C46 C47 C48 C44 C45 C26 C27 C30 Intertiet	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 0.0541 0.05477 0.0541 0.0649 0.0525 0.0640 0.0525 0.0640 0.0528 0.0640 0.0528 0.0649 0.0528 0.0649 0.0528 0.0649 0.0528 0.0449 0.0529 0.0422 0.0330 0.0449 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0420 0.0524 0.0525 0.0420 0.0524 0.0525 0.0420 0.0524 0.0525 0.0440 0.0525 0.0524 0.0525 0.0440 0.0525 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0440 0.0525 0.0440 0.0525 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0557 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0557 0
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1030 0.1030 0.1210 0.1210 0.1210 0.1210 0.1211 0.1443 0.4451 40.99 0.6556 0.0382 -0.4982 0.0686 0.0382 -0.4982 0.0686 0.0382 -0.359 0.0443 -0.359 0.4443 0.4266 0.3285 0.1087 0.1086 0.4443 0.4266 0.3285 0.1087 0.1086 0.1087 0.1086 0.1092 0.1087 0.1051 0.00550 0.00550 0.00550 0.00	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C48 C25 S26 C27 S28 S29 C30 O31 C32 C33 O34 H37 H38 H39 O44 C33 O34 H37 C33 O34 H37 H38 H39 O41 C42 C43 O44 C45 C46 C47 C48 C25 S26 C27 C28 S29 C30 C47 C48	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0641 0.0649 -0.5206 0.0525 0.0640 0.0525 0.0640 0.0525 0.0640 0.0649 0.3669 -0.5284 0.3469 -0.3067 0.4372 -0.2398 -0.1378 0.4222 0.0330 -0.422 0.0429 0.4222 0.0330 0.4222 0.0429 0.4221 0.0524 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1422 0.1443 0.1421 0.1421 0.1443 0.1421 0.1443 0.1421 0.1443 0.1421 0.1443 0.1421 0.1441 0.1421 0.1441 0.1421 0.1441 0.1421 0.1441 0.1421 0.1441 0.14
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C1} \\ $	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1074 0.1030 0.1030 0.1210 0.1216 0.1037 0.1210 0.1216 0.1245 0.1245 0.0293 0.0656 -0.499 A 0.0656 0.0651 0.0652 0.0662 -0.5139 0.0662 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5139 0.0682 -0.5135 0.0682 -0.5135 0.0682 -0.5135 0.0682 0.057 0.1057 0.005	H36 H37 H38 H39 H40 O41 C42 C43 C25 S26 C27 C28 C27 C28 C27 C33 C32 C33 C34 H37 H38 H37 H38 H36 H37 H38 D44 C42 C32 C33 D41 C42 C44 C45 C46 C47 C46 C47 C28 S29 S26 C27 C30 C31	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 0.0541 0.0649 0.0525 0.06640 0.0525 0.06640 0.0526 0.06640 0.0649 0.0449 0.0524 0.0649 0.0524 0.0544 0.0651 0.1215 0.1205 0.1205 0.1205 0.0649 0.0524 0.0549 0.0549 0.0549 0.0549 0.0549 0.0524 0.0549 0.0524 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0549 0.0552 0.0449 0.0554 0.0549 0.0554 0.0549 0.05540000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C3} \\ {\rm C11} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C11} \\ {\rm C11} \\ {\rm C12} \\ {\rm C11} \\ {\rm$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1030 0.1210 0.1210 0.1210 0.1216 0.1443 0.1451 40.99 40.953 0.0666 -0.4982 -0.5159 0.0283 0.0665 0.0382 -0.5149 0.0382 -0.359 0.4443 0.4266 0.3285 0.1087 0.1086 0.1087 0.1081 0.1051 0.0055	H36 H37 H38 H39 H40 O41 C42 C43 C44 C47 C48 C47 C48 C25 S26 C27 S28 C30 O31 C32 C33 O34 H37 H38 H39 H40 O41 C42 C33 O34 H38 H39 O44 C42 C43 O44 C42 C44 C45 C46 C47 C48 C47 C48 C25 S26 C30 C31 C32	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1114\\ 0.1115\\ 0.1125\\ 0.1225\\ 0.1225\\ 0.1220\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3699\\ \hline 0.3670\\ 0.4372\\ -0.2384\\ 0.34699\\ \hline 0.3670\\ 0.4372\\ -0.3378\\ 0.4222\\ 0.0330\\ -0.4372\\ -0.3378\\ 0.4222\\ 0.0330\\ -0.4222\\ 0.0330\\ -0.5150\\ 0.447\\ 0.1422\\ 0.1101\\ 0.0524\\ -0.5143\\ 0.0624\\ -0.5140\\ 0.0524\\ -0.522\\ 0.3500\\ \hline \hline 0.0478\\ -0.522\\ 0.3500\\ \hline \hline 0.0478\\ -0.522\\ 0.3500\\ \hline \hline 0.0478\\ -0.522\\ 0.3500\\ \hline 0.0478\\ -0.522\\ 0.3500\\ \hline 0.0428\\ -0.5239\\ \hline 0.0329\\ \hline 0.0439\\ \hline 0.0334\\ -0.6137\\ \hline 0.0334\\ -0.6334\\ 0.0634\\ -0.6334\\ 0.0634\\ -0.6334\\ 0.0634\\ \hline 0.0439\\ \hline \end{array}$
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm O7} \\ {\rm C7} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C2} \\ {\rm C12} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C12} \\ {\rm $	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1074 0.1030 0.1210 0.1030 0.1210 0.1216 0.1037 0.1216 0.1245 0.0293 0.0656 -0.499 A 0.0656 -0.4982 0.0662 -0.5159 0.0662 -0.5143 0.0862 -0.3359 0.0682 -0.359 0.0862 -0.359 0.0862 -0.359 0.0862 -0.359 0.0862 -0.359 0.0862 -0.359 0.0862 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.0336 0.0356 0.0356 0.0357 0.	H36 H37 H38 H39 H40 O41 C42 C43 C25 S26 C27 C28 C27 C28 C27 C33 C32 C33 C44 C45 C46 O47 C48 C27 C30 O31 C32 C33 C46 O41 C42 C43 D44 C45 C46 O47 C46 C47 C30 C31 C32 C33	0.1424 0.1114 0.1114 0.1115 0.1225 0.1210 0.0541 0.05477 0.0541 0.0649 -0.5206 0.0525 0.06640 -0.5284 0.3469 -0.3346 -0.3346 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.4372 0.0544 0.0544 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.1215 0.1
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm Z} = \\ \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H23} \\ {\rm H24} \\ {\rm H20} \\ {\rm H21} \\ {\rm H20} \\ {\rm H20} \\ {\rm H21} \\ {\rm H16} \\ {\rm H10} \\ {\rm H10} \\ {\rm H21} \\ {\rm H20} \\$	-0.3066 0.4262 0.3257 0.1046 0.1044 0.1074 0.1079 0.1030 0.1030 0.1030 0.1210 0.1210 0.1210 0.1210 0.1210 0.1216 0.1443 0.4451 40.99 0.6556 -0.4982 0.0656 -0.4982 0.0682 -0.4982 0.0682 -0.4982 0.0682 -0.4982 0.0682 -0.359 0.0822 0.03225 0.03225 0.4443 -0.3295 0.4245 0.4266 0.3285 0.4266 0.3285 0.1087 0.1051 0.00555 0.00555 0.00555 0.00555 0.00555 0.00555 0.00555 0.00555 0.00555	H36 H37 H38 H39 H40 O41 C42 C43 C44 C47 C48 C47 C48 C25 S26 C27 C33 O34 H35 H37 H38 H39 H40 O44 C33 O34 H38 H39 O44 C42 C43 O44 C45 C46 C47 C48 C42 C44 C45 C46 C47 C48 C44 C45 S26 C30 C31 C32 C33 C34	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3670 0.4372 -0.2388 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.4222 0.0350 0.4224 0.1101 0.1201 0.1215 0.1215 0.1225 0.1443 0.0524 -0.5263 0.0524 -0.5252 0.0524 0.0524 -0.5253 0.0524 -0.5252 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 -0.5253 0.0524 0.0524 -0.5253 0.0524 0.0524 0.0525 0.0547 0.0547 0.0525 0.0525 0.0525 0.0525 0.0525 0.0525 0.0547 0.0525 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C8} \\ {\rm C10} \\ $	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1074 0.1030 0.1210 0.1030 0.1210 0.1216 0.1216 0.1216 0.1245 0.0293 0.0656 -0.499 A 0.0656 0.0651 0.0652 0.0651 0.0662 -0.5149 0.0862 -0.5149 0.0862 -0.51359 0.0662 0.1087 0.1259 0.1087 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0087 0.0087 0.0087 0.0086 0.0086 0.0087 0.0087 0.0086 0.0086 0.0086 0.0086 0.0086 0.0086 0.0087 0.0087 0.0087 0.0087 0.0086 0.0087 0.0086 0.0087 0.0087 0.0086 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0086 0.0087 0.0087 0.0087 0.0087 0.0086 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.0087 0.	H36 H37 H38 H39 H40 O41 C42 C43 C25 S26 C27 C28 C27 C28 C27 C28 C27 C30 O31 C32 C33 O44 C45 C48 H39 H40 O41 C42 C33 O44 C45 C46 O47 C46 O47 C46 C47 C28 S29 C30 O31 C32 C33 O34 D35	$\begin{array}{c} 0.1424\\ 0.1124\\ 0.1114\\ 0.1115\\ 0.1225\\ 0.1220\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3469\\ -0.33067\\ 0.3469\\ -0.33067\\ 0.4372\\ 0.4372\\ 0.4372\\ 0.3398\\ -0.1378\\ 0.4372\\ 0.4372\\ 0.4372\\ 0.06330\\ -0.5160\\ 0.0449\\ 0.0524\\ 0.0524\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0624\\ -0.5140\\ 0.0634\\ -0.5394\\ -0.3366\\ 0.4410\\ -0.3394\\ -0.3366\\ 0.4410\\ -0.3394\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5394\\ -0.5149\\ 0.0634\\ -0.5394\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5149\\ 0.0634\\ -0.5346\\ -0.$
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm Z} = - \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H12} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm H23} \\ {\rm H22} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C12} \\ {$	-0.3066 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1079 0.1030 0.1037 0.1030 0.1021 0.1210 0.1210 0.1210 0.1210 0.1211 0.1443 0.4451 40.99 0.6556 -0.4982 0.0656 -0.4982 0.0682 -0.4982 0.0682 -0.4982 0.0682 -0.4982 0.0682 -0.359 0.0682 -0.3285 0.0282 0.4443 -0.3285 0.1087 0.1086 0.1097 0.1051 0.0056 0.	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 S26 C27 C33 C34 H35 H37 C33 C34 H37 C33 C34 H37 C33 C34 H38 H39 H40 O41 C42 C33 C34 H37 H38 H39 O41 C42 C45 C46 C47 C48 C44 C45 S26 C27 C28 S29 C30 C31 C25 S26 C33	$\begin{array}{c} 0.1424\\ 0.1114\\ 0.1114\\ 0.1115\\ 0.1125\\ 0.1225\\ 0.1225\\ 0.1226\\ 0.0541\\ 0.0649\\ -0.5206\\ 0.0525\\ 0.0640\\ -0.5284\\ 0.3699\\ \hline 0.3672\\ -0.5284\\ 0.34699\\ \hline 0.3672\\ -0.5284\\ 0.3459\\ \hline 0.4222\\ 0.0330\\ -0.4372\\ -0.3378\\ 0.4222\\ 0.0330\\ -0.4222\\ 0.0330\\ -0.5162\\ 0.0422\\ 0.0630\\ 0.4222\\ 0.1101\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5140\\ 0.0524\\ -0.5390\\ \hline 0.0699\\ 0.4412\\ 0.0691\\ -0.529\\ 0.3500\\ \hline 0.0428\\ -0.529\\ 0.3500\\ \hline 0.0428\\ -0.529\\ 0.3500\\ \hline 0.0428\\ -0.529\\ 0.0634\\ -0.5346\\ -0.524\\ -0.5346\\ -0.5346\\ -0.5346\\ -0.5346\\ -0.5346\\ -0.5346\\ 0.0439\\ 0.0534\\ \hline 0.5346\\ -0.5346\\ 0.1428\\ 0.0439\\ 0.0534\\ \hline 0.5346\\ 0.1428\\ 0.1428\\ \hline 0.1428\\ 0.1428\\ 0.1428\\ \hline 0.1428\\ 0.1$
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H16} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C4} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C9} \\ {\rm C11} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C6} \\ {\rm C9} \\ {\rm C11} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C1} \\ {\rm C1} \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C1} \\ {\rm C2} \\ {\rm C1} \\ {\rm C$	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1077 0.1030 0.1210 0.1210 0.1216 0.1216 0.1243 0.1451 40.99 Å 0.0565 0.0565 0.0565 0.0565 0.0661 0.0662 -0.4982 0.0662 -0.5149 0.06867 0.1087 0.1057 0.05147 0.0326 0.0376 0.0444 0.0376 0.0466 0.0376 0.0376	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C27 C28 C27 C33 O34 H37 H38 H39 H40 O44 C45 C26 C27 C33 O44 C45 C46 O41 C42 C43 O44 C45 C26 S26 C27 S28 S29 C30 O41 C42 C25 S26 C27 S28 S29 O31 C32 S33 S44	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 -0.3388 -0.1378 0.4372 -0.3387 -0.4372 -0.3387 -0.4372 -0.3387 0.4372 -0.5160 0.0449 0.0437 0.0524 -0.5140 0.0524 -0.5149 0.0651 0.0524 -0.33069
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm Z} = \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H12} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm C3} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C10} \\ {\rm C12} \\ {\rm C12}$	-0.3066 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1020 0.1210 0.1210 0.1210 0.1210 0.1212 0.1443 0.1445 1 40.99 4 -0.5159 0.0282 -0.4982 0.0686 -0.4982 0.0382 -0.5149 0.0382 -0.1359 -0.3582 -0.359 0.4443 -0.3285 0.1087 0.1097 0.1086 0.1097 0.1081 0.1097 0.1081 0.1097 0.1081 0.1081 0.1097 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1081 0.1085 0.0086 0.0085 0.008	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C48 C25 S26 C27 C33 O34 H37 H38 H39 O44 C37 C30 O31 C32 C33 O44 H37 H38 H39 O44 C42 C43 O44 C45 C46 C47 C48 C25 S26 C31 C32 C33 C34 H35 H36 H37 H36 H37	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2398 0.4322 -0.3378 0.4222 0.0330 -0.4372 -0.3378 0.4222 0.0330 0.4222 0.0330 0.4222 0.0437 0.4372 0.0429 0.4222 0.0350 0.4222 0.0429 0.4221 0.1443 0.1422 0.1443 0.0524 -0.5260 0.0524 -0.5250 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0524 0.0525 0.0525 0.0547 0.0548 0.0548 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0548 0.0530 0.0530 0.0548 0.05300 0.05300 0.05300 0.05300 0.0530000000000
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C3} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C3} \\ {\rm C10} \\ {\rm C10} \\ {\rm C2} \\ {\rm C3} \\ {\rm C10} \\ {\rm C10} \\ {\rm C2} \\ {\rm C3} \\ {\rm C10} \\ {\rm C11} \\ {\rm C10} \\ {$	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1077 0.1030 0.1210 0.1210 0.1216 0.1216 0.1216 0.1245 0.0293 0.0656 0.0651 0.0651 0.0651 0.0662 -0.4982 0.0662 -0.5149 0.087 0.1259 0.087 0.1259 0.087 0.1087 0.0376 0.0376 0.0376 0.0376 0.0376 0.0376 0.0376 0.0376 0.0326	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C27 C28 C27 C30 C31 C32 C33 O44 C45 C46 O47 C33 O44 C45 C46 O47 C43 O44 C45 C46 O47 C43 O44 C45 S26 C27 S28 S29 C42 C43 O44 C45 S26 C27 S28 S29 O31 C22	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 0.5347 0.0544 0.0524 0.0541 0.0524 0.0547 0.125 0.125 0.125 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.1423 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.125 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0547 0.0549 0.0547 0.0557 0.0547 0.0557 0.0547 0.0557 0.0547 0.0557 0.0547 0.05570000000000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm z} = \\ \hline \\ {\rm c2} \\ {\rm c3} \\ {\rm c3} \\ {\rm c3} \\ {\rm c4} \\ {\rm c5} \\ {\rm c6} \\ {\rm 07} \\ {\rm c3} \\ {\rm c3} \\ {\rm c4} \\ {\rm c5} \\ {\rm c6} \\ {\rm 07} \\ {\rm c3} \\ {\rm c3} \\ {\rm c4} \\ {\rm c5} \\ {\rm c6} \\ {\rm 07} \\ {\rm c6} \\ {\rm c7} $	-0.3066 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1020 0.1210 0.1210 0.1210 0.1210 0.1212 0.1443 0.1445 0.4451 40.99 Å -0.5159 0.0282 -0.4982 0.0686 -0.4982 0.0382 -0.5149 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0255 0.1085 0.1097 0.1051 0.0355 0.0365 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0376 0.0355 0.0356 0.0355 0.0355 0.0356 0.03555 0.03555 0.03555 0.03555 0.03555 0.03555 0.03555 0.03555 0.	H36 H37 H38 H39 H40 O41 C42 C43 C46 O47 C48 C25 S29 C30 C31 C32 C33 O34 H37 H38 H39 O44 C42 C33 O34 H37 H38 H39 O44 C42 C33 O34 H37 C48 C25 S26 C32 C33 O31 C25 S26 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2398 0.4322 -0.3378 0.4222 0.0330 -0.4372 -0.3378 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.4222 0.0350 0.4223 0.1443 0.1422 0.1401 0.1201 0.1201 0.1201 0.1215 0.1215 0.1215 0.0524 -0.5262 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0525 0.0524 0.0525 0.0525 0.0547 0.0548 0.0547 0.0548 0.0548 0.0548 0.0548 0.0548 0.0548 0.0548 0.0548 0.0538 0.0548 0.0538 0.0548 0.0538 0.0548 0.0538 0.0548 0.0538 0.0548 0.0538 0.0538 0.0548 0.0538 0.0538 0.0548 0.05380 0.05380 0.05380 0.05380 0.05380 0.05480 0.0548000
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm H14} \\ {\rm H12} \\ {\rm H22} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C13} \\ {\rm C12} \\ {\rm C13} \\ {\rm C14} \\ {\rm C12} \\ {\rm C13} \\ {\rm C14} \\ {\rm C15} \\ {\rm C16} $	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1077 0.1030 0.1210 0.1210 0.1216 0.1216 0.1216 0.1245 0.0293 0.0656 0.0651 0.0651 0.0651 0.0662 -0.4982 0.0662 -0.5149 0.0867 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1057 0.0376 -0.5147 0.0326 -0.3259 0.0428 0.0428 0.0428 0.0428 0.0325 0.0428 0.0325 0.0428 0.0325 0.0428 0.0325 0	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C27 C28 C27 C33 O34 H37 H36 H37 H38 H39 H40 C41 C42 C43 O44 C45 C33 O44 C45 C26 C27 S28 C39 O41 C42 C44 C45 C27 S28 S29 C30 O31 C32 C33 O44 C35 S29 C30	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 -0.3386 -0.1378 0.4372 -0.3387 -0.1378 0.4372 -0.3388 -0.1378 0.4372 -0.5160 0.0437 0.4372 -0.517 0.4372 -0.517 0.4372 -0.517 0.4372 -0.517 0.4222 0.0830 -0.5142 0.0524 -0.5149 0.0534 -0.3366 0.4100 0.6534 -0.3366 0.4102 0.0534 -0.3366 0.4100 0.0534 -0.3366 0.4125 0.5346 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 -0.5346 -0.5346 -0.5346 -0.5356 -0.5356 -0.5356 -0.5556
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C11} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm H16} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H22} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C7} \\ {\rm C12} \\ {\rm C11} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \end{array}$	-0.3066 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1021 0.1210 0.1210 0.1210 0.1210 0.1211 0.1443 0.1445 0.4451 40.99 Å -0.5159 0.0282 -0.4982 0.0686 -0.4982 0.0382 -0.5149 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0255 0.1065 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.0376 -0.5193 0.0366 0.0382 -0.5149 0.0551 0.0666 0.1097 0.1051 0.1051 0.1051 0.1051 0.0376 -0.5193 0.0365 0.0365 0.0376 -0.5193 0.0376 -0.5193 0.0376 -0.5193 0.0376 -0.5193 0.0376 -0.3376 -0.3599 0.0376 -0.3599 0.0387 -0.3599 0.0376 -0.3599 0.0376 -0.3599 0.0376 -0.3599 0.0325 0.0376 -0.3599 0.0325 0.0376 -0.3599 0.0325 0.0325 0.0376 -0.3599 0.0325 0.0325 0.0376 -0.3599 0.0325 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S29 C30 C31 C32 C33 O34 H35 H37 C33 O34 H35 H37 C42 C33 O34 H37 C48 C47 C48 C30 O41 C42 C45 C46 C47 C48 C44 C45 C46 C47 C48 C45 C46 C47 C48 C41 C52	0.1124 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2388 -0.1378 0.4222 0.0330 -0.4372 -0.2388 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.4222 0.0350 0.4222 0.0427 0.1443 0.1215 0.0524 -0.5140 0.0524 -0.5250 0.0524 -0.5550 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0524 0.0552 0.0524 0.0557
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C12} \\ {\rm C3} \\ {\rm O4} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C3} \\ {\rm C12} \\ {\rm C13} \\ {\rm C12} \\ {\rm C13} \\ {\rm C14} \\ {\rm C11} \\ {\rm C12} \\ {\rm C13} \\ {\rm C14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ \end{array}$	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1077 0.1030 0.1210 0.1210 0.1216 0.1216 0.1243 0.1451 40.99 Å 0.0556 0.0563 0.0565 0.0565 0.0661 0.0682 -0.4892 0.0682 -0.51359 0.0682 -0.51359 0.0682 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.1057 0.0666 -0.5147 0.0326 -0.5147 0.0544 -0.5147 0.0325 0.0428 -0.5147 0.0329 0.0428 -0.3299 0.0326 -0.5147 0.0325 0.0428 -0.3299 0.0428 -0.3299 0.0326 -0.5147 0.0326 -0.5147 0.0325 0.0428 -0.3299 0.0428 -0.3299 0.0259 0.0259 0.0259 0.0326 -0.5147 0.0329 0.0259 0.0428 -0.3299 0.0259 0.0259 0.0259 0.0259 0.0326 -0.5147 0.0325 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259 0.0428 -0.3259	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S26 C27 C33 O34 H37 H38 H39 H40 O44 C45 C26 C23 O34 H39 H40 O41 C42 C43 O44 C45 C27 C33 O44 C45 C27 S28 S29 C33 O41 C42 C28 S29 C30 O31 C32 C33 C34	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 -0.3388 -0.1378 0.4372 -0.3387 0.4372 -0.3387 0.4372 -0.3388 0.4322 0.4372 -0.5150 0.4372 0.443 0.0554 -0.5547 0.1215 0.0561 0.0554 -0.5149 0.0534 -0.3350 0.4142 0.0534 -0.3350 0.4142 0.0534 -0.3350 0.4224 0.0534 -0.3346 0.0534 -0.3346 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5346 -0.5346 -0.5346 -0.5346 -0.5550 -0.5477 -0.5550 -0.5477 -0.5547 -0.55500 -0.5550 -0.5550 -0.55500 -0.55500 -0.55500 -0.55500 -0.55
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm I2} \\ {\rm I2} \\ {\rm I2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H1$	-0.3066 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1070 0.1210 0.1210 0.1210 0.1210 0.1211 0.1443 0.1445 0.4451 40.99 Å -0.5159 0.0282 -0.4982 0.0686 -0.4982 0.0382 -0.5149 0.0382 -0.1359 -0.3589 0.0382 -0.1359 -0.359 0.0382 -0.1359 0.0382 -0.1359 0.0285 0.1086 0.1097 0.1085 0.1097 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.0376 0.0385 0.0666 0.0376 0.0387 -0.5199 0.0385 0.0666 0.0387 -0.5296 0.0387 -0.5199 0.0387 -0.5199 0.0387 -0.5296 0.0387 -0.3599 0.0376 -0.3599 0.0325 0.0376 -0.3599 0.0325 0.0376 -0.3599 0.0325 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355 0.0355	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 C31 C32 C33 O34 H35 H37 H38 H39 O41 C42 C32 C33 O34 H37 C48 C25 S26 C37 C38 C39 C31 C44 C45 C46 C47 C48 C47 C48 C32 C33 C34 H35	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.6471 0.0641 0.0649 -0.5206 0.0525 0.0640 0.0525 0.0640 0.0525 0.0640 0.0526 0.0526 0.0640 0.4372 -0.3388 -0.1388 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.0429 0.0524 0.1215 0.0524 -0.5140 0.0524 -0.5250 0.0524 -0.5253 0.0524 0.0524 0.0524 -0.5253 0.0524 0.0525 0.0547 0.0547 0.0525 0.0547 0.0547 0.0557 0.0547 0.0557 0.0547 0.0557 0.0547 0.0557 0.0547 0.0554 0.0524 0.0552 0.0547 0.0554 0.0554 0.0554 0.0554 0.0552 0.0554 0.0552 0.0554 0.0554 0.0552 0.0554 0.0554 0.0552 0.0554 0.0556 0.0556 0.0556 0.0556 0.0
$ \begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm S13} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C10} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm C10} \\ {\rm C10} \\ {\rm C11} \\ $	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1074 0.1030 0.1210 0.1210 0.1216 0.1216 0.1216 0.1245 0.0293 0.0656 0.0651 0.0651 0.0682 -0.4822 0.0682 -0.5149 0.0862 -0.5149 0.0862 -0.5149 0.0862 -0.5159 0.0662 -0.5159 0.0662 -0.5159 0.0662 -0.5159 0.0662 0.0682 -0.5159 0.0682 0.0684 0.0685 0.0686 0.0376 0.0376 0.0329 0.03282 0.0329 0.03282 0.0328	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S26 C27 C33 O34 H37 H36 H37 H38 H39 H40 C41 C42 C33 O44 C45 C26 C27 C30 O41 C42 C43 O44 C45 C27 S28 S29 C30 O31 C42 C33 O34 H37 H38 H39 H38 H39 H30	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 0.5347 0.0524 -0.5140 0.06691 0.0654 -0.3366 0.4410 -0.5346 0.4378 -0.33069 0.4410 0.0524 -0.33069 0.4410 0.0534 -0.3306 0.4410 0.0534 -0.3306 0.4410 0.0534 -0.3366 0.4410 0.0534 -0.3366 0.4410 0.0534 -0.3346 0.0534 -0.3346 0.0534 -0.5346 -0.5346 -0.5356 -0.5400 -0.5546 -0.5546 -0.5550 -0.5400 -0.5546 -0.5546 -0.5546 -0.5546 -0.5550 -0.5546 -0.55500 -0.5550 -0.5550 -0.5550 -0.55
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm Z} = \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm C11} \\ {\rm C12} \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C11} \\ {\rm C12} \\ {\rm C13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H24} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H22} \\ {\rm C3} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C6} \\ {\rm C7} \\ {\rm C7} \\ {\rm C10} \\ {\rm C11} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H10} \\ {\rm $	-0.306 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1210 0.1210 0.1210 0.1210 0.1210 0.1210 0.1210 0.1210 0.1243 0.4451 40.99 Å -0.5159 0.0263 -0.4982 0.0686 -0.4982 0.0382 -0.5149 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0382 -0.359 0.0666 0.3257 0.1065 0.1067 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.1051 0.0355 0.0666 -0.3370 0.0666 0.3257 0.0666 0.0387 -0.5194 0.0376 -0.3370 0.0666 0.0376 -0.3376 -0.339 0.0666 -0.3376 -0.3299 0.0387 -0.5194 0.0387 -0.359 0.0666 -0.3299 0.0387 -0.5194 0.0387 -0.3299 0.4243 0.0666 -0.3376 -0.3299 0.4284 0.0387 -0.3299 0.4284 0.0387 -0.3299 0.4284 0.0387 -0.3299 0.4284 0.0387 -0.3299 0.4282 0.3259 0.0387 -0.3299 0.4282 0.3259 0.0387 -0.3299 0.4282 0.0387 -0.3299 0.4285 0.0666 -0.3299 0.0387 -0.3299 0.4285 0.0666 -0.3299 0.0387 -0.3299 0.0387 -0.3299 0.0387 -0.3299 0.4285 0.0666 -0.3299 0.0387 -0.3299 0.0287 -0.3299 0.4285 0.0666 -0.3299 0.0287 -0.3299 0.0287 -0.3299 0.4282 0.0387 -0.3299 0.4285 0.0666 -0.3299 0.0387 -0.3299 0.0287 -0.3299 0.0287 -0.3299 0.4282 0.3259 0.0387 -0.3299 0.4282 0.3259 0.0387 -0.3299 0.4282 0.3259 0.0387 -0.3299 0.4282 0.3259 0.	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H37 H38 H39 O41 C42 C32 C33 O34 H37 C48 C25 S26 C37 C38 C39 C31 C44 C45 C46 C47 C48 C41 C42 C32 C33 C34 H35	0.1124 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.641 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2388 -0.378 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.0429 0.0429 0.0524 -0.5140 0.0524 -0.526 0.0524 -0.5250 0.0524 0.0524 -0.5550 0.0524 -0.5550 0.0524 -0.5550 0.0524 0.0524 -0.5550 0.0524 0.0525 0.0524 0.0524 0.0524 0.0524 0.0552 0.0524 0.0524 0.0524 0.0524 0.0525 0.0524 0.0525 0.0524 0.0525 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555 0.0555
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm C2} \\ {\rm C3} \\ {\rm O4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C3} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ {\rm Z} = \\ {\rm C1} \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C6} \\ {\rm C7} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm C14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H12} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H12} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H12} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H12} \\ {\rm H10} \\ $	-0.3066 0.4262 0.3257 0.1044 0.1044 0.1074 0.1046 0.1047 0.1030 0.1030 0.1210 0.1030 0.1210 0.1216 0.1043 0.1443 0.1451 40.99 Å -0.5159 0.0565 0.0651 0.0652 -0.4982 0.0662 -0.4982 0.0662 -0.5149 0.0862 -0.5149 0.0862 -0.5149 0.1087 0.1086 0.0326 0.0326 -0.5398 0.0326 -0.5399 0.0326 0.030	H36 H37 H38 H39 H40 O41 C42 C43 C25 C26 C27 C28 C27 C28 C27 C28 C27 C30 C31 C32 C33 O44 C45 C26 C27 C30 O31 C32 C33 O44 C46 O47 C43 D44 C45 S26 C37 C38 H39 H40 O41 C42 C33 O31 C32 C33 O41 C42 C43 H38 H39	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 0.0525 0.0660 0.0525 0.0660 0.0526 0.0649 0.0649 0.0649 0.0649 0.0388 0.04372 0.3369 0.4372 0.3388 0.04372 0.1423 0.0649 0.0524 0.0544 0.0544 0.0544 0.0524 0.0541 0.0541 0.0524 0.0541 0.0541 0.0524 0.0541 0.0541 0.0552 0.1425 0.0541 0.0544 0.0525 0.0440 0.0525 0.0547 0.1423 0.0544 0.0524 0.0544 0.0524 0.0544 0.0554 0.0541 0.0554 0.0541 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0554 0.0555
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm Z} = \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C3} \\ {\rm H16} \\ {\rm H17} \\ {\rm C12} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C6} \\ {\rm O7} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H10} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H21} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H19} \\ {\rm H21} \\ {\rm H21} \\ {\rm H21} \\ {\rm H22} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H19} \\ {\rm H10} \\ {\rm H1$	-0.306 0.4262 0.3257 0.1046 0.3257 0.1046 0.1074 0.1074 0.1079 0.1030 0.1210 0.1210 0.1210 0.1210 0.1210 0.1212 0.1443 0.1451 40.99 Å -0.5159 0.0283 0.0656 -0.4982 0.0685 -0.4982 0.0382 -0.5149 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0382 -0.3159 0.0666 0.3257 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.1085 0.0335 0.0666 0.5296 0.0387 -0.519 0.0385 0.0666 -0.3370 0.0666 0.0376 -0.3376 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.0387 -0.3259 0.4266 0.0387 -0.3259 0.0387 -0.3259 0.4288 0.0666 -0.3299 0.4282 0.0387 -0.3289 0.4288 0.0666 -0.3299 0.4282 0.0387 -0.3289 0.0387 -0.3289 0.0387 -0.3289 0.4285 0.0387 -0.3289 0.0387 -0.3289 0.0387 -0.3289 0.0387 -0.3289 0.0387 -0.3289 0.0387 -0.3289 0.0325 0.0376 -0.3289 0.0325 0.0376 -0.3289 0.0267 0.0276 -0.3289 0.0267 0.0276 -0.3289 0.0267 0.0276 -0.3289 0.0267 0.0276	H36 H37 H38 H39 H40 O41 C42 C43 C25 S26 C27 C28 C33 D34 H35 H36 H37 C33 D34 H35 H36 H37 C33 D34 H38 H39 H40 O41 C42 C33 D34 H37 C48 C25 S26 C37 C38 C44 C45 C36 D31 C43 C44 C45 C46 H37 H38 H39 H40 C46	0.1424 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.6471 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2388 -0.378 0.4322 -0.2388 -0.378 0.4322 -0.3388 -0.4322 0.4372 -0.3388 0.4222 0.0330 0.4222 0.0330 0.4222 0.0330 0.4222 0.0350 0.4222 0.0350 0.0429 0.0527 -0.5413 0.0624 -0.5140 0.0524 -0.5284 0.0524 -0.5284 0.0524 -0.5250 0.0428 0.3500 -0.3305 0.4224 0.0350 0.0428 0.3500 -0.3369 0.4214 0.0524 -0.5413 0.0652 0.0524 -0.5413 0.0652 0.0524 -0.5369 0.4410 0.0524 -0.5413 0.0652 0.0524 -0.5369 0.4410 0.0524 -0.5369 0.4254 0.03500 -0.3369 0.4254 0.03500 -0.3369 0.4254 0.0354 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5349 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0534 -0.5520 0.0429 0.0429 0.0529 0.0429 0.0529 0.0429 0.0529 0.0520 0
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H15} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm S11} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C12} \\ {\rm C3} \\ {\rm C3} \\ {\rm H14} \\ {\rm H19} \\ {\rm H22} \\ {\rm H24} \\ \hline \\ {\rm C12} \\ {\rm C3} \\ {\rm C6} \\ {\rm C9} \\ {\rm C10} \\ {\rm C12} \\ {\rm C3} \\ {\rm C12} \\ {\rm C3} \\ {\rm C10} \\ {\rm C12} \\ {\rm C12} \\ {\rm C13} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ \end{array}$	-0.3066 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1074 0.1074 0.1030 0.1210 0.1210 0.1216 0.1212 0.1216 0.1216 0.1243 0.1443 0.4451 40.99 Å 0.0565 0.0561 0.0565 0.0661 0.0682 -0.4892 0.0682 -0.5149 0.087 0.1057 0.1087 0.1	H36 H37 H38 H39 H40 O41 C42 C43 C42 C43 C44 C45 C27 C28 S26 C27 C33 O34 H35 H36 H37 H38 H39 H40 O44 C45 C27 C33 O34 H35 H36 H37 H38 H39 O41 C42 C25 S26 C27 S28 S29 C33 O31 C32 C33 O34 H38 H39 H37 H38 H39	0.1424 0.1114 0.1114 0.1115 0.1225 0.1220 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3469 -0.3367 0.4372 0.0534 -0.5547 0.0524 0.0525 0.0525 0.0525 0.0527 0.5347 0.1423 0.0534 -0.5140 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.3350 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5149 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5346 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0534 -0.5540 0.0554 0.0554 0.0555 0.055
$\begin{array}{c} {\rm C12} \\ {\rm S13} \\ {\rm H14} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ {\rm Z} = \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C3} \\ {\rm C4} \\ {\rm C5} \\ {\rm C6} \\ {\rm O7} \\ {\rm C10} \\ {\rm S11} \\ {\rm C12} \\ {\rm C13} \\ {\rm H16} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H190} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ \hline \\ \hline \\ {\rm C2} \\ {\rm C3} \\ {\rm C6} \\ {\rm C7} \\ {\rm C8} \\ {\rm C9} \\ {\rm C10} \\ {\rm C10} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C2} \\ {\rm C3} \\ {\rm O1} \\ {\rm C1} \\ {\rm C1} \\ {\rm C1} \\ {\rm H16} \\ {\rm H17} \\ {\rm H18} \\ {\rm H19} \\ {\rm H20} \\ {\rm H21} \\ {\rm H21} \\ {\rm H22} \\ {\rm H23} \\ {\rm H24} \\ {\rm H21} \\ {\rm H24} \\ {\rm H21} \\ {\rm H24} \\ {\rm H21} \\ {\rm H24} \\ {\rm H21} \\ {\rm H24} \\ {\rm $	-0.306 0.4262 0.3257 0.1044 0.1074 0.1074 0.1074 0.1079 0.1030 0.1210 0.1210 0.1210 0.1210 0.1210 0.1210 0.1210 0.1212 0.1443 0.4451 40.99 Å -0.5159 0.0263 -0.4651 0.0382 -0.5149 0.0382 -0.5149 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0382 -0.3519 0.0666 0.3285 0.1087 0.1087 0.1087 0.1087 0.1087 0.1085 0.1087 0.1085 0.3036 0.4443 -0.5193 0.4443 -0.5199 0.4443 0.4266 0.3285 0.0666 -0.3376 -0.519 0.0387 -0.519 0.0387 -0.519 0.0386 0.0387 -0.3376 -0.5296 0.3259 0.4488 -0.3259 0.4488 -0.3259 0.4266 0.0387 -0.5191 0.0366 -0.3376 -0.5296 0.3259 0.4282 0.3259 0.4285 0.0387 -0.5296 0.3259 0.4285 0.0387 -0.5296 0.3259 0.4285 0.0387 -0.5296 0.3259 0.4285 0.0387 -0.5296 0.3259 0.4285 0.4485 0.3259 0.4285 0.1025	H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H37 H38 H39 O41 C42 C32 C33 O34 H37 C48 C25 S26 C37 C38 C44 C45 C37 C38 C39 C31 C44 C45 C46 C47 C48 C44 C45	0.1124 0.1114 0.1114 0.1115 0.1225 0.1225 0.1225 0.0541 0.0649 -0.5206 0.0525 0.0640 -0.5284 0.3649 -0.3667 0.4372 -0.2398 -0.378 0.4322 -0.2398 -0.378 0.4322 -0.2398 -0.4322 -0.3367 0.4372 -0.2398 -0.4222 0.0830 -0.4222 0.0830 -0.4222 0.0830 -0.4222 0.0830 -0.4222 0.1443 0.1422 0.1421 0.0524 -0.5140 0.0524 -0.5280 0.0524 -0.5220 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5230 0.0524 -0.5250 0.04254 0.0524 -0.5230 0.0524 -0.5250 0.04254 0.0524 -0.5300 0.04254 0.0429 0.0534 -0.5349 -0.5349 -0.5349 -0.5349 -0.5349 -0.5349 -0.5350 0.0425 0.04254 0.0429 0.0534 -0.5349 -0.5349 -0.5349 -0.5349 -0.5349 -0.5349 -0.5349 -0.5350 -0.525 0.0425 0.0425 0.0425 0.0425 0.0425 0.0425 0.0425 0.0525 0.0425 0.0425 0.0425 0.0429 0.0554 0.0555

Table E.2: Partial Charge Distribution of +1 Oxidized Rotaxane when the Center of Mass of the CBPQT⁴⁺ Ring Moves from z = 10.92 Å (TTF side) to z = 44.83 Å (DNP side)

z =	:10.92 Å														
01	-0.5374	C25	-0.3310	C49	-0.1512	H73	0.1519	C97	-0.0909	C121	-0.1317	H145	0.1823	C169	-0.0971
C2	0.0394	S26	0.2497	C50	-0.0588	H74	0.1514	H98	0.1431	C122	0.1110	H146	0.1469	C170	-0.1002
C3	0.0616	C27	-0.2626	C51	-0.0466	H75	0.1168	C99	0.0421	C123	-0.1532	H147	0.1452	H171	0.1218
04	-0.5052	C28	-0.1540	C52	-0.0661	H76	0.1171	C100	0.0541	C124	0.1519	H148	0.1186	H172	0.1212
C5	0.0829	S29	0.2401	C53	-0.0671	H77	0.1193	C101	-0.0975	N125	-0.4077	H149	0.1218	C173	-0.1747
C6	0.0353	C30	0.0903	C54	-0.0439	H78	0.1191	H102	0.1466	C126	-0.1712	H150	0.1853	N174	-0.4084
07	-0.5164	031	-0.5120	C55	-0.0603	H79	0.1230	C103	-0.1017	C127	0.0969	H151	0.1816	C175	0.1714
C8	0.0927	C32	0.0465	C56	-0.1435	H80	0.1230	H104	0.1446	C128	-0.1219	H152	0.1803	C176	-0.1317
C9	-0.1515	C33	0.0470	C57	0.4246	H81	0.3399	C105	0.0567	C129	-0.1218	H153	0.1503	C177	0.1167
C10	-0.2775	034	-0.5247	H58	0.1252	H82	0.1811	C106	-0.1020	C130	0.0899	H154	0.1542	C178	-0.1522
S11	0.2587	H35	0.1257	H59	0.1257	H83	0.1865	H107	0.1386	C131	-0.1031	H155	0.1818	C179	0.1564
C12	-0.3311	H36	0.1027	H60	0.1181	H84	0.1578	C108	-0.0973	C132	-0.0964	C156	0.1058	H180	0.1891
S13	0.2507	H37	0.1114	H61	0.1182	H85	0.1651	H109	0.1461	C133	-0.1727	C157	-0.1276	H181	0.1639
H14	0.3272	H38	0.1184	H62	0.1180	H86	0.1778	C110	0.0290	N134	-0.4048	C158	0.1595	H182	0.1434
H15	0.0995	H39	0.1252	H63	0.1182	H87	0.1695	C111	-0.0947	C135	0.1653	N159	-0.4078	H183	0.1669
H16	0.1011	H40	0.1155	H64	0.1440	H88	0.1680	H112	0.1344	C136	-0.1252	C160	0.1422	H184	0.1751
H17	0.1060	041	-0.5109	H65	0.1442	H89	0.1741	C113	-0.1187	C137	0.1114	C161	-0.1505	H185	0.1891
H18	0.1040	C42	0.0286	066	-0.4718	C90	-0.0908	H114	0.1312	C138	-0.1392	H162	0.1584	H186	0.1308
H19	0.0955	C43	0.0606	C67	-0.0012	H91	0.1425	C115	0.3246	C139	0.1589	H163	0.1816	H187	0.1362
H20	0.0862	044	-0.5109	C68	0.0653	C92	-0.1101	C116	-0.1194	H140	0.1723	C164	-0.1681	H188	0.1831
H21	0.1097	C45	0.0575	069	-0.4994	H93	0.1579	H117	0.1370	H141	0.1453	C165	0.0897	H189	0.1804
H22	0.1212	C46	0.0132	C70	0.0593	C94	0.3479	C118	-0.0939	H142	0.1544	C166	-0.1148	H190	0.1638
H23	0.0940	047	-0.4878	C71	0.0207	C95	-0.1098	H119	0.1375	H143	0.1790	C167	-0.1156	H191	0.1374
H24	0.1214	C48	0.4187	072	-0.4878	H96	0.1573	C120	0.1569	H144	0.1823	C168	0.0949	Total	5.0000
z =	15.66 Å														
01	-0.4907	C25	-0.3683	C49	-0.1507	H73	0.1522	C97	-0.0941	C121	-0.1283	H145	0.1870	C169	-0.1049
C2	0.0201	S26	0.2822	C50	-0.0585	H74	0.1517	H98	0.1382	C122	0.1036	H146	0.1508	C170	-0.1067
C3	0.0653	C27	-0.2754	C51	-0.0459	H75	0.1175	C99	0.0413	C123	-0.1539	H147	0.1494	H171	0.1294
04	-0.5034	C28	-0.1483	C52	-0.0663	H76	0.1178	C100	0.0483	C124	0.1542	H148	0.1144	H172	0.1288
C5	0.0709	S29	0.2428	C53	-0.0669	H77	0.1199	C101	-0.1009	N125	-0.4064	H149	0.1135	C173	-0.1673
C6	0.0396	C30	0.0855	C54	-0.0433	H78	0.1197	H102	0.1407	C126	-0.1591	H150	0.1828	N174	-0.4099
07	-0.5136	031	-0.5192	C55	-0.0598	H79	0.1253	C103	-0.1071	C127	0.0841	H151	0.1801	C175	0.1459
C8	0.0912	C32	0.0505	C56	-0.1434	H80	0.1253	H104	0.1346	C128	-0.1115	H152	0.1802	C176	-0.1335
C9	-0.1368	C33	0.0603	C57	0.4247	H81	0.3417	C105	0.0505	C129	-0.1132	H153	0.1510	C177	0.1083
C10	-0.2459	034	-0.5334	H58	0.1238	H82	0.2073	C106	-0.1073	C130	0.0919	H154	0.1561	C178	-0.1531
S11	0.2609	H35	0.0995	H59	0.1242	H83	0.1612	H107	0.1255	C131	-0.1145	H155	0.1812	C179	0.1590
C12	-0.3060	H36	0.1100	H60	0.1177	H84	0.1585	C108	-0.1007	C132	-0.1147	C156	0.0940	H180	0.1886
S13	0.2820	H37	0.1037	H61	0.1177	H85	0.1657	H109	0.1392	C133	-0.1630	C157	-0.1150	H181	0.1625
H14	0.3395	H38	0.1057	H62	0.1179	H86	0.1782	C110	0.0269	N134	-0.4148	C158	0.1129	H182	0.1374
H15	0.1215	H39	0.0978	H63	0.1180	H87	0.1702	C111	-0.0989	C135	0.1671	N159	-0.3998	H183	0.1679
H16	0.1214	H40	0.1019	H64	0.1443	H88	0.1687	H112	0.1306	C136	-0.1308	C160	0.1590	H184	0.1808
H17	0.1113	041	-0.5132	H65	0.1445	H89	0.1746	C113	-0,1230	C137	0.0977	C161	-0.1393	H185	0.1869
H18	0.1115	C42	0.0305	066	-0.4718	C90	-0.0941	H114	0.1114	C138	-0.1556	H162	0.1668	H186	0.1457
H19	0.1018	C43	0.0601	C67	-0.0012	H91	0.1377	C115	0.3097	C139	0.1516	H163	0.1925	H187	0.1445
H20	0.1019	044	-0.5107	C68	0.0647	C92	-0.1118	C116	-0.1240	H140	0.1826	C164	-0.1637	H188	0.1881
H21	0.1178	C45	0.0579	069	-0.4978	H93	0.1539	H117	0.1170	H141	0.1572	C165	0.0764	H189	0.1810
H22	0.1187	C46	0.0125	C70	0.0592	C94	0.3429	C118	-0.0981	H142	0.1576	C166	-0.1223	H190	0.1766
H23	0.1280	047	-0.4862	C71	0.0194	C95	-0.1116	H119	0.1337	H143	0.1865	C167	-0.1204	H191	0.1470
H24	0.1299	C48	0.4194	072	-0.4806	H96	0.1531	C120	0.1656	H144	0.1827	C168	0.0817	Total	5.0000
<i>z</i> =	18.75 Å														
01	-0 4694	C25	-0.3207	C49	-0 1498	H73	0 1538	C97	-0 1005	C121	-0 1249	H145	0 1867	C169	-0 1077
C2	0.0155	\$26	0.2837	C50	-0.0585	H74	0.1532	H08	0.1221	C122	0.0927	H146	0.1506	C170	=0 1063
C3	0.0589	C27	-0.2968	C51	-0.0453	H75	0 1222	C99	0.0352	C123	-0 1435	H147	0 1515	H171	0 1130
0.0	-0.4810	C28	-0.1570	C52	=0.0660	H76	0.1222	C100	0.0440	C124	0.1561	H148	0.1190	H172	0.1126
C5	0.0593	920	0.3045	C53	=0.0671	H77	0.1220	C101	-0 1071	N125	-0.4085	H140	0.1185	C173	-0 1774
CG	0.0403	C30	0.0754	C54	=0.0426	H78	0 1230	H102	0 1302	C126	=0 1631	H150	0 1864	N174	-0 4027
07	-0 5144	031	-0.5167	C55	-0.0597	H79	0 1121	C103	-0 1124	C127	0.0607	H151	0 1878	C175	0 1594
CS	0.0864	C32	0.0590	C56	-0 1431	H80	0 1119	H104	0 1125	C128	-0 1159	H152	0 1739	C176	-0 1306
C9	-0 1356	C33	0.0573	C57	0 4253	H81	0 3337	C105	0.0350	C129	-0 1188	H153	0 1381	C177	0.0921
C10	-0 2392	034	-0 5496	858	0 1178	H82	0 2145	C106	-0 1123	C130	0.0630	H154	0 1610	C178	-0 1481
S11	0.3563	H35	0 1119	H59	0 1184	H83	0 1659	H107	0 1002	C131	-0 1028	H155	0 1920	C179	0 1515
C12	-0.3035	H36	0 1059	H60	0 1156	H84	0 1603	C108	-0 1067	C132	-0 1020	C156	0.0886	H180	0 1924
S13	0.3465	H37	0.0924	H61	0.1155	H85	0.1664	H109	0.1279	C133	-0.1647	C157	-0.1274	H181	0.1622
H14	0.3463	H38	0.0924	H62	0.1167	H86	0.1787	C110	0.0336	N134	-0.4124	C158	0.1640	H182	0.1392
H15	0.1300	H39	0.0947	H63	0.1167	H87	0.1724	C111	-0.1020	C135	0.1654	N159	-0.4032	H183	0.1845
H16	0.1301	H40	0.0963	H64	0.1445	H88	0.1703	H112	0.1303	C136	-0.1209	C160	0.1527	H184	0.1863
H17	0.1213	041	-0.5207	H65	0.1448	H89	0.1758	C113	-0.1384	C137	0.0972	C161	-0.1458	H185	0.1893
H18	0.1214	C42	0.0381	066	-0.4717	C90	-0.1007	H114	0.0788	C138	-0.1494	H162	0.1632	H186	0.1456
H19	0.1155	C43	0.0585	C67	-0.0020	H91	0.1223	C115	0.3010	C139	0.1568	H163	0.1936	H187	0.1454
H20	0.1156	044	-0.5109	C68	0.0616	C92	-0.1159	C116	-0.1392	H140	0.1808	C164	-0.1765	H188	0.1917
H21	0.1220	C45	0.0602	069	-0.4809	H93	0.1399	H117	0.0782	H141	0.1413	C165	0.0740	H189	0.1860
H22	0.1230	C46	0.0108	C70	0.0526	C94	0.3315	C118	-0.1010	H142	0.1621	C166	-0.1055	H190	0.1858
H23	0.1376	047	-0.4847	C71	0.0312	C95	-0.1158	H119	0.1314	H143	0.1920	C167	-0.1056	H191	0.1405
H24	0.1388	C48	0.4206	072	-0.5125	H96	0.1387	C120	0.1613	H144	0.1899	C168	0.0767	Total	5.0000
_ z =	23.27 Å														
01	-0.4773	C25	-0.3072	C49	-0.1512	H73	0.1523	C97	-0.1066	C121	-0.1309	H145	0.1785	C169	-0.1157
C2	0.0164	S26	0.3874	C50	-0.0596	H74	0.1519	H98	0.1029	C122	0.1013	H146	0.1449	C170	-0.1109
C3		007	-0 2490	051		H75	0 1179	C99	0.0216	0102	-0.1426	H147		U171	0 1128
04	0.0622	627	0.2100	0.01	-0.0474		0.1170		0.0210	0123		111-11	0.1437	11/1	0.1120
C5	0.0622 -0.4917	C28	-0.1455	C52	-0.0474 -0.0662	H76	0.1178	C100	0.0461	C123	0.1529	H148	0.1437 0.1178	H172	0.1159
C6	0.0622 -0.4917 0.0641	C28 S29	-0.1455	C52 C53	-0.0474 -0.0662 -0.0674	H76 H77	0.1181 0.1215	C100 C101	0.0461 -0.1123	C123 N125	0.1529 -0.4153	H148 H149	0.1437 0.1178 0.1264	H172 C173	0.1159 -0.1641
	0.0622 -0.4917 0.0641 0.0371	C27 C28 S29 C30	-0.1455 0.3775 0.0695	C52 C53 C54	-0.0474 -0.0662 -0.0674 -0.0444	H76 H77 H78	0.1178 0.1181 0.1215 0.1212	C100 C101 H102	0.0461 -0.1123 0.1261	C123 C124 N125 C126	0.1529 -0.4153 -0.1504	H148 H149 H150	0.1437 0.1178 0.1264 0.1829	H171 H172 C173 N174	0.1120 -0.1641 -0.4101
07	0.0622 -0.4917 0.0641 0.0371 -0.5149	C28 S29 C30 031	-0.1455 0.3775 0.0695 -0.5174	C52 C53 C54 C55	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605	H76 H77 H78 H79	0.1178 0.1181 0.1215 0.1212 0.1327	C100 C101 H102 C103	0.0461 -0.1123 0.1261 -0.1229	C123 C124 N125 C126 C127	0.1529 -0.4153 -0.1504 0.0644	H148 H149 H150 H151	0.1437 0.1178 0.1264 0.1829 0.1841	H171 C173 N174 C175	0.1120 -0.1159 -0.1641 -0.4101 0.1624
07 C8	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863	C27 C28 S29 C30 D31 C32	-0.1455 0.3775 0.0695 -0.5174 0.0639	C52 C53 C54 C55 C56	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443	H76 H77 H78 H79 H80	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327	C100 C101 H102 C103 H104	0.0461 -0.1123 0.1261 -0.1229 0.0832	C123 C124 N125 C126 C127 C128	0.1529 -0.4153 -0.1504 0.0644 -0.1194	H148 H149 H150 H151 H152	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665	H171 H172 C173 N174 C175 C176	0.1120 0.1159 -0.1641 -0.4101 0.1624 -0.1213
07 C8 C9	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863 -0.1382	C27 C28 S29 C30 D31 C32 C33	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484	C52 C53 C54 C55 C56 C57	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241	H76 H77 H78 H79 H80 H81	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481	C100 C101 H102 C103 H104 C105	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294	C123 C124 N125 C126 C127 C128 C129	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188	H148 H149 H150 H151 H152 H153	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428	H171 H172 C173 N174 C175 C176 C177	0.1120 0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037
07 C8 C9 C10	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863 -0.1382 -0.2393	C27 C28 S29 C30 O31 C32 C33 O34	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525	C52 C53 C54 C55 C56 C57 H58	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121	H76 H77 H78 H79 H80 H81 H82	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267	C100 C101 H102 C103 H104 C105 C106	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286	C123 C124 N125 C126 C127 C128 C129 C130	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661	H148 H149 H150 H151 H152 H153 H154	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620	H171 H172 C173 N174 C175 C176 C177 C178	0.1120 0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390
07 C8 C9 C10 S11	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863 -0.1382 -0.2393 0.4225	C27 C28 S29 C30 O31 C32 C33 O34 H35	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391	C52 C53 C54 C55 C56 C57 H58 H59	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1119	H76 H77 H78 H79 H80 H81 H82 H83	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657	C100 C101 H102 C103 H104 C105 C106 H107	0.0210 0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615	C123 C124 N125 C126 C127 C128 C129 C130 C131	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016	H147 H148 H149 H150 H151 H152 H153 H154 H155	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884	H171 H172 C173 N174 C175 C176 C177 C178 C179	0.1129 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564
07 C8 C9 C10 S11 C12	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361	C52 C53 C54 C55 C56 C57 H58 H59 H60	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1119 0.1135	H76 H77 H78 H79 H80 H81 H82 H83 H84	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657 0.1583	C100 C101 H102 C103 H104 C105 C106 H107 C108	0.0210 0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020	H148 H149 H150 H151 H152 H153 H154 H155 C156	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180	0.1129 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1806
07 C8 C9 C10 S11 C12 S13	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034 \end{array}$	C27 C28 S29 C30 031 C32 C33 034 H35 H36 H37	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1119 0.1135 0.1138	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85	0.1173 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657 0.1583 0.1644	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109	0.0210 0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568	H148 H149 H150 H151 H152 H153 H154 H155 C156 C157	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181	0.11159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1545
07 C8 C9 C10 S11 C12 S13 H14	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\end{array}$	C27 C28 S29 C30 031 C32 C33 034 H35 H36 H37 H38	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62	-0.0474 -0.0662 -0.0674 -0.0404 -0.0605 -0.1443 0.4241 0.1121 0.1121 0.1135 0.1135 0.1138 0.1157	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657 0.1657 0.1683 0.1644 0.1773	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110	0.0210 0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159	C123 C124 N125 C126 C127 C128 C129 C129 C130 C131 C132 C133 N134	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568 -0.4089	H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530	H171 H172 C173 N174 C175 C176 C176 C177 C178 C179 H180 H181 H182	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1806 0.1545 0.1509
07 C8 C9 C10 S11 C12 S13 H14 H15	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1090	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.1421 0.1121 0.1135 0.1138 0.1157 0.1159	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87	0.1118 0.1181 0.1215 0.1212 0.1327 0.3481 0.2267 0.1657 0.1583 0.1644 0.1773 0.1716	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159 -0.1181	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568 -0.4089 0.1539	H149 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H181 H182 H183	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1806 0.1545 0.1509 0.1758
07 C8 C9 C10 S11 C12 S13 H14 H15 H16	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863 -0.1382 -0.2393 0.4225 -0.3165 0.4034 0.3436 0.1274 0.1272	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1090 0.1037	C51 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1135 0.1138 0.1157 0.1159 0.1430	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1583 0.1657 0.1583 0.1644 0.1773 0.1716 0.1694	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159 -0.1181 0.0914	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568 -0.4089 0.1539 -0.1153	H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498	H171 H172 C173 N174 C175 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1505 0.1509 0.1758 0.1758
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17	0.0622 -0.4917 0.0641 0.0371 -0.5149 0.0863 -0.1382 -0.2393 0.4225 -0.3165 0.4034 0.3436 0.1274 0.1272 0.1169	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 Q41	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1037 -0.5282	C51 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1119 0.1135 0.1138 0.1157 0.1159 0.1430 0.1430	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657 0.1583 0.1644 0.1773 0.1716 0.1694 0.1741	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159 -0.1181 0.0914 -0.9373	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137	$\begin{array}{c} 0.1529 \\ -0.4153 \\ -0.1504 \\ 0.0644 \\ -0.1194 \\ -0.1188 \\ 0.0661 \\ -0.1016 \\ -0.1020 \\ -0.1568 \\ -0.4089 \\ 0.1539 \\ -0.1153 \\ 0.1007 \end{array}$	H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498 -0.1540	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H183 H184 H185	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1806 0.1545 0.1509 0.1758 0.1839 0.1839
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18	0.0622 -0.4917 0.0641 -0.5149 0.0863 -0.1382 -0.2393 0.4225 -0.3165 0.4034 0.3436 0.1274 0.1272 0.1169 0.1174	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1090 0.1037 -0.5282 0.0433	C51 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1135 0.1138 0.1138 0.1157 0.1159 0.1430 -0.4732	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H86 H87 H88 S(20)	0.1118 0.1181 0.1215 0.1212 0.1327 0.3481 0.2267 0.1657 0.1657 0.1653 0.1644 0.1716 0.1694 0.1741 -0.071	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159 -0.1181 0.0914 -0.1373 0.0975	C124 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138	0.1529 -0.4153 -0.1504 -0.1504 -0.1194 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568 -0.4089 0.1539 -0.1153 0.1007 -0.1484	H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498 -0.1540 0.1540	H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H181 H182 H183 H184 H185 H186	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1806 0.1545 0.1509 0.1758 0.1839 0.1841 0.1463
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\\ 0.3436\\ 0.1272\\ 0.1169\\ 0.1174\\ 0.1105\\ \end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1090 0.1037 -0.5282 0.0433 0.0586	C51 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 O66 C67	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1138 0.1138 0.1157 0.1159 0.1430 0.1430 -0.4732 -0.0007	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91	0.1118 0.1181 0.1215 0.1212 0.1327 0.3481 0.2267 0.1657 0.1653 0.1644 0.1773 0.1716 0.1694 0.1741 -0.1071 0.1009	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115	0.0461 -0.1123 0.1261 -0.1229 0.0832 0.0294 -0.1286 0.0615 -0.1143 0.1244 0.0159 -0.1181 0.0914 -0.1373 0.0975	C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138	0.1529 -0.4153 -0.1504 0.0644 -0.1194 -0.1188 0.0661 -0.1016 -0.1020 -0.1568 -0.4089 0.1539 -0.1153 0.1007 -0.1484 0.1561	H148 H149 H150 H151 H152 H153 H154 H155 C156 C156 C157 C158 N159 C160 C161 H162 H163	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498 -0.1540 0.1422 0.1448	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H187	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1545 0.1509 0.1758 0.1839 0.1841 0.1463 0.1442
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19 H20	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\\ 0.1272\\ 0.1169\\ 0.1174\\ 0.1105\\ 0.1111\\ \end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1037 -0.5282 0.0433 0.0586 -0.5118	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1135 0.1138 0.1157 0.1159 0.1430 0.1430 -0.4732 -0.0007	H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91 C92	0.1118 0.1181 0.1215 0.1212 0.1327 0.1327 0.3481 0.2267 0.1657 0.1657 0.1683 0.1644 0.1773 0.1716 0.1694 0.1741 -0.1071 0.1009 -0.21212	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116	$\begin{array}{c} 0.0461\\ -0.1123\\ 0.1261\\ -0.1229\\ 0.0832\\ 0.0294\\ -0.1286\\ 0.0615\\ -0.1143\\ 0.1244\\ 0.0159\\ -0.1181\\ 0.0914\\ -0.1373\\ 0.0975\\ 0.2941\\ -0.1409\end{array}$	C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140	$\begin{array}{c} 0.1529 \\ -0.4153 \\ 0.1504 \\ 0.0644 \\ -0.1194 \\ -0.1188 \\ 0.0661 \\ -0.1016 \\ -0.1020 \\ -0.1568 \\ -0.4089 \\ 0.1539 \\ -0.1153 \\ 0.1007 \\ -0.1484 \\ 0.1561 \\ 0.1506 \end{array}$	H144 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498 -0.1448 0.1422 0.1747 -0.1625	H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H187 H188	0.1159 -0.1641 -0.4101 0.1624 -0.1213 0.1037 -0.1390 0.1564 0.1509 0.1758 0.1839 0.1841 0.1463 0.1442
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19 H20 H21	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\\ 0.3436\\ 0.1274\\ 0.1272\\ 0.1169\\ 0.1174\\ 0.1105\\ 0.1111\\ 0.1235\end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1090 0.1037 -0.5282 0.0433 0.0586 -0.5118 0.0609	C52 C53 C54 C55 C56 C56 H59 H60 H61 H62 H63 H64 H65 O66 C67 C68 O69	-0.0474 -0.0662 -0.0674 -0.0444 -0.0605 -0.1443 0.4241 0.1121 0.1119 0.1135 0.1138 0.1157 0.1159 0.1430 0.1430 0.1430 -0.4732 -0.0007 0.0638 -0.5000	H76 H77 H78 H77 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91 C92 H93	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.1327 0.1327 0.1327 0.1583 0.1664 0.1773 0.1716 0.1694 0.1741 -0.1071 0.1009 -0.1212 0.1295	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117	$\begin{array}{c} 0.0461\\ -0.1123\\ 0.1261\\ -0.1229\\ 0.0832\\ 0.0294\\ -0.1286\\ 0.0615\\ -0.1143\\ 0.1244\\ 0.0159\\ -0.1181\\ 0.0914\\ -0.1373\\ 0.0975\\ 0.2941\\ -0.1409\\ 0.1658\end{array}$	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141	$\begin{array}{c} 0.1529 \\ -0.4153 \\ -0.1504 \\ 0.0644 \\ -0.1194 \\ -0.1188 \\ 0.0661 \\ -0.1016 \\ -0.1020 \\ -0.1568 \\ -0.4089 \\ 0.1539 \\ -0.1153 \\ 0.1007 \\ -0.1484 \\ 0.1561 \\ 0.1606 \\ 0.1223 \end{array}$	H144 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 H162 H163 C164 H163 C165	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1540 0.1442 0.1540 0.1442 0.1542 0.1542 0.1625 0.1542 0.1543 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1542 0.1545 0.1555 0.0555 0.1555 0.0555 0.0555 0.1555 0.05	H171 C173 N174 C175 C176 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H187 H186 H187	$\begin{array}{c} 0.1159\\ -0.1641\\ -0.4101\\ 0.1624\\ -0.1213\\ 0.1037\\ -0.1390\\ 0.1564\\ 0.1806\\ 0.1545\\ 0.1509\\ 0.1758\\ 0.1839\\ 0.1841\\ 0.1463\\ 0.1442\\ 0.1815\\ 0.1806 \end{array}$
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\\ 0.1272\\ 0.1169\\ 0.1174\\ 0.1105\\ 0.1111\\ 0.1235\\ 0.1241\end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46	-0.1455 0.3775 0.0695 -0.5174 0.0639 0.0484 -0.5525 0.1391 0.1361 0.0987 0.1019 0.1037 -0.5282 0.0433 0.0586 -0.5118 0.0609 0.0118	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 D66 C67 C68 D66 C67 C68 D66 C70	$\begin{array}{c} -0.0474\\ -0.0662\\ -0.0674\\ -0.0444\\ -0.0605\\ -0.1443\\ 0.4241\\ 0.1121\\ 0.1135\\ 0.1135\\ 0.1138\\ 0.1157\\ 0.1159\\ 0.1430\\ -0.4732\\ -0.0007\\ 0.0638\\ -0.5000\\ 0.0605\end{array}$	H76 H77 H78 H77 H80 H81 H82 H83 H84 H85 H86 H87 H88 H89 C90 H91 C92 H93 C94	0.1178 0.1181 0.1215 0.1212 0.1327 0.1327 0.1327 0.1657 0.1683 0.1644 0.1773 0.1716 0.1694 0.1741 -0.1071 0.1009 -0.1212 0.1295 0.3217	C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C111 H112 C113 H114 C115 C116 H117 C118	$\begin{array}{c} 0.0461\\ -0.1123\\ 0.1261\\ -0.1229\\ 0.0832\\ 0.0294\\ -0.1286\\ 0.0615\\ -0.1143\\ 0.1244\\ 0.0159\\ -0.1181\\ 0.0914\\ -0.1373\\ 0.0975\\ 0.2941\\ -0.1409\\ 0.1058\\ -0.1256\end{array}$	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142	$\begin{array}{c} 0.1529\\ -0.4153\\ -0.1504\\ 0.0644\\ -0.1194\\ -0.1188\\ 0.0661\\ -0.1020\\ -0.1568\\ -0.4089\\ 0.1553\\ -0.1153\\ 0.1007\\ -0.1484\\ 0.1561\\ 0.1606\\ 0.1223\\ 0.1615\end{array}$	H144 H149 H150 H151 H152 H153 H154 H155 C156 C157 C156 C157 C160 C161 H162 H163 C164 C165 C166	0.1437 0.1178 0.1264 0.1829 0.1841 0.1665 0.1428 0.1620 0.1884 0.0892 -0.1099 0.1530 -0.4097 0.1498 -0.1540 0.1422 0.1747 -0.1625 0.0908 -0.1177	H171 C173 N174 C175 C176 C177 C178 C179 H180 H181 H182 H183 H184 H185 H186 H187 H188 H189 H190	$\begin{array}{c} 0.1159\\ -0.1641\\ -0.4101\\ 0.1624\\ -0.1213\\ 0.1037\\ -0.1390\\ 0.1564\\ 0.1806\\ 0.1545\\ 0.1509\\ 0.1758\\ 0.1839\\ 0.1841\\ 0.1463\\ 0.1442\\ 0.1815\\ 0.1806\\ 0.1642\end{array}$
07 C8 C9 C10 S11 C12 S13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23	$\begin{array}{c} 0.0622\\ -0.4917\\ 0.0641\\ 0.0371\\ -0.5149\\ 0.0863\\ -0.1382\\ -0.2393\\ 0.4225\\ -0.3165\\ 0.4034\\ 0.3436\\ 0.1274\\ 0.1272\\ 0.1169\\ 0.1174\\ 0.1105\\ 0.1111\\ 1.2235\\ 0.1241\\ 0.1244\end{array}$	C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C43 O44 C45 C46 O47	-0.1455 -0.1455 -0.6695 -0.5174 -0.6399 -0.4644 -0.5525 -0.1391 -0.1361 -0.987 -0.1019 -0.1090 -0.1037 -0.523 -0.0433 -0.6866 -0.5118 -0.6609 -0.4865	C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H65 O66 C67 C68 O69 C70 C71	$\begin{array}{c} -0.0474\\ -0.0662\\ -0.0674\\ -0.0444\\ -0.0605\\ -0.1443\\ 0.4241\\ 0.1121\\ 0.1119\\ 0.1135\\ 0.1138\\ 0.1157\\ 0.1159\\ 0.1430\\ 0.1430\\ -0.4732\\ -0.0007\\ 0.0638\\ -0.5000\\ 0.0605\\ 0.0099\end{array}$	176 177 178 179 180 181 182 183 184 185 184 185 186 187 188 189 C90 191 C92 193 C94 C95	0.1181 0.1215 0.1225 0.1227 0.1327 0.3481 0.2267 0.1553 0.1563 0.1716 0.1684 0.1771 0.1099 -0.1212 0.1295 0.3287	C100 C101 H102 C103 H104 C105 C106 H107 C106 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118 H119	$\begin{array}{c} 0.0246\\ 0.0461\\ -0.1123\\ 0.1261\\ -0.1229\\ 0.0832\\ 0.0294\\ -0.1286\\ 0.0615\\ -0.1143\\ 0.1286\\ 0.0615\\ -0.1143\\ 0.0159\\ -0.1181\\ 0.0914\\ -0.1373\\ 0.0975\\ 0.2941\\ -0.1409\\ 0.1058\\ -0.1256\\ 0.1084\\ \end{array}$	C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C137 C138 C137 H140 H141 H142	$\begin{array}{c} 0.1529\\ -0.4153\\ -0.1504\\ 0.0644\\ -0.1194\\ -0.1194\\ -0.1188\\ 0.0661\\ -0.1020\\ -0.1568\\ -0.4089\\ 0.1539\\ -0.1153\\ 0.1007\\ -0.1484\\ 0.1561\\ 0.1606\\ 0.1223\\ 0.1615\\ 0.1848\end{array}$	H144 H149 H150 H1551 H1552 H153 H154 H155 C156 C157 C158 N159 C160 C161 H163 C164 C165 C165 C165 C167	$\begin{array}{c} 0.1437\\ 0.1178\\ 0.1264\\ 0.1829\\ 0.1841\\ 0.1665\\ 0.1428\\ 0.1620\\ 0.1884\\ 0.0892\\ -0.1099\\ 0.1530\\ -0.4097\\ 0.1498\\ -0.1540\\ 0.1442\\ 0.1747\\ -0.1625\\ 0.0908\\ -0.1177\\ -0.1147\end{array}$	H1712 C173 N174 C175 C176 C1776 C1777 C1778 C179 H1800 H181 H182 H183 H184 H185 H186 H185 H1886 H187 H1888 H1899 H1901	$\begin{array}{c} 0.1129\\ -0.1641\\ -0.4101\\ 0.1624\\ -0.1213\\ 0.1037\\ -0.1390\\ 0.1564\\ 0.1806\\ 0.1545\\ 0.1509\\ 0.1758\\ 0.1839\\ 0.1841\\ 0.1463\\ 0.1442\\ 0.1815\\ 0.1806\\ 0.1642\\ 0.1429\end{array}$

01	28.17 A														
01	-0.4928	C25	-0.3046	C49	-0.1541	H73	0.1543	C97	-0.1288	C121	-0.1220	H145	0.1850	C169	-0.1009
C2	0.0234	S26	0.4139	C50	-0.0587	H74	0.1539	H98	0.0887	C122	0.1014	H146	0.1400	C170	-0.1037
C3	0.0599	C27	-0.2438	C51	-0.0484	H75	0.1127	C99	0.0142	C123	-0.1415	H147	0.1348	H171	0.1237
04	-0.4841	C28	-0.1407	C52	-0.0655	H76	0.1129	C100	0.0258	C124	0.1478	H148	0.1240	H172	0.1212
C5	0.0624	S29	0.4096	C53	-0.0675	H77	0.1139	C101	-0.1343	N125	-0.4094	H149	0.1230	C173	-0.1658
C6	0.0370	C30	0.0736	C54	-0.0430	H78	0.1136	H102	0.1045	C126	-0.1666	H150	0.1750	N174	-0.4128
07	-0.5153	031	-0.5188	C55	-0.0610	H79	0.1016	C103	-0.1331	C127	0.0705	H151	0.1866	C175	0.1636
C8	0.0854	C32	0.0549	C56	-0.1402	H80	0.1015	H104	0.1012	C128	-0.1168	H152	0.1679	C176	-0.1239
C9	-0.1351	C33	0.0401	C57	0.4263	H81	0.3260	C105	0.0236	C129	-0.1133	H153	0.1395	C177	0.1022
C10	-0.2356	034	-0.5219	H58	0.1073	H82	0.2266	C106	-0.1334	C130	0.0800	H154	0.1579	C178	-0.1448
S11	0.4361	H35	0.1461	H59	0.1030	H83	0.1881	H107	0.1035	C131	-0.1032	H155	0.1848	C179	0.1494
C12	-0.3111	H36	0.1439	H60	0.1173	H84	0.1474	C108	-0.1352	C132	-0.1022	C156	0.0961	H180	0.1838
\$13	0 4220	H37	0 1078	H61	0 1186	H85	0 1624	H109	0 1016	C133	-0 1749	C157	-0 1184	H181	0 1511
H14	0.3384	1138	0 1059	862	0 1194	186	0 1809	C110	0.0147	N134	-0 4049	C158	0 1/08	H182	0 1447
114	0.3364	1120	0.1033	102	0.1194	100	0.1009	0110	0.0147	0125	-0.4049	0158 N150	0.1498	1102	0.1447
n15	0.1202	n59	0.1271	103	0.1201	107	0.1009		-0.1260	0135	0.1463	N159	=0.4024	H103	0.1000
H16	0.1200	H40	0.1257	H64	0.1384	H88	0.1700	H112	0.0908	C136	-0.1216	C160	0.1512	H184	0.1852
H17	0.1174	041	-0.5212	H65	0.1373	H89	0.1804	C113	-0.1250	C137	0.0953	C161	-0.1455	H185	0.1821
H18	0.1179	C42	0.0389	066	-0.4639	C90	-0.1297	H114	0.1357	C138	-0.1466	H162	0.1578	H186	0.1414
H19	0.1128	C43	0.0634	C67	-0.0075	H91	0.0843	C115	0.3218	C139	0.1509	H163	0.1864	H187	0.1374
H20	0.1134	044	-0.5154	C68	0.0711	C92	-0.1272	C116	-0.1265	H140	0.1669	C164	-0.1733	H188	0.1880
H21	0.1246	C45	0.0541	069	-0.4999	H93	0.1343	H117	0.1336	H141	0.1448	C165	0.0757	H189	0.1782
H22	0.1252	C46	0.0205	C70	0.0572	C94	0.3257	C118	-0.1270	H142	0.1545	C166	-0.1127	H190	0.1710
H23	0.1465	047	-0.4931	C71	0.0379	C95	-0.1257	H119	0.0866	H143	0.1841	C167	-0.1171	H191	0.1443
H24	0.1473	C48	0.4154	072	-0.5359	H96	0.1366	C120	0.1617	H144	0.1849	C168	0.0705	Total	5.0000
z = z	32.22 Å														
01	-0.4888	C25	-0.3055	C49	-0.1591	H73	0.1520	C97	-0.1275	C121	-0.1238	H145	0.1815	C169	-0.1070
C2	0.0209	S26	0.4325	C50	-0.0615	H74	0.1511	H98	0.0994	C122	0.0918	H146	0.1477	C170	-0.1063
C3	0.0612	C27	-0.2413	C51	-0.0541	H75	0.1187	C99	0.0162	C123	-0.1400	H147	0.1457	H171	0.1174
04	-0 4864	C28	-0 1392	C52	-0.0651	H76	0 1194	C100	0.0346	C124	0 1501	H148	0 1262	H172	0 1212
C5	0.0626	529	0 4228	C53	-0.0661	H77	0 1210	C101	-0 1438	N125	-0 4156	H149	0 1336	C173	-0 1661
CG	0.0371	C30	0.0786	C54	=0.0505	H78	0 1210	H102	0.0426	C126	=0 1551	H150	0 1796	N174	=0.4137
07	=0.5154	031	=0.5166	C55	=0.0636	H70	0 1235	C103	=0 1115	C127	0.0779	H151	0 1805	C175	0 1586
C8	0.0853	C32	0.0495	C56	-0 1444	H80	0.1232	H104	0 1242	C128	=0.1164	H152	0.1832	C176	-0.1316
C0	-0.1255	002	0.0433	000	0.11111	100	0.1202	C105	0.1242	C120	-0 1191	U1E2	0.1602	C177	0.1010
C10	-0.0255	024	-0 5076	1007	0.4200	101	0.0422	C106	-0.1146	C120	0.0794	1100	0.1500	0170	-0 1442
Q11	0.2000	134	0.02/0	100	0.0303	1102	0.2210	H107	0.1021	C121	-0 1024	H1CC	0.1701	0170	0.1514
C10	-0 2107	426	0.1404	109 PE0	0.10500	103 404	0.2000	C100	-0 1050	0120	-0 1005	0150	0.1191	h100	0.1014
012	0.0107	100	0.1442	100	0.1002	104	0.1570	1100	0.1202	0132	-0 1566	0100	-0.10530	1100	0.1023
513	0.4314	100	0.1131	100	0.1028	100	0.15/0	1109	0.003/	N124	-0.1000	010/	-0.1251	1010	0.109/
H14	0.3394	138	0.1130	162	0.1188	186	0.1749	0110	0.0170	N134	-0.4416	0158	0.1505	n182	0.1343
H15	0.1225	n39	0.1248	no3	0.11/4	181	0.1543	0111	-0.1060	0135	0.1656	N159	-0.4109	n183	0.1678
H16	0.1223	n40	0.1234	104	0.1322	188	0.1622	n112	0.1050	0136	-0.1168	0160	0.1495	n184	0.1790
H17	0.1169	U41	-0.5431	H65	U.1335	н89	0.1736	C113	-0.1203	0137	0.0869	C161	-0.1488	H185	0.1821
H18	0.11/3	042	0.0453	066	-0.4/10	090	-0.1240	n114	0.1299	0138	-0.1544	n162	0.1559	n186	0.1412
H19	0.1123	C43	0.0711	C67	-0.0009	H91	0.1012	C115	0.3175	C139	0.1468	H163	0.1816	H187	0.1412
H20	0.1129	044	-0.5149	C68	0.0642	C92	-0.0937	C116	-0.1215	H140	0.1717	C164	-0.1648	H188	0.1839
H21	0.1246	C45	0.0499	069	-0.4920	H93	0.0693	H117	0.1298	H141	0.1432	C165	0.0763	H189	0.1797
H22	0.1252	C46	0.0298	C70	0.0569	C94	0.2897	C118	-0.1063	H142	0.1565	C166	-0.1187	H190	0.1686
H23	0.1473	047	-0.5010	C71	0.0213	C95	-0.1365	H119	0.1007	H143	0.1827	C167	-0.1169	H191	0.1470
H24	0.1481	C48	0.4068	072	-0.4864	H96	0.0984	C120	0.1604	H144	0.1832	C168	0.0781	Total	5.0000
z = z	36.84 Å														
01	-0.4780	C25	-0.3059	C49	-0.1708	H73	0.1457	C97	-0.1141	C121	-0.1377	H145	0.1861	C169	-0.1115
C2	0.0175	S26	0.4552	C50	-0.0703	H74	0.1447	H98	0.1227	C122	0.0804	H146	0.1496	C170	-0.1092
C3	0.0589	C27	-0.2386	C51	-0.0652	H75	0.1199	C99	0.0371	C123	-0.1468	H147	0.1497	H171	0.1291
04	-0.4819	C28	-0.1377	C52	-0.0665	H76	0.1207	C100	0.0304	C124	0.1499	H148	0.1126	H172	0.1299
C5	0.0596	\$29	0.4418	C53	-0.0610	H77	0.1233	C101	-0.1140	N125	-0.4076	H149	0.1137	C173	-0.1610
C6	0.0362	C30	0.0814	C54	-0.0741	H78	0.1233	H102	0.0808	C126	-0.1646	H150	0.1855	N174	-0.4067
07	-0.5155	031	-0.5159	C55	-0.0691	H79	0 1265	C103	-0 1116	C127	0.0770	H151	0 1835	C175	0 1615
C8	0.0846	C32	0 0445	C56	-0 1540	H80	0 1262	H104	0 1197	C128	-0 1148	H152	0 1824	C176	-0 1219
C9	-0 1353	C33	0.0490	C57	0 4100	H81	0.3451	C105	0.0416	C129	-0 1141	H153	0 1570	C177	0.0846
C10	-0 2343	034	-0.5312	858	0.0939	H82	0 2313	C106	-0 1124	C130	0.0807	H154	0 1618	C178	-0 1451
S11	0 4658	H35	0 1491	H59	0.0920	H83	0 2184	H107	0 1214	C131	-0 1084	H155	0 1857	C179	0 1586
C12	=0.3100	1100	0 1467	H60	0.0901	H84	0 1078	C108	=0 1160	C132	-0 1080	C156	0.0831	H180	0 1874
\$13	0 4476	H37	0 1121	H61	0.0930	H85	0 1442	H109	0 1027	C133	-0 1689	C157	-0 1190	H181	0 1657
H14	0 3433	1138	0 1122	862	0.0941	186	0 1674	C110	0.0234	N134	=0.4066	C158	0 1610	H182	0 1364
1114	0.0400	1100	0.1122	102	0.0341	1100	0.10/1	0110	0.0204	MIO-	0.2000	0100	0.1010	11102	
H15	0 1279	830	0 1253	1 163	0 0937	487	0 1083	C111	-0 1057	C135	0 1597	N150	-0 4106	#183	0.1700
H15 H16	0.1279	H39 H40	0.1253	H63	0.0937	H87 H88	0.1083	C111	-0.1057	C135	0.1597	N159 C160	-0.4106	H183	0.1700
H15 H16 H17	0.1279 0.1276 0.1205	H39 H40 041	0.1253 0.1237 -0.5481	H63 H64 H65	0.0937 0.1124 0.1158	H87 H88 H89	0.1083 0.1394 0.1627	C111 H112 C113	-0.1057 0.1091 -0.1230	C135 C136 C137	0.1597	N159 C160 C161	-0.4106 0.1547 -0.1469	H183 H184 H185	0.1700 0.1841 0.1794
H15 H16 H17	0.1279 0.1276 0.1205	H39 H40 041	0.1253 0.1237 -0.5481	H63 H64 H65	0.0937 0.1124 0.1158	H87 H88 H89	0.1083 0.1394 0.1627	C111 H112 C113	-0.1057 0.1091 -0.1230	C135 C136 C137	0.1597 -0.1349 0.0777	N159 C160 C161	-0.4106 0.1547 -0.1469	H183 H184 H185	0.1304 0.1700 0.1841 0.1794
H15 H16 H17 H18	0.1279 0.1276 0.1205 0.1210	H39 H40 041 C42	0.1253 0.1237 -0.5481 0.0559	H63 H64 H65 066	0.0937 0.1124 0.1158 -0.4831	H87 H88 H89 C90	0.1083 0.1394 0.1627 -0.1141	C111 H112 C113 H114	-0.1057 0.1091 -0.1230 0.1205	C135 C136 C137 C138	0.1597 -0.1349 0.0777 -0.1475	N159 C160 C161 H162	-0.4106 0.1547 -0.1469 0.1640	H183 H184 H185 H186	0.1700 0.1841 0.1794 0.1426
H15 H16 H17 H18 H19	0.1279 0.1276 0.1205 0.1210 0.1160	H39 H40 041 C42 C43	0.1253 0.1237 -0.5481 0.0559 0.0590	H63 H64 H65 D66 C67	0.0937 0.1124 0.1158 -0.4831 0.0074	H87 H88 H89 C90 H91	0.1083 0.1394 0.1627 -0.1141 0.1261	C111 H112 C113 H114 C115	-0.1057 0.1091 -0.1230 0.1205 0.3116	C135 C136 C137 C138 C139	0.1597 -0.1349 0.0777 -0.1475 0.1513	N159 C160 C161 H162 H163	-0.4106 0.1547 -0.1469 0.1640 0.1891	H183 H184 H185 H186 H187	0.1304 0.1700 0.1841 0.1794 0.1426 0.1423
H15 H16 H17 H18 H19 H20	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167	H39 H40 041 C42 C43 044	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199	H63 H64 H65 D66 C67 C68	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615	H87 H88 H89 C90 H91 C92	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430	C111 H112 C113 H114 C115 C116	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237	C135 C136 C137 C138 C139 H140	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805	N159 C160 C161 H162 H163 C164	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589	H183 H184 H185 H186 H187 H188	0.1304 0.1700 0.1841 0.1794 0.1426 0.1423 0.1812
H15 H16 H17 H18 H19 H20 H21	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267	H39 H40 041 C42 C43 044 C45	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565	H63 H64 H65 D66 C67 C68 D69	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869	H87 H88 H89 C90 H91 C92 H93	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746	C111 H112 C113 H114 C115 C116 H117	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218	C135 C136 C137 C138 C139 H140 H141	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545	N159 C160 C161 H162 H163 C164 C165	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704	H183 H184 H185 H186 H187 H188 H189	0.1304 0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830
H15 H16 H17 H18 H19 H20 H21 H22	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272	H39 H40 041 C42 C43 044 C45 C46	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451	H63 H64 H65 066 C67 C68 069 C70	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559	H87 H88 H89 C90 H91 C92 H93 C94	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033	C111 H112 C113 H114 C115 C116 H117 C118	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055	C135 C136 C137 C138 C139 H140 H141 H142	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1513 0.1805 0.1545 0.1606	N159 C160 C161 H162 H163 C164 C165 C166	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188	H183 H184 H185 H186 H187 H188 H189 H190	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685
H15 H16 H17 H18 H19 H20 H21 H22 H23 H24	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272 0.1502	H39 H40 041 C42 C43 044 C45 C46 047	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189	H63 H64 H65 066 C67 C68 069 C70 C71	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194	H87 H88 H89 C90 H91 C92 H93 C94 C95 U00	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087	C135 C136 C137 C138 C139 H140 H141 H142 H143 U144	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857	N159 C160 C161 H162 H163 C164 C165 C166 C166 C167	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193	H183 H184 H185 H186 H187 H188 H189 H190 H191	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350
H15 H16 H17 H18 H19 H20 H21 H22 H23 H24	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272 0.1502 0.1511	H39 H40 041 C42 C43 044 C45 C46 047 C48	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783	H63 H64 H65 066 C67 C68 069 C70 C71 072	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total	$\begin{array}{c} 0.1700\\ 0.1841\\ 0.1794\\ 0.1426\\ 0.1423\\ 0.1812\\ 0.1830\\ 0.1685\\ 0.1350\\ 5.0000\\ \end{array}$
H15 H16 H17 H18 H19 H20 H21 H22 H23 H24 z = 4	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272 0.1502 0.1511 40.99 Å	H39 H40 D41 C42 C43 D44 C45 C46 D47 C48	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783	H63 H64 H65 O66 C67 C68 069 C70 C71 072	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000
$ \begin{array}{c} \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \hline \begin{array}{c} z = - \\ 01 \\ \hline \end{array} \end{array} $	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1267 0.1272 0.1502 0.1511 40.99 Å -0.4992	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783	H63 H64 H65 O66 C67 C68 O69 C70 C71 O72 C49	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C121	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000
H15 H16 H17 H18 H19 H20 H21 H22 H23 H24 Z = - 01 C2 C C2 C2 C2 C2 C2 C	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272 0.1502 0.1511 40.99 Å -0.4992 0.0230	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C25	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336	H63 H64 H65 D66 C67 C68 D69 C70 C71 072 C49 C50 C75	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.055	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.1395 0.1302 0.1316	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C97	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0322	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C122	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1396 0.1037 -0.1396	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H145 H146	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400	H183 H184 H185 H185 H186 H187 H188 H189 H190 H191 Total	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091
$\begin{array}{c} \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \hline \\ \hline $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1511\\ \hline 40.99 {\rm \AA} \\ -0.4992\\ 0.0230\\ 0.0623\\ 0.062$	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C27 C27	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0559 0.0559 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415	H63 H64 H65 C67 C68 D69 C70 C71 072 C49 C50 C50	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0659 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0954	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 U72	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0984	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306	C135 C136 C137 C138 C139 H140 H141 H142 H143 H143 H144 C121 C122 C123 C123	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1823 -0.1396 0.1037 -0.1447	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146 H147 H146	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1386	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H171	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091 0.1123
$\begin{array}{c} \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \hline \\ \textbf{C2} \\ \textbf{C3} \\ \textbf{04} \\ \textbf{C4} \\ \textbf{C7} \\ \end{array}$	0.1279 0.1276 0.1205 0.1210 0.1160 0.1167 0.1267 0.1272 0.1502 0.1511 40.99 Å -0.4992 0.0230 0.0623 -0.4923	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C46 C47 C25 S26 C27 C28 S26 C27 C28	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0550 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3052 -0.3052 0.4336 -0.2415 -0.1401	H63 H64 H65 066 C67 C68 069 C70 C71 072 C71 072 C49 C50 C51 C52 C52	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0744 0.0744	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.1395 0.1302 0.1316 0.0984 0.0972	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C120 C127 H98 C99 C100	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1087 0.1590 -0.0937 -0.0937 0.1388 0.0306 0.0635	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1396 0.0137 -0.1447 0.1508	N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H146 H147 H148	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 -0.1193 0.1771 0.1400 0.1386 0.1248	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C172	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091 0.1123 0.1112
	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1511\\ 40.99\ \mathring{A}\\ -0.4992\\ 0.0230\\ 0.0623\\ -0.4923\\ 0.0644\\ 0.0272\end{array}$	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C46 C47 C48 C25 S26 C27 C28 S29 C22	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.2415 -0.1401 0.4192	H63 H64 H65 066 C67 C68 069 C70 C71 072 C72 C50 C51 C52 C52 C53	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0744 -0.0847 -0.0847	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76 H77 H76	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0972 0.1055	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C100 C101	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306 0.0635 -0.1005	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C124	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1396 0.1037 -0.1447 0.1508 -0.4065	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H147 H148 H149 H149 H147	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1386 0.1248 0.1268	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 X72	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091 0.1123 0.1116 -0.1672
	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1511\\ 40.99\ \dot{A}\\ \hline -0.4992\\ 0.0230\\ 0.0623\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.552\end{array}$	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 C32	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.4192 0.0748	H63 H64 H65 D66 C67 C68 069 C70 C71 072 C49 C50 C51 C52 C53 C54 C53 C54	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0744 -0.0744 -0.0847 -0.1236	H87 H88 H89 C90 H91 C92 H93 C92 H93 C95 H96 H73 H74 H75 H76 H77 H78	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0972 0.1055 0.1047	C111 H112 C113 H114 C115 C116 H117 C120 C120 C97 H98 C99 C100 C101 H102 C101 H102 C101	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306 0.0635 -0.1005 0.1441	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C126	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1396 0.1037 -0.1447 0.1508 -0.4065 -0.1595	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H150	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1386 0.1248 0.1268 0.1769	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C177	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091 0.1123 0.1116 -0.1672 -0.4123 0.5000
	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1267\\ 0.1502\\ 0.1511\\ 0.1511\\ 0.0230\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0551\\ \end{array}$	H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.4192 0.0748 -0.5161	H63 H64 H65 D66 C67 C68 D69 C70 C71 D72 C49 C50 C51 C52 C53 C54 C55	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0744 -0.0847 -0.1236 -0.0831 -0.0845 -0.0854 -0.074 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0744 -0.0847 -0.0744 -0.0847 -0.0744 -0.0847 -0.0744 -0.0744 -0.0744 -0.0744 -0.0744 -0.0744 -0.0744 -0.0744 -0.0747 -0.0744 -0.0747 -0.0744 -0.07577 -0.07577 -0.07577 -0.075777 -0.0757777 -0.0757777777777777777777777777777777777	H87 H88 H89 C90 H91 C92 H93 C94 C94 C94 C94 H96 H73 H74 H75 H76 H77 H78 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0972 0.1047 0.0988	C111 H112 C113 H114 C115 C116 H117 C120 C120 C120 C127 H98 C99 C100 C101 H102 C101 H102 C103	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306 0.0635 -0.1005 0.1441 -0.0929 0.5755	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C127	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1857 0.1823 -0.1396 0.1037 -0.1447 0.1508 -0.4065 -0.1595 0.0680	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H150 H151	-0.4106 0.1547 -0.1640 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1386 0.1248 0.1268 0.1769 0.1839 0.1839	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175	0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1091 0.1123 0.1116 -0.1672 0.1629
$\begin{array}{c} \rm H15 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \hline z = - \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm 04 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C6 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C6 \\ \rm C6 \\ \rm C6 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1511\\ 40.99 \mbox{ Å}\\ -0.4992\\ 0.0230\\ 0.0623\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0858\\ -0.3752\end{array}$	H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S26 C27 C28 S29 C30 031 C32 C22	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.4192 0.0748 -0.5161 0.0531	H63 H64 H65 C67 C68 069 C70 C71 072 C50 C51 C52 C52 C52 C52 C54 C55 C54 C55 C55	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0954 -0.0954 -0.0847 -0.0847 -0.0831 -0.1755 0.2062	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76 H77 H78 H79 H80 UP0	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1316 0.0972 0.1302 0.1316 0.0972 0.1055 0.1047 0.0988 0.0991 0.2020	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C120 C100 C101 H102 C103 H104 C107	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306 0.0635 -0.1005 0.1441 -0.0929 0.1535	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1827 -0.1396 0.1037 -0.1447 0.1508 -0.4065 -0.1595 0.0680 -0.1229	N159 C160 C161 H162 H163 C164 C165 C166 C166 C167 C168 H145 H145 H145 H147 H148 H149 H150 H151 H152 Ptc2	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1386 0.1248 0.1268 0.1769 0.1839 0.1668	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C175	-0.1304 0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 -0.1085 -0.1091 0.1123 0.1116 -0.1672 -0.1342 0.1629 -0.1334
$\begin{array}{c} \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \hline \\ \text{C2} \\ \text{C3} \\ \text{O4} \\ \text{C5} \\ \text{C6} \\ \text{O7} \\ \text{C8} \\ \text{C9} \\ \text{C9} \\ \hline \end{array}$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1511\\ 40.99 \\ \overline{A}\\ -0.4992\\ 0.0233\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0658\\ -0.1350\\ -0.3551\\ 0.0658\\ \end{array}$	H39 H40 O41 C42 C43 C43 C45 C46 O47 C48 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 C32 C32 C34	0.12253 0.1227 0.5481 0.0559 0.0559 0.0559 0.0659 0.0451 -0.5199 0.0655 0.0451 -0.5189 0.0453 -0.5189 0.3783 -0.3352 0.4336 0.4336 0.4336 0.4326 0.4326 0.4326 0.4326 0.4355 0.0748 -0.5161 0.0254 0.0551	Н63 Н64 Н65 О66 С67 С68 069 С70 С71 072 С59 С50 С51 С52 С53 С54 С55 С55 С56 С55	0.0937 0.1124 0.1158 0.0158 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.2062 -0.2062 -0.9954 -0.0954 -0.0954 -0.0831 -0.0831 -0.1755 0.3903 0.4007	H87 H88 H89 C30 H91 C92 H93 C94 C35 H96 H73 H74 H73 H74 H75 H76 H77 H78 H77 H78 H79 H80 H81 H29 H80 H81 H29 H29 H29 H29 H29 H29 H29 H29 H29 H29	0.1083 0.1394 0.1627 -0.141 0.1261 0.746 0.3033 -0.1395 0.0776 0.1302 0.1302 0.1302 0.0984 0.09972 0.1085 0.1047 0.1088 0.1047 0.0988	C111 H112 C113 H114 C115 C116 H117 C120 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C107	-0.1057 0.1091 -0.1230 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1087 0.1087 0.1087 0.1087 0.1087 0.1086 0.0937 0.1388 0.0306 0.0635 -0.10929 0.1441 -0.0929 0.1535	C135 C136 C137 C138 C137 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C126 C127 C128 C129 C129 C129 C129	0.1597 -0.1349 0.0777 -0.1475 0.1615 0.1805 0.1606 0.1857 0.1823 -0.1396 0.1037 -0.1396 0.1037 -0.1447 0.1508 -0.1508 -0.1595 0.0660 -0.1297 -0.1157	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H150 H151 H152 H152 H152	-0.4106 0.1547 -0.1469 -0.1640 0.1891 -0.1589 -0.1183 -0.1183 -0.1193 -0.1193 -0.1193 -0.1193 -0.1193 -0.1193 -0.1286 0.1288 0.1288 0.1769 0.1283 0.1769 0.1639 0.1639 0.1649 0.1649 0.1649 0.1649 0.1288 0.1769 0.1288 0.1769 0.1283 0.1	H183 H184 H185 H186 H187 H188 H189 H190 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C177	-0.1300 0.1700 0.1841 0.1724 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1483 0.1485 5.0000 -0.1085 -0.1091 0.1123 0.1116 -0.1091 0.1126 -0.1224 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1330 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1520 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1629 -0.1350 0.1520 -0.1350 0.1520 -0.1350 0.1520 -0.1550 -0.15
	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1205\\ 0.1210\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1501\\ 0.1267\\ 0.1272\\ 0.1501\\ 0.0230\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0633\\ 0.0644\\ 0.0370\\ 0.05151\\ 0.0858\\ -0.1350\\ 0.0355\\ 0.03253\\ 0.0464\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.03253\\ 0.0464\\ 0.0370\\ 0.03253\\ 0.0464\\ 0.0370\\ 0.03253\\ 0.0465\\ 0.03253\\ 0.0465\\ 0.03253\\ 0.0465\\ 0.0325\\ 0.0465\\ 0.0325\\ 0.0465\\ 0.035\\ 0.035\\ 0.035\\ 0.035\\ 0.005\\ 0.035\\ 0.005\\ 0.035\\ 0.005\\ 0.035\\ 0.005\\ 0$	H39 H40 041 C42 C43 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031 C32 C33 034 C32 C33 C32 C33 C34 C32 C33 C34 C32 C33 C33 C34 C33 C32 C33 C33 C33 C33 C33 C33 C33 C33	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5189 0.0451 -0.5189 0.3783 -0.4336 0.4336 0.4336 0.4336 0.4336 0.4352 0.07415 0.07415 0.07541 0.0254 -0.5665 0.0264 -0.5665	H63 H64 H65 D66 C67 C68 D69 C70 C71 072 C71 072 C50 C51 C52 C53 C54 C55 C56 C57 H58 μе о	0.0937 0.1124 0.1158 0.1158 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4869 0.0559 0.0194 -0.4767 -0.1216 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0847 -0.0847 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0851 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0055 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0855 -0.0055 -0.0855 -0.0855 -0.0074 -0.0855 -0.0955 -0.08555 -0.0855 -0.0855 -0.08555 -0.08555 -0.08555 -0.08555 -0.08555 -0	H87 H88 H89 C30 H91 C32 H93 C94 C95 H96 H73 H74 H75 H76 H77 H78 H77 H78 H77 H78 H77 H78 H79 H80 H81 H82 H82	0.1083 0.1394 0.1627 -0.1141 -0.1430 0.0746 0.3033 -0.1395 0.3070 0.1316 0.0984 0.0972 0.1055 0.1045 0.0984 0.0991 0.3248 0.0991 0.3248	C111 H112 C113 H114 C115 C116 H117 C120 C97 H98 C99 C100 C101 H102 C103 H102 C103 H105 C105 C106	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1237 0.1218 -0.1055 0.1087 0.1388 0.3306 0.3366 0.3366 0.3366 0.3365 -0.1005 0.1441 -0.0929 0.1535 0.0647 -0.0929	C135 C136 C137 C138 C137 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C120 C129 C130 C121	0.1597 -0.1390 0.0777 -0.1475 0.1513 0.1805 0.1505 0.1606 0.1887 0.1887 0.1037 -0.1447 0.1037 -0.1447 0.1037 -0.1508 -0.4665 -0.1657 0.06650 -0.1657	N159 C160 C161 H162 H163 C164 C165 C166 C166 C166 H145 H146 H147 H148 H149 H150 H151 H151 H153 H154 L153 H154 L153	-0.4106 0.1547 -0.1469 0.1640 0.1889 -0.1589 0.0704 -0.1183 -0.1193 0.0704 -0.1183 0.1771 0.1400 0.1386 0.1268 0.1268 0.1268 0.1289 0.1668 0.1349 0.1655 0.1349	H183 H184 H185 H186 H187 H188 H189 H191 Total C169 C170 C170 C170 H171 H172 C173 N174 C175 C176 C177 C177 C177 C177	0.1330 0.1700 0.1841 0.1734 0.1426 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 5.0000 5.0000 0.1116 0.1123 0.1116 0.1672 0.1672 0.1672 0.1672
$\begin{array}{c} \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \hline \\ \hline \\ \hline \\ z = - \\ \hline \\ c1 \\ c2 \\ c3 \\ c4 \\ c5 \\ c6 \\ c7 \\ c8 \\ c9 \\ c10 \\ s11 \\ c1 \\ c1 \\ c1 \\ c1 \\ c1 \\ c1 \\ c$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.1501\\ 0.0623\\ -0.4923\\ 0.0623\\ -0.4923\\ 0.0623\\ 0.0643\\ -0.3150\\ -0.5151\\ 0.0088\\ -0.1350\\ -0.350\\ 0.04466\\ -0.3253\\ 0.4466\\ -0.3253\\ -0.325\\ -$	H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031 C32 C33 034 H35 C33 D34 H35	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.5161 0.0254 -0.5065 0.0462 0.0524	H63 H64 H65 O66 C67 C68 O69 C70 C71 072 C49 C50 C51 C52 C53 C54 C55 C54 C55 C56 C57 H58 H59 H59 H20	0.0937 0.1124 0.1124 0.1158 -0.4803 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0154 -0.4767 -0.1216 -0.94767 -0.2052 -0.21216 -0.0744 -0.0744 -0.0831 -0.1755 0.3903 0.1096 0.1145 0.0021	H87 H88 H89 C90 H91 C92 H93 C94 C94 C94 H96 H96 H73 H74 H75 H76 H77 H78 H79 H80 H81 H82 H83 H82 H83	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0994 0.0984 0.0991 0.2279 0.2229	C111 H112 C113 H114 C115 C116 H117 C120 C120 C100 C100 C101 H102 C103 H104 C106 H107 C106 H107 C106 C106 H107 C105	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.3116 -0.1237 0.1237 0.1238 -0.1055 0.1065 0.0937 0.1388 0.3066 0.0937 0.1388 0.3066 0.0929 0.1441 -0.0929 0.1552 0.5547 -0.0929	C135 C136 C137 C138 C137 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C130 C130 C137 C137 C137 C137 C137 C137 C138 C137 C137 C137 C138 C137 C137 C138 C137 C121 C122 C123 C122 C123 C124 C122 C123 C124 C122 C123 C124 C122 C123 C124 C127 C128 C127 C128 C127 C128 C127 C128 C127 C128 C127 C127 C128 C127 C127 C128 C127 C127 C128 C127 C127 C128 C127 C127 C127 C128 C127 C127 C128 C127 C127 C127 C128 C127 C127 C127 C127 C128 C127 C127 C127 C127 C127 C127 C127 C127	0.1597 -0.1397 0.0777 0.1475 0.1513 0.1805 0.1545 0.1606 0.1887 0.1823 -0.1397 -0.1397 -0.1447 0.1508 -0.1037 -0.1447 0.1508 -0.1036 -0.1299 -0.1157 0.0685 -0.0689 -0.0595 -0.0699	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H145 H145 H148 H149 H150 H151 H152 H153 H154 H155 C155	-0.4106 0.1547 -0.1469 0.1640 0.1889 -0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1188 -0.1188 0.0710 -0.1193 0.0710 -0.1193 0.0710 -0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1547 0.1547 0.15570000000000000000000000000000000000	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C176 C177 C178 C179 H100	0.1304 0.1700 0.1841 0.1724 0.1426 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1455 0.1350 0.1350 0.1350 0.1350 0.1152 0.1085 -0.1085 -0.1085 0.1167 -0.1672 0.1423 0.1672 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1423 0.1424 0.1425 0.1424 0.1424 0.1424 0.1425 0.1424 0.1424 0.1425 0.1425 0.1424 0.1424 0.1426 0.1424 0.1425 0.1425 0.1425 0.1427 0.1447 0.1447 0.1447 0.1447 0.1447 0.1457000000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm 04 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C12 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ \rm C10 \\ \rm C10 \\ \rm S111 \\ \rm C10 \\ $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1267\\ 0.1272\\ 0.1501\\ 0.1501\\ 0.0220\\ 0.0220\\ 0.0220\\ 0.0220\\ 0.0220\\ 0.0220\\ 0.0220\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0876\\ -0.3550\\ -0.3353\\ 0.4466\\ -0.3107\\ 0.4257\\ 0.0425\\ 0.045\\ 0.045\\ 0.045\\ 0.045\\ 0.045\\ $	H39 H40 041 C42 C43 044 C45 C46 C47 C48 C25 S26 C27 C28 S29 C30 C32 C33 C32 C33 C32 C33 C34 H35 H36 H35 H36	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3415 -0.4336 -0.4336 -0.44192 0.0748 -0.5161 0.0254 -0.5065 0.0254 -0.5065 0.0254 -0.5065	H63 H64 H65 D66 C67 C68 D69 C70 C71 D72 C49 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 Pec	0.0937 0.1124 0.1158 0.1158 0.0074 0.0615 0.0559 0.0559 0.0559 0.0559 0.0559 0.0559 0.0747 -0.4869 0.0559 0.01954 -0.4767 -0.2262 -0.0984 -0.0984 -0.0984 0.0847 -0.236 0.0393 0.1995 0.3993 0.1996	H87 H88 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76 H77 H78 H77 H78 H77 H78 H77 H78 H79 H80 H81 H82 H83 H84 Per	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.1302 0.1316 0.1316 0.0984 0.0972 0.1065 0.0988 0.0991 0.3248 0.3229 0.2279 0.2015	C111 H112 C113 H114 C115 C116 H117 C120 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H107 C108	-0.1057 0.1091 0.1205 0.3116 -0.1230 0.1205 0.1218 -0.1237 0.1218 -0.1055 0.1087 0.1388 0.0306 0.0635 -0.1005 0.1348 0.0306 0.0635 -0.1005 0.1441 -0.0929 0.1555 0.1455 0.0647 -0.0921 0.1555 0.0647 -0.0931 0.1555 0.0647 -0.0931 0.054 0.054 0.054 0.054 0.055 0.054 0.055 0.005 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.055 0.005 0.05500000000	C135 C136 C137 C138 C139 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C120 C131 C131 C131 C132 C122	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1543 0.1805 0.1646 0.1887 0.1887 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1037 -0.1447 0.1508 0.0680 -0.1229 -0.1555 0.0680 -0.1229 -0.1555	N159 C160 C161 H162 H163 C164 C165 C166 C165 C166 H146 H147 H146 H147 H146 H147 H149 H150 H151 H152 H153 H155 C156 C155 C156 C157	-0.4106 0.1547 0.1540 0.1640 0.1689 0.0704 -0.1188 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1400 0.1386 0.1248 0.1268 0.1289 0.1655 0.1349 0.1655 0.1349	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C179 H180 H191 H192 C179 H192 H192 H192 H192 H192 H192 H192 H19	-0.1334 0.1730 0.1740 0.1784 0.1734 0.1426 0.1423 0.1423 0.1423 0.1423 0.1423 0.1425 0.1425 0.1425 0.1425 0.1425 0.1685 0.1091 0.1116 -0.1672 -0.1672 0.1672 0.1672 0.1672 0.1672 0.1570 0.1577 0.1570
	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0523\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4923\\ 0.0624\\ 0.0370\\ -0.5151\\ 0.0858\\ -0.1350\\ -0.3150\\ 0.0858\\ -0.3150\\ 0.0858\\ -0.3150\\ 0.0858\\ -0.285\\ 0.4466\\ -0.3150\\ 0.285\\ 0.28$	H39 H40 041 C42 C43 044 C45 C46 047 C48 C25 S26 C27 C28 S29 C30 031 C32 C33 034 H36 H37 H32 C32	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0531 0.0555 0.0551 0.0551 0.0555 0.0551 0.0555 0.0551 0.05550 0.05550 0.05550 0.05550 0.055500000000	H63 H64 H65 O66 C67 C68 O69 C70 O71 O72 C49 C50 C51 C52 C53 C54 C55 C55 C56 C57 H58 H59 H60 H61 H22	0.0937 0.1124 0.1158 0.1158 0.0074 0.0615 0.0559 0.0194 -0.2662 -0.1216 -0.0954 -0.0954 -0.0954 -0.0954 0.0954 0.00954 0.1236 0.0954 0.1096 0.1096 0.1096 0.1096 0.1096 0.1096 0.1096 0.1096 0.1096 0.00979 0.00979 0.00979	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H76 H77 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 -0.1430 0.0746 0.3033 -0.1395 0.1316 0.1316 0.0984 0.0972 0.1055 0.1047 0.0984 0.0991 0.2279 0.2279 0.2015 0.09350	C111 H112 C113 H114 C115 C116 H117 C120 C107 H99 C120 C107 H99 C100 C101 C102 C103 H104 C105 C106 H107 C108 H109 C112	-0.1057 0.1091 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1087 0.1388 0.0306 0.0937 0.1388 0.0306 0.0937 0.1388 0.0306 0.0655 0.1441 -0.0929 0.1535 0.0541 0.0931 0.552 -0.0931 0.552 0.0051 0.552 0.0546 0.0051 0.552 0.055 0.055 0.055 0.055 0.1055 0.1055 0.1057 0.1055 0.1057 0.1057 0.1055 0.1057 0.1055 0.1057 0.1055 0.1057 0.1055 0.1057 0.1055 0.1057 0.1057 0.1055 0.1057 0.1057 0.1057 0.1055 0.1057 0.1057 0.1055 0.1057 0.0057 0.1057 0.0057 0.1055 0.0057 0.1055 0.0057	C135 C136 C137 C138 C139 H140 H141 H141 H143 H144 C121 C122 C123 C124 N125 C124 C127 C128 C129 C130 C131 C132 C133 C132 C133 C132 C133 C135 C135 C135 C135 C135 C135 C137 C135 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C137 C138 C139 C139 C138 C139 C139 C139 C139 C138 C139 C139 C138 C139 C139 C138 C139 C138 C139 C139 C138 C139 C138 C139 C138 C139 C138 C139 C139 C138 C139 C139 C138 C139 C139 C138 C139 C139 C139 C138 C139 C139 C139 C139 C138 C139 C139 C139 C139 C139 C139 C139 C139	$\begin{array}{c} 0.1597\\ -0.1349\\ 0.0777\\ -0.1475\\ 0.1513\\ 0.1805\\ 0.1545\\ 0.1606\\ 0.1887\\ 0.1823\\ 0.1823\\ 0.1823\\ 0.1823\\ 0.1823\\ 0.1823\\ 0.1823\\ 0.1825\\ 0.0405\\ -0.1229\\ -0.1447\\ 0.0685\\ -0.1229\\ -0.1555\\ -0.0949\\ -0.0555\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.155\\ -0.0949\\ -0.055\\ -0.0949\\ -0.095\\ -0.0949\\ -0.004\\ -0.00$	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H146 H145 H146 H147 H148 H147 H148 H147 H151 H151 H151 H153 H154 H155 C156 C156 C157 C157 C157 C157 C157 C157 C157 C157	-0.4106 0.1547 -0.1469 0.1640 0.1881 -0.1589 0.0704 -0.1183 -0.1193 0.0704 0.1193 0.0704 0.1193 0.0704 0.1193 0.1193 0.1202 0.1268 0.1268 0.1268 0.1268 0.1268 0.1268 0.1655 0.1838 0.1655	H183 H184 H185 H186 H186 H187 H188 H189 H190 H191 Total Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 C177 C178 C179 H180 H181 H190 H181 H190 H181 H190 H190 H181 H190 H181 H190 H190 H190 H190 H190 H190 H190 H19	0.1303 0.1700 0.1841 0.1794 0.1426 0.1426 0.1423 0.1812 0.1830 0.1685 0.1350 5.0000 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1672 -0.14123 0.11123 0.11123 0.1157 0.1527 0.1503 0.1503
$\begin{array}{c} \rm H15 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H22 \\ \rm H24 \\ \hline \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1222\\ 0.1501\\ 0.1502\\ 0.1511\\ 40.99 \mbox{ A} \\ -0.4923\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0624\\ 0.0370\\ -0.5151\\ 0.0376\\ -0.3553\\ 0.0486\\ -0.3353\\ 0.4466\\ -0.3107\\ 0.4265\\ 0.3362\\ 0.4265\\ 0.3362\\ 0.4466\\ 0.0425\\ 0.3362\\ 0.0426\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0362\\ 0.0425\\ 0.0025\\ $	H39 H40 041 C42 C43 044 C45 C46 C45 C46 C47 C48 C25 S26 C27 C28 S29 C30 031 C32 C33 034 H35 H36 H37 H38	0.1253 0.1237 -0.5481 0.0559 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3411 -0.34192 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.1457 0.1457 0.1286 0.1286	H63 H64 H65 O66 C67 C68 O69 C70 C71 O72 C49 C50 C51 C52 C53 C54 C55 C55 C56 C55 C56 C57 H58 H59 H61 H62 H52	0.0937 0.1124 0.1158 0.0158 0.0074 0.0615 0.0659 0.0559 0.0154 0.0154 0.0154 0.0154 0.0154 0.0154 0.01747 0.0262 0.1216 0.0744 0.0274 0.02847 0.02831 0.3903 0.1145 0.3903 0.1196 0.3903	H87 H88 H89 C90 H91 C92 H93 C94 H96 H96 H73 H74 H75 H76 H77 H78 H76 H77 H78 H80 H81 H82 H83 H84 H85 H85 H85	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0972 0.1055 0.0972 0.1055 0.3248 0.3256 0.3356 0.3356 0.3248 0.3248 0.3256 0.3256 0.3256 0.3356 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.34566 0.345666 0.345666666666666666666666666666666666666	C111 H112 C113 H114 C115 C116 H117 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C105 C106 C106 C107 C108 C107 C107 C108 C107 C107 C108 C107 C108 C107 C108 C107 C107 C108 C107 C108 C107 C108 C107 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C108 C107 C107 C108 C107 C108 C107 C107 C107 C107 C107 C107 C107 C107	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1237 0.1237 0.1287 0.1055 0.1590 -0.19937 0.1388 0.0365 -0.1005 0.0635 -0.1005 0.1441 -0.0929 0.1535 0.0547 -0.0931 0.1535 0.0547 -0.1002 0.1506 0.0400 -0.0591	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C123 C124 C126 C127 C128 C126 C127 C128 C129 C131 C131 C133 N134 C135 C135 C135 C135 C135 C135 C136 C137 C138 C137 C138 C139 C138 C139 C136 C137 C138 C139 C138 C139 C138 C139 C139 C138 C122 C122 C123 C124 C122 C123 C124 C122 C123 C124 C122 C123 C124 C129 C129 C129 C129 C129 C129 C129 C129	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1505 0.1545 0.1565 0.15857 0.15857 0.1037 -0.1447 0.1037 -0.1447 0.1508 0.0680 -0.1055 0.0680 -0.1555 0.0685 -0.1157 0.0555 -0.938 -0.938 -0.938 -0.938	N159 C1600 C161 H162 H163 C164 C165 C166 C167 C168 H145 H145 H145 H147 H148 H149 H150 H151 H152 H153 H155 C156 C157 C158	-0.4106 0.1547 -0.1469 0.1640 0.1881 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1389 0.1288 0.1288 0.1288 0.1288 0.1288 0.1349 0.1655 0.1349 0.1655 0.1349	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C179 H171 H172 C175 C176 C177 C176 C177 C177 C177 H181 H181 H181 H181 H182	0.1533 0.1700 0.1841 0.1794 0.1426 0.1423 0.1423 0.1423 0.1423 0.1426 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1165 0.1091 0.11123 0.11679 0.1679 0.1579 0.1579 0.1579
$\begin{array}{c} \rm H15 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline z = - \\ 01 \\ \rm C2 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm S12 \\ \rm S13 \\ \rm H14 \\ \rm H15 \\ \rm H14 \\ \rm H15 \\ \rm H14 \\ \rm H15 \\ \rm C12 \\ \rm S13 \\ \rm S14 \\ \rm H14 \\ \rm H15 \\ \rm S14 \\ \rm S16 \\ $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1205\\ 0.1210\\ 0.1167\\ 0.1267\\ 0.1267\\ 0.1267\\ 0.1272\\ 0.1501\\ 0.1272\\ 0.1501\\ 0.1272\\ 0.1511\\ 0.0127\\ 0.1511\\ 0.0230\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0643\\ 0.0370\\ -0.5151\\ 0.0858\\ -0.355\\ 0.4664\\ 0.0370\\ -0.2353\\ 0.4664\\ 0.0370\\ -0.355\\ 0.4255\\ 0.3252\\ 0.1161\\ 0.3252\\ 0.1161\\ 0.3255\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.1161\\ 0.0325\\ 0.032$	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 C33 O34 H36 H37 H38 H39 H36	0.12253 0.1227 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5189 0.0451 -0.5189 0.4336 -0.2415 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.5655 0.0254 -0.5655 0.1457 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284	H63 H64 H65 O66 C67 C68 O69 C70 C71 O72 C49 C50 C51 C52 C53 C54 C55 C56 C55 C56 C57 H58 H60 H61 H62 H63 H62 H63	0.0937 0.1128 0.1158 0.1158 0.0074 0.0615 0.0659 0.0194 -0.4869 0.0559 0.0194 -0.4767 -0.1216 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 0.0953 0.1096 0.1195 0.0992 0.0979 0.0878 0.0878	H87 H88 H89 C90 H91 C92 H93 C94 C95 H96 H73 H74 H75 H75 H75 H75 H75 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H86 H87 C92 C92 C92 C92 C92 C92 C92 C92 C92 C92	0.1083 0.1394 0.1627 -0.1141 -0.1430 0.0746 0.3033 -0.1395 0.3033 -0.1395 0.1316 0.0994 0.0972 0.1055 0.1047 0.0984 0.0991 0.3248 0.2279 0.2015 0.0939 0.0850 0.0535 0.1508	C111 H112 C113 H114 C115 C116 H117 C118 H119 C107 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C100 C111 H112 C115 H112 C115 C115 C115 C115 C115 C115 C115 C	-0.1057 0.1091 0.1205 0.3116 -0.1230 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1238 0.0305 0.1388 0.0306 0.1388 0.0306 0.1388 0.0306 0.1431 -0.0929 0.1555 0.0644 0.0547 -0.0931 0.1555 0.0641 0.0547 -0.002 0.1556 0.0440 0.0460 0.0467	C135 C136 C137 C138 C139 H140 H141 H142 H143 H143 H143 H143 H143 H143 H144 C121 C122 C123 C124 C127 C128 C127 C128 C127 C128 C127 C130 H140 H141 H142 H143 H143 H143 H143 H143 H143 H143 H143	0.1597 -0.1390 0.0777 -0.1475 0.1513 0.1805 0.1545 0.1606 0.1887 0.1887 0.1887 0.1037 -0.1447 0.1037 -0.1496 -0.1595 0.0680 -0.1595 0.0685 -0.0555 -0.0949 -0.1555 -0.949 -0.4102 0.1555	N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H151 H151 H151 H155 H155 H155 H155 C156 C157 C158 N159 C100 C101 H145 H155 H155 H155 H155 H155 H155 H15	-0.4106 0.1547 -0.1469 0.1640 0.1881 -0.1589 0.0704 -0.1183 -0.1193 0.0704 0.1193 0.1771 0.1193 0.1248 0.1268 0.1268 0.1268 0.1268 0.1268 0.1268 0.1268 0.1655 0.1349 0.1655 0.1594 0.1247 0.0757 -0.1247 0.1665	H183 H184 H185 H186 H187 H188 H189 H190 H190 H190 H190 H171 C169 C170 H171 C173 N174 C175 C176 C177 C178 C177 H180 H181 H182 H182 H182 H182 H182 H182 H182	0.1300 0.1700 0.1841 0.1794 0.1426 0.1842 0.1812 0.1812 0.1830 0.1855 0.1350 5.0000 5.0000 5.0000 5.0000 0.1123 0.1116 0.1123 0.1123 0.1123 0.1570 0.1503 0.1503 0.1579 0.1842
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H15 \\ \rm H16 \\$	0.1279 0.1276 0.1276 0.1205 0.1210 0.1160 0.1160 0.1267 0.1227 0.1222 0.1502 0.1502 0.1502 0.0623 -0.4923 0.0623 -0.4923 0.0624 0.0370 0.0684 0.0370 0.0684 0.0364 0.0370 0.0684 0.0364 0.0364 0.0364 0.0364 0.0466 -0.3107 0.4265 0.3262 0.4265 0.3262 0.4265 0.3262 0.4265 0.3362 0.4466 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.3362 0.4265 0.4272 0.0370 0.0410 0.0370 0.0466 0.0370 0.0460 0.0370 0.0460 0.0370 0.0460 0.0370 0.0460 0.0470 0.0400 0.04700 0.04700 0.0470000000000	H39 H40 O41 C42 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C37 C28 S29 C33 C32 C33 C31 C32 C33 C34 H35 H36 H37 H38 H39 H40 C42 C42 C42 C42 C42 C42 C42 C42 C42 C42	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 0.0748 -0.5161 0.0524 -0.5161 0.0524 -0.5161 0.0524 -0.5161 0.1224 0.1226 0.1226	H63 H64 H65 D667 C68 D69 C70 C71 072 C49 C50 C51 C52 C53 C54 C55 C56 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H63 H64	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0154 -0.0194 -0.0767 -0.2262 -0.1216 -0.0744 -0.0847 -0.1226 0.01744 -0.0847 -0.1236 0.0145 0.0831 0.1145 0.3903 0.1145 0.0878 0.0928 0.0928	H87 H88 H89 C90 H91 C92 H93 C94 H96 H73 H74 H75 H76 H77 H78 H77 H77 H78 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H87 H88	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1316 0.0972 0.1055 0.0972 0.1055 0.0988 0.2979 0.2015 0.2015 0.2215 0.2215 0.08980 0.2215	C111 H112 C113 H114 C115 C116 H117 C118 H119 C106 H109 C100 H102 C103 H104 C106 H107 C106 H107 C106 H107 C106 H109 C110 H112 C111 H112 C112 H112 C113 H114 H112 H115 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H116 H117 H117	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1055 0.1237 0.1287 0.1065 0.1067 0.1590 -0.0937 0.1388 0.0306 0.0635 -0.1005 0.0455 0.0457 -0.0929 0.1532 -0.1002 0.1532 -0.1002 0.1508 -0.0640	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H143 H144 H143 H144 C121 C122 C123 C124 C122 C123 C124 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C135 C136 C137 C135 C136 C137 C138 H140 H140 H141 H142 H142 H142 H143 H140 H142 H143 H142 H143 H140 H142 H143 H140 H143 H140 H143 H140 H143 H140 H142 H143 H140 H143 H140 H143 H142 H143 H140 H143 H142 H143 H142 H143 H142 H143 H142 H143 H142 H143 H140 H143 H140 H143 H142 H143 H140 H143 H143 H140 H143 H143 H142 H143 H143 H143 H143 H143 H143 H143 H143	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1505 0.1543 0.1545 0.1545 0.1545 0.1523 0.1237 -0.1396 0.1037 -0.1037 -0.1037 -0.1037 -0.1005 0.0555 0.06800 -0.1257 0.0555 -0.1157 0.0555 -0.1532 -0.1532 -0.1552 -0.1532 -0.1552 -0.1532 -0.1552 -0.1552 -0.1552 -0.1552 -0.1552 -0.1552 -0.1553 -0.1555 -0.1	N159 C160 C161 H162 H162 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 C157 C158 C160 C161 H162 H162 H162 H162 H163 H162 H163 H163 H163 H163 H163 H163 H163 H163	-0.4106 0.1547 -0.1463 0.1640 0.1889 0.0704 -0.1188 -0.1589 0.0704 -0.1193 0.0701 0.1771 0.1400 0.1386 0.1248 0.1248 0.1288 0.1289 0.1289 0.1839 0.1650 -0.1247 0.1650 -0.1244 0.1650 -0.24144 0.0444	H183 H184 H185 H186 H187 H188 H189 H190 Total Total C169 C170 H171 H172 C173 N174 C176 C177 C178 C177 C178 C179 H180 H181 H181 H181 H183 H184 H183 H184 H185	0.1333 0.1700 0.1841 0.1794 0.1426 0.1423 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1350 0.1685 0.1167 0.1091 0.1123 0.1629 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1573 0.1577 0.1574 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C6 \\ \rm C7 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1260\\ 0.1167\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1501\\ 0.0230\\ 0.0632\\ 0.0644\\ 0.0230\\ 0.0642\\ 0.0370\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0856\\ -0.3352\\ 0.0466\\ -0.3352\\ 0.0466\\ -0.3362\\ 0.03862\\ $	H39 H40 O41 C42 C43 O44 C45 C46 O47 C48 C25 S26 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H35 H36 H37 H38 H39 O44 C42 C43 C45 C46 O47 C46 C47 C46 O47 C46 O47 C46 C47 C46 C47 C46 O47 C46 C47 C47 C46 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3436 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.5161 0.0521 0.0254 0.1487 0.1286 0.1287 0.1286 0.1286 0.1287 0.1286 0.1286 0.1286 0.1286 0.1287 0.1286	H63 H64 H65 O66 C67 C68 O69 C70 C71 O72 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H64 H64 H64 H65	0.0937 0.1124 0.1158 0.1158 0.0074 0.0615 0.0559 0.0194 -0.4869 0.0559 0.0194 -0.4865 0.0194 -0.4765 0.0194 -0.1216 -0.0954 -0.0947 -0.1236 0.0994 0.0847 -0.1235 0.0994 0.0994 0.0393 0.1096 0.3903 0.1195 0.0992 0.0979 0.0878 0.0936 0.0936 0.0936 0.0936 0.0936	H87 H88 H89 C90 H93 C92 H93 C95 H96 H73 H76 H77 H78 H79 H80 H81 H82 H83 H84 H85 H86 H87 H88 H88 H88 H88 H88 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 0.3033 -0.1395 0.3033 -0.1316 0.9984 0.9984 0.9994 0.9994 0.0972 0.1065 0.0995 0.0995 0.0995 0.3248 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9991 0.3456 0.9972 0.00774 0.1356 0.9972 0.007740000000000	C111 H112 C113 H114 C115 C116 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H109 C100 C101 H107 C108 H109 C110 C111 H112 C113 H112 H122 H122 H122 H122 H122 H122 H	-0.1057 0.1091 0.1091 0.1205 0.3116 -0.1237 0.1218 -0.1237 0.1218 -0.1055 0.1087 0.1388 0.0306 0.1388 0.0306 0.1388 0.0306 0.1388 0.0306 0.1464 -0.0929 0.1555 0.0642 -0.0931 0.1555 0.0640 0.0640 0.0440 0.0440 0.0466 0.0466 0.0467 0.1002	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 C123 C124 C127 C128 C127 C128 C129 C130 C130 C131 C132 C133 C135 C135 C135 C137 C135 C136 C137 C138 C137 C138 C137 C138 C137 C138 C139 C136 C137 C138 C137 C138 C139 C136 C137 C138 C139 C138 C139 C138 C139 C139 C138 C139 C138 C139 C138 C139 C139 C138 C139 C139 C139 C138 C139 C139 C139 C139 C139 C139 C139 C139	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1606 0.1887 0.1887 0.1087 -0.1396 -0.1087 -0.1037 -0.1447 0.1508 -0.4065 -0.1655 -0.4055 -0.4055 -0.4055 -0.4055 -0.4055 -0.4055 -0.4055 -0.4122 -0.4127 0.555 -0.4122 -0.4127 -0	N159 C160 C161 H162 C164 C165 C166 C166 C166 H146 H147 H148 H149 H150 H151 H155 H154 H155 C156 C156 C157 C158 N159 C158 N159 C160 C161 H162 H155 H155 C156 C161 H162 H162 H162 H162 H162 H162 H162 H	-0.4106 0.1547 0.1549 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1193 0.0710 0.1193 0.1193 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1339 0.1655 0.1349 0.1655 0.1349 0.1655 0.1247 0.1247 0.1655	H183 H184 H185 H186 H185 H186 H187 H188 H190 H191 Total C169 C170 H171 Total C170 H172 C173 N174 C175 C176 C176 C177 C177 H180 H181 H182 H183 H184 H185 H182 H183 H184 H185 H182 H183 H184 H185 H182 H183 H184 H185 H185 H185 H185 H185 H185 H185 H185	0.1333 0.1700 0.1841 0.1794 0.1426 0.1426 0.1423 0.1812 0.1423 0.1830 0.1425 0.1830 0.1685 0.1350 0.1685 0.1091 0.1123 0.1116 0.1672 0.
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H24 \\ \hline \\ z = - \\ 01 \\ c \\ $	0.1279 0.1276 0.1276 0.1205 0.1210 0.1160 0.1160 0.1167 0.1227 0.1227 0.1502 0.1502 0.1502 0.1501 0.0623 -0.4992 0.0220 0.0623 -0.4923 0.0643 0.0370 -0.5151 0.0382 0.0466 -0.3150 0.4265 0.3262 0.4265 0.4272 0.0370 0.0370 0.0370 0.0350 0.0465 0.0350 0.0465 0.0350 0.0465 0.0350 0.0465 0.0350 0.0465 0.0350 0.0465 0.0350 0.4466 0.1180 0.1180 0.0426 0.0466 0.0426 0.04660000000000	H39 H40 O41 C42 C43 O44 C45 C46 O47 C25 S26 C27 C28 S29 C30 O31 C32 C32 C33 O34 H35 H36 H37 H38 H39 H40 O41 C42 C42 C42 C42 C43 C44 C44 C44 C44 C44 C44 C44 C44 C44	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.5161 0.0254 -0.5164 0.0521 0.0254 -0.5164 0.0524 -0.5164 0.1284 0.1284 0.1285 0.1284 0.1285 0.1284 0.1285 0.1284 0.1285 0.1	H63 H64 H65 O66 C67 C68 O69 C70 C71 072 C49 C50 C51 C52 C53 C54 C55 C55 C55 C55 C55 C55 C55 C55 C55	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0744 -0.0847 -0.0831 -0.1256 0.0145 0.0393 0.1145 0.0979 0.878 0.0979 0.878 0.0988 0.0988 0.0988	H87 H88 H89 C90 H93 C92 H93 C94 C95 H96 H77 H78 H77 H78 H80 H81 H82 H83 H84 H85 H86 H87 H88 C90	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1316 0.0972 0.1316 0.0972 0.1055 0.0972 0.1055 0.0988 0.2279 0.2015 0.2215 0.2215 0.2015 0.0886 0.5088 0.2279 0.2015 0.0886 0.508 0.508 0.508 0.5075 0.0856 0.508 0.508 0.5075 0.0856 0.508 0.0754 0.0856 0.0754 0.0856 0.0758 0.0758 0.0075 0.0858 0.0758 0.0075 0.000	C111 H112 C113 H114 C115 C116 H117 C120 C107 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C107 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C106 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C105 C107 H107 C107 C107 H107 C107 H107 C107 C107 H107 C107 C107 H107 C107 C107 H107 C107 C107 C107 C107 C107 C107 C107 C	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1055 0.1067 0.1590 -0.0937 0.1388 0.0635 -0.1005 0.0306 0.0647 -0.0929 0.1453 0.1550 -0.1508 -0.1508 -0.1508 -0.1550	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C133 C136 C137 C138 C136 C137 C135 C136 C137 C138 C137 C138 C139 C139 C139 C139 C139 C139 C139 C139	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1505 0.1543 0.1545 0.1545 0.1545 0.1523 0.1237 -0.1495 -0.1037 -0.1037 -0.1037 -0.1037 -0.1037 -0.1055 0.06650 -0.1252 -0.1157 0.0555 -0.0949 -0.1532 -0.1532 -0.1532 -0.1532 -0.1532 -0.1532 -0.1532 -0.1427 -0.1427 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1479 -0.1532 -0.1427 -0.1479 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1427 -0.1532 -0.1427 -	N159 C160 C161 H162 C164 C165 C166 C166 C167 C168 H145 H145 H146 H147 H148 H149 H150 H151 H152 H153 H155 C156 C157 C158 S159 C160 C161 H159 C161 C161 H145 H155 H155 H155 H155 H155 H155 H15	-0.4106 0.1547 0.1540 0.1640 0.1889 0.0704 -0.1188 -0.1589 0.0704 -0.1188 -0.1188 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1650 -0.1247 0.1650 -0.1247 0.1494 -0.1494 -0.1495 0.1495	H183 H184 H185 H186 H185 H186 H187 H189 H190 H191 Total Total C169 C170 H171 H172 C173 N174 C176 C177 C177 C177 C177 C177 H180 H181 H183 H184 H183 H184 H184 H184 H184 H184 H184 H184 H184	0.1300 0.1700 0.1841 0.1734 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1428 0.1483 0.1485 0.1485 0.1485 0.1485 0.14123 0.1116 0.1685 0.1692 0.1423 0.1577 0.1577 0.1574 0.1573 0.1579 0.1574 0.1573 0.1579 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1574 0.1575 0.15770000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm C2 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H10 \\$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1501\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0644\\ 0.0370\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0856\\ -0.2353\\ 0.0466\\ -0.3107\\ 0.4265\\ 0.3362\\ 0.1181\\ 0.3622\\ 0.1181\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1097\\ 0.0057\\ 0.0$	H39 H40 O41 C42 C43 O44 C45 C46 C46 C25 S26 C47 C48 C27 C28 S29 C33 C33 C33 C33 C33 C33 C33 C33 C33 C3	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3415 -0.3052 0.4336 -0.44336 -0.44192 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5055 0.14857 0.1284 -0.1296 0.1305 0.1284 -0.5271 0.1284 -0.5271 0.05857	H63 H64 H64 H65 D66 C67 C70 C71 O72 C70 C70 C71 O72 C70 C71 C72 C50 C50 C51 C51 C52 C53 C54 C55 C56 C57 C56 H59 H60 H61 H61 H61 H61 H65 H65 H65 H65 H65 H65 H65 H65 H65 H65	0.0337 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.262 -0.1216 -0.0954 -0.0744 -0.0847 -0.0954 -0.0847 -0.1236 -0.0954 -0.1236 0.3903 0.1145 0.3903 0.1996 0.3936 0.0878 0.0992 0.0878 0.0936 0.0936 0.0936 0.0936 0.0936 0.0936	H87 H88 H89 C30 C32 H33 C32 H33 C32 H73 H74 H75 H76 H77 H78 H77 H78 H77 H78 H77 H78 H80 H81 H82 H85 H86 H89 H85 H86 H87 H88 H89 C30 C30 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.3033 -0.1316 0.1316 0.1316 0.0984 0.0972 0.1065 0.0988 0.0991 0.3248 0.0993 0.3248 0.0993 0.3248 0.0993 0.3248 0.0993 0.3248 0.0993 0.3248 0.0954 0.1107 1.1158 0.11588 0.11475 0.0939	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H012 C103 H104 C105 C105 C106 H107 C108 H107 C108 H107 C110 H112 C113 H114 C115 C116 H117 C118 H112 C115 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C118 H112 C120 C97 H98 C99 C100 C100 C100 C100 C100 C100 C100	-0.1057 0.1061 0.1091 0.1205 0.3116 -0.1230 0.1218 -0.1237 0.1218 -0.1055 0.1087 0.1580 -0.1087 0.1388 0.0306 0.0635 -0.1005 0.1388 0.0306 0.0647 -0.0929 0.1555 0.0647 -0.0921 0.1505 0.0647 -0.0921 0.1505 0.0647 -0.0921 0.1505 0.0647 -0.0921 0.1505 0.0647 -0.0921 0.1505 0.0647 -0.0921 0.1505 0.1002 0.1505 0.1001 0.1505 0.1001 0.150 0.100100000000	C135 C136 C137 C138 C139 H140 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 C132 C133 C134 C135 C136 C137 C138 C136 C137 C138 C139 C139 C139 C139 C130 C137 C138 C139 C136 C137 C138 C137 C138 C139 C136 C137 C138 C139 C139 C136 C137 C138 C139 C139 C139 C139 C139 C139 C139 C139	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1606 0.1887 0.1887 0.1637 -0.1487 0.1037 -0.1487 0.1037 -0.1447 0.1037 -0.1508 -0.4065 -0.1555 -0.4065 -0.1555 -0.4065 -0.938 -0.1555 -0.402 0.5555 -0.402 0.1532 -0.4120 -0.1427 0.1202 -0.1427 0.1202 -0.1427 0.1202 -0.1427 -0.1517 -0.1517 -0.1527 -0	N159 C160 C161 H162 C164 C165 C166 C166 C166 H146 H147 H146 H147 H147 H148 H149 H151 H153 H154 H155 C156 C156 C157 C158 N159 C160 C161 H165 H155 H155 C156 C161 H165 H155 H155 H155 C161 H165 H165 H165 H165 H165 H165 H165 H	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.11771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1389 0.1655 0.1349 0.1655 0.1349 0.1655 0.1349 0.1650 -0.4120 0.1650 -0.4120 0.1477 0.1477 0.1477	H183 H184 H185 H186 H185 H186 H187 H188 H190 H191 Total C169 C170 H171 Total C170 H172 C173 H172 C173 H172 C175 C176 C177 C178 H180 H180 H182 H183 H184 H185 H186 H185 H186 H185 H186 H186 H185 H186 H187 H187 H187 H187 H187 H187 H187 H187	-0.1930 0.1700 0.1841 0.1794 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1682 0.1682 0.1682 0.1672 0.177 0.1772
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H16 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \end{array}$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.0623\\ -0.4923\\ 0.0623\\ -0.4923\\ 0.0623\\ -0.4923\\ 0.0643\\ -0.35161\\ 0.0370\\ -0.5151\\ 0.0683\\ 0.04285\\ 0.3362\\ 0.4285\\ 0.3362\\ 0.4285\\ 0.3362\\ 0.1180\\ 0.1149\\ 0.104\\ \end{array}$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C48 C46 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	$\begin{array}{c} 0.1253\\ 0.1237\\ -0.5481\\ 0.0559\\ 0.0590\\ -0.5199\\ 0.0565\\ 0.0451\\ -0.5199\\ 0.3783\\ \hline \\ -0.3783\\ \hline \\ -0.3783\\ \hline \\ -0.3052\\ 0.4336\\ -0.2415\\ -0.1401\\ 0.0748\\ -0.5161\\ 0.0748\\ -0.5616\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ 0.1284\\ -0.5515\\ \hline \end{array}$	H63 H64 H65 C67 C70 C71 C72 C49 C70 C71 C72 C55 C56 C55 C55 C55 C55 C55 C55 C55 C57 H58 H59 H60 H61 H62 H63 H64 C77 C77 C77 C77 C77 C77 C77 C77 C77 C7	$\begin{array}{c} 0.0937\\ 0.1124\\ 0.1124\\ 0.1158\\ -0.4831\\ 0.0074\\ 0.0615\\ -0.4869\\ 0.0559\\ 0.0559\\ 0.0559\\ 0.0194\\ -0.4767\\ \hline 0.2052\\ -0.1216\\ -0.0954\\ -0.0744\\ -0.0954\\ -0.0954\\ -0.0954\\ 0.0933\\ 0.1296\\ 0.1145\\ 0.0992\\ 0.0878\\ 0.0939\\ 0.0878\\ 0.0939\\ -0.5136\\ 0.0988\\ 0.0159\\ -0.5136\\ 0.01765\\ \hline \end{array}$	H87 H88 H89 H89 H91 C30 C34 C34 C34 C34 C35 H73 H74 H73 H74 H75 H76 H77 H77 H77 H77 H77 H77 H78 H80 H81 H81 H82 H83 H84 H87 H81 H82 H83 H84 H87 C30 C30 C30 C30 C30 C30 C30 C30 C30 C30	0.1083 0.1394 0.1627 -0.1141 -0.1430 0.0746 0.3033 -0.1395 0.3033 -0.1395 0.1316 0.9984 0.977 0.1055 0.1047 0.9984 0.9991 0.3248 0.2279 0.2015 0.09991 0.3248 0.2279 0.2015 0.09991 0.3248 0.2279 0.2015 0.09991 0.3248 0.0754 0.1147 0.1147 0.1147 0.1147 0.0934 0.0754 0.1147 0.1147 0.1147 0.0934 0.1147 0.1147 0.1147 0.0934 0.1154 0.1155 0.1141 0.0934 0.0755 0.0754 0.0754 0.0755 0.0754 0.0754 0.0755 0.0754 0.0755 0.0754 0.0754 0.0755 0.0754 0.0754 0.0755 0.0754 0.0754 0.0755 0.0754 0.0754 0.0754 0.0755 0.07540000000000000000000000000000000000	C111 H112 C113 H114 C115 C116 C116 H117 C118 H119 C120 C100 C100 C101 H102 C103 H102 C103 H104 C105 C106 H109 C110 C111 H112 C113 H114 C113 H114 C115 C116 C116 C116 C116 C116 C116 C116	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.10937 0.1388 0.3066 0.0937 0.1388 0.3066 0.0932 0.1441 -0.0929 0.1441 0.1532 -0.1902 0.1566 0.4440 -0.90847 -0.1656 0.1658 -0.1658 -0.1658	C135 C136 C137 C138 C139 H140 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140	$\begin{array}{c} 0.1597\\ -0.1349\\ 0.0777\\ -0.1475\\ 0.1513\\ 0.1805\\ 0.1545\\ 0.1505\\ 0.1545\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1037\\ -0.1447\\ 0.0655\\ -0.1595\\ 0.0680\\ -0.1229\\ -0.1555\\ -0.0949\\ -0.1555\\ -0.0949\\ -0.1555\\ -0.0949\\ -0.1555\\ -0.0949\\ -0.1555\\ -0.1555\\ -0.1552\\ -0.1427\\ 0.1552\\ -0.1427\\ 0.1552\\ -0.1427\\ 0.1555\\ -0.1427\\ 0.1555\\ -0.1651\\ -0.1557\\ -0.1651\\ -0.1557\\ -0.1651\\ -0.1557\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575\\ -0.1575$	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H146 H146 H147 H148 H149 H150 H151 H151 H151 H152 H153 H154 H155 C156 C157 C158 C160 C161 H162 H162 H162 H162 H162 H162 H163	-0.4106 0.1547 -0.1469 0.1640 0.1889 0.0704 -0.1188 -0.1589 0.0704 -0.1193 0.0710 0.1771 0.1400 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1769 0.1339 0.1655 0.1650 -0.1247 0.1650 -0.4127 0.1494 0.1495 0.1495	H183 H184 H185 H186 H185 H186 H187 H189 H190 H191 Total Total C169 C170 C170 C170 C177 C178 C177 C177 C177 C177 C177 H181 H182 H184 H184 H184 H187 H188	0.1304 0.1704 0.1784 0.1426 0.1784 0.1426 0.1423 0.1812 0.1830 0.1350 5.0000 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1334 0.1162 -0.1570 0.1570 0.1570 0.1577 0.1804 0.1875
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H21 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H11 \\ \rm H10 \\$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1222\\ 0.1501\\ 0.1502\\ 0.1501\\ 0.0230\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0370\\ 0.0355\\ 0.0055\\ 0.005\\ 0.00$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C48 C47 C48 C44 C44 C45 C45 C45 C45 C45 C45 C45 C45	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3452 -0.3452 -0.3452 -0.2415 -0.2415 -0.1401 0.0524 -0.5161 0.0254 -0.5161 0.0254 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.0587 -0.5181 0.0587 0.0587 -0.51841 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 -0.5571 0.0587 0.05770 0.05770 0.05770 0.05770 0.05770000000000	H63 H64 H65 C67 C68 C67 C70 C69 C70 C71 072 C50 C71 072 C50 C51 C52 C53 C54 C55 C56 C57 H58 H59 H60 H61 H62 H63 H64 H64 H65 C67 C68 B06 B06 B06 B06 B06 B06 B06 B07 C72 C72 C72 C72 C72 C72 C72 C72 C72 C7	$\begin{array}{c} 0.0937\\ 0.1124\\ 0.1158\\ -0.4831\\ 0.0074\\ 0.0615\\ -0.4869\\ 0.0559\\ 0.0559\\ 0.0164\\ -0.4767\\ -0.2362\\ -0.1216\\ -0.0744\\ -0.0847\\ -0.0744\\ -0.0847\\ -0.1236\\ -0.0784\\ 0.0992\\ 0.3903\\ 0.1996\\ 0.1996\\ 0.0992\\ 0.0978\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0878\\ 0.0992\\ 0.0998\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.0388\\ 0.03$	H87 H88 H89 H89 H89 H89 H81 H81 H81 H73 H74 H76 H77 H76 H77 H77 H76 H77 H77 H81 H81 H81 H81 H83 H84 H85 H86 H87 H88 H88 H87 H88 H87 H88 H87 H87 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0776 0.1316 0.0974 0.1316 0.0974 0.0972 0.1055 0.0972 0.1055 0.0988 0.0998 0.3248 0.3450 0.3450 0.3450 0.3448 0.3248 0.3450 0.3450 0.3448 0.3450 0.3450 0.3448 0.3450 0.3450 0.3448 0.3450 0.3450 0.3448 0.3450 0.3450 0.3448 0.3450 0.3450 0.3450 0.3448 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3448 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.3450 0.34500000000000000000000000000000000000	C111 H112 C113 H114 C115 C116 C116 C116 H117 C120 C27 H98 C99 C100 C101 C100 C100 C100 C100 C100	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1237 0.1237 0.1237 0.1287 0.1287 0.1590 -0.0937 0.1388 0.3065 -0.1005 0.0635 -0.1005 0.0547 -0.0929 0.1555 0.0547 -0.0929 0.1555 0.0547 -0.0931 0.1558 0.0547 -0.1558 0.0568 -0.1667 0.1665 0.1665	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1666 0.1857 0.1685 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1447 0.1037 -0.1447 0.1555 0.0680 -0.1055 -0.1055 -0.1055 -0.1055 -0.1427 0.1555 -0.4102 0.1527 0.1527 0.1657 0.1657	N159 C160 C161 H162 C164 C165 C166 C166 C166 H145 H146 H147 H148 H149 H150 H151 H155 H155 C156 C157 C158 N159 C160 C1612 H163 C164 C165	$\begin{array}{c} -0.4106\\ 0.1547\\ -0.1469\\ 0.1540\\ 0.1589\\ 0.0704\\ -0.1188\\ -0.1589\\ 0.0704\\ -0.1188\\ -0.1193\\ 0.0710\\ 0.1711\\ 0.1400\\ 0.1348\\ 0.1248\\ 0.1248\\ 0.1248\\ 0.1248\\ 0.1248\\ 0.1248\\ 0.1248\\ 0.1349\\ 0.1655\\ 0.1349\\ 0.1655\\ 0.1349\\ 0.1655\\ 0.1349\\ 0.1655\\ 0.1349\\ 0.1655\\ 0.1349\\ 0.1655\\ 0.1449\\ 0.1440\\ -0.1477\\ 0.1650\\ -0.1248\\ -0.1477\\ 0.1650\\ -0.1248\\ -0.1477\\ 0.1650\\ -0.1268\\ -0.1268\\ -0.1268\\ -0.1278\\ -0.1268\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1278\\ -0.1288\\ -0.1278\\ -0.1288\\ -0.1278\\ -0.1288\\ -0.1278\\ -0.1288\\ -0.1278\\ -0.128$	H183 H184 H185 H186 H186 H186 H187 H189 H190 H191 Total C169 C170 H171 Total C170 H172 C173 N174 C175 C176 C177 C178 C177 C178 C179 H180 H181 H182 H183 H184 H185 H187 H185 H187 H187 H187 H187 H187 H187 H187 H187	0.1530 0.1730 0.1841 0.1734 0.1426 0.1423 0.1423 0.1423 0.1423 0.1425 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1685 0.1685 0.1691 0.1116 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1570 0.1577 0.1570 0.1577 0.1577 0.1574 0.15770 0.15770 0.15770 0.15770000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H22 \\ \rm H24 \\ \rm H22 \\ \rm H24 \\ \rm H22 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm O1 \\ \rm C12 \\ \rm S13 \\ \rm H16 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1226\\ 0.1226\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ 0.0624\\ 0.00230\\ 0.0623\\ 0.0624\\ 0.0370\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0858\\ -0.1350\\ 0.0648\\ 0.0370\\ -0.2353\\ 0.4466\\ -0.3150\\ 0.04285\\ 0.3466\\ -0.3150\\ 0.04285\\ 0.3466\\ 0.1361\\ 0.1145\\ 0.1149\\ 0.1027\\ 0.1104\\ 0.1237\\ 0.1243\\ 0.1243\\ \end{array}$	H39 H40 O41 K42 C42 C43 C45 C46 C46 C46 C46 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C46 C46 C46 C46 C46 C46 C46 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	$\begin{array}{c} 0.1253\\ 0.1227\\ -0.5481\\ 0.0559\\ 0.0590\\ -0.5199\\ 0.0565\\ 0.0451\\ -0.5189\\ 0.3783\\ \hline \\ -0.5189\\ 0.3783\\ \hline \\ -0.5183\\ -0.4012\\ 0.0748\\ -0.5163\\ 0.0551\\ 0.0551\\ 0.0551\\ 0.1284\\ 0.1285\\ 0.1651\\ 0.1284\\ 0.1285\\ 0.1651\\ 0.1284\\ 0.1285\\ 0.1284\\ 0.1285\\ 0.1284\\ 0.1285\\ 0.1284\\ 0.1285\\ 0.1284\\ 0.1285\\ $	H63 H64 H65 C67 C68 C67 C71 072 C59 C71 072 C50 C51 C52 C55 C55 C55 C55 C55 C55 C56 C56 H59 H60 H61 H62 H63 H64 H65 B66 C77 C68 C77 C68 C77 C68 C75 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4863 0.0559 0.0194 -0.4767 -0.1216 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 0.0992 0.0992 0.0979 0.0878 0.0936 0.0928 0.0936 0.0936 0.0936 0.0936 0.0936 0.0936 0.0936 0.0936 0.0123 0.0765 -0.5080 0.0643	H87 H88 H89 H89 H91 C30 C34 C34 C34 C34 C34 C35 H73 H74 H77 H78 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 -0.1261 -0.1430 0.0746 0.3033 -0.1395 0.3077 0.1316 0.9984 0.9972 0.1055 0.1047 0.9984 0.9991 0.3248 0.3248 0.2279 0.0058 0.0991 0.3248 0.2279 0.0058 0.0991 0.3248 0.2279 0.0058 0.0991 0.3248 0.2279 0.00591 0.1477 0.1477 0.1475 0.0939 0.1508 0.0754 0.1475000000000000000000000000000000000000	C111 H112 C113 H114 C115 C116 H119 C120 C99 C100 C101 H102 C103 H104 C105 C106 H107 C108 H109 C110 C111 H112 C113 H114 C115 C116 H117 C118	-0.1057 0.1091 -0.1230 0.3116 -0.1245 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1388 0.3306 0.3366 0.3366 0.3365 -0.1005 0.1348 0.3306 0.4441 -0.9929 0.1535 0.547 -0.0931 0.5452 0.545 0.0647 -0.0931 0.555 0.0440 -0.0867 0.1565 0.3524 -0.1075 0.3552 -0.1075 0.1665 -0.1665 -0.0862	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H143 H144 C121 C122 C123 C124 C127 C128 C127 C128 C127 C129 C130 C130 C131 C132 C133 H140 H141 C135 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C136 C137 C138 C139 C136 C137 C138 C139 C139 C139 C139 C139 C139 C139 C139	$\begin{array}{c} 0.1597\\ -0.1390\\ 0.0777\\ -0.1475\\ 0.1777\\ -0.1475\\ 0.1513\\ 0.1805\\ 0.1553\\ 0.1605\\ 0.1605\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1887\\ 0.1037\\ -0.1447\\ 0.1037\\ -0.1447\\ 0.0685\\ -0.4065\\ -0.1657\\ -0.9948\\ -0.1555\\ -0.9948\\ -0.1555\\ -0.9948\\ -0.1555\\ -0.4102\\ 0.1552\\ -0.4102\\ 0.1552\\ -0.4102\\ 0.1552\\ -0.4102\\ 0.1552\\ -0.4102\\ 0.1552\\ -0.4102\\ 0.1555\\ -0.4102\\ 0.1555\\ -0.4102\\ 0.1555\\ -0.4102\\ 0.1555\\ -0.4102\\ 0.1555\\ -0.4102\\ 0.1557\\ -0.4102\\ 0.1557\\ -0.157\\ 0.1651\\ 0.1364\\ 0.1657\\ -0.157\\ 0.1657\\ 0.1657\\ 0.1657\\ 0.1657\\ 0.167\\ 0.1657\\$	N159 C160 C161 H162 H163 C164 C165 C166 C167 C167 C167 H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C166 C161 C164 C165 C166 C161 C164 C165 C166 C166 C167 C168 H145 H145 H145 H145 H145 H145 H155 H155	-0.4106 0.1547 -0.1469 0.1640 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1183 -0.1193 0.0704 0.1771 0.1400 0.1386 0.1268 0.1268 0.1268 0.1268 0.1289 0.1665 0.1339 0.1665 0.1339 0.1655 0.1349 0.1577 -0.1247 0.1655 0.1424 0.1427 -0.1424 0.1427 0.1427 0.1427 0.1427 0.1429 0.1427 0.1447 0	H183 H184 H185 H186 H185 H186 H187 H188 H190 H191 Total C169 C170 H171 Total C170 H172 C173 N174 C175 C176 C176 C177 C178 C177 C178 C177 H180 H1812 H182 H183 H185 H186 H185 H186 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H187	$\begin{array}{c} 0.1330\\ 0.1700\\ 0.1841\\ 0.1794\\ 0.1426\\ 0.1794\\ 0.1426\\ 0.1830\\ 0.1812\\ 0.1830\\ 0.1850\\ 0.1350\\ 5.0000\\ 5.0000\\ 5.0000\\ 1.0001\\ 0.1133\\ 0.1081\\ 0.1123\\ 0.1116\\ 0.1672\\ -0.4123\\ 0.1116\\ 0.1672\\ -0.4123\\ 0.1570\\ 0.1570\\ 0.1570\\ 0.1570\\ 0.1623\\ 0.1570\\ 0.1804\\ 0.1573\\ 0.1804\\ 0.1573\\ 0.1804\\ 0.1573\\ 0.1805\\ 0.1776\\ 0.1473\\ 0.1805\\ 0.1792\\ 0.1805\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1892\\ 0.1792\\ 0.1792\\ 0.1892\\ 0.179$
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0230\\ 0.0623\\$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C47 C48 C27 C28 S29 C30 C37 C28 S29 C30 C31 C32 C33 C33 H35 H35 H35 H37 H38 H37 H38 H40 O41 C42 C42 C42 C43 C45 C45 C42 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	$\begin{array}{c} 0.1253\\ 0.1227\\ -0.5481\\ 0.0550\\ -0.5199\\ 0.0565\\ 0.0451\\ -0.5199\\ 0.3783\\ \hline \end{array}$	H63 H64 H65 C67 C68 C67 C70 C71 C72 C69 C70 C71 C72 C53 C54 C55 C54 C55 C54 C55 C54 C55 C54 C55 H59 H60 H61 H61 H62 H63 H64 H65 C67 C70 C71 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0194 -0.0194 -0.0744 -0.0287 -0.1216 -0.0744 -0.0236 -0.1216 0.01947 -0.1236 0.01947 -0.1236 0.0145 0.0145 0.0145 0.0145 0.0393 0.1145 0.0392 0.0378 0.03878 0.0392 0.03878 0.0392 0.0392 0.0392 0.0392 0.0392 0.0392 0.0393 0.1393 0.0393 0	H87 H88 H89 C30 C30 H31 H31 C32 C34 H33 C34 H33 H74 H75 H36 H77 H76 H77 H77 H76 H77 H77 H78 H77 H78 H76 H81 H82 H83 H84 H85 H85 H85 H85 H85 H85 H85 H73 H74 H76 H77 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0992 0.1055 0.0972 0.1045 0.0988 0.2279 0.2015 0.3248 0.2279 0.2015 0.3248 0.2279 0.2015 0.3248 0.2279 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0989 0.2015 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0077 0.005 0.0077 0.005 0.005 0.0076 0.0076 0.0077 0.005 0.0077 0.005 0.0076 0.0076 0.0076 0.0076 0.0076 0.0077 0.005 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0076 0.0077 0.0077 0.005 0.0076 0.0076 0.0076 0.0076 0.0077 0.0076 0.00770 0.00770 0.00770 0.00770 0.00770 0.007700000000	C111 H112 C113 H114 C115 C116 C116 C117 C118 H117 C120 C97 H98 C99 C100 C101 C101 C101 C103 H102 C103 H102 C103 H102 C103 H102 C105 C106 C106 C106 C107 C108 H112 C116 C106 C107 C107 C108 C107 C100 C101 C101 C101 C101 C100 C100	-0.1057 0.1001 -0.1230 0.3116 -0.1237 0.1218 -0.1055 0.1237 0.1237 0.1237 0.1237 0.1237 0.1550 -0.0937 0.1550 -0.0937 0.1388 0.0306 0.0305 -0.00929 0.1353 0.0547 -0.0929 0.1553 0.1558 0.1568 -0.1665 0.1665 0.1665 0.1568	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C122 C122 C122 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H141 H143	$\begin{array}{c} 0.1597\\ -0.1349\\ 0.0777\\ -0.1475\\ 0.1613\\ 0.1513\\ 0.1805\\ 0.1543\\ 0.1543\\ 0.1543\\ 0.1543\\ 0.1543\\ 0.1037\\ -0.1447\\ 0.1427\\ 0.1427\\ 0.1508\\ -0.4065\\ -0.1037\\ -0.1447\\ 0.1508\\ 0.0680\\ -0.1037\\ -0.157\\ 0.0594\\ -0.0938\\ -0.1557\\ 0.1522\\ -0.1427\\ 0.1527\\ 0.1527\\ 0.1527\\ 0.1364\\ 0.1657\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1364\\ 0.1057\\ 0.1057\\ 0.105$	N159 C160 C161 H162 C165 C166 C166 C166 C167 H145 H146 H147 H148 H149 H149 H151 H155 H153 H155 C156 C167 C158 N159 C160 C161 H162 H163 C164 C165 C166 C166 C166 C166 C166 C166 C167	-0.4106 0.1547 0.1540 0.1640 0.1881 -0.1589 0.0704 -0.1188 -0.1138 0.0710 0.1771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1650 -0.1247 0.1650 -0.1247 0.1494 0.1494 0.1495 0.1494 0.1495 0.1494 0.1495 0.1495 0.1495 0.1495 0.1495 0.1495 0.1497 0.1495 0.1497 0.1495 0.1497 0.1495 0.1497 0.1497 0.1495 0.1497 0.1495 0.1497 0.1495 0.1497 0.1495 0.1	H183 H184 H185 H186 H185 H186 H187 H189 H190 Total Total C169 C170 H171 H172 C173 N174 C176 C177 C178 C179 H180 H181 H182 H181 H182 H180 H187 H187 H187 H187 H187 H187 H187 H187	0.1333 0.1700 0.1841 0.1794 0.1426 0.1423 0.1423 0.1423 0.1423 0.1426 0.1423 0.1426 0.1423 0.1685 0.1380 0.1685 0.1380 0.1116 0.1123 0.1116 0.1113 0.1116 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1570 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579 0.1839 0.1776 0.1477 0.1839 0.1776 0.1477 0.1829 0.1775 0.1829 0.1775
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H12 \\ \rm H21 \\ \rm H22 \\ \rm H24 \\ \rm H24 \\ \end{array}$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1267\\ 0.1272\\ 0.1272\\ 0.1501\\ 0.1501\\ 0.0230\\ 0.0350\\$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C27 C28 S29 O47 C48 C27 C28 S29 C27 C28 S29 C30 O47 C48 H37 H36 H37 H36 H37 H40 O41 C43 C45 C44 C43 C45 C46 C42 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3415 -0.3352 0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.5415 -0.5655 0.0254 -0.5655 0.1284 -0.5271 0.1285	H63 H64 H65 C67 C68 C70 C70 C71 C72 C69 C70 C71 C72 C50 C52 C53 C52 C55 C56 C55 C56 C57 H59 H60 H61 H62 H63 H64 H64 H65 C77 C67 C77 C72 C77 C72 C77 C77 C77 C77 C77 C7	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.4767 -0.1216 -0.0954 -0.0744 -0.0847 -0.0847 -0.1236 0.0395 0.3903 0.1145 0.3903 0.1996 0.3952 0.0765 -0.5080 0.0182 0.0765 -0.5080	H87 H88 H89 H89 H89 H81 H81 H81 H83 C34 H83 C34 H74 H75 H77 H76 H77 H77 H77 H77 H77 H77 H78 H81 H81 H81 H81 H83 H84 H85 H86 H87 H81 H82 H83 H82 H91 H81 H81 H83 H81 H83 H84 H84 H85 H84 H85 H85 H85 H84 H85 H84 H85 H85 H85 H85 H85 H85 H85 H85 H85 H85	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1316 0.0972 0.1316 0.0984 0.0972 0.1055 0.1316 0.0988 0.0991 0.3248 0.0993 0.3248 0.0993 0.3248 0.0939 0.0850 0.1508 0.0754 0.1119 0.1475 -0.0938 0.1407 -0.1182 0.1348	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H012 C102 C103 H104 C105 C106 H107 C108 H107 C108 H107 C111 H112 C113 H114 C115 C116 H117 C118 H119 C120	-0.1057 0.1061 0.1205 0.3116 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1087 0.1087 0.1388 0.0306 0.0635 -0.1005 0.1388 0.0306 0.0635 -0.1005 0.1441 -0.0929 0.1555 0.0440 -0.0931 0.1552 -0.1067 0.1667 0.3524 -0.1075 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.3524 -0.1075 0.1666 0.1555	C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C127 C128 C129 C130 C131 C132 C133 C132 C133 C134 C135 C136 C137 C138 C139 H140 H141 H142 H142 H144	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1606 0.1887 0.1887 0.1887 0.1887 0.1887 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.4065 -0.11229 -0.4055 -0.4055 -0.4055 -0.4102 0.5555 -0.4102 0.1120 -0.4127 0.1522 0.1120 -0.1427 0.1527 0.1552 -0.4120 0.1527 0.1551 0.1561 0.1557 0.1555 0.1557 0.1555 0.1557 0.1555 0.1557 0.1577 0.15570000000000000000000000000000000000	N159 C160 C161 H162 H162 C164 C165 C166 C166 H146 H147 H147 H147 H147 H148 H149 H151 H155 C156 C156 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C167 C168	-0.4106 0.1547 -0.1469 0.1640 0.189 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1171 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1268 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1247 0.1247 0.1220 0.0247 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.0250 0.02500 0.0250000000000	H183 H184 H185 H186 H185 H186 H187 H188 H190 H191 Total C169 C170 H171 Total C170 H171 C175 C176 C177 C178 C177 C177 H180 H181 H182 H183 H184 H185 H186 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H188 H187 H187	0.1333 0.1700 0.1841 0.1794 0.1426 0.1426 0.1423 0.1812 0.1426 0.1426 0.1425 0.1426 0.1425 0.1426 0.1426 0.1426 0.1426 0.1682 0.1682 0.1682 0.1091 0.1123 0.1617 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1673 0.1672 0.1672 0.1672 0.1673 0.1672 0.1673 0.1672 0.1673 0.1674 0.1672 0.1673 0.1677 0.1673 0.1677 0.1672 0.1673 0.1677 0.1673 0.1677 0.1672 0.1673 0.1677 0.1673 0.1677 0.1672 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1673 0.1677 0.1672 0.1673 0.1677 0.1776 0.1777 0.1672 0.1772 0.1574 0.15770 0.15770 0.15770000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H22 \\ \rm H24 \\ \rm Z = - \end{array}$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1226\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.1501\\ 0.0623\\ -0.4923\\ 0.0623\\ 0.0623\\ -0.4923\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0083\\ 0.0646\\ -0.3150\\ 0.04285\\ 0.3362\\ 0.4466\\ -0.3352\\ 0.4466\\ 0.3362\\ 0.3362\\ 0.3362\\ 0.1180\\ 0.1149\\ 0.1243\\ 0.1149\\ 0.104\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1465\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1145\\ 0.1144\\ 0.1237\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1473\\ 0.1465\\ 0.1473\\ 0.$	H39 H40 O41 C42 C42 C45 C45 C45 C45 C46 C47 C48 C47 C48 C27 C27 C28 C30 O31 C32 C32 C30 O31 H35 H37 H38 H37 H38 H37 H38 H39 H40 O41 C42 C43 C43 C42 C43 C42 C43 C45 C43 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.2415 -0.1401 0.0748 -0.5161 0.0254 -0.505 0.1482 0.1284	H63 H64 H65 C67 C68 C67 C70 C71 072 C69 C70 C71 072 C55 C54 C55 C55 C54 C55 C56 C56 C56 H59 H60 H61 H62 H63 H64 H65 C66 C67 C70 C70 C71 C54 C55 C70 C72 C54 C72 C54 C72 C54 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0559 0.0194 -0.4767 -0.1216 -0.0744 -0.0744 -0.0831 -0.0744 -0.0831 -0.1755 0.1906 0.1145 0.0939 0.1145 0.0939 0.0145 0.0939 0.0878 0.0938 0.0938 0.0938 0.0936 0.0938 0.0125 0.0765 -0.5136 0.0765 -0.5580 0.0765 -0.5580 0.0765 -0.5580 0.0765 -0.5580 0.0765 -0.5580 0.0765 -0.5580 0.0588 0.0588 0.0588 0.0588 0.0588 0.0765 -0.5580 0.0588 0.058	H87 H88 H89 CS0 H89 H81 H89 CS0 CS5 H73 H74 H77 H76 H86 H77 H77 H77 H77 H78 H80 H81 H77 H78 H80 H81 H82 H83 H84 H85 H86 H87 H87 H87 H87 H87 H87 H87 H87 H87 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0984 0.0972 0.1055 0.1047 0.9888 0.0972 0.1055 0.1047 0.2279 0.2015 0.2279 0.2015 0.03930 0.2279 0.2015 0.03930 0.1475 -0.0934 0.1119 0.1475 0.1475 0.1475 0.3263 -0.1188 0.3263 -0.1184	Cill Hil2 Cil3 Hil4 Cil5 Cil6 Hil7 Cil8 Hil9 Ci20 C97 H98 C99 Ci00 Ci01 Hi02 Ci00 Ci01 Hi02 Ci03 Hi02 Ci03 Hi02 Ci03 Hi14 Ci15 Ci06 Hi07 Ci06 Hi07 Ci06 Hi07 Ci06 Hi07 Ci06 Hi17 Ci18 Hi14 Ci15 Ci06 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H98 Ci20 Ci07 H115 H114 H114 H112 Ci16 Ci06 Ci07 H107 H107 H107 H107 H107 Ci07 H107 H107 H107 Ci07 Ci07 Ci07 Ci07 Ci07 Ci07 Ci07 Ci	-0.1057 0.1061 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 -0.1005 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0424 -0.0929 0.1552 -0.1002 0.1508 -0.1653 0.5568 -0.1075 0.1665 -0.0857 0.1508 -0.1075 0.1665 -0.0857 0.1508 -0.0175 0.1665 -0.0857 0.1508 -0.058 0.558 -0.1508 -0.058 -0.1508 -0.058 -0.1508 -0.058 -0.1508 -0.058 -0.1508 -0.1558 -0.058 -0.1558 -0	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C127 C127 C127 C127 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H141 H141 H141 H141 H141 H141	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1503 0.1543 0.1543 0.1545 0.1545 0.1545 0.1823 -0.1396 0.1037 -0.1423 -0.1396 0.1037 -0.1423 -0.1508 -0.1655 -0.229 -0.1157 0.0555 -0.4102 0.1535 -0.1552 -0.1552 -0.1552 -0.1555 -0.1427 -0.1555 -	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H145 H146 H147 H148 H149 H150 H151 H151 H151 H151 H155 C156 C157 C158 S159 C160 C161 C161 C165 C166 C167 C165 C166 C167 C165 C166 C167 C165 C166 C167 C166 C167 C166 C167 C168	-0.4106 0.1547 0.1640 0.1640 0.1889 0.0704 -0.1188 -0.1589 0.0704 -0.1193 0.0710 0.1771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1769 0.1839 0.1655 0.1839 0.1655 0.1838 0.0757 0.1650 -0.1247 0.1650 -0.1247 0.1494 0.1495 0.1494 0.1495 0.1495 0.1495 0.1211 -0.1639 0.0805 -0.2111 -0.112 0.0808	H183 H184 H185 H186 H185 H186 H187 H188 H189 H190 H191 Total Total C169 C170 H190 H191 Total Total Total H172 C173 C176 C177 C178 C176 C177 C178 C176 C177 H180 H181 H182 H183 H184 H183 H184 H185 H186 H187 H188 H189 H189 H189 H189 H189 H189 H189	0.1304 0.1704 0.1784 0.1426 0.1794 0.1426 0.1812 0.1812 0.1812 0.1830 0.1350 5.0000 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 -0.1085 0.1123 0.1123 0.1123 0.1123 0.1123 0.1570 0.1570 0.1570 0.1577 0.1804 0.1579 0.1842 0.1879 0.1473 0.1875 0
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm 04 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C9 \\ \rm C12 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H12 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H22 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H23$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0635\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0355\\$	H39 H40 041 C42 C43 044 C45 C46 C25 S26 C37 C28 S29 C30 031 H35 H36 H37 H38 H39 H40 041 C45 C46 C45 C46 C47 C48	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 -0.4451 -0.3452 0.4336 -0.2441 -0.244 -0.5161 0.0254 -0.1401 0.0254 -0.5161 0.0254 -0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.5567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0564 0.0567 -0.51284 0.0564 0.0567 -0.5271 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.5271 0.0567 -0.5577 0.0567 -0.51284 0.0567 -0.5271 0.0567 -0.5271 0.0567 -0.51284 0.0567 -0.51284 0.0567 -0.5271 0.0567 -0.51284 0.0567 -0.5271 0.0567 -0.5271 0.0567 -0.51284 0.0567 -0.5271 0.0567 -0.51284 0.05777 0.05777 0.05777 0.05777 0.057777 0.057777777777	H63 H64 H65 C67 C68 C67 C70 C69 C70 C71 072 C50 C51 C52 C53 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H65 C67 C70 C68 C77 C68 C77 C68 C77 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0159 -0.0194 -0.4767 -0.2362 -0.1216 -0.0744 -0.0744 -0.0744 -0.0744 -0.0744 -0.1236 0.03903 0.1145 0.0392 0.0392 0.0992 0.0992 0.0992 0.0992 0.0992 0.0995 0.0992 0.0995 0.00765 0.00765 0.00386 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0059 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0074 0.0095 0.0059 0.0059 0.0059 0.0054 0.0074 0.0074 0.0092 0.0097 0.00590000000000	H87 H88 H89 H89 H89 H89 H81 H81 H81 H73 H74 H75 H86 H77 H77 H76 H77 H77 H81 H81 H81 H83 H84 H85 H86 H87 H88 H88 H89 H81 H82 H83 H84 H83 H84 H83 H84 H83 H84 H84 H85 H85 H86 H87 H87 H87 H87 H87 H87 H87 H87 H87 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0376 0.1316 0.0972 0.1055 0.0972 0.1055 0.0972 0.1055 0.0988 0.0972 0.1065 0.3248 0.2279 0.3248 0.3248 0.3248 0.3248 0.3248 0.3248 0.3248 0.1508 0.1508 0.1508 0.1147 0.1407 -0.1348 0.3263 0.1314 0.1314	C111 H112 C113 H114 C115 C116 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C103 H104 C105 C106 H107 C108 H119 C110 C111 H112 C113 H114 C115 C116 C116 C116 H117 C118 H119 C120 C97 C97	-0.1057 0.1061 0.1230 0.2205 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1287 0.1590 -0.0937 0.1388 0.3065 -0.1005 0.6635 -0.1005 0.0647 -0.0929 0.1555 0.0547 -0.0931 0.1558 0.0567 -0.1665 0.1665 0.1665 0.1655 0.1665 0.1655 0.1555 0.1655 0.1557 0.1557	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H142 H144 C121 C121 C121 C121	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1645 0.1666 0.1857 0.1037 -0.1447 0.1037 -0.1487 0.1037 -0.1447 0.1037 -0.1447 0.1037 -0.1447 0.1508 0.0680 -0.1055 0.0680 -0.1557 0.0555 -0.1655 -0.1427 0.1555 -0.4102 0.1527 0.1657 0.1364 0.1364 0.1364 0.1367 0.1392	N159 C160 C161 H162 H162 C164 C165 C166 C166 H145 H146 H147 H148 H149 H151 H155 H151 H155 C156 C156 C157 C158 N159 C160 C1612 H163 C164 C165 C166 C167 C168 H145	-0.4106 0.1547 -0.1469 0.1640 0.1881 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.0710 0.1771 0.1400 0.1384 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1494 0.1465 0.1494 0.1477 0.1655 0.1477 0.1655 0.1477 0.1655 0.1477 0.1655 0.1211 -0.1477 0.1655 0.1477 0.1655 0.1212 0.0858 -0.1211 0.0858	H183 H184 H185 H186 H186 H186 H187 H189 H190 H191 Total C169 C170 H171 C175 C176 C177 C178 C177 C178 C177 C177 H180 H181 H182 H183 H184 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H186 H187 H187 H188 H188 H187 H187 H187 H188 H188	-0.1930 0.1700 0.1841 0.1794 0.1426 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1685 0.1685 0.1690 0.1116 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1570 0.1570 0.1570 0.1570 0.1577 0.1804 0.1577 0.1804 0.1579 0.1776 0.1477 0.1804 0.1776 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.1579 0.1477 0.1804 0.14770000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H15 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H24 \\ \rm H24 \\ \rm H21 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1226\\ 0.1226\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ 0.0644\\ 0.0370\\ -0.555\\ 0.0644\\ 0.0370\\ -0.555\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0644\\ 0.0370\\ -0.255\\ 0.0124\\ 0.000\\$	H39 H40 O41 H40 C42 C43 C45 C46 C45 C46 C46 C47 C48 C47 C48 C47 C48 C47 C48 C48 C48 C48 C48 C48 C48 C49 C42 C44 C42 C42 C42 C44 C42 C42 C43 C42 C42 C43 C42 C42 C43 C42 C42 C43 C44 C42 C43 C44 C42 C43 C44 C42 C45 C42 C45 C42 C45 C42 C45 C46 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C47 C48 C47 C47 C47 C47 C47 C47 C47 C47 C47 C47	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.3482 0.0748 -0.2415 0.0748 -0.5161 0.0254 -0.5051 0.0254 -0.5051 0.1254	H63 H64 H66 C67 C68 C67 C68 C70 C71 072 C50 C71 072 C50 C71 C72 C55 C53 C54 C55 C55 C55 C55 C55 C55 C55 C56 H59 H60 H61 H62 H63 H64 H65 C70 C72 C56 C72 C56 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4863 0.0559 0.0194 -0.4765 -0.1216 -0.0954 -0.2062 -0.1216 -0.0954 -0.0954 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0964 0.0992 0.0979 0.0992 0.0979 0.0936 0.0988 0.0988 0.0988 0.0988 0.0386 -0.5380 0.0643 0.0659 0.0659 0.0659 0.0194 0.0775 0.0075	H87 H88 H89 H89 H81 H81 C30 C34 C34 C34 C34 C34 H73 H74 H73 H74 H77 H78 H81 H77 H78 H81 H81 H81 H82 H83 H84 H85 H86 H87 H81 H82 H83 C30 C30 C30 C30 C30 H73 H74 H74 H75 H77 H78 H77 H78 H77 H77 H78 H77 H77 H78 H77 H77	0.1083 0.1394 0.1627 -0.1141 -0.1261 0.3033 -0.3395 0.3033 -0.3395 0.3707 0.1316 0.9984 0.9972 0.1055 0.1045 0.09972 0.1055 0.1045 0.09988 0.0991 0.3248 0.2279 0.08860 0.3248 0.2279 0.08860 0.1508 0.0939 0.08650 0.1508 0.1508 0.1119 0.11475 -0.0934 0.11475 0.1122 0.13263 0.1326	C111 H112 C113 H114 C115 C116 C116 C116 H17 C118 H17 C120 C120 C100 C100 C101 H102 C100 C100 C101 H102 C105 C106 H107 C106 H109 C110 C111 H112 C113 H104 C115 C116 H107 C118 H109 C110 C111 H112 C118 H119 C120 C107 H98	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1055 0.1087 -0.1055 0.306 0.635 -0.0937 0.1388 0.0306 0.635 0.0306 0.635 0.0441 -0.0929 0.1532 0.1552 0.1441 0.1552 0.1568 0.0457 -0.0857 0.1568 -0.0175 0.1653 0.3524 -0.0075 0.1568 -0.0175 0.1568 -0.0257 0.1568 -0.0257 0.1568 -0.0257 0.1568 -0.0257 0.1568 -0.0257 0.1558 -0.0257 -	C135 C136 C137 C138 C137 C138 C139 H140 H141 H142 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H144 H144 H142 H143 H144 H144 H144 H144 H144 H144 H144	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1606 0.1887 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.1507 0.0680 -0.1229 -0.1557 0.0685 -0.1655 -0.4002 0.5555 -0.4002 0.5555 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5557 -0.4120 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5577 0.5777 0.5777 0.57777 0.57777 0.577777 0.57777777777	N159 C160 C161 H162 H163 C164 C165 C166 C167 C167 C167 H145 H146 H147 H148 H149 H150 H151 H152 H153 H154 H155 C156 C157 C158 N159 C160 C161 H162 H163 C164 C165 C166 C167 C168 H145 H146	-0.4106 0.1547 -0.1469 0.1640 0.1881 -0.1589 0.0704 -0.1188 -0.1193 0.0704 0.1711 0.1400 0.1386 0.1248 0.1248 0.1268 0.1268 0.1349 0.1665 0.1349 0.1655 0.1399 0.1655 0.1577 -0.1247 0.1595 0.0757 -0.1247 0.1495 0.	H183 H184 H185 H186 H187 H188 H189 H190 Total C169 C170 H171 H172 C176 C177 C176 C177 H183 H184 H185 H186 H187 H188 H189 H189 H180 H181 H182 H188 H189 H190 H191	0.1330 0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1830 0.1685 0.1380 5.0000 5.0009 -0.1091 0.1123 0.1116 0.1672 -0.1091 0.1123 0.1116 0.1672 -0.1672 -0.1672 -0.1672 -0.1672 0.1570 0.1570 0.1570 0.1570 0.1570 0.1570 0.1573 0.1805 0.1579 0.1822 0.1776 0.1473 0.1805 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1776 0.1825 0.1854 0.1854 0.1854 0.0988 -0.1125
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm 04 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C12 \\ \rm C3 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H12 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm H15 \\ \rm H16 \\ \rm H17 \\ \rm H10 \\ \rm H23 \\ \rm H13 \\ \rm H10 $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1501\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0485\\ -0.1350\\ 0.0486\\ -0.3107\\ 0.0485\\ 0.3362\\ 0.1180\\ 0.1145\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1181\\ 0.1180\\ 0.1181\\ 0.1180\\ 0.1181\\ 0.1180\\ 0.1181\\ 0.1180\\ 0.1145\\ 0.1181\\ 0.1183\\ 0.1237\\ 0.1243\\ 0.1483\\ A\\ 1.483\\ A\\ 1.483\\ A\\ 0.0679\\ 0.1433\\ 0.0674\\ 0.0679\\ 0.1433\\ 0.0674\\ 0.0679\\ 0.0633\\ 0.0124\\ 0.0679\\ 0.0674\\ 0.0679\\ 0.0674$	H39 H40 041 C42 C43 044 C45 C46 C47 C48 C27 C28 S29 C30 031 H35 H36 H37 H38 H39 H40 041 C42 C43 C44 C45 C46 O47 C48 C44 C45 C46 C47 C28 S26 C27	0.1253 0.1227 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 0.1284 0.1284 0.1284 -0.5271 0.1284 -0.5271 0.0499 0.0587 -0.5188 0.1284 -0.5271 0.0429 0.0587 -0.5188 0.1284 -0.5271 0.0429 0.0587 -0.5128 0.1284 -0.5271 0.0429 0.0587 -0.5128 0.1284 -0.5271 0.0429 0.0587 -0.5128 0.0544 0.0545 0.0544 0.0545 0.0544 0.0545 0.0545 0.0545 0.0545 0.0545 0.0556 0.0556 0.0556 0.0557 0.0545 0.05570 0.05570 0.05570 0.05570 0.05570000000000	H63 H64 H65 C67 C68 C67 C70 C69 C70 C71 072 C50 C71 072 C51 C52 C53 C54 C55 C55 C56 C57 H58 H66 H59 H66 H61 H62 H63 H64 H65 C67 C71 C72 C72 C50 C72 C51 C52 C54 C54 C55 C72 C54 C54 C54 C54 C54 C54 C54 C54 C54 C54	0.0937 0.1124 0.1158 0.1158 0.074 0.6615 0.0659 0.0559 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0383 0.1096 0.3803 0.1095 0.0887 0.0392 0.03878 0.0392 0.0392 0.0392 0.0395 0.0395 0.0395 0.0386 0.0386 0.0388 0.0395 0.0388 0.0399 0.0388 0.03980 0.03980000000000000000000000000	H87 H88 H89 K89 K90 K95 H91 K93 K94 K93 K94 K93 H94 H93 K94 K74 H75 H76 H77 H77 H78 H77 H79 H81 H82 H83 H84 H83 H84 H87 H88 H86 H87 H88 H88 H87 H88 H87 H82 H83 H84 H83 H84 H85 H85 H86 H87 H73 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H75 H74 H74 H75 H74 H75 H74 H75 H74 H75 H76 H77 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0972 0.1055 0.0972 0.1055 0.0972 0.1055 0.0988 0.0992 0.1055 0.3248 0.3248 0.3248 0.3248 0.3248 0.3248 0.11508 0.1119 0.1125 0.11348 0.1123 0.11223 0.11223 0.11226	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C102 C100 C101 C102 C103 H102 C103 H107 C105 C106 H107 C109 C110 C110 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C99 C99	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1287 0.1550 -0.0937 0.1388 0.06635 -0.1005 0.06435 -0.0929 0.1535 0.1558 0.1558 -0.1067 0.1568 -0.1067 0.1568 -0.1067 0.1568 -0.1665 -0.0652 0.1558 -0.1655 0.1558 -0.1655 0.1558 -0.1655 0.1558 -0.1655 0.1558 -0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.067 0.1558 -0.1657 0.1558 -0.1657 0.1558 -0.0662 0.1558 -0.0642 -0.0704 0.1531 -0.0948 0.0343 -0.0948 0.0343 -0.0948 -0.0948 -0.0343 -0.0345 -0.0348 -0.0348 -0.0348 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C1612 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1463 0.1640 0.1589 0.0704 -0.11589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1348 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1247 0.1650 -0.1211 -0.1477 0.1650 -0.1211 0.0898	H183 H184 H185 H186 H187 H189 H190 H191 Total C169 C170 H171 C175 C177 C178 H182 H182 H183 H184 H185 H180 H181 H182 H183 H184 H185 H189 H190 H181 H182 H183 H184 H185 H189 H190 Total C169 C169 C169 H171	0.1330 0.1730 0.1734 0.1234 0.1234 0.1426 0.1423 0.1423 0.1425 0.1423 0.1426 0.1425 0.1425 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1685 0.1685 0.169 0.1116 0.1672 0.1570 0.1577 0.1572 0.1574 0.1572 0.1574 0.1575
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C7 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H15 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm H22 \\ \rm C3 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C4 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C4 \\ \rm C4 \\ \rm C4 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C4 \\ \rm C4 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ 0.0624\\ 0.00230\\ 0.0623\\ 0.0624\\ 0.00230\\ 0.0623\\ 0.0644\\ 0.00370\\ -0.535\\ 0.0644\\ 0.00370\\ -0.535\\ 0.4466\\ -0.3150\\ 0.04285\\ 0.3466\\ 0.1350\\ 0.1425\\ 0.1481\\ 0.1180\\ 0.1180\\ 0.1149\\ 0.1237\\ 0.1243\\ 0.1423\\ 0.1423\\ 0.1423\\ 0.1423\\ 0.1423\\ 0.1423\\ 0.1423\\ 0.0679\\ -0.3638\\ 1.0003\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ -0.485\\ 0.0579\\ -0.4846\\ -0.485\\ -0.485\\ -0.486\\ -0.485\\ -0.486\\ -0.485\\ -0.486\\ -0.485\\ -0.486\\ -0.486\\ -0.486\\ -0.585\\ -0.586\\ -0.58$	H39 H40 O41 H40 C42 C43 C45 C46 C45 C46 C46 C27 C28 C32 C32 C32 C32 C32 C33 C32 C32 C33 H36 H37 H38 H36 H37 H38 H36 H37 H38 H36 C45 C45 C45 C45 C45 C45 C45 C45 C45 C45	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.2415 -0.2415 0.0748 -0.2415 0.0521 0.0521 0.0524 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.1284 0.1284 0.1287 0.1287 0.1287 0.1287 0.5515 0.0566 -0.5158 0.0566 -0.5233 0.05451 -0.3478	H63 H64 H65 C67 C68 C67 C68 C69 C70 C71 072 C50 C71 C72 C52 C55 C55 C55 C55 C55 C56 C56 C57 C56 H59 H60 H61 H62 H63 H64 H65 C67 C68 B C70 C72 C68 C72 C72 C68 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4863 0.0559 0.0194 -0.4765 -0.1216 -0.0954 -0.1216 -0.0954 -0.0954 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 -0.0847 0.0995 0.0995 0.0992 0.0992 0.0992 0.0992 0.0979 0.0878 0.0988 0.1039 -0.5080 0.0182 0.0765 -0.5080 0.0182 0.0765 -0.5080 0.0182 0.0182 0.0182 0.0182 0.0182 0.0182 0.0182 0.0182 0.0182 0.0286 -0.5080 0.0182 0.0286 -0.5080 0.0192 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 -0.5080 0.0194 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0.0998 0.0991 0.3248 0.0991 0.3248 0.2279 0.0399 0.0850 0.0399 0.0558 0.0774 0.1192 0.1475 -0.0939 0.1475 -0.0328 0.1192 0.1326 0.1318 0.1326 0.1326 0.1326 0.1326 0.1326	C111 H112 C113 H114 C115 C116 H119 C120 C97 H98 C99 C100 C101 H102 C105 C106 H109 C100 C101 H107 C108 H109 C110 C111 H111 C113 H114 C115 C116 H119 C120 C97 H98 C99 C97 H98 C120 C97 H98 C120 C97 H98 C120 C97 H98 C120 C120 C120 C97 H98 C120 C120 C120 C120 C120 C120 C120 C120	-0.1057 0.1057 0.1091 -0.1230 0.3116 -0.1245 0.3116 -0.1237 0.1218 0.1218 0.1237 0.1055 0.1087 0.1388 0.0306 0.0635 -0.1005 0.1388 0.0306 0.0635 -0.1005 0.1441 -0.0929 0.1535 0.0640 0.0640 0.0440 0.0440 0.0467 0.1552 0.1667 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0467 0.1553 0.0569 0.1535	C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 C127 C128 C127 C128 C127 C128 C127 C128 C127 C129 C130 C131 C132 C133 H140 H141 H142 H143 H144 H142 H144	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1606 0.1887 0.1887 0.1887 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.4065 -0.1657 0.0685 -0.4005 -0.11557 0.0555 -0.4102 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1551 0.1554 0.1555 -0.4120 0.1552 -0.4120 0.1551 0.1555 -0.4120 0.1552 -0.4120 0.1551 0.1555 -0.4120 0.1551 0.1555 -0.4120 0.1551 0.1555 -0.4120 0.1552 -0.4120 0.1551 0.1555 -0.4120 0.1552 -0.4120 0.1552 -0.4120 0.1551 0.1555 -0.4120 0.1552 -0.4120 0.1551 0.1555 -0.4120 0.1552 -0.4120 0.1555 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.4120 0.1557 -0.	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$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ c_2 \\ c_3 \\ 04 \\ c_5 \\ c_6 \\ 07 \\ c_6 \\ 07 \\ c_6 \\ 07 \\ c_6 \\ 07 \\ c_8 \\ c_9 \\ c_1 \\ c_1 \\ c_2 \\ c_3 \\ 04 \\ c_6 \\ 07 \\ c_1 \\ c_1 \\ c_2 \\ c_3 \\ 04 \\ H16 \\ H17 \\ H18 \\ H19 \\ H20 \\ H21 \\ H22 \\ H23 \\ H24 \\ C_5 \\ c$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.0230\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.05161\\ 0.0426\\ 0.3362\\ 0.3362\\ 0.3466\\ 0.3107\\ 0.4466\\ 0.3107\\ 0.4466\\ 0.3362\\ 0.3362\\ 0.3362\\ 0.3362\\ 0.1161\\ 0.1145\\ 0.1237\\ 0.14483\\ 0.14483\\ 0.1465\\ 0.1473\\ 1.1483\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0579\\ -0.4846\\ 0.0538\\ -0.0538\\ 0.0538\\ -0$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C47 C48 C27 C28 S29 C30 O31 C42 C32 C32 C33 C32 C32 C33 H36 C42 C43 C44 C45 C42 C44 C45 C42 C44 C45 C42 C45 C47 C48 C48 C47 C48 C47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 0.0748 -0.5161 0.0521 0.0254 -0.5161 0.0254 0.1482 0.1482 0.1487 0.1284 -0.5249 0.1284 -0.5249 0.1284 -0.5247 0.1284 -0.5247 0.1284 -0.5247 0.04297 0.05637 -0.5158 0.05647 0.0564 0.0564 0.05647 -0.5138 0.05647 -0.5138 0.05647 -0.5138 0.05647 -0.5139 0.05647 -0.5139 0.05647 -0.5139 0.05647 -0.5233 0.3478	H63 H64 H65 C67 C68 C67 C70 C71 072 C69 C70 C71 C72 C53 C54 C55 C54 C55 C54 C55 C56 C57 H59 H60 H61 H62 H64 H65 H64 H65 C67 C70 C71 C71 C52 C53 C70 C72 C53 C70 C72 C54 C72 C54 C72 C54 C72 C54 C72 C54 C72 C54 C72 C55 C74 C55 C74 C72 C55 C74 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C72 C55 C74 C55 C77 C75 C74 C55 C77 C75 C56 C77 C75 C74 C56 C77 C75 C74 C56 C57 C77 C56 C77 C77 C77 C56 C77 C77 C56 C77 C77 C77 C77 C77 C77 C77 C77 C77 C7	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0154 -0.4869 0.0559 0.0194 -0.4767 -0.2262 -0.1216 -0.0744 -0.0744 -0.0236 -0.1236 -0.0236 -0.0236 0.0393 0.1045 0.0393 0.1145 0.0392 0.0378 0.0392 0.0378 0.0392 0.0386 -0.5380 -0.5830 -0.5330 -0.5350 -0.5350 -0.535000 -0.535000 -0.535000 -0.53500	H87 H88 H89 CS0 H89 CS0 H91 CS2 CS4 H93 CS4 H93 CS4 H93 CS4 H93 H73 H74 H75 H76 H77 H73 H75 H76 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0992 0.1055 0.0972 0.1055 0.0972 0.1055 0.0988 0.2279 0.2015 0.0988 0.2279 0.2015 0.0988 0.2279 0.2015 0.0988 0.2279 0.2015 0.0988 0.2279 0.2015 0.0988 0.2217 0.1055 0.3248 0.2279 0.2015 0.0988 0.2217 0.1055 0.3248 0.2279 0.2015 0.0988 0.2119 0.2115 0.0988 0.2119 0.2015 0.0988 0.2119 0.2015 0.0988 0.2119 0.2015 0.0988 0.2119 0.2015 0.0988 0.2119 0.2015 0.0988 0.2119 0.2015 0.00592 0.2119 0.219	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 C101 C101 C103 H102 C103 H102 C103 H102 C103 H102 C105 C106 H107 C105 C106 H107 C105 C106 H117 C116 H112 C116 C105 C106 H107 C107 H112 C116 C105 C106 H117 C116 C105 C106 C107 H112 C105 C106 C107 H112 C105 C106 C107 H112 C105 C107 H112 C105 C107 H112 C105 C107 H112 C107 H112 C107 H112 C107 C107 H112 C107 C107 C107 C107 C107 C107 C107 C107	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.1218 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1550 -0.0937 0.1589 0.0306 0.0305 -0.00937 0.1388 0.0305 -0.0057 0.1532 -0.1002 0.1508 -0.1658 0.1568 0.15	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C122 C122 C122 C124 C122 C122	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1865 0.1867 0.1823 -0.1396 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.1037 -0.1507 0.157 0.157 0.157 0.1527 0.1527 0.1527 0.1364 0.1364 0.1364 0.1372 -0.1396 0.1872	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H151 H155 H155 C156 C167 C168 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1463 0.1640 0.1881 -0.1589 0.0704 -0.1188 -0.1138 0.0710 0.1771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1650 -0.1247 0.1650 -0.1247 0.1495 0.1494 0.1494 0.1497 0.1493 0.1494 0.1497 0.1493 0.1288 0.757 -0.1247 0.1493 0.1288 0.757 -0.1247 0.1493 0.1288 0.1212 0.1888 0.1226 0.1226 0.1226 0.1226	H183 H184 H185 H186 H187 H189 H191 Total C169 C170 H171 H172 C173 N174 H175 C176 C177 C178 H180 H182 H182 H184 H185 H180 H181 H182 H184 H185 H180 H181 H182 H183 H184 H185 H189 H190 Total C169 C170 H171 H172 C173	0.1333 0.1700 0.1841 0.1794 0.1426 0.1423 0.1423 0.1423 0.1423 0.1426 0.1423 0.1426 0.1423 0.1426 0.1423 0.1426 0.1423 0.1685 0.1380 0.1116 0.1091 0.1123 0.1679 0.1679 0.1679 0.1679 0.1679 0.1679 0.1570 0.1579 0.15770000000000000000000000000000000000
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H12 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm I \\ \rm I \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm O7 \\ \rm C6 \\ \rm C6 \\ \rm I \\ \rm C \\ \rm C$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1267\\ 0.1227\\ 0.1272\\ 0.1502\\ 0.1501\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0230\\ 0.0370\\ 0.05151\\ 0.0370\\ 0.05151\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0350\\ 0.0353\\ 0.0446\\ 0.1243\\ 0.1243\\ 0.0579\\ 0.1243\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0579\\ 0.0354\\ 0.0538\\ 0.0414\\ 0.0579\\ 0.0354\\ 0.0538\\ 0.0414\\ 0.0579\\ 0.0354\\ 0.0538\\ 0.0414\\ 0.0579\\ 0.0354\\ 0.0538\\ 0.0354\\ 0.0538\\ 0.0414\\ 0.0579\\ 0.0579\\ 0.0354\\ 0.0578\\ 0.057$	H39 H40 O41 C42 C43 C45 C46 C46 C46 C46 C47 C48 C27 C28 C30 C32 C33 C32 C33 C32 C33 C32 C33 C32 C33 C32 C33 C34 H35 H36 H37 C45 C45 C45 C47 C48 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C47 C48 C47 C48 C47 C48 C47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3415 -0.3052 0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.4336 -0.5158 0.0254 -0.5271 0.1284 -0.5271 0.1296 0.1305 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0.1887 0.1887 0.1887 0.1887 0.1887 0.1828 -0.4065 -0.4065 -0.4065 -0.4065 -0.4065 -0.4055 0.0680 -0.1120 -0.4122 0.555 -0.4102 0.555 -0.4102 0.1527 0.1527 0.1527 0.1552 -0.4120 0.1527 0.1555 0.1527 0.1555 0.1527 0.1555 0.1527 0.1555 0.1527 0.1552 0.1557 0.1557 0.1557 0.1557 0.1552 0.1557 0.1551 0.1551 0.1551 0.1557 0.1551 0.1551 0.1557 0.1557 0.1551 0.1557 0.157	N159 C160 C161 H162 H162 C164 C165 C166 C166 H146 H147 H147 H148 H149 H151 H155 C156 C156 C157 C158 N159 C156 C161 H163 C164 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1469 0.1640 0.1891 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.11771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1268 0.1389 0.1655 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1424 0.1427 0.1655 0.1427 0.1650 0.1427 0.1639 0.1477 0.1639 0.1477 0.1477 0.1639 0.1228 0.1228 0.1228 0.1228 0.1228 0.1228 0.1238 0.1228 0.1238 0.1247 0.1247 0.1247 0.1247 0.1248 0.1247 0.1248 0.1	H183 H184 H185 H186 H186 H186 H188 H189 H190 H191 Total 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$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H19 \\ \rm H21 \\ \rm H18 \\ \rm H19 \\ \rm H19 \\ \rm H21 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4992\\ 0.0623\\ -0.4992\\ 0.0370\\ -0.5151\\ 0.0382\\ 0.0446\\ 0.1149\\ 0.1097\\ 0.1149\\ 0.1097\\ 0.1149\\ 0.1097\\ 0.1149\\ 0.1097\\ 0.1144\\ 0.1237\\ 0.1465\\ 0.1149\\ 0.1097\\ 0.1463\\ 0.1443\\ -0.4636\\ 0.0579\\ -0.4638\\ 0.06579\\ -0.4638\\ 0.06579\\ -0.4638\\ 0.0658\\ 0.0638\\ 0.0638\\ 0.0638\\ 0.0638\\ 0.0638\\ 0.0414\\ -0.5150\\ 0.0538\\ 0.0144\\ 0.0579\\ -0.4838\\ 0.0414\\ -0.5150\\ 0.0538\\ 0.0144\\ -0.5150\\ 0.0538\\ 0.0144\\ -0.5150\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.00144\\ -0.5150\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0144\\ -0.5150\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ 0.0579\\ -0.4838\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0578\\ -0.515\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ 0.0014\\ -0.5150\\ 0.0014\\ -0.510$	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C27 C28 S29 C27 C28 S29 C30 O31 H37 H38 H37 H38 H37 H38 H37 C42 C43 C42 C43 C44 C45 C42 C43 C45 C45 C45 C47 C48 C48 C47 C48 C48 C48 C47 C48 C48 C47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.401 0.0748 -0.2415 -0.0748 -0.5161 0.0254 -0.5161 0.0524 -0.5161 0.0524 -0.5161 0.1284 0.1	H63 H64 H64 H65 C67 C70 C69 C70 O72 C71 O72 C50 C71 C72 C53 C54 C55 C54 C55 C54 C55 C54 C55 C70 C71 H61 H62 H63 H64 H65 H66 C67 C70 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0559 0.0194 -0.2767 -0.2262 -0.1216 -0.0954 -0.0744 -0.0847 -0.0954 0.0744 -0.0847 -0.1236 0.0145 0.0145 0.0145 0.0831 -0.1256 0.0145 0.0878 0.0393 0.1145 0.0992 0.0145 0.0992 0.0145 0.0992 0.0388 0.0386 -0.5136 0.0386 -0.5136 0.0386 -0.5136 0.0386 -0.5136 0.0386 -0.5380 -0.5380 -0.5120 -0.1192 -0.0750 -0.	H87 H88 H89 CS0 H89 CS0 H81 H73 H74 H75 H76 H77 H78 H76 H77 H78 H77 H80 H81 H76 H77 H88 H85 H86 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H78 H77 H78 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 0.3033 -0.395 0.3033 -0.1395 0.3074 0.3033 -0.1316 0.0970 0.1316 0.0972 0.1055 0.0972 0.1055 0.0972 0.1045 0.2079 0.2015 0.2019 0.2215 0.2015 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2215 0.2015 0.2215 0.2015 0.3263 -0.1188 0.1314 0.1223 0.1223 0.1326 0.1326 0.1326 0.1326 0.1324	C111 H112 C113 H114 C115 C116 H117 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 H107 C101 H112 C115 C116 H117 C120 C101 H112 C120 C101 H112 C120 C101 H112 C120 C101 H112 C120 C101 H112 C120 C101 C115 H114 C115 C120 C101 H112 C120 C101 C115 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C120 C101 C101	-0.1057 0.1061 -0.1230 0.2125 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0306 0.1532 -0.1002 0.1508 0.1508 -0.1508 0.1555 -0.1665 0.1665 0.1555 -0.0855 0.1665 0.1555 -0.0948 0.1331 0.0345 0.035	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C122 C122 C124 C126 C127 C128 C126 C127 C128 C129 C130 C131 C132 C133 N134 C136 C136 C136 C136 C136 C137 C138 C139 H140 H141 H141 H141 H142 H143 H144 H142 H143 H144 H142 H143 H144 H144	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1505 0.1543 0.1563 0.1865 0.1867 0.1823 -0.1396 0.1037 -0.1447 0.1037 -0.1447 0.1508 0.0680 -0.1037 -0.1447 0.1509 -0.1292 -0.1157 0.0655 -0.4102 0.1527 0.1527 0.1527 0.1657 0.1905 0.1667 0.1905	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H151 H155 C156 C167 C158 C157 C158 N159 C160 C161 H162 H163 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 -0.1467 0.1547 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1183 0.0710 0.1771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1655 -0.1247 0.1650 -0.4120 0.1494 -0.1495 0.1494 0.1495 0.1495 0.1495 0.1288 0.0268 0.1226 0.1226 0.1226 0.1237 0.1280 0.1226 0.1237 0.1280 0.1226 0.1237 0.1285 0.1285 0.1285 0.1285 0.1285 0.12880 0.1226 0.1226 0.1285 0.128	H183 H184 H186 H186 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 H181 H182 H184 H185 H186 H187 H188 H189 H190 Total	0.1333 0.1700 0.1841 0.1794 0.1426 0.1423 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1483 0.1485 0.1485 0.1485 0.1485 0.1485 0.1412 0.1412 0.1412 0.1412 0.1412 0.1412 0.1427 0.1477 0.1427 0.1477 0.1427 0.1427 0.1477 0.1427 0.1477 0.1427 0.1477 0.1427 0.1477 0.1427 0.1477 0.1427 0.1477 0.
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H21 \\ \rm H22 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H23 \\ \rm H21 \\ \rm H23 \\ \rm H23 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C7 \\ \rm C8 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C1 \\ \rm$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1267\\ 0.1272\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ -0.4923\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0382\\ 0.0448\\ 0.037\\ 0.1243\\ 0.1097\\ 0.1243\\ 0.1097\\ 0.1243\\ 0.1455\\ 0.1443\\ 0.1483\\ 0.1483\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0538\\ 0.0414\\ -0.5150\\ 0.0414\\ -0.5150\\ 0.0830\\ $	H39 H40 041 C42 C43 044 C45 C46 C25 S26 C27 C28 S29 C30 031 H35 H36 H37 H38 H39 H40 041 C45 C46 C45 C46 C47 C48 C25 S26 C43 C44 C45 C46 C47 C48 C27 C28 S29 C32 C32	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.4451 -0.4336 -0.4419 -0.4336 -0.4419 -0.4336 -0.4419 0.0748 -0.5161 0.0254 -0.524 -0.5161 0.0254 -0.5271 0.1284 0.1286 0.1285 0.1285 0.1285 0.1285 0.0564 -0.5271 0.0565 -0.5271 0.05657 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.05567 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0557 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5271 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 -0.5275 0.0577 0.0577 0.0577 0.0577 0.0577 0.0577 0.05777 0.05777 0.05777 0.05777 0.057777 0.057777777777	H63 H64 H64 H65 C67 C68 G69 C70 C71 072 C69 C71 072 C53 C54 C55 C54 C55 C56 C57 H58 H60 H61 H62 H63 H64 H65 C67 C71 C72 C53 C72 C54 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 0.1158 0.0074 0.0615 0.0659 0.0559 0.0559 0.0559 0.0559 0.0559 0.0559 0.0784 0.0784 0.0784 0.0784 0.0784 0.0784 0.0393 0.1145 0.0393 0.1996 0.0393 0.1145 0.0992 0.0878 0.0393 0.1145 0.0992 0.0783 0.0992 0.0785 0.0386 0.0393 0.0992 0.0785 0.0386 0.0386 0.0395 0.0395 0.0395 0.0395 0.0395 0.0395 0.0395 0.0386 0.0386 0.0395 0.0395 0.0395 0.0386 0.0386 0.0386 0.0386 0.0386 0.0395 0.0386 0.0395 0.0386 0.0395 0.0386 0.0392 0.0392 0.0392 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0393 0.0395 0.0386 0.	H87 H88 H89 H89 H89 H89 H89 H81 H81 H73 H74 H75 H76 H77 H80 H81 H81 H83 H84 H87 H88 H87 H88 H88 H87 H88 H88 H87 H88 H88	0.1083 0.1394 0.1627 -0.1141 0.1261 0.3033 -0.1395 0.3033 -0.1395 0.3033 -0.1316 0.1316 0.9844 0.9972 0.1055 0.1316 0.9924 0.0972 0.1065 0.9939 0.3248 0.2279 0.1065 0.3248 0.3248 0.3248 0.3248 0.3248 0.1508 0.1508 0.1508 0.1508 0.1508 0.1508 0.1508 0.1508 0.1508 0.1192 0.1192 0.1324 0.1326 0.1324 0.1326 0.1324 0.1326 0.1324 0.1326 0.136	C111 H112 C113 H114 C115 C116 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 C106 C106 C106 C106 C106 C106 C107 H109 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C101 H102 C100 C100 C101 H102 C100 C100 C100 C100 C100 C100 C100 C	-0.1057 -0.1057 0.1091 -0.1230 0.3116 -0.1237 0.1218 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1388 -0.0937 -0.1388 0.0365 -0.1005 0.1434 -0.0929 0.1535 -0.1007 0.1506 -0.0667 0.1505 0.0640 -0.0667 0.1505 0.0667 0.1505 0.0667 0.1505 0.1555 -0.0948 0.1331 0.0342 -0.0992 0.1331 0.0342 -0.0992 0.1331 0.0342 -0.0342 -0.0948 0.1321 -0.0992 0.1336 0.1321 -0.0992 0.1336 0.1321 -0.0992 0.1326 -0.1331 -0.0342 -0.0342 -0.0342 -0.0345	C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C124 N134 C133 N134 C133 C136 C137 C138 C136 C137 C138 C139 H140 H141 H142 H141 H142 H142 H141 C121 C122 C123 C124 H144 H144 H144 H144 H144 H144 H144 H	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1636 0.1887 0.1887 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1447 0.1508 -0.4065 -0.4065 -0.4065 -0.1655 0.0988 -0.1657 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1551 -0.1394 0.1384 0.1384 0.1384 0.1395 0.1872	N159 C160 C161 H162 H162 C164 C165 C166 C167 C168 H146 H147 H148 H149 H151 H155 C156 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1469 0.1640 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1348 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1494 0.1655 0.1497 0.1655 0.1497 0.1655 0.1497 0.1655 0.1211 -0.1635 0.1221 0.0898	H183 H184 H185 H186 H186 H186 H187 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178 H180 H180 H182 H183 H184 H185 H182 H183 H184 H185 H185 H189 H190 Total	-0.1930 0.1700 0.1841 0.1794 0.1426 0.1423 0.1812 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1500 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1679 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579 0.1579 0.1427 0.1625 0.125 0.125 0.125 0.125 0.127 0.1625 0.127 0.127 0.127 0.1675 0.167
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C6 \\ \rm O7 \\ \rm S11 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H14 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C9 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H10 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H22 \\ \rm H23 \\ \rm C3 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C9 \\ \rm H10 \\ \rm $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1501\\ 0.0623\\ -0.4932\\ 0.0623\\ -0.4932\\ 0.0623\\ -0.4923\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0283\\ 0.4466\\ -0.3352\\ 0.4466\\ -0.3352\\ 0.4466\\ 0.0323\\ 0.4466\\ 0.3362\\ 0.1180\\ 0.1142\\ 0.1243\\ 0.1423\\ 0.1445\\ 0.1144\\ 0.1237\\ 0.1104\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.1237\\ 0.1144\\ 0.5579\\ -0.4636\\ 0.0638\\ 0.0614\\ 44.83\\ A\\ -0.4636\\ 0.0579\\ -0.4636\\ 0.0538\\ 0.0588\\ 0.0588\\ 0.0588\\ 0.0588\\ 0.0588\\ 0.0588\\ 0.0588\\ 0.05$	H39 H40 041 C42 C45 C46 C47 C48 C27 C28 C27 C28 C30 D31 C32 C33 H36 H37 H38 H39 H40 C41 C42 C43 C44 C45 C46 C47 C48 C41 C42 C43 C44 C45 C46 C47 C48 S29 C30 C31 C32 C33	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.2415 -0.1401 0.0748 -0.5161 0.0254 -0.505 0.1482 0.1284 0.1285 0.1284 0.1285	H63 H64 H65 C67 C68 C67 C70 C71 072 C69 C70 C71 072 C50 C51 C52 C54 C55 C56 C57 C70 C74 H59 H60 H61 H62 H63 H64 H64 H65 H60 C67 C70 C70 C70 C72 C55 C70 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0559 0.0559 0.0194 -0.0767 -0.2062 -0.1216 -0.0764 -0.0744 -0.0831 -0.0744 -0.0831 -0.1755 0.3903 0.1145 0.0939 0.1145 0.0939 0.01123 0.0939 0.01123 0.0939 0.01123 0.0939 0.01123 0.0326 0.0388 0.01122 0.0760 -0.5380 -0.5380 -0.5380 -0.0386 -0.0386 -0.0386 -0.0386 -0.0386 -0.0385 -0.	H87 H88 H89 K30 K30 H73 H74 H75 H36 H77 H78 H77 H78 H80 H81 H85 H86 H77 H78 H87 H88 H85 H86 H87 H88 H87 H88 H87 H87 H87 H87 H87 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0972 0.1055 0.0972 0.1055 0.0972 0.2015 0.2279 0.2015 0.2215 0.2015 0.3248 0.2215 0.2015 0.3248 0.2015 0.0754 0.1199 0.1475 -0.0934 0.1199 0.1475 0.1348 0.1314 0.1314	C111 H112 C113 H114 C115 C116 H117 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C106 H107 C106 H107 C106 H107 C101 H112 C116 H117 C116 H117 C116 H117 C116 H117 C126 C106 H107 C106 C106 C101 C101 H107 C106 C106 C101 C101 H107 C106 C106 C106 C101 H107 C106 C106 C101 C107 H107 C106 C106 C106 C101 H117 C106 C106 C106 C101 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 H117 C116 C116 H117 C116 C116 C116 H117 C116 C116 C116 C116 C116 C116 C116 C	-0.1057 0.1061 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.3066 0.0937 0.1388 0.3066 0.0937 0.1388 0.3066 0.0937 0.1580 0.3066 0.0929 0.1441 -0.0929 0.1555 -0.1065 -0.0654 -0.1075 0.1665 -0.1653 0.1508 0.1508 -0.1508 0.1508 0.1508 -0.1508 0.1538 0.1548 0.	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C133 C134 C135 C136 C137 C138 C139 H140 H141 H141 H141 H142 H143 H144 H143 H144 H143 H144 H144 H143 H144 H143 H144 H143 H144 H144	0.1597 -0.1394 0.0777 -0.1475 0.1513 0.1805 0.1523 0.1543 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1823 0.1037 -0.1425 0.1037 -0.1405 0.1528 -0.1998 0.0938 -0.10938 -0.1527 0.1559 0.1657 0.0465 0.1559 0.1657 0.0465 0.1559	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H145 H146 H147 H148 H149 H150 H151 H152 H153 H155 C156 C157 C168 C157 C168 C167 C166 C167 C168 H145 H146 H147 H162 H163 C164 C167 C168 H145 H146 H145 H146 H145 H145 H145 H145 H146 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1469 0.1640 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1193 0.0701 0.1771 0.1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1655 0.1839 0.1650 -0.1247 0.1650 -0.1247 0.1650 -0.1247 0.1650 -0.1247 0.1650 0.1247 0.1495 0.1495 0.1249 0.12410 0.12410 0.12410000000000000000000000000000000000	H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C176 C177 C176 C177 H183 H184 H183 H184 H185 H186 H187 H188 H189 H180 H190 H191 Total C169 C170 H171 Total C169 C170 H171 C175 C176 C177	0.1300 0.1700 0.1841 0.1704 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1380 0.1380 0.1380 0.1380 0.1380 0.1380 0.1380 0.1123 0.1123 0.1123 0.1123 0.1672 0.1672 0.1673 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1805 0.1874 0.1875 0.1874 0.1875 0.1874 0.1875 0.1875 0.1874 0.1875 0.1874 0.1875 0.1874 0.1875 0.1874 0.1875 0.
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm 04 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm C12 \\ \rm C3 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C11 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H20 \\ \rm H21 \\ \rm H20 \\ \rm H10 \\ \rm H10 \\ \rm H10 \\ \rm H20 \\ $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1261\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.0230\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0633\\ 0.0446\\ 0.370\\ 0.0370\\ 0.1350\\ 0.4465\\ 0.3362\\ 0.362\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1180\\ 0.1183\\ 0.0448\\ 0.0179\\ 0.1237\\ 0.1243\\ 0.0174\\ 0.1638\\ 0.0124\\ 0.0653\\ 0.0638\\ 0.0124\\ 0.0538\\ 0.0124\\ 0.0538\\ 0.0124\\ 0.0538\\ 0.0124\\ 0.0538\\ 0.0124\\ 0.0538\\ 0.0633\\ 0$	H39 H40 O41 C42 C43 O44 C45 C46 C47 C48 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H39 H39 H39 H39 H39 H39 H39 H39 H30 O41 C45 C46 C47 C38 S26 C37 C38 C32 C33 C34	0.1253 0.1227 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 -0.2415 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.5271 0.0499 0.0587 -0.5128 0.0544 0.0542 0.0547 -0.5233 0.3478	H63 H64 H64 H65 C67 C70 C69 C70 C71 072 C50 C71 072 C51 C52 C53 C54 C55 C56 C57 H58 H66 H61 H62 H66 C67 C70 C72 C72 C54 C55 C70 C72 C54 C71 C64 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 0.1158 0.074 0.6615 0.0659 0.0559 0.0159 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0194 0.0383 0.1096 0.3833 0.1096 0.3833 0.1096 0.3833 0.1096 0.3836 0.0887 0.0992 0.0878 0.0992 0.0878 0.0992 0.01122 0.0878 0.0396 0.0182 0.0395 0.0386 0.0396 0.0386 0.0396 0.0386 0.0396 0.0386 0.0396 0.0386 0.0386 0.0396 0.0386 0.	H87 H88 H89 H89 H89 H89 H89 C30 H91 H73 H74 H75 H76 H77 H78 H76 H77 H78 H81 H81 H81 H81 H82 H85 H86 H87 H88 H89 H81 H82 H83 H84 H87 H83 H84 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H88 H87 H87	0.1083 0.1394 0.1627 -0.1141 0.1261 0.3033 -0.1395 0.3033 -0.1395 0.3033 -0.1316 0.9984 0.9984 0.9984 0.9984 0.3248 0.1150 0.3248 0.3248 0.3248 0.3248 0.3248 0.1508 0.1508 0.1508 0.1508 0.1141 0.1326 0.1348 0.1326 0.1334 0.1336 0.1334	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C103 H104 C105 C106 C101 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C101 C101 C115 C116 H117 C118 H119 C120 C101 C117 C118 H119 C120 C101 C101 C101 H112 C101 C101 C101 C101 C101 C101 C101 C	-0.1057 0.1061 -0.1230 0.205 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1550 -0.0937 0.1388 0.0365 -0.1005 0.6635 -0.1005 0.1541 -0.0929 0.1535 -0.1058 -0.1558 -0.0962 0.1558 -0.1558 -0.0962 0.1558 -0.0948 0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0932 -0.1321 -0.0058 -0.0064 -0.1321 -0.0058 -0.0064 -0.1321 -0.0058 -0.0064 -0.0058 -0.0	C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C124 N125 C126 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H144 H144 C121 C122 C123 C124 C126 C127 C128 C129 C120 C120 C120 C121 C122 C123 C124 C121 C122 C123 C124 C121 C122 C123 C124 C121 C122 C123 C124 C121 C122 C123 C124 C129 C130 C120 C120 C120 C120 C120 C120 C120 C12	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1635 0.1636 0.1857 0.1637 -0.1396 -0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.1055 0.0680 -0.1255 0.0680 -0.1555 -0.1655 -0.1657 0.1527 0.1527 0.1567 0.1394 -0.1394 0.1384 0.1384 0.1384 0.1384 0.1384 0.1384 0.1384 0.1384 0.1384 0.1395 0.1384 0.1395 0.1397 0.15777 0.157777 0.15777777777777777777777777777777777777	N159 C160 C161 H162 C161 C164 C165 C166 C167 C168 H145 H146 H147 H155 C156 C157 C158 N159 C160 C161 C165 C157 C158 N155 C156 C166 C167 C168 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1463 0.1640 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1183 -0.1193 0.0710 0.1193 0.0710 0.1288 0.1288 0.1288 0.1288 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1490 0.1655 0.1211 0.0898 0.1221 0.0898	H183 H184 H185 H186 H186 H186 H186 H187 H188 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C177 C178 C177 C178 H180 H181 H182 H183 H184 H185 H187 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C173 N174 C175 C176 C176 C177 C178	-0.1930 0.1730 0.1734 0.1426 0.1734 0.1426 0.1423 0.1426 0.1423 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1685 0.1685 0.1685 0.1685 0.1691 0.1116 -0.1672 -0.1672 0.1574 0.1672 0.1574 0.1579 0.1574 0.1672 0.1574 0.1579 0.1574 0.1257 0.1254 0.1257 0.1257 0.1257 0.1257 0.1257 0.1257 0.1257 0.1257 0.1277 0.1
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm H16 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H14 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H21 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm Z = - \\ \rm 01 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C0 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C9 \\ \rm C10 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C9 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C9 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1226\\ 0.1220\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0643\\ 0.0623\\ 0.0653\\ 0.0653\\ 0.0653\\ 0.4285\\ 0.3502\\ 0.1160\\ 0.1140\\ 0.1237\\ 0.1149\\ 0.1037\\ 0.1104\\ 0.1237\\ 0.1149\\ 0.1037\\ 0.1104\\ 0.1233\\ 0.1465\\ 0.1149\\ 0.1037\\ 0.1104\\ 0.1233\\ 0.1465\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0638\\ 0.0124\\ 0.0679\\ -0.483\\ A\\ 0.0614\\ 0.0538\\ 0.0124\\ 0.0038\\ 0.0$	H39 H40 O41 C42 C43 C45 C45 C45 C45 C46 C47 C48 C47 C48 C47 C48 C32 C32 C32 C32 C33 C32 C32 C33 C34 H35 C46 C47 C42 C42 C42 C43 C42 C43 C42 C43 C43 C44 C43 C44 C43 C44 C43 C44 C44	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3052 0.4336 -0.2415 -0.3401 0.0748 -0.2415 0.0748 -0.5161 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5065 0.1482 0.1284 0.0565 0.0567 0.0567 0.0567 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-0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0055 -0.0057 -0	H87 H88 H89 H89 H89 CS0 H89 CS0 H91 CS2 H93 CS5 H96 H73 H74 H77 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1627 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1316 0.0974 0.0972 0.1055 0.0972 0.1055 0.0972 0.1055 0.0994 0.0972 0.1055 0.0972 0.1055 0.0994 0.0992 0.0988 0.0991 0.3248 0.0991 0.3248 0.0993 0.055 0.0774 0.1305 0.1508 0.0754 0.1192 0.1475 -0.0938 0.1316 0.1192 0.1326 0.0972 0.1326 0.0972 0.1326 0.0972 0.1326 0.0972 0.1326 0.0972 0.1326 0.0972 0.0072 0.0072 0.00754 0.1326 0.1326 0.1326 0.00754 0.1326 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.1025 0.0055 0.0055 0.0055 0.0055 0.0055 0.0055 0.00	Cill Hil2 Cil3 Hil4 Cil5 Cil6 Cil6 Cil7 Hil7 Cil8 Hil7 Cil2 Ci00 Ci01 Hi02 Ci00 Ci01 Hi02 Ci03 Hi04 Ci05 Ci06 Hi07 Ci06 Hi07 Cil18 Hi19 Ci20 Ci01 Hi02 Ci03 Hi04 Ci05 Ci06 Hi07 Ci118 Hi19 Ci20 Ci01 Ci05 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C129 C130 C131 C137 C138 C139 C130 C131 C137 C138 C139 C130 C137 C138 C139 C130 C131 C137 C138 C139 C130 C130 C131 C137 C128 C129 C130 C131 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C139 C130 C137 C138 C137 C137 C137 C137 C137 C137 C137 C137	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1606 0.1887 0.1887 0.1887 0.1887 0.1887 0.1887 0.1887 0.1887 0.1887 0.1508 -0.4065 -0.1997 0.0680 -0.1229 -0.1157 0.0555 -0.402 0.555 -0.402 0.555 -0.4120 0.1557 0.0558 0.0420 0.1557 0.0427 0.1557 0.0420 0.1559 0.0411 0.04	N159 C160 C161 H162 C164 C165 C166 C167 C168 H145 H146 H147 H148 H149 H150 H151 H155 C156 C157 C158 C157 C158 C156 C157 C158 C157 C158 H162 H162 H162 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1469 0.1540 0.1589 0.7640 0.771 0.1589 0.7704 -0.1133 0.7710 -0.1133 0.7710 -1400 0.1386 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1655 0.1650 -0.4127 0.4149 0.0777 0.1455 0.0757 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H183 H184 H185 H186 H187 H188 H189 H190 H191 Total C169 C170 H171 H172 C175 C176 C177 C178 H183 H184 H185 H186 H187 H188 H189 H180 H181 H182 H184 H185 H186 H187 H188 H189 H180 H181 Total Total C169 C170 H171 H172 C173 N174 C175 C176 C177 C178	0.1330 0.1700 0.1841 0.1794 0.1426 0.1841 0.1794 0.1426 0.1812 0.1812 0.1830 0.1425 0.1805 0.1085 0.1085 0.1085 0.1081 0.1116 0.1123 0.1116 0.1123 0.1116 0.1672 0.1672 0.1573 0.1579 0.1804 0.1579 0.1805 0.1579 0.1829 0.1792 0.1529 0.1792 0.1579 0.1827 0.1257 0.127 0.127 0.127 0.127 0.1573 0.127 0.1573 0.127 0.1573 0.127 0.1573 0.127 0.1573 0.127 0.1574 0.1575 0.127 0.1575 0.127 0.1575 0.127 0.1575 0.1129 0.1575 0.1129 0.1575 0.1129 0.1575 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575 0.1125 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575 0.1127 0.1575
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline c_2 \\ c_3 \\ \rm 04 \\ c_5 \\ c_6 \\ 07 \\ c_6 \\ 07 \\ c_6 \\ 07 \\ c_8 \\ c_9 \\ c_1 \\ c_1 \\ c_2 \\ c_3 \\ 04 \\ c_5 \\ c_6 \\ c_7 \\ c_8 \\ c_9 \\ c_1 \\ c_1 \\ c_2 \\ c_3 \\ 04 \\ c_5 \\ c_6 \\ c_1 \\ c_1 \\ c_2 \\ c_3 \\ c_6 \\ c_7 \\$	0.1279 0.1276 0.1276 0.1205 0.1210 0.1160 0.1160 0.1167 0.1227 0.1502 0.0623 0.0623 0.0623 0.0623 0.0624 0.0623 0.0624 0.0623 0.0624 0.0623 0.0624 0.0623 0.0624 0.0623 0.0624 0.0370 0.0625 0.	H39 H40 O41 C42 C43 C45 C46 C45 C46 C47 C48 C27 C28 S29 C30 O31 C32 C33 C32 C33 C32 C33 C34 H35 H36 C42 C44 C45 C44 C45 C44 C45 C44 C45 C44 C45 C45	0.1253 0.1227 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 -0.2415 0.0748 -0.5161 0.0521 0.0254 -0.5161 0.0254 -0.5161 0.1284 -0.5161 0.1284 -0.5247 0.1284 -0.5233 0.3478 -0.5427 0.05637 -0.5128 0.0564 0.0566 0.0	H63 H64 H64 H65 C67 C70 C69 C70 C71 C72 C71 C72 C71 C72 C53 C54 C55 C56 C57 C76 H59 H60 C77 H59 H60 C77 C71 C72 C74 C55 C74 C55 C75 C74 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 0.1158 0.074 0.6615 0.0675 0.0559 0.0159 0.0154 0.0164 0.0744 0.0744 0.0744 0.0744 0.0744 0.0744 0.0744 0.0745 0.1245 0.0831 0.1145 0.0831 0.1145 0.0833 0.1096 0.1145 0.0831 0.0878 0.0833 0.1096 0.1145 0.0878 0.0835 0.0878 0.0878 0.0878 0.0878 0.0878 0.0878 0.0888 0.0392 0.0878 0.0888 0.0393 0.0925 0.0386 0.0	H87 H88 H89 CS0 H89 CS0 H91 CS2 CS4 H93 CS4 H93 CS4 H93 CS4 H73 H74 H75 H76 H77 H78 H83 H84 H83 H84 H85 H85 H86 H87 H83 H88 H88 H88 H87 H73 H74 H75 H76 H77 H77 H77 H79 H80 H81 H77 H79 H81 H75 H76 H77 H77 H77 H79 H81 H81 H82 H77 H77 H79 H81 H82 H77 H77 H79 H81 H81 H82 H77 H77 H77 H77 H77 H79 H81 H81 H81 H73 H74 H75 H75 H76 H77 H77 H77 H77 H77 H77 H77 H77 H77	0.1083 0.1394 0.1627 -0.1141 0.1261 -0.1430 0.0746 0.3033 -0.1395 0.0770 0.1302 0.1316 0.0972 0.1055 0.0972 0.1055 0.0972 0.1055 0.0988 0.0992 0.1045 0.0998 0.3248 0.2279 0.3248 0.3248 0.3248 0.3248 0.3248 0.3248 0.3248 0.1119 0.1407 -0.1332 0.1348 0.1123 0.1348 0.1223 0.1326 0.1314	C111 H112 C113 H114 C115 C116 H119 C120 C97 H98 C99 C100 C101 C101 C102 C103 H104 C105 C106 H107 C108 H117 C116 H117 C116 H117 C116 H117 C120 C101 H112 C120 C101 H112 C120 C101 H114 C120 C101 H112 C120 C101 H112 C120 C101 C101 C101 C101 C101 C101 C	-0.1057 0.1061 -0.1230 0.1205 0.3116 -0.1237 0.1218 -0.1055 0.1087 0.1590 -0.0937 0.1388 0.0305 -0.1005 0.0635 -0.1005 0.1388 0.0305 -0.1005 0.1388 0.0355 -0.1005 0.1532 -0.1002 0.1532 -0.1007 0.1508 -0.1655 0.1665 -0.0652 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1665 0.1532 -0.1007 0.1532 -0.1007 0.1532 -0.1007 0.1568 0.1552 -0.0067 0.1568 0.1552 -0.0067 0.1568 0.1552 -0.0067 0.1568 0.1555 0.1665 0.1665 0.1535 -0.1655 0.1535 -0.1067 0.1535 -0.1067 0.1535 -0.1067 0.1535 -0.1067 0.1535 -0.1067 0.1535 -0.1065 0.1535 -0.1067 0.1535 -0.1067 0.1535 -0.0048 0.1313 -0.00948 0.1313 -0.00948 0.1331 -0.0999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.00999 0.1383 -0.009999 0.1383 -0.00999 -0.0099 -0.0	C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 C121 C122 C122 C122 C124 N125 C126 C127 C128 C129 C130 C131 C132 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H144 H144 H143 H144 H144 H143 H144 H144	0.1597 -0.1349 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1865 0.1857 0.1825 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.1595 0.0680 -0.1595 0.0680 -0.1229 -0.157 0.0555 -0.4022 0.1555 -0.4102 0.1555 -0.4102 0.1527 0.1527 0.1527 0.1364 0.1364 0.1364 0.1364 0.1364 0.1657 0.1319 0.1651 0.1005 0.1651 0.10151 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1651 0.1027 0.1027 0.1017 0.1027 0.1017 0.1027 0.10	N159 C160 C161 H162 C165 C166 C167 C168 H145 H146 H147 H148 H149 H155 C156 C167 C168 C167 C168 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 0.1640 0.1589 0.0704 -0.11589 0.0704 -0.11589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1348 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1650 -0.1247 0.1650 -0.1211 0.6650 -0.1211 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-0.1672 -0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1672 0.1570 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1805 0.1577 0.1804 0.1577 0.1804 0.1577 0.1804 0.1577 0.1805 0.1877 0.1877 0.1875 0.1877 0.1875 0.1877 0.1875 0.1855 0.18
$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm Z = - \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C6 \\ \rm C7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C3 \\ \rm C1 \\ $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1226\\ 0.1226\\ 0.1220\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ -0.4992\\ 0.0220\\ 0.0623\\ 0.0644\\ 0.0623\\ 0.0644\\ 0.0623\\ 0.0644\\ 0.0633\\ 0.4466\\ -0.1350\\ 0.1446\\ 0.1149\\ 0.1243\\ 0.1445\\ 0.1149\\ 0.1243\\ 0.1445\\ 0.1149\\ 0.1243\\ 0.1445\\ 0.1149\\ 0.1243\\ 0.1445\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0638\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0638\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0638\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0638\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0538\\ 0.0124\\ 0.0679\\ -0.4846\\ 0.0538\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0538\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0538\\ 0.0124\\ 0.0579\\ -0.4846\\ 0.0538\\ 0.0124\\ 0.0579\\ -0.3255\\ 0.0417\\ 0.0259\\ -0.3255\\ 0.4373\\ -0.2964\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0417\\ 0.0256\\ 0.0356\\ 0.0358\\ 0.0258\\ 0.0358\\ 0.0226\\ 0.0328\\ 0.0226\\ 0.0328\\ 0.0226\\ 0.0328\\ 0.0028\\$	H39 H40 041 C42 C43 C44 C45 C46 C47 C48 C27 C30 C31 C32 C33 C44 C45 C30 C31 C32 C33 C46 C47 C48 C41 C42 C43 C44 C45 C46 C47 C28 S29 C30 C31 C25 S26 C37 C38 S29 C30 C31 C32 C33 C34 C35 C36 C37 C38 C39 C31	0.1253 0.1237 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5189 0.3783 -0.3052 0.4336 -0.2415 -0.3401 0.0748 -0.2415 0.0748 -0.5161 0.0748 -0.5161 0.0551 0.1254 -0.505 0.1452 0.1254 -0.5158 0.0566 -0.5233 0.0566 -0.5233 0.05451 -0.3478 -0.3478 -0.3478 -0.3556 0.4251 -0.3478 -0.5555 0.0356 -0.5158 0.0557 -0.5158 0.0556 -0.5158 0.0556 -0.5158 0.0556 -0.5158 0.0556 -0.5158 0.0556 -0.5158 0.0556 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0576 -0.5158 0.0556	H63 H64 H65 C67 C68 C67 C71 072 C50 C71 072 C50 C51 C52 C53 C54 C55 C56 C57 C70 H58 H69 H61 H65 C67 C70 C71 C72 C68 H59 H60 C70 C71 C68 H59 H61 H51 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0194 -0.4767 -0.2052 -0.2052 -0.21216 -0.0984 -0.4767 -0.236 -0.0984 -0.0744 -0.0847 -0.0847 -0.0847 -0.1236 0.0395 0.3903 0.1145 0.3903 0.1996 0.3936 0.0396 0.0182 0.0755 -0.5080 0.0182 0.0182 0.0182 0.0182 0.0182 0.0182 0.0386 -0.5380 -0.53	H87 H88 H89 H89 H89 H89 H81 H81 H81 H74 H75 H76 H77 H76 H77 H78 H77 H81 H81 H81 H84 H85 H87 H91 H82 H83 H74 H75 H96 H87 H77 H78 H81 H74 H76 H77 H77 H81 H81 H74 H76 H77 H77 H81 H81 H81 H76 H77 H77 H81 H81 H81 H76 H77 H77 H81 H81 H81 H76 H77 H77 H81 H81 H81 H76 H77 H77 H81 H81 H81 H77 H77 H78 H81 H81 H77 H77 H77 H77 H77 H77 H77 H77 H77 H7	0.1083 0.1394 0.1627 -0.1141 0.1627 -0.1430 0.3033 -0.1395 0.3033 -0.1395 0.3037 0.1316 0.9944 0.9944 0.9972 0.1055 0.1316 0.9982 0.0972 0.1065 0.1065 0.1065 0.0991 0.3248 0.0991 0.3248 0.2279 0.1065 0.3248 0.2279 0.1065 0.3248 0.3248 0.3248 0.3248 0.3243 0.1192 0.1192 0.1475 0.1326 0.1314 0.1326 0.1314	C111 H112 C113 H114 C115 C116 C116 C116 H17 C118 H17 C120 C297 H98 C99 C100 C100 C101 H102 C105 C106 H102 C105 C106 H109 C110 C111 H112 C113 H104 C105 C106 H109 C110 C111 H112 C118 H109 C110 C111 H112 C128 H109 C100 C111 H112 C128 H109 C100 C111 H112 C128 H109 C100 C111 H112 C128 H104 C126 H107 C128 H104 C126 H107 C128 H104 C126 H107 C128 H107 C128 H104 C126 H107 C128 H107 H107 C128 H107 C128 H107 H107 C128 H107 H107 C128 H107 H107 H107 H107 H107 H107 H107 H107	-0.1057 0.1061 -0.1230 0.3116 -0.1237 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1055 0.1067 0.0937 0.1550 -0.0065 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0306 0.0421 -0.0929 0.1553 0.1441 -0.0929 0.1553 0.1568 -0.1056 0.1552 -0.1056 0.1552 -0.1055 0.1552 -0.00647 -0.0852 0.1555 0.1558 -0.1075 0.1558 -0.1075 0.1558 -0.1075 0.1558 -0.00852 0.1558 -0.00852 0.1533 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.0345 0.1333 0.0345 0.0566 0.1331 -0.0992 0.1356 0.1333 -0.1035 0.1558 -0.1035 0.1333 0.0546 -0.0992 0.1333 -0.1035 0.1333 -0.1035 0.1331 -0.0346 0.0546 -0.0992 0.1333 -0.1035 0.1331 -0.0346 0.0546 -0.0992 0.1333 -0.1035 0.1331 -0.0350 0.1331 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$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \hline \\ \rm C2 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H16 \\ \rm H17 \\ \rm H22 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H16 \\ \rm H17 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm C5 \\ \rm C6 \\ \rm O7 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm O4 \\ \rm C5 \\ \rm C6 \\ \rm C9 \\ \rm C10 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C1 \\ \rm C1 \\ \rm C1 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm C7 \\ \rm C1 \\ \rm $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1501\\ 0.1267\\ 0.1502\\ 0.0230\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0370\\ 0.0382\\ 0.0373\\ 0.0443\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.4636\\ 0.0124\\ 0.0579\\ -0.3636\\ 0.0124\\ 0.0573\\ -0.3636\\ 0.0124\\ 0.0533\\ -0.3204\\ 0.0333\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.4333\\ -0.2954\\ 0.4373\\ -0.2954\\ 0.3243\\ 0.0343\\ 0.0343\\ -0.2455\\ 0.3443\\ 0.0343\\ -0.2455\\ 0.3443\\ 0.0343\\ -0.2454\\ 0.0343\\ -0.2455\\ 0.3443\\ 0.0343\\ -0.2454\\ 0.0343\\ -0.2455\\ 0.3443\\ -0.1349\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1342\\ -0.1320\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.245\\ -0.343\\ -0.344\\ -0.575\\ -0.343\\ -0.245\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.345\\ -0.34$	H39 H40 O41 H40 C42 C43 C45 C46 C46 C46 C47 C48 C47 C48 C47 C48 C27 C30 C37 C32 C33 C32 C33 C32 C33 C32 C33 C34 H35 H36 O41 C42 C45 C45 C45 C47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	0.1253 0.1237 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.4301 0.0543 -0.4419 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 0.1286 0.1286 0.1286 0.1286 0.1286 0.1286 0.1286 0.1286 0.1287 -0.5188 0.0566 -0.5271 0.05487 -0.5188 0.0566 -0.5271 0.05487 -0.5188 0.0566 -0.2390 0.0567 -0.2390 -0.5188 0.0566 -0.2390 -0.5188 0.0566 -0.2390 -0.5188 0.0566 -0.2390 -0.5188 0.0566 -0.1349 0.0571 0.0561 0.0571 0.0561 0.0356 -0.1349 0.0571 0.0551 0.0356 -0.1349 0.0515 0.0555 0.0356 -0.1349 0.1215 0.0555 0.0356 -0.1349 0.0551 0.0555 0.0356 -0.1349 0.0571 0.0551 0.0556 -0.1349 0.0571 0.0556 -0.1349 0.0571 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1349 0.0556 -0.1457 0.0557 -0.2356 -0.1457 0.0557 -0.2576 -0.1457 0.0557 -0.2576 -0.1457 0.0557 -0.2576 -0.1457 0.0557 -0.2576 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1457 0.0556 -0.1256 0.0571 0.0556 -0.1256 0.0571 0.0556 -0.1256 0.0571 0.0556 -0.1256 0.0556 -0.1255 0.0556 0.0555 0.0556 0.0555 0.0555 0.0555 0.0555 0.0556 0.0555	H63 H64 H64 H65 C67 C68 G69 C70 C71 072 C50 C71 C72 C51 C52 C53 C54 C55 C55 C55 C55 C56 H59 H60 H61 H62 C67 C70 C71 C72 C50 C70 C71 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C75 C72 C55 C75 C72 C55 C75 C72 C55 C75 C72 C55 C75 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C72 C55 C75 C72 C55 C74 C55 C75 C55 C75 C75 C72 C55 C75 C72 C55 C75 C75 C72 C55 C75 C72 C55 C75 C75 C72 C55 C75 C72 C55 C72 C55 C75 C72 C55 C75 C72 C55 C75 C75 C75 C75 C75 C75 C75 C75 C75	0.0937 0.1124 0.1158 0.1158 0.015 0.0074 0.0615 0.0659 0.0559 0.0559 0.0559 0.0559 0.0559 0.0559 0.0559 0.0559 0.0569 0.0569 0.0569 0.0569 0.0569 0.0569 0.0569 0.0847 0.0683 0.0992 0.0831 0.0992 0.0831 0.0992 0.0878 0.0992 0.0878 0.0992 0.0878 0.0992 0.0785 0.0992 0.0785 0.0386 0.0393 0.0395 0.01122 0.0653 0.0386 0.	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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \rm H23\\ \rm H24\\ \rm H23\\ \rm H24\\ \rm H23\\ \rm H24\\ \rm C2\\ \rm C3\\ \rm C6\\ \rm O7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm H18\\ \rm H19\\ \rm H22\\ \rm H23\\ \rm H14\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H190\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm C3\\ \rm C6\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm C3\\ \rm C6\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm C6\\ \rm C6\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm C6\\ \rm C6\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm C12\\ \rm C3\\ \rm H14\\ \rm H16\\ \rm H16$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0230\\ 0.0623\\ -0.4992\\ 0.0230\\ 0.0623\\ -0.4992\\ 0.0230\\ 0.0623\\ -0.4923\\ 0.0623\\ -0.4923\\ 0.0623\\ -0.4923\\ 0.0633\\ -0.4923\\ 0.0633\\ 0.0370\\ -0.5151\\ 0.0283\\ 0.4466\\ -0.3102\\ 0.0283\\ 0.4466\\ -0.3362\\ 0.3362\\ 0.1180\\ 0.1145\\ 0.1149\\ 0.1027\\ 0.1044\\ 0.1237\\ 0.1104\\ 0.1237\\ 0.1104\\ 0.1237\\ 0.1104\\ 0.1237\\ 0.1465\\ 0.3632\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0579\\ -0.4653\\ 0.0538\\ 0.0414\\ -0.5150\\ 0.0538\\ 0.0414\\ -0.5150\\ 0.0538\\ 0.0414\\ -0.5150\\ 0.0329\\ 0.03255\\ 0.3453\\ 0.3443\\ 0.1349\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1348\\ 0.1349\\ 0.1348\\ 0.1$	H39 H40 041 C42 C43 044 C45 C46 C47 C48 C27 C28 S29 C30 031 B37 H36 H37 H38 H39 H40 041 C42 C43 C44 041 C42 C43 H36 H37 H38 H39 H40 041 C42 C43 C44 044 C45 C27 S28 C27 S28 C33 034 H36 H37 H38 H39 H36 H37	0.1253 0.1227 -0.5481 0.0559 0.0559 0.0550 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.4336 -0.2415 -0.2415 -0.2415 -0.2415 0.0254 0.0748 -0.5161 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline C2\\ \rm C3\\ \rm O4\\ \rm C5\\ \rm C6\\ \rm O7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm S11\\ \rm C12\\ \rm C3\\ \rm S11\\ \rm H16\\ \rm H17\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline L2\\ \rm C3\\ \rm C6\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C5\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C5\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C5\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C5\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C1\\ \rm C1\\ \rm C1\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C6\\ \rm C7\\ \rm C3\\ \rm C3\\ \rm C4\\ \rm C5\\ \rm C6\\ \rm C7\\ \rm C3\\ \rm C3\\ \rm C1\\ \rm C1\\$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1261\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1222\\ 0.1502\\ 0.1501\\ 0.1262\\ 0.0230\\ 0.0623\\ 0.0633\\$	H39 H40 H40 O41 C42 C43 O44 C45 C25 S26 C27 C28 S29 C30 O31 D34 H35 H36 H36 H37 H38 H39 H40 O41 C45 S26 C33 C34 H37 H38 H39 H40 O41 C45 C26 S26 C31 C32 C32 S29 C30 D31 C32 C32 C33 C34 H35 H36 H37 H38 H39 H40 D41 H36	0.1253 0.1227 -0.5481 0.0559 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 0.3783 -0.2415 -0.2415 0.0748 -0.1401 0.4192 0.0748 -0.1401 0.4192 0.0748 -0.1412 0.0748 -0.5161 0.0254 -0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.1284 0.5561 0.0567 -0.5183 0.0564 0.0567 -0.5183 0.0564 0.0567 -0.5183 0.0564 0.05667 -0.2390 0.0567 -0.1349 0.0567 -0.1349 0.0571 0.0356 -0.2390 -0.1349 0.0571 0.0356 -0.1349 0.0771 -0.512 0.0551 0.0512 0.0551 0.0551 0.0551 0.0551 0.0551 0.0551 0.0551 0.0551 0.0556 -0.1349 0.0771 -0.512 0.0551 0.0551 0.0556 -0.1349 0.0771 0.0551 0.0551 0.0557 -0.1349 0.0571 0.0551 0.0557 -0.1349 0.0571 0.0551 0.0556 -0.1349 0.0711 -0.512 0.0556 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0.1563 0.1666 0.1887 0.1687 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1487 0.1037 -0.1487 0.1508 -0.4065 -0.4065 -0.4065 -0.4065 -0.1555 0.0680 -0.1555 -0.993 -0.1555 -0.993 -0.1555 -0.993 -0.1555 -0.4102 0.1527 0.1527 0.1527 0.1557 0.1527 0.1557 0.1572 0.1572 0.1551 -0.1572 0.1551 -0.1571 0.1581 -0.1551 -0.1657 0.0880 -0.1657 0.1657 0.0880 -0.1657 0.1657 0.0880 -0.1657 0.1657 0.0880 -0.1657 0.1657	N159 C160 C161 H162 C161 C164 C165 C166 C167 C168 H145 H146 H147 H151 H155 C156 C157 C168 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 -0.1469 0.1540 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1188 -0.1193 0.0710 0.1771 0.1400 0.1384 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1439 0.1655 0.1439 0.1655 0.1420 0.1421 0.1655 0.1211 0.0858 0.1221 0.1238 0.1221 0.1238 0.1223 0.1880 0.1228 0.1221 0.1385 0.1228 0.1238 0.1221 0.1385 0.1238 0.1238 0.1238 0.1238 0.1238 0.1228 0.1211 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline c_2\\ c_3\\ c_4\\ c_5\\ c_6\\ 07\\ c_6\\ 07\\ c_8\\ c_9\\ c_1\\ c_1\\ c_2\\ c_3\\ c_6\\ c_6\\ c_7\\ c_8\\ c_9\\ c_1\\ c_1\\ c_1\\ c_2\\ c_3\\ c_6\\ c_6\\ c_7\\ c_8\\ c_9\\ c_1\\ c_1\\ c_2\\ c_3\\ c_6\\ c_6\\ c_7\\ c_8\\ c_9\\ c_1\\ c_1\\ c_2\\ c_3\\ c_6\\ c_6\\ c_7\\ c_8\\ c_9\\ c_1\\ c_1\\ c_2\\ c_3\\ c_6\\ c_9\\ c_1\\ c_1\\ c_2\\ c_3\\ c_1\\ c_1\\ c_1\\ c_1\\ c_1\\ c_1\\ c_1\\ c_1$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1501\\ 0.1502\\ 0.0623\\ -0.4932\\ 0.0623\\ -0.4932\\ 0.0623\\ -0.4932\\ 0.0623\\ 0.0643\\ -0.3510\\ 0.0623\\ 0.0644\\ 0.0370\\ -0.5151\\ 0.0083\\ 0.0466\\ -0.3150\\ 0.0466\\ -0.3352\\ 0.4466\\ -0.3352\\ 0.4466\\ -0.3352\\ 0.4466\\ 0.1242\\ 0.0579\\ -0.4635\\ 0.1149\\ 0.1074\\ 0.1024\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.4635\\ 0.0124\\ 0.0579\\ -0.3255\\ 0.04373\\ -0.2964\\ 0.4175\\ 0.3449\\ 0.1346\\ 0.1242\\ 0.072\\ 0.072\\ 0.072\\ 0.072\\ 0.000\\ $	H39 H40 H40 O41 C42 C42 C45 C46 C47 C48 C27 C28 C30 D31 C32 C33 D34 H35 H36 H37 H38 H39 H40 O41 C42 C43 C44 C45 C45 C46 C47 C42 C43 O41 C44 C45 C45 C26 C27 C28 S29 C30 O31 C22 C33 O34 H36 H37 H37 H38 H38 H39 H36 H37 H37 H38 H38 H39 H38 H39 H37 H38 H38 H39 H37 H38 H38	0.1253 0.1237 -0.5481 0.0559 0.0559 0.0559 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.2415 -0.565 0.1284 0.1285 0.1284 0.1285 0	H63 H64 H64 H65 C67 C70 C68 C67 C71 072 C69 C70 C71 C72 C72 C71 C72 C72 C72 C73 C72 C73 C74 C75 C75 C75 C75 C76 H61 H62 C77 C76 C70 C71 C72 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 -0.4831 0.0074 0.0615 -0.4869 0.0559 0.0559 0.0559 0.0559 0.0194 -0.4767 -0.2062 -0.1216 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0954 -0.0847 -0.0954 -0.0847 -0.0954 -0.0847 -0.0954 0.0145 0.0979 0.1205 0.0145 0.0979 0.0145 0.0979 0.0145 0.0979 0.0145 0.0979 0.0145 0.0979 0.0145 0.0979 0.0326 0.0988 0.01122 0.0366 -0.5380 -0.5380 -0.5380 -0.0588 0.01122 0.0760 -0.0588 0.01122 0.0760 -0.0386 -0.0	H87 H88 H89 K30 K30 H73 H74 H75 H36 H77 H78 H77 H78 H77 H78 H80 H81 H83 H84 H85 H85 H85 H85 H87 H83 H84 H85 H87 H85 H87 H85 H87 H87 H85 H87 H87 H88 H89 K39 K32 K34 K35 K34 K35 K35 K35 K35 K35 K35 K35 K35 K35 K35	0.1083 0.1394 0.1627 -0.1141 0.1627 -0.1430 0.0746 0.3033 -0.1395 0.0776 0.1302 0.1316 0.0972 0.1055 0.1047 0.0988 0.2075 0.1047 0.2015 0.1083 0.1119 0.1407 -0.1188 0.1123 0.1223 0.1223 0.1025 0.100	C111 H112 C113 H114 C115 C116 H117 C120 C120 C120 C120 C120 C120 C120 C120	-0.1057 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline C2\\ \rm C3\\ \rm 04\\ \rm C5\\ \rm C6\\ \rm 07\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm H14\\ \rm H16\\ \rm H17\\ \rm H22\\ \rm H22\\ \rm H23\\ \rm H24\\ \rm H22\\ \rm H23\\ \rm H26\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H26\\ \rm H16\\ \rm H16$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1216\\ 0.1265\\ 0.1205\\ 0.1267\\ 0.1267\\ 0.1267\\ 0.1267\\ 0.1267\\ 0.1267\\ 0.1272\\ 0.0230\\ 0.0623\\ 0.0633\\ 0.0623\\ 0.0633\\ 0.0623\\ 0.0633\\$	H39 H40 O41 C42 C43 O44 C45 C46 C47 C48 C27 C28 S29 C30 O31 C32 C33 O34 H35 H36 H37 H38 H40 O41 C42 C25 S26 C37 C38 C39 H40 O41 C42 C35 S26 C37 C28 S29 C30 O31 C32 C33 C34 H37 H38 H37 H38 H37 H38 H39 H40	0.1253 0.1227 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3452 0.4336 -0.2415 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline z= -\\ 01\\ 01\\ 01\\ 02\\ c3\\ c3\\ c3\\ c4\\ c5\\ c6\\ 07\\ c8\\ c9\\ c10\\ c12\\ s13\\ \rm H14\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline z= -\\ 01\\ c5\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c5\\ c6\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c5\\ c6\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c5\\ c6\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c5\\ c6\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c5\\ c6\\ c6\\ c7\\ c8\\ c9\\ c10\\ c12\\ c3\\ c3\\ c12\\ c12\\ c3\\ c12\\ c12\\ c12\\ c12\\ c12\\ c12\\ c12\\ c12$	0.1279 0.1276 0.1276 0.1205 0.1216 0.1205 0.1210 0.1160 0.1160 0.1267 0.1227 0.1502 0.1502 0.1501 0.0623 -0.4992 0.0220 0.0623 -0.4923 0.0624 0.0623 0.0643 0.0623 0.0644 0.0370 -0.5151 0.0623 0.4285 0.3625 0.4285 0.4285 0.4285 0.4285 0.4285 0.4285 0.4285 0.4285 0.4285 0.1149 0.1149 0.1149 0.1144 0.1144 0.1144 0.1144 0.1144 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline c_2\\ \rm c_3\\ \rm 04\\ \rm C5\\ \rm c_6\\ \rm 07\\ \rm c_6\\ \rm 07\\ \rm C6\\ \rm 07\\ \rm C6\\ \rm 07\\ \rm C6\\ \rm 07\\ \rm C6\\ \rm 07\\ \rm C12\\ \rm C3\\ \rm H14\\ \rm H16\\ \rm H17\\ \rm H22\\ \rm H23\\ \rm H24\\ \rm H22\\ \rm H23\\ \rm H24\\ \rm H22\\ \rm H23\\ \rm H15\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm C12\\ \rm C3\\ \rm C6\\ \rm C6\\ \rm C6\\ \rm C7\\ \rm C6\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C12\\ \rm C3\\ \rm H14\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H19\\ \rm H10\\ \rm H10$	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1276\\ 0.1205\\ 0.1210\\ 0.1267\\ 0.1205\\ 0.1160\\ 0.1160\\ 0.1167\\ 0.1267\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0624\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0623\\ 0.0644\\ 0.0370\\ 0.0623\\$	H39 H40 O41 C42 C43 O44 C45 C46 C47 C48 C27 C28 S26 C30 O31 H36 H37 H38 H37 H38 H39 H40 C41 C42 C43 C44 C45 C46 C47 C48 C44 C45 C27 C28 S29 C30 C32 C33 C34 H35 H36 H37 H38 H39 H40 O41 C42 C43 H37 H38 H39	0.1253 0.1227 -0.5481 0.05590 -0.5199 0.05650 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 0.1482 0.1482 0.1482 0.1482 0.1487 0.1284 -0.5031 0.0587 -0.5128 0.0587 -0.5128 0.0587 -0.5128 0.0587 -0.5128 0.0544 0.05637 -0.5128 0.0564 0.0564 0.05637 -0.51349 0.0564 0.2396 -0.5233 0.3478	H63 H64 H64 H65 C67 C68 C67 C70 C71 C72 C69 C70 C71 C72 C53 C54 C55 C56 C57 C74 H59 H60 C74 H59 H60 C77 C71 C72 C71 C72 C74 C55 C76 C77 C72 C72 C72 C72 C72 C72 C72 C72 C72	0.0937 0.1124 0.1158 0.1158 0.074 0.6615 0.0674 0.6659 0.0559 0.0194 0.0767 0.0262 0.0194 0.0744 0.0744 0.0744 0.0744 0.0744 0.0744 0.0745 0.02831 0.1145 0.0831 0.1145 0.0831 0.1145 0.0833 0.1096 0.0835 0.0838 0.0393 0.0992 0.0878 0.0393 0.0992 0.0878 0.0393 0.0992 0.0878 0.0393 0.0393 0.0393 0.0395 0.0386 0.	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$\begin{array}{c} \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H20 \\ \rm H21 \\ \rm H22 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm H23 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm C4 \\ \rm C5 \\ \rm C6 \\ \rm 07 \\ \rm C8 \\ \rm C9 \\ \rm C10 \\ \rm S11 \\ \rm C12 \\ \rm S13 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H22 \\ \rm H24 \\ \rm C2 \\ \rm C3 \\ \rm 01 \\ \rm C2 \\ \rm C3 \\ \rm C6 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm C3 \\ \rm C6 \\ \rm C9 \\ \rm C10 \\ \rm C12 \\ \rm C3 \\ \rm H14 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H16 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H19 \\ \rm H19 \\ \rm H16 \\ \rm H17 \\ \rm H18 \\ \rm H19 \\ \rm H19 \\ \rm H19 \\ \rm H19 \\ \rm H10 \\ \rm H11 \\ \rm H19 \\ \rm H10 \\ \rm $	$\begin{array}{c} 0.1279\\ 0.1276\\ 0.1226\\ 0.1226\\ 0.1220\\ 0.1210\\ 0.1160\\ 0.1167\\ 0.1227\\ 0.1227\\ 0.1227\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.1502\\ 0.0623\\ 0.0623\\ 0.0624\\ 0.0623\\ 0.0624\\ 0.0623\\ 0.0624\\ 0.0623\\ 0.0644\\ 0.0623\\ 0.0658\\ 0.0658\\ 0.0658\\ 0.0658\\ 0.0658\\ 0.0658\\ 0.0644\\ 0.0658\\ 0.0658\\ 0.0424\\ 0.1465\\ 0.1149\\ 0.1243\\ 0.1465\\ 0.1149\\ 0.1243\\ 0.1243\\ 0.0679\\ -0.4843\\ 0.0624\\ 0.0638\\ 0.0638\\ 0.0414\\ 0.0579\\ -0.35150\\ 0.0638\\ 0.0124\\ 0.0579\\ -0.355\\ 0.0446\\ 0.0538\\ 0.0124\\ 0.0579\\ -0.3255\\ 0.0443\\ 0.0638\\ 0.0414\\ 0.0538\\ 0.0244\\ 0.0579\\ -0.3255\\ 0.0443\\ 0.0638\\ 0.0414\\ 0.5150\\ 0.0838\\ 0.0414\\ 0.5150\\ 0.0838\\ 0.0414\\ 0.5150\\ 0.0838\\ 0.0414\\ 0.0579\\ -0.3255\\ 0.0443\\ 0.0579\\ -0.2355\\ 0.0443\\ 0.0579\\ -0.2355\\ 0.0443\\ 0.0579\\ -0.2355\\ 0.0443\\ 0.0538\\ 0.0414\\ 0.1540\\ 0.0838\\ 0.0414\\ 0.1540\\ 0.0838\\ 0.0414\\ 0.0538\\ 0.0441\\ 0.1240\\ 0.1346\\ 0.1346\\ 0.1346\\ 0.1242\\ 0.1242\\ 0.1240$	H39 H40 H40 O41 H40 O41 C42 C43 C45 C46 C47 C48 C25 S26 S26 C27 C30 O31 C32 C27 C30 O31 C32 C33 O34 H36 H37 H38 H39 H40 O41 C42 C25 S26 C27 C28 S29 H30 O41 C42 C46 O47 C47 C28 S29 C30 O31 C32 C33 O34 H37 H38 H39 H40 O41 C42 C33 O34 H37 H38 H37 H38 H37 H38 H37 H39 H37	0.1253 0.1227 -0.5481 0.0559 0.0590 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3052 0.4336 -0.2415 -0.1401 0.0748 -0.2415 0.0748 -0.2415 0.0748 -0.2415 0.0748 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.1254 0.1254 0.1264 0.1264 0.1264 0.1284 0.1284 0.1284 0.1284 0.1284 0.0565 0.1482 0.0566 0.1482 0.0566 0.1482 0.0566 0.1284 -0.5158 0.0566 -0.5233 0.03478 -0.33478 -0.3356 -0.3478 -0.3356 -0.3478 -0.3556 0.0356 -0.5158 0.0556 0.1435 0.0556 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.1435 0.0556 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.0356 -0.5158 0.0556 0.0356 0.0356 -0.5181 0.0556 0.0356 0.0557 0.0556 0.0557 0.05	H63 H64 H65 C67 C68 C67 C70 C71 072 C50 C71 072 C50 C51 C52 C55 C55 C55 C55 C55 H59 H60 H61 H62 C67 C70 C71 C55 C55 C70 C71 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 C55 C70 C72 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$\begin{array}{c} \rm H16\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline c_2\\ \rm C_3\\ \rm 04\\ \rm C_5\\ \rm C_6\\ \rm 07\\ \rm C_8\\ \rm C_9\\ \rm C10\\ \rm C_1\\ \rm C2\\ \rm C_6\\ \rm 07\\ \rm C_8\\ \rm C9\\ \rm C10\\ \rm H16\\ \rm H17\\ \rm H18\\ \rm H19\\ \rm H20\\ \rm H21\\ \rm H22\\ \rm H23\\ \rm H24\\ \hline c_5\\ \rm C_6\\ \rm 07\\ \rm C_8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C4\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C10\\ \rm C1\\ \rm C1\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C1\\ \rm C1\\ \rm C1\\ \rm C1\\ \rm C2\\ \rm C3\\ \rm C6\\ \rm C7\\ \rm C8\\ \rm C9\\ \rm C1\\ \rm C1\\$	0.1279 0.1276 0.1276 0.1205 0.1210 0.1160 0.1160 0.1167 0.1267 0.1222 0.1502 0.1502 0.0502 0.0623 0.0623 0.0623 0.0623 0.0623 0.0623 0.0623 0.0623 0.0623 0.0624 0.0370 0.0370 0.0446 0.0370 0.0466 0.0370 0.4466 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0.0559 -0.5199 0.0565 0.0451 -0.5199 0.3783 -0.3783 -0.3783 -0.3452 0.4336 -0.2415 -0.2415 0.0254 -0.2415 0.0254 -0.1401 0.0531 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.0254 -0.5161 0.1284 0.1284 0.1284 0.1284 0.1284 0.5271 0.0499 0.0587 -0.5129 0.0542 0.0542 0.0542 0.0542 0.0254 -0.5233 0.3478 -0.5233 0.3478 -0.5233 0.3478 -0.523 0.0429 0.0551 0.0254 -0.2305 0.1284 0.0557 -0.5184 0.0542 0.0557 -0.5129 0.0557 -0.5365 0.0557 -0.5538 0.0512 0.0552 0.0425 0.0512 0.0552 0.0425 0.0552 0.0425 0.0552 0.0552 0.0552 0.0552 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0552 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5536 0.0711 0.0557 -0.5530 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0.2279 0.1065 0.3248 0.1192 0.1192 0.1336 0.1326 0.1326 0.1326 0.1326 0.1223 0.1047 0.1047 0.1021 0.1047 0.1021 0.1047 0.1051 0.1021 0.1047 0.1022 0.1021 0.1047 0.1022 0.0779 0.1025 0.1021 0.1047 0.1022 0.1021 0.1047 0.1021 0.1047 0.1022 0.0779 0.1025 0.1021 0.1047 0.1022 0.0030 0.1047 0.0095 0.1021 0.0095 0.1022 0.1012 0.1022 0.1012 0.1022 0.1012 0.1022 0.1012 0.1025 0.1007 0.1000 0.1007 0.1000 0.10000000000	C111 H112 C113 H114 C115 C116 H117 C118 H119 C120 C97 H98 C99 C100 C101 H102 C103 H104 C105 C106 H107 C103 H107 C103 H107 C103 H107 C100 C110 C111 H112 C113 H114 C120 C97 H98 C99 C100 C101 H107 C120 C107 H107 C120 C107 H107 C120 C107 H107 C120 C107 H107 C120 C107 H107 C120 C107 C108 H109 C120 C107 C108 H109 C120 C107 C108 H107 C120 C107 C108 H107 C120 C107 C108 H107 C120 C107 C108 H107 C108 H107 C107 C108 H107 C107 C108 H107 C100 C110 C110 C110 C110 C110 C110 C	-0.1057 0.1067 0.1031 0.1230 0.2205 0.3116 -0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1237 0.1388 -0.3055 -0.0937 0.1388 0.3365 -0.1005 0.6635 -0.1005 0.6635 -0.1005 0.1541 -0.0929 0.1535 -0.1007 0.1565 0.1665 0.1535 -0.0948 0.1331 0.0345 0.0345 0.1331 0.0345 0.1335 0.1355 0.1355 0.1664 0.1355 0.1355 0.1464 0.0345 0.1355 0.1465 0.1331 0.0345 0.1335 0.1355 0.1465 0.1355 0.1355 0.1355 0.1465 0.1355 0.1355 0.1355 0.1467 0.0992 0.1355 0.1467 0.0992 0.1355 0.1467 0.0992 0.1355 0.1467 0.0917 0.1465 0.377 0.1467 0.0315 0.356 0.1467 0.1467 0.0315 0.355 0.1467 0.1467 0.0929 0.1355 0.355 0.1467 0.1535 0.1555	C135 C136 C137 C138 C139 H140 H141 H142 C121 C122 C123 C124 N125 C126 C127 C128 C129 C130 C131 C132 C124 N125 C126 C127 C128 C133 N134 C135 C136 C137 C138 C139 H140 H141 H142 H143 H144 H143 H144 H143 H144 H144 H143 H144 H143 H144 H143 H144 H143 H144 H144	0.1597 -0.1397 0.0777 -0.1475 0.1513 0.1805 0.1563 0.1666 0.1887 0.1587 0.1687 0.1037 -0.1447 0.1037 -0.1447 0.1037 -0.1447 0.1508 -0.4065 -0.4065 -0.1555 0.0680 -0.1257 0.0555 -0.1655 -0.9949 -0.993 -0.1557 0.1522 -0.1402 0.1522 -0.1402 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1527 0.1551 -0.1457 0.1551 -0.1657 0.1872 -0.1657 0.0880 -0.1657 0.1657 0.0880 -0.1657 0.16	N159 C160 C161 H162 C161 C164 C165 C166 C167 C168 H146 H147 H148 H149 H150 H151 H155 C156 C157 C158 N159 C160 C161 H163 C164 C165 C166 C167 C168 H145 H145 H145 H145 H145 H145 H145 H145	-0.4106 0.1547 0.1640 0.1589 0.0704 -0.1188 -0.1589 0.0704 -0.1183 -0.1193 0.0710 0.1771 0.1400 0.1384 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1248 0.1349 0.1655 0.1349 0.1655 0.1349 0.1655 0.1434 0.1400 0.1655 0.1420 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1655 0.1421 0.1427 0.1655 0.1421 0.1427 0.1655 0.1421 0.1427 0.1655 0.1421 0.1427 0.1655 0.1421 0.1588 0.0888 0.1226 0.1121 0.1585 0.159 0.1411 0.1559 0.4153 0.1559 0.4153 0.1559 0.4153 0.1559 0.4153 0.1553 0.1559 0.4153 0.1553 0.1553 0.1559 0.1687 0.1553 0.1553 0.1553 0.1559 0.1687 0.1553 0.1555 0.	H183 H184 H185 H186 H186 H186 H187 H188 H190 H191 Total C169 C170 H171 Total C173 H172 C173 H172 C173 H172 C177 C178 C177 C178 C177 H180 H181 H182 H183 H184 H185 H187 H185 H189 H190 H191 Total C169 C170 H171 Total C169 C177 C178 H180 H191 Total H181 H182 H183 H184 H185 H181 H181 H182 H183 H184 H183 H184 H183 H184 H185 H186 H187 H181 H182 H183 H184 H183 H184 H185 H186 H187 H181 H182 H181 H181 H182 H183 H184 H183 H184 H185 H186 H187 H181 H182 H183 H184 H183 H184 H185 H186 H187 H188 H187 H188 H188 H186 H187 H188 H188 H186 H187 H182 H181 H182 H183 H184 H183 H184 H185 H186 H187 H188 H180 H181 H182 H181 H182 H181 H182 H183 H184 H183 H184 H185 H186 H187 H182 H181 H182 H183 H184 H185 H187 H182 H183 H184 H185 H186 H187 H187 H187 H187 H187 H187 H187 H187	-0.1930 0.1730 0.1734 0.1734 0.1426 0.1734 0.1426 0.1734 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1426 0.1687 0.1687 0.1687 0.1672 0.1579 0.1527 0.1584 0.1584 0.1584 0.1584 0.1584 0.1587 0.1584 0.1584 0.1584 0.1587 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.1584 0.1587 0.158

Table E.3:	Partial Charge	Distribution o	f + 2 Oxid	ized Rot	axane w	when the	e Center	of Mass	of t	the
$CBPQT^{4+}$	Ring Moves from	m $z = 10.92$ Å	(TTF sid	e) to $z =$	44.83 Å	(DNP	side)			

| z = | 10.92 A |

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--|--|---|
| 01 | -0.4596 | C25

 | -0.3297 | C49 | -0.1448 | H73
 | 0.1605
 | C97 | -0.0890 | C121 | -0.1310
 | H145 | 0.1870 | C169 | -0.0978
 |
| C2 | 0.0112 | S26

 | 0.2671 | C50 | -0.0570 | H74
 | 0.1600
 | H98 | 0.1477 | C122 | 0.1127
 | H146 | 0.1497 | C170 | -0.1009
 |
| C3 | 0.0601 | C27

 | -0.2613 | C51 | -0.0393 | H75
 | 0.1526
 | C99 | 0.0436 | C123 | -0.1525
 | H147 | 0.1491 | H171 | 0.1214
 |
| 04 | -0.5032 | C28

 | -0.1534 | C52 | -0.0648 | H76
 | 0.1532
 | C100 | 0.0567 | C124 | 0.1549
 | H148 | 0.1198 | H172 | 0.1226
 |
| C5 | 0.0762 | S29

 | 0.2547 | C53 | -0.0642 | H77
 | 0.1534
 | C101 | -0.0954 | N125 | -0.4061
 | H149 | 0.1228 | C173 | -0.1764
 |
| C6 | 0.0345 | C30

 | 0.0905 | C54 | -0.0415 | H78
 | 0.1531
 | H102 | 0.1515 | C126 | -0.1737
 | H150 | 0.1899 | N174 | -0.4069
 |
| 07 | -0.5166 | 031

 | -0.5123 | C55 | -0.0562 | H79
 | 0 1677
 | C103 | -0.0997 | C127 | 0 0954
 | H151 | 0 1862 | C175 | 0 1722
 |
| C8 | 0.0915 | C32

 | 0.0442 | C56 | =0 1448 | 80
 | 0 1678
 | H104 | 0 1501 | C128 | =0 1221
 | H152 | 0 1827 | C176 | =0 1327
 |
| C0 | -0.1514 | C22

 | 0.0442 | 000 | 0.1140 | 100
 | 0.2747
 | C105 | 0.1501 | C120 | -0.1217
 | U1E2 | 0.162/ | 0170 | 0.1176
 |
| C10 | -0.1314 | 024

 | -0 5221 | 1007 | 0.4249 | 101
 | 0.3747
 | C105 | -0.1000 | C129 | -0.1217
 | 1155 | 0.1514 | 0179 | -0.1521
 |
| 010 | -0.2703 | 0.34

 | -0.5221 | 100 | 0.1280 | 102
 | 0.1000
 | 0100 | -0.1000 | 0130 | 0.0000
 | 1154 | 0.1580 | 0170 | -0.1521
 |
| S11 | 0.2751 | H35

 | 0.1293 | H59 | 0.1286 | H83
 | 0.1931
 | H107 | 0.1437 | 0131 | -0.1042
 | H155 | 0.1862 | 0179 | 0.1577
 |
| C12 | -0.3321 | H36

 | 0.1063 | H60 | 0.1244 | H84
 | 0.1679
 | C108 | -0.0952 | C132 | -0.0977
 | C156 | 0.1078 | H180 | 0.1938
 |
| S13 | 0.2665 | H37

 | 0.1132 | H61 | 0.1245 | H85
 | 0.1747
 | H109 | 0.1514 | C133 | -0.1743
 | C157 | -0.1274 | H181 | 0.1680
 |
| H14 | 0.3545 | H38

 | 0.1204 | H62 | 0.1238 | H86
 | 0.1779
 | C110 | 0.0305 | N134 | -0.4037
 | C158 | 0.1623 | H182 | 0.1435
 |
| H15 | 0.1376 | H39

 | 0.1284 | H63 | 0.1239 | H87
 | 0.1767
 | C111 | -0.0926 | C135 | 0.1664
 | N159 | -0.4063 | H183 | 0.1691
 |
| H16 | 0.1391 | H40

 | 0.1186 | H64 | 0.1506 | H88
 | 0.1773
 | H112 | 0.1390 | C136 | -0.1257
 | C160 | 0.1454 | H184 | 0.1794
 |
| H17 | 0.1185 | 041

 | -0.5087 | H65 | 0.1508 | H89
 | 0.1737
 | C113 | -0.1172 | C137 | 0.1125
 | C161 | -0.1501 | H185 | 0.1940
 |
| H18 | 0.1161 | C42

 | 0.0274 | 066 | -0.4813 | C90
 | -0.0889
 | H114 | 0.1361 | C138 | -0.1401
 | H162 | 0.1623 | H186 | 0.1345
 |
| H19 | 0 1033 | C43

 | 0.0556 | C67 | 0.0039 | H91
 | 0 1472
 | C115 | 0 3280 | C139 | 0 1597
 | H163 | 0 1873 | H187 | 0 1400
 |
| H20 | 0.0933 | 044

 | =0.5029 | C68 | 0.0341 | C02
 | =0.1086
 | C116 | -0 1179 | H140 | 0 1757
 | C164 | =0.1709 | H188 | 0 1880
 |
| 1120 | 0.1125 | C4E

 | 0.0020 | 060 | -0.4204 | 102
 | 0.1605
 | U117 | 0.1401 | H140 | 0.1/60
 | 0104 | 0.1705 | 1100 | 0.1960
 |
| 1121 | 0.1155 | 040

 | 0.0004 | 005 | -0.4294 | 004
 | 0.1025
 | 0110 | 0.1421 | 1141 | 0.1400
 | 0100 | 0.0882 | 1105 | 0.1602
 |
| HZZ | 0.1256 | 040

 | 0.0061 | 070 | 0.0396 | 694
 | 0.3505
 | 0110 | -0.0918 | H142 | 0.1607
 | 0100 | -0.1152 | H190 | 0.1690
 |
| H23 | 0.0969 | 047

 | -0.4769 | 071 | -0.0059 | 095
 | -0.1083
 | H119 | 0.1421 | H143 | 0.1861
 | C167 | -0.1159 | H191 | 0.1410
 |
| H24 | 0.1266 | C48

 | 0.4245 | 072 | -0.3868 | H96
 | 0.1617
 | C120 | 0.1602 | H144 | 0.1879
 | C168 | 0.0939 | Total | 6.0000
 |
| z = | 15.66 A |

 | | | |
 |
 | | | |
 | | | |
 |
| 01 | -0.4118 | C25

 | -0.3665 | C49 | -0.1464 | H73
 | 0.1600
 | C97 | -0.0898 | C121 | -0.1283
 | H145 | 0.1896 | C169 | -0.1049
 |
| C2 | -0.0008 | S26

 | 0.2876 | C50 | -0.0571 | H74
 | 0.1594
 | H98 | 0.1472 | C122 | 0.1048
 | H146 | 0.1525 | C170 | -0.1068
 |
| C3 | 0.0505 | C27

 | -0.2751 | C51 | -0.0409 | H75
 | 0.1521
 | C99 | 0.0460 | C123 | -0.1534
 | H147 | 0.1511 | H171 | 0.1288
 |
| 04 | -0.4609 | C28

 | -0.1483 | C52 | -0.0654 | H76
 | 0.1527
 | C100 | 0.0523 | C124 | 0.1553
 | H148 | 0.1144 | H172 | 0.1285
 |
| C5 | 0.0477 | S29

 | 0.2488 | C53 | -0.0652 | H77
 | 0.1523
 | C101 | -0.0960 | N125 | -0.4058
 | H149 | 0.1136 | C173 | -0.1689
 |
| CG | 0.0412 | C30

 | 0.0854 | C54 | -0.0423 | H78
 | 0.1520
 | H102 | 0.1493 | C126 | -0.1604
 | H150 | 0.1854 | N174 | -0.4098
 |
| 07 | -0 5142 | 031

 | -0 5195 | C55 | -0.0564 | H79
 | 0 1701
 | C103 | -0 1033 | C127 | 0.0836
 | H151 | 0 1830 | C175 | 0 1471
 |
| 01 | 0.0142 | C30

 | 0.0501 | CEC | =0 1/465 | 11/3
 | 0.1701
 | H104 | 0.1000 | C100 | =0 1117
 | H150 | 0.1000 | C176 | =0 1996
 |
| 00 | -0 1274 | 032

 | 0.0501 | 000 | -0.1400 | 100
 | 0.1/03
 | 0105 | 0.1443 | C100 | -0.1117
 | 1110Z | 0.1000 | 0177 | -0.1330
 |
| 09 | -0.13/4 | 033

 | 0.05/6 | | 0.4244 | пб1
UCC
 | 0.3/5/
 | 0105 | 0.0568 | 0129 | -0.1134
 | 1153 | 0.1505 | 0170 | 0.1091
 |
| C10 | -0.2447 | U34

 | -0.5305 | H58 | 0.1278 | H82
 | 0.2056
 | C106 | -0.1036 | C130 | 0.0914
 | H154 | 0.1585 | C178 | -0.1533
 |
| S11 | 0.2712 | н35

 | 0.1005 | H59 | 0.1285 | н83
 | 0.1630
 | H107 | 0.1350 | C131 | -0.1145
 | H155 | 0.1841 | C179 | 0.1599
 |
| C12 | -0.3073 | H36

 | 0.1114 | H60 | 0.1213 | H84
 | 0.1655
 | C108 | -0.0957 | C132 | -0.1148
 | C156 | 0.0951 | H180 | 0.1917
 |
| S13 | 0.2908 | H37

 | 0.1058 | H61 | 0.1214 | H85
 | 0.1726
 | H109 | 0.1481 | C133 | -0.1643
 | C157 | -0.1149 | H181 | 0.1645
 |
| H14 | 0.3667 | H38

 | 0.1080 | H62 | 0.1211 | H86
 | 0.1762
 | C110 | 0.0275 | N134 | -0.4148
 | C158 | 0.1142 | H182 | 0.1376
 |
| H15 | 0.1570 | H39

 | 0.0998 | H63 | 0.1211 | H87
 | 0.1755
 | C111 | -0.0957 | C135 | 0.1679
 | N159 | -0.3991 | H183 | 0.1691
 |
| H16 | 0.1568 | H40

 | 0.1040 | H64 | 0.1485 | H88
 | 0.1758
 | H112 | 0.1360 | C136 | -0.1310
 | C160 | 0.1602 | H184 | 0.1837
 |
| H17 | 0.1359 | 041

 | -0.5065 | H65 | 0.1487 | H89
 | 0.1723
 | C113 | -0.1210 | C137 | 0.0987
 | C161 | -0.1393 | H185 | 0.1901
 |
| H18 | 0.1362 | C42

 | 0.0258 | 066 | -0.4837 | C90
 | -0.0896
 | H114 | 0.1188 | C138 | -0.1556
 | H162 | 0.1687 | H186 | 0.1478
 |
| H19 | 0 1282 | C43

 | 0.0591 | C67 | 0.0046 | H91
 | 0 1468
 | C115 | 0 3156 | C139 | 0 1524
 | H163 | 0 1956 | H187 | 0 1465
 |
| 820 | 0 1282 | 044

 | =0.5105 | C68 | 0.0344 | C02
 | =0 1073
 | C116 | =0 1221 | H140 | 0 1830
 | C164 | =0.1654 | H188 | 0 1913
 |
| 1120 | 0.1202 | C4E

 | 0.0100 | 060 | -0.4200 | 102
 | 0.1642
 | u117 | 0.12/1 | H140 | 0.1664
 | 0104 | 0.0761 | 1100 | 0.1911
 |
| n21
1100 | 0.1259 | 045

 | 0.0568 | 069 | =0.4322 | n95
 | 0.1643
 | n117 | 0.1245 | H141 | 0.1564
 | 0165 | 0.0761 | 1109 | 0.1841
 |
| H22 | 0.1269 | 646

 | 0.0079 | 070 | 0.0408 | 094
 | 0.3521
 | C118 | -0.0948 | H142 | 0.1604
 | C166 | -0.1223 | H190 | 0.1783
 |
| | // | 11/1/2

 | -0.4802 | I C71 | -0.0071 | I C95
 | -0.1071
 | I H119 | 0 1392 | H143 | 0.1900
 | C167 | -0.1204 | H191 | 0.1474
 |
| H23 | 0.1331 | 041

 | | | |
 |
 | | 011002 | |
 | | | |
 |
| H23
H24 | 0.1351 | C48

 | 0.4241 | 072 | -0.3773 | H96
 | 0.1634
 | C120 | 0.1670 | H144 | 0.1857
 | C168 | 0.0815 | Total | 6.0000
 |
| $\frac{H23}{H24}$ | 0.1351
0.1350
18.75 Å | C48

 | 0.4241 | 072 | -0.3773 | Н96
 | 0.1634
 | C120 | 0.1670 | H144 | 0.1857
 | C168 | 0.0815 | Total | 6.0000
 |
| H23
H24
z =
01 | 0.1331
0.1350
18.75 Å
-0.4309 | C48

 | -0.3153 | 072
C49 | -0.3773 | H96
 | 0.1634
 | C120
C97 | -0.0949 | H144
C121 | -0.1244
 | C168
H145 | 0.0815 | Total
C169 | 6.0000
 |
| H23
H24
z =
01
C2 | 0.1331
0.1350
18.75 Å
-0.4309
0.0058 | C48
C25
S26

 | -0.3153
0.3018 | 072
C49
C50 | -0.3773
-0.1456
-0.0552 | H96
H73
H74
 | 0.1634
 | C120
C97
H98 | -0.0949
0.1370 | H144
C121
C122 | -0.1244
0.0941
 | C168
H145
H146 | 0.0815 | Total
C169
C170 | -0.1077
-0.1065
 |
| $H23 \\ H24 \\ z = 01 \\ C2 \\ C3 \\ C3 \\ C3 \\ C3 \\ C2 \\ C3 \\ C3$ | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513 | C48
C25
S26
C27

 | -0.3153
0.3018
-0.2962 | 072
C49
C50
C51 | -0.3773
-0.1456
-0.0552
-0.0406 | H96
H73
H74
H75
 | 0.1634
0.1594
0.1588
0.1402
 | C120
C97
H98
C99 | -0.0949
0.1370
0.0473 | H144
C121
C122
C123 | -0.1244
0.0941
-0.1429
 | C168
H145
H146
H147 | 0.0815 | Total
C169
C170
H171 | 6.0000
-0.1077
-0.1065
0.1134
 |
| $H23 \\ H24 \\ z = 01 \\ C2 \\ C3 \\ 04 \\ 04 \\ c2 \\ c3 \\ c4 \\ c4 \\ c5 \\ c5 \\ c5 \\ c5 \\ c5 \\ c5$ | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589 | C25
S26
C27
C28

 | -0.3153
0.3018
-0.2962
-0.1575 | 072
C49
C50
C51
C52 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649 | H96
H73
H74
H75
H76
 | 0.1634
0.1594
0.1588
0.1402
0.1407
 | C120
C97
H98
C99
C100 | -0.0949
0.1370
0.0473
0.0461 | H144
C121
C122
C123
C124 | -0.1244
0.0941
-0.1429
0.1581
 | C168
H145
H146
H147
H148 | 0.0815
0.1908
0.1534
0.1535
0.1180 | Total
C169
C170
H171
H172 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
 |
| H23
H24 | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589 | C25
S26
C27
C28

 | -0.3153
0.3018
-0.2962
-0.1575 | 072
C49
C50
C51
C52
C52 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661 | H96
H73
H74
H75
H76
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
 | C120
C97
H98
C99
C100 | -0.0949
0.1370
0.0473
0.0461 | H144
C121
C122
C123
C124
N125 | -0.1244
0.0941
-0.1429
0.1581
 | C168
H145
H146
H147
H148
H140 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177 | Total
C169
C170
H171
H172
C172 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
 |
| $ \begin{array}{c} H23 \\ H24 \\ \hline z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \end{array} $ | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371 | C25
S26
C27
C28
S29
C20

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752 | 072
C49
C50
C51
C52
C53
C54 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661 | H96
H73
H74
H75
H76
H77
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
 | C120
C97
H98
C99
C100
C101 | -0.0949
0.1370
0.0473
0.0461
-0.1007 | H144
C121
C122
C123
C124
N125
C124 | 0.1857
-0.1244
0.0941
-0.1429
0.1581
-0.4080
0.1640
 | C168
H145
H146
H147
H148
H149
U150 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177 | Total
C169
C170
H171
H172
C173 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
 |
| $ \begin{array}{r} H23 \\ H24 \\ \hline z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \end{array} $ | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371 | C25
S26
C27
C28
S29
C30

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752 | 072
C49
C50
C51
C52
C53
C54 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381 | H96
H73
H74
H75
H76
H77
H78
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1422
 | C120
C97
H98
C99
C100
C101
H102
C102 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408 | H144
C121
C122
C123
C124
N125
C126
C126 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
 | C168
H145
H146
H147
H148
H149
H150 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901 | Total
C169
C170
H171
H172
C173
N174 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
 |
| H23
H24
Z ==
01
C2
C3
04
C5
C6
07 | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151 | C25
S26
C27
C28
S29
C30
D31

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172 | 072
C49
C50
C51
C52
C53
C54
C55 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555 | H96
H73
H74
H75
H76
H77
H78
H79
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
 | C120
C97
H98
C99
C100
C101
H102
C103 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100 | H144
C121
C122
C123
C124
N125
C126
C127 | 0.1857
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
 | C168
H145
H146
H147
H148
H149
H150
H151 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918 | Total
C169
C170
H171
H172
C173
N174
C175 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
 |
| $ \begin{array}{r} H23 \\ H24 \\ \hline z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ \end{array} $ | 0.1331
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845 | C48
C25
S26
C27
C28
S29
C30
D31
C32

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582 | 072
C49
C50
C51
C52
C53
C54
C55
C56 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0381
-0.0555
-0.1422 | H96
H73
H74
H75
H76
H77
H78
H79
H80
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
 | C120
C97
H98
C99
C100
C101
H102
C103
H104 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252 | H144
C121
C122
C123
C124
N125
C126
C127
C128 | 0.1857
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
 | C168
H145
H146
H147
H148
H149
H150
H151
H152 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735 | Total
C169
C170
H171
H172
C173
N174
C175
C176 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
-0.1304
 |
| $ \begin{array}{r} H23 \\ H24 \\ \hline z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ \end{array} $ | 0.1330
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335 | C48
C25
S26
C27
C28
S29
C30
D31
C32
C33

 | -0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0553 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177 | -0.1077 -0.1065 0.1134 0.1124 -0.1802 -0.4006 0.1628 -0.1304 0.0951
 |
| $ \begin{array}{r} H23 \\ H24 \\ z = \\ 01 \\ C2 \\ C3 \\ 04 \\ C5 \\ C6 \\ 07 \\ C8 \\ C9 \\ C10 \\ \end{array} $ | 0.1350
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348 | C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34

 | -0.3153
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0553
-0.5475 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106 | -0.1670
-0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099 | H144
C121
C122
C123
C124
N125
C126
C126
C127
C128
C129
C130 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1370
0.1643 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178 | 6.0000 -0.1077 -0.1065 0.1134 0.1124 -0.1802 -0.4006 0.1628 -0.1304 0.0951 -0.1477
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ \hline 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872 | C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35

 | -0.3153
0.3241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0553
-0.5475
0.1154 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0669
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
 | C168
H145
H146
H147
H148
H149
H150
H151
H151
H152
H153
H154
H155 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179 | $\begin{array}{c} -0.1077 \\ -0.1065 \\ 0.1134 \\ 0.1124 \\ -0.1802 \\ -0.4006 \\ 0.1628 \\ -0.1304 \\ 0.0951 \\ -0.1477 \\ 0.1541 \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ \hline 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \end{array}$ | 0.1351
0.1350
18.75 A
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872
-0.3088 | C48
C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35
H36

 | -0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0553
-0.5475
0.1154
0.1090 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C55
C56
C57
H58
H59
H60 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254
0.1207 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
H84
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108 | -0.0949
0.1670
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
-0.1017
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960
0.0902 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C177
C178
C179
H180 | $\begin{array}{c} 6.0000 \\ \hline \\ -0.1077 \\ -0.1065 \\ 0.1134 \\ 0.1124 \\ -0.1802 \\ -0.4006 \\ 0.1628 \\ -0.1304 \\ 0.0951 \\ -0.1477 \\ 0.1541 \\ 0.1976 \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ \hline 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872
-0.3088
0.3748 | C48
C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35
H36
H37

 | -0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0553
-0.5475
0.1154
0.1090
0.0939 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254
0.1207
0.1205 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
H84
H85
 | 0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
0.1748
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003
0.1387 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133 | -0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
-0.1017
-0.1670
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960
0.0902
-0.1275 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179
H180
H181 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
-0.1304
0.0951
-0.1477
0.1541
0.1976
0.1655
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872
-0.3088
0.3748
0.3748
0.3590 | C48
C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35
H36
H37
H38

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0563
-0.5475
0.1154
0.1090
0.0939
0.0943 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254
0.1207
0.1205 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
H84
H85
H86
 | 0.1634
0.1584
0.1588
0.1402
0.1407
0.1424
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
0.1748
0.1816
 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003
0.1387
0.0331 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133
N134 | -0.1287
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
-0.1017
-0.1670
-0.4107
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157
C158 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960
0.0902
-0.1275
0.1669 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179
H180
H181
H182 | $\begin{array}{c} 6.0000 \\ \hline \\ \hline \\ -0.1077 \\ -0.1065 \\ 0.1134 \\ 0.1124 \\ -0.1802 \\ -0.4006 \\ 0.1628 \\ -0.1304 \\ 0.0951 \\ -0.1477 \\ 0.1541 \\ 0.1976 \\ 0.1655 \\ 0.1384 \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H23} \\ \text{Z} = \\ \hline z = \\ 01 \\ 02 \\ 03 \\ 04 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 07 \\ 05 \\ 05$ | 0.1351
0.1350
18.75 A
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872
-0.3088
0.3748
0.3590
0.1468 | C48
C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35
H36
H37
H38
H39

 | -0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.6172
0.0563
-0.5475
0.1154
0.1090
0.0939
0.0943
0.0970 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62
H63 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0649
-0.0661
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254
0.1207
0.1205
0.1210
0.1210 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H81
H82
H83
H84
H85
H86
H87
 |
0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
0.1748
0.1816
0.1781 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110
C111 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003
0.1387
0.0331
-0.0991 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133
N134
C135 | -0.1287
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
-0.1017
-0.1670
-0.4107
0.1678
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157
C158
N159 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960
0.0902
-0.1275
0.1669
-0.4024 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179
H180
H181
H182
H183 | $\begin{array}{c} 6.0000 \\ \hline \\ \hline \\ -0.1077 \\ -0.1065 \\ 0.1134 \\ 0.1124 \\ -0.1802 \\ -0.4006 \\ 0.1628 \\ -0.1304 \\ 0.0951 \\ -0.1477 \\ 0.1541 \\ 0.1976 \\ 0.1655 \\ 0.1384 \\ 0.1861 \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H23} \\ \text{Z} = \\ \hline 2 \\ \text{C1} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S111} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \end{array}$ | 0.1351
0.1350
18.75 A
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3748
0.3590
0.1467 | C48
C48
C25
S26
C27
C28
S29
C30
031
C32
C33
034
H35
H36
H37
H38
H39
H40

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0583
-0.5475
0.1154
0.1090
0.0939
0.0943
0.0970
0.0981 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62
H63
H64 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0661
-0.0681
-0.0381
-0.0555
-0.1422
0.4293
0.1247
0.1254
0.1207
0.1205
0.1210
0.1210
0.1488 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H81
H82
H85
H86
H85
H86
H87
H88
 |
0.1634
0.1594
0.1588
0.1402
0.1407
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
0.1748
0.1816
0.1781
0.1786 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110
C111
H112 | -0.0949
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003
0.1387
0.0331
-0.0991
0.1350 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133
N134
C135
C136 | 0.1887
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1025
-0.1017
-0.4107
0.1678
-0.4107
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C156
C157
C158
N159
C160 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1370
0.1643
0.1960
0.0902
-0.1275
0.1669
-0.4024
0.1551 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C177
C178
C179
H180
H181
H182
H183
H184 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
-0.1304
0.0951
-0.1477
0.1541
0.1976
0.1655
0.1384
0.1861
0.1904
 |
| $\begin{array}{c} \text{H23} \\ \text{H23} \\ \text{Z} = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \end{array}$ | 0.1351
0.1350
18.75 A
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.2348
0.3872
-0.3088
0.3748
0.3590
0.1465
0.1467
0.1322 | C48
C48
C25
S26
C27
C28
S29
C30
C32
C33
C32
C33
C34
H35
H35
H37
H38
H39
H40
OA1

 | 0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0553
-0.5475
0.1154
0.1090
0.0939
0.0943
0.0970
0.0981
-0.592 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62
H63
H64
H65 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0661
-0.0881
-0.0555
-0.1422
0.4293
0.1247
0.1264
0.1207
0.1205
0.1210
0.1488
0.1491 | H96
H73
H74
H75
H76
H77
H78
H77
H78
H77
H80
H81
H82
H83
H84
H85
H86
H87
H88
H89
 |
0.1634
0.1594
0.1598
0.1402
0.1407
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1671
0.1748
0.1816
0.1781
0.1788 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110
C111
H112
C113 | 0.1670
0.1670
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1099
0.1126
-0.1003
0.1387
0.0331
-0.0991
0.1370 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C127
C128
C120
C130
C131
C132
C133
N134
C135
C136
C137 | 0.1887
0.1887
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1220
0.0627
-0.1025
-0.1017
-0.1670
-0.4107
0.1678
-0.1199
0.0997
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157
C158
N159
C160
C161 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1177
0.1901
0.1918
0.1735
0.1643
0.1960
0.0902
-0.1275
0.1669
-0.4024
0.1551
-0.1454 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179
H180
H181
H182
H183
H184 | 6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
-0.1304
0.0951
-0.1477
0.1541
0.1976
0.1685
0.1384
0.1904
0.1904
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \end{array}$ | 0.1351
0.1350
18.75 A
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
0.0845
-0.1335
-0.2348
0.3872
-0.3088
0.3748
0.3590
0.1466
0.1467
0.1322 | C48
C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O31
C32
C33
O31
H35
H36
H35
H36
H37
H38
H39
H40
O41
C42

 | -0.4241
-0.3153
0.3018
-0.2962
-0.1575
0.3241
0.0752
-0.5172
0.0582
0.0553
-0.5475
0.1154
0.1090
0.0943
0.0943
0.0981
-0.5092
0.0981 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62
H63
H64
H65 | -0.3773
-0.1456
-0.0552
-0.0406
-0.0661
-0.0585
-0.1422
0.4293
0.1247
0.1254
0.1207
0.1205
0.1210
0.1210
0.1488
0.1491
-0.4767 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
H84
H85
H84
H85
H86
H87
H88
H89
C90
 |
0.1634
0.1584
0.1588
0.1402
0.1402
0.1402
0.1424
0.1422
0.1626
0.1627
0.3718
0.2233
0.1706
0.1674
0.1706
0.1776
0.1776
0.1776 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110
C111
H112
C113
H114 | 0.1670
0.1670
0.1370
0.0473
0.0461
-0.1007
0.1408
-0.1100
0.1252
0.0445
-0.1099
0.1126
-0.1003
0.1387
0.0331
-0.0991
0.1350
-0.1372
0.0855 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133
N134
C135
C136
C137
C138 | 0.1857
-0.1244
0.0941
-0.1429
0.1581
-0.4080
-0.1649
0.0604
-0.1167
-0.1200
0.0627
-0.1017
-0.1017
-0.4107
0.1678
-0.1199
0.0997
-0.1486
 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157
C158
C156
C157
C158
N159
C160
C161
H162 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1180
0.1901
0.1901
0.1918
0.1735
0.1370
0.1963
0.1370
0.1960
0.0902
-0.1275
0.1669
-0.4024
0.1651
-0.1454 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C179
H180
H181
H182
H183
H184
H185 | $\begin{array}{c} 6.0000\\ \hline\\ \hline\\ -0.1077\\ -0.1065\\ 0.1134\\ -0.1802\\ -0.4006\\ 0.1628\\ -0.1304\\ 0.0951\\ -0.1477\\ 0.1541\\ 0.1976\\ 0.1655\\ 0.1384\\ 0.1861\\ 0.1904\\ 0.1941\\ 0.1941\\ 0.1941\\ \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
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-0.1335
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0.1324 | C48
C48
C25
S26
C27
C28
S29
C30
O31
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O31
C32
C33
O34
H35
H36
H37
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O41
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 | 0.4241
-0.3153
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C49
C50
C51
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C56
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C67 | -0.3773
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1.776 | C120
C97
H98
C99
C100
C101
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C110
C111
H112
C113
H114
C115 | 0.1670
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-0.0031
-0.0391
-0.3055
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C121
C122
C123
C124
N125
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C127
C128
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C132
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N134
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C136
C137
C138
C139 |
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H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C157
C158
N159
C160
C161
H162
H163 | 0.0815
0.1908
0.1534
0.1535
0.1180
0.1180
0.1901
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-0.1275
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-0.4024
0.1670
0.1670
0.1978 | Total
C169
C170
H171
H172
C173
N174
C176
C176
C177
C178
C179
H180
H181
H182
H183
H184
H185
H186
H185
H186 |
6.0000
-0.1077
-0.1065
0.1134
0.1124
-0.1802
-0.4006
0.1628
-0.1304
0.0951
-0.1477
0.1645
0.1384
0.1861
0.1904
0.1479
0.1479 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ z = \\ \hline 01 \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H20} \\ \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
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-0.5151
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-0.1335
-0.2348
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-0.3088
0.3590
0.1468
0.1467
0.1322
0.1324
0.1265 | C48
C25
S26
C27
C28
S29
C30
O31
C32
C33
O34
H35
H36
H37
H38
H39
H40
O41
C42
C43
O44

 | 0.4241
-0.3153
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-0.2962
-0.1575
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-0.5472
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0.0981
-0.5992
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0.0583 | 072
C49
C50
C51
C52
C53
C54
C55
C56
C57
H58
H59
H60
H61
H62
H63
H64
H65
O66
C67
C68 | -0.3773
-0.1456
-0.0552
-0.0669
-0.0649
-0.0649
-0.0555
-0.1422
0.4293
0.1244
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0.1488
0.1491
-0.4767
0.0002
0.0469 | H96
H73
H74
H75
H76
H77
H78
H79
H80
H81
H82
H83
H84
H85
H86
H87
H88
H86
H87
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H89
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H91
C92
 |
0.1634
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0.2233
0.1706
0.1671
0.1748
0.1816
0.1786
0.1776
-0.997
0.1373
-0.1976 | C120
C97
H98
C99
C100
C101
H102
C103
H104
C105
C106
H107
C108
H109
C110
C111
H112
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C116 | 0.1670
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0.0356
0.0855
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0.0356 | H144
C121
C122
C123
C124
N125
C126
C127
C128
C129
C130
C131
C132
C133
N134
C135
C136
C136
C137
C138
C139
H140 | 0.1857
-0.1244
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-0.4080
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-0.1200
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-0.1025
-0.1017
-0.1025
-0.1017
-0.4107
0.1640
-0.4109
0.0997
-0.12996
0.1580
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 | C168
H145
H146
H147
H148
H149
H150
H151
H152
H153
H154
H155
C156
C156
C157
C158
N159
C160
C161
H162
H163
C164 | 0.0815
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0.1911
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-0.4024
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-0.1678 | Total
C169
C170
H171
H172
C173
N174
C175
C176
C177
C178
C177
C178
C179
H181
H182
H181
H182
H184
H185
H186
H187 | $\begin{array}{c} 6.0000 \\ \hline \\ \hline \\ -0.1077 \\ -0.1065 \\ 0.1134 \\ 0.1124 \\ -0.1802 \\ -0.4006 \\ 0.1628 \\ -0.1304 \\ 0.0951 \\ -0.1477 \\ 0.1541 \\ 0.1976 \\ 0.1655 \\ 0.1384 \\ 0.1861 \\ 0.1904 \\ 0.1941 \\ 0.1479 \\ 0.1479 \\ 0.1479 \\ 0.1479 \\ 0.1479 \end{array}$
 |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H21} \end{array}$ | 0.1351
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18.75 Å
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-0.4589
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-0.5151
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0.1265 | C48
C48
C25
S26
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C28
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C30
O31
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C33
O34
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H36
H37
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C49
C50
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H58
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C68 | -0.3773
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| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \text{Z} = \\ \hline 01 \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C7} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H21} \\ \text{H22} \\ \text{H22} \end{array}$ | 0.1351
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H38
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O44
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C45
C47

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Total | $\begin{array}{c} 6.0000\\ \hline\\ \hline\\ -0.1077\\
-0.1065\\ 0.1134\\ 0.1124\\ -0.1802\\ -0.4006\\ 0.1628\\ -0.1304\\ 0.0951\\ -0.1477\\ 0.1541\\ 0.1976\\ 0.1655\\ 0.1384\\ 0.1861\\ 0.1904\\ 0.1941\\ 0.1941\\ 0.1479\\ 0.1947\\ 0.1947\\ 0.19467\\ 0.1900\\ 0.1873\\ 0.1384\\ 6.0000\\ \end{array}$ |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ z = \\ \hline \\ c1 \\ c2 \\ c3 \\ c4 \\ c5 \\ c6 \\ c7 \\ c8 \\ c9 \\ c10 \\ s11 \\ c12 \\ s13 \\ H14 \\ H16 \\ H17 \\ H18 \\ H19 \\ H20 \\ H21 \\ H22 \\ H23 \\ H24 \\ \hline z = \\ z = \\ \end{array}$ | 0.1351
0.1350
18.75 Å
-0.4309
0.0058
0.0513
-0.4589
0.0506
0.0371
-0.5151
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-0.2348
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23.27 Å | C48
C48
C25
S26
C27
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S29
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O31
C32
C33
O34
H35
H36
H37
H38
H39
H40
O41
C41
C42
C43
O44
C45
C46
O47
C47
C48

 | 0.4241
-0.3153
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-0.2962
-0.1575
0.0752
-0.5172
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-0.5475
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-0.5475
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-0.5092
-0.5105
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-0.4814
0.4242 | 072
C49
C50
C51
C52
C53
C54
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C56
C57
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H62
H63
H64
H65
O66
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C70
C71 | -0.3773
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C97
H98
C99
C100
C101
H102
C103
H104
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C137
C138
C136
C137
H140
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H142
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H144 |
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H154
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C158
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C168 | 0.0815
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C173
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C176
C177
C178
C179
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H186
H187
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H191
Total | $\begin{array}{c} 6.0000\\ \hline\\ -0.1077\\ -0.1065\\
0.1134\\ 0.1124\\ -0.4006\\ 0.1628\\ -0.1304\\ 0.0951\\ -0.1477\\ 0.1541\\ 0.1976\\ 0.1655\\ 0.1384\\ 0.1976\\ 0.1861\\ 0.19941\\ 0.19941\\ 0.1991\\ 0.1479\\ 0.1967\\ 0.1990\\ 0.1873\\ 0.1394\\ 6.0000\\ \end{array}$ |
| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \hline z = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ 07 \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{C12} \\ \text{S13} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H190} \\ \text{H21} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \text{H2} \\ $ | 0.1351
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| $\begin{array}{l} \text{H23} \\ \text{H24} \\ \textbf{z} = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C10} \\ \text{S111} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H22} \\ \text{H23} \\ \text{H24} \\ \textbf{z} = \\ \begin{array}{c} \textbf{z} \\ \text{C2} \\ \text{C2} \\ \end{array} \end{array}$ | $\begin{array}{c} 0.1350\\ 0.1350\\ 18.75 \\ A\\ \hline \\ -0.4309\\ 0.0058\\ 0.0518\\ -0.4589\\ 0.0506\\ 0.0371\\ -0.5151\\ 0.0845\\ -0.1335\\ -0.2348\\ 0.3872\\ -0.3088\\ 0.3748\\ 0.3590\\ 0.1468\\ 0.1467\\ 0.1322\\ 0.1324\\ 0.1263\\ 0.1265\\ 0.1281\\ 0.1281\\ 0.1281\\ 0.1449\\ 0.1442\\ 23.27 \\ A\\ \hline \\ -0.3942\\ -0.0049 \end{array}$ | C48
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| $\begin{array}{c} \text{H23} \\ \text{H24} \\ \text{H24} \\ \text{Z} = \\ 01 \\ \text{C2} \\ \text{C3} \\ 04 \\ \text{C5} \\ \text{C6} \\ \text{C9} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C9} \\ \text{C10} \\ \text{C11} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H16} \\ \text{H17} \\ \text{H18} \\ \text{H19} \\ \text{H22} \\ \text{H24} \\ \text{H22} \\ \text{H24} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C6} \\ \text{C7} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C9} \\ \text{C9} \\ \text{C10} \\ \text{C12} \\ \text{C2} \\ \text{C3} \\ \text{C6} \\ \text{C9} \\ \text{C6} \\ \text{C9} \\ \text{C10} \\ \text{C12} \\ \text{C12} \\ \text{C12} \\ \text{C2} \\ \text{C10} \\ \text{C11} \\ \text{C12} \\ C$ | $\begin{array}{c} 0.1350\\ 0.1350\\ 18.75 \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \$ | C48 C25 S26 C27 C27 C27 C30 031 C32 C33 034 H35 H36 H37 H38 H39 H40 041 C42 C43 C44 C45 C46 C47 C48 C25 S29 C30 C31 C32 C33 C34 H35 H36 H37

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| $\begin{array}{l} \text{H23} \\ \text{H24} \\ \text{H24} \\ \text{Z} = \\ 01 \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C5} \\ \text{C6} \\ \text{C6} \\ \text{C9} \\ \text{C10} \\ \text{C12} \\ \text{S13} \\ \text{H14} \\ \text{H15} \\ \text{H17} \\ \text{H16} \\ \text{H17} \\ \text{H22} \\ \text{H2} \\ \text{H2} \\ \text{C3} \\ \text{C4} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C1} \\ \text{C2} \\ \text{C3} \\ \text{C4} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C9} \\ \text{C1} \\ \text{C1} \\ \text{C2} \\ \text{C8} \\ \text{C9} \\ \text{C1} \\ \text{C2} \\ \text{C1} \\ \text{C1} \\ \text{C2} \\ \text{C3} \\ \text{C6} \\ \text{C6} \\ \text{C7} \\ \text{C8} \\ \text{C9} \\ \text{C9} \\ \text{C1} \\ \text{C2} \\ \text{C1} \\ \text{C1} \\ \text{C1} \\ \text{C2} \\ \text{C1} \\ \text{C1}$ | 0.1351
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C10	-0.2332	034	-0.5200	H58	0.1076	H82	0.2323	C106	-0.1371	C130	0.0794	H154	0.1658	C178	-0.1430
C12	-0.3124	H36	0.1819	H60	0.1035	H84	0.1968	C108	-0.1379	C131 C132	-0.1027	C156	0.1936	H180	0.1849
S13	0.4493	H37	0.1083	H61	0.1209	H85	0.1667	H109	0.1040	C133	-0.1788	C157	-0.1158	H181	0.1572
H14 H15	0.3650	H38 H39	0.1065	H62 H63	0.1216	H86 H87	0.1810	C110 C111	0.0145	N134 C135	-0.4020	C158 N159	0.1575	H182 H183	0.1502
H16	0.1553	H40	0.1296	H64	0.1403	H88	0.1748	H112	0.0899	C136	-0.1202	C160	0.1581	H184	0.1925
H17	0.1383	041	-0.5186	H65	0.1392	H89	0.1798	C113	-0.1243	C137	0.0995	C161	-0.1429	H185	0.1883
H18 H19	0.1388	C42 C43	0.0370	C67	-0.4704	H91	0.0828	C115	0.1392	C138 C139	-0.1449	H162 H163	0.1663	H186 H187	0.1464 0.1418
H20	0.1342	044	-0.5159	C68	0.0583	C92	-0.1266	C116	-0.1260	H140	0.1745	C164	-0.1780	H188	0.1953
H21 H22	0.1329	C45 C46	0.0530	069	-0.4865 0.0546	H93 C94	0.1388	H117 C118	0.1371	H141 H142	0.1511	C165 C166	0.0743	H189 H190	0.1853
H23	0.1543	040	-0.4897	C71	0.0055	C95	-0.1249	H119	0.0851	H143	0.1940	C167	-0.1162	H191	0.1508
H24	0.1552	C48	0.4184	072	-0.4303	H96	0.1410	C120	0.1697	H144	0.1921	C168	0.0696	Total	6.0000
 01	-0.3980	C25	-0.3054	C49	-0.1606	H73	0.1530	C97	-0.1312	C121	-0.1218	H145	0.1901	C169	-0.1064
C2	-0.0036	S26	0.4775	C50	-0.0619	H74	0.1520	Н98	0.1004	C122	0.0983	H146	0.1535	C170	-0.1059
C3	0.0410	C27	-0.2371	C51	-0.0552	H75	0.1212	C99	0.0139	C123	-0.1366	H147	0.1514	H171	0.1181
C5	0.0350	S29	0.4663	C53	-0.0656	H77	0.1213	C100	-0.1447	N125	-0.4110	H140 H149	0.1364	C173	-0.1715
C6	0.0356	C30	0.0791	C54	-0.0516	H78	0.1241	H102	0.0384	C126	-0.1602	H150	0.1881	N174	-0.4089
07 C8	-0.5164	C32	-0.5174 0.0438	C55	-0.0640	H79 H80	0.1284 0.1282	H104	-0.1106	C127 C128	-0.1153	H151 H152	0.1895	C175 C176	-0.1300
C9	-0.1355	C33	0.0444	C57	0.4200	H81	0.3463	C105	0.0490	C129	-0.1167	H153	0.1559	C177	0.1033
C10	-0.2316	034	-0.5262	H58	0.0979	H82	0.2354	C106	-0.1136	C130	0.0770	H154	0.1626	C178	-0.1408
C12	-0.3105	H36	0.1530	H60	0.1059	H84	0.1306	C108	-0.1254	C132	-0.1198	C156	0.1003	H180	0.1931
S13	0.4727	H37	0.1141	H61	0.1026	H85	0.1558	H109	0.0825	C133	-0.1619	C157	-0.1232	H181	0.1689
H14 H15	0.3719 0.1645	H38 H39	0.1141 0.1303	H62 H63	0.1208 0.1190	н86 H87	0.1749 0.1506	C110 C111	0.0169 -0.1056	N134 C135	-0.4368 0.1749	C158 N159	0.1597 -0.4061	H182 H183	0.1447 0.1795
H16	0.1642	H40	0.1289	H64	0.1301	H88	0.1619	H112	0.1069	C136	-0.1145	C160	0.1576	H184	0.1890
H17 H18	0.1486	041 C42	-0.5426 0.0426	H65 066	0.1317	H89 C90	0.1745	C113 H114	-0.1195 0.1325	C137 C138	0.0939	C161 H162	-0.1455 0.1655	H185 H186	0.1898
H19	0.1453	C43	0.0742	C67	-0.0012	H91	0.1028	C115	0.3176	C139	0.1545	H163	0.1926	H187	0.1488
H20	0.1458	044	-0.5155	C68	0.0623	C92	-0.0977	C116	-0.1208	H140	0.1808	C164	-0.1701	H188	0.1918
H21 H22	0.1375	C45 C46	0.0462	C70	-0.4876	H93 C94	0.2893	C118	-0.1326	H141 H142	0.1502	C165 C166	-0.1174	H189 H190	0.1895
H23	0.1590	047	-0.5037	C71	0.0188	C95	-0.1412	H119	0.1023	H143	0.1962	C167	-0.1156	H191	0.1571
H24	0.1599	C48	0.4038	072	-0.4743	H96	0.1001	C120	0.1697	H144	0.1924	C168	0.0763	Total	6.0000
 01	-0.4047	C25	-0.3037	C49	-0.1695	H73	0.1516	C97	-0.1109	C121	-0.1370	H145	0.1938	C169	-0.1116
C2	-0.0006	S26	0.4528	C50	-0.0675	H74	0.1506	H98	0.1291	C122	0.0856	H146	0.1561	C170	-0.1090
C3 04	-0.4281	C27 C28	-0.2397	C51 C52	-0.0619	H75 H76	0.1285	C99 C100	0.0365	C123 C124	-0.1449 0.1550	H147 H148	0.1557	H171 H172	0.1261
C5	0.0343	S29	0.4388	C53	-0.0607	H77	0.1327	C101	-0.1113	N125	-0.4040	H149	0.1147	C173	-0.1650
C6	0.0397	C30	0.0780	C54	-0.0691	H78	0.1327	H102	0.0946	C126	-0.1681	H150	0.1941	N174	-0.4031
C8	0.0802	C32	0.0481	C56	-0.1493	H80	0.1427	H104	0.1333	C127	-0.1140	H151 H152	0.1913	C176	-0.1202
C9	-0.1366	C33	0.0367	C57	0.4137	H81	0.3579	C105	0.0420	C129	-0.1134	H153	0.1610	C177	0.0892
C10 S11	-0.2361	U34 H35	-0.5186	H58 H59	0.0956	H82 H83	0.2245	C106 H107	-0.1055 0.1354	C130 C131	-0.1089	H154 H155	0.1716	C178 C179	-0.1430 0.1644
C12	-0.3073	H36	0.1480	H60	0.0877	H84	0.1096	C108	-0.1132	C132	-0.1080	C156	0.0873	H180	0.1945
S13	0.4451	H37	0.1205	H61	0.0942	H85	0.1519	H109	0.1178	C133	-0.1739	C157	-0.1181	H181	0.1742
H14 H15	0.1602	H39	0.1213	H63	0.0952	H87	0.1109	C110 C111	-0.0991	C135	0.1685	N159	-0.4073	H182 H183	0.1435
H16	0.1598	H40	0.1274	H64	0.1139	H88	0.1475	H112	0.1283	C136	-0.1334	C160	0.1582	H184	0.1932
H17 H18	0.1473	041 C42	-0.5463	H65 066	0.1162	H89 C90	-0.1705	C113 H114	-0.1149	C137 C138	-0.1450	C161 H162	-0.1453	H185 H186	0.1840
H19	0.1441	C43	0.0603	C67	0.0026	H91	0.1321	C115	0.3285	C139	0.1584	H163	0.1946	H187	0.1500
H20	0.1445	044	-0.5202	C68	0.0563	C92	-0.1414	C116	-0.1156	H140	0.1869	C164	-0.1616	H188	0.1854
H21 H22	0.1344	C45	0.0456	C70	0.0502	C94	0.3086	C118	-0.0989	H141 H142	0.1682	C166	-0.1181	H105 H190	0.1744
H23	0.1523	047	-0.5189	C71	0.0096	C95	-0.1378	H119	0.1280	H143	0.1943	C167	-0.1187	H191	0.1395
H24	40.99 Å	C48	0.3799	072	-0.4415	нэр	0.0834	C120	0.1653	H144	0.1891	C168	0.0696	lotal	6.0000
01	-0.4191	C25	-0.3040	C49	-0.2109	H73	0.1354	C97	-0.0927	C121	-0.1382	H145	0.1877	C169	-0.1084
C2	0.0021	S26	0.4539	C50	-0.1242	H74 H75	0.1369	H98	0.1407	C122	0.1099	H146	0.1482	C170	-0.1090
04	-0.4442	C28	-0.1400	C52	-0.0743	H76	0.1078	C100	0.0630	C124	0.1589	H148	0.1245	H172	0.1148
C5	0.0424	S29	0.4385	C53	-0.0846	H77	0.1187	C101	-0.1008	N125	-0.4022	H149	0.1267	C173	-0.1729
07	-0.5156	031	-0.5165	C55	-0.1240	п/8 Н79	0.1179	C103	-0.0926	C126	0.0661	H151	0.18/1 0.1921	C175	0.1725
C8	0.0817	C32	0.0505	C56	-0.1732	H80	0.1305	H104	0.1551	C128	-0.1213	H152	0.1783	C176	-0.1312
C10	-0.1360	034	-0.5059	H58	0.3922	H81 H82	0.3486	C105 C106	-0.0928	C129 C130	-0.1141 0.0536	H153 H154	0.1445	C177	-0.1537
S11	0.4681	H35	0.1522	H59	0.1145	H83	0.2092	H107	0.1548	C131	-0.0937	H155	0.2015	C179	0.1597
C12 S13	-0.3100 0.4479	H36 H37	0.1497 0.1289	н60 Н61	0.0996 0.0980	H84 H85	0.0942	C108 H109	-U.1004 0.1512	C132 C133	-0.0937 -0.1610	C156 C157	0.0818 -0.1220	н180 H181	0.1937 0.1627
H14	0.3635	H38	0.1302	H62	0.0847	H86	0.1551	C110	0.0436	N134	-0.4062	C158	0.1745	H182	0.1643
H15 H16	0.1537	H39 H40	0.1332	H63 H64	0.0911	H87 H88	0.0745	C111 H112	-0.0868	C135	0.1621	N159 C160	-0.4080	H183 H184	0.1927
H17	0.1398	041	-0.5276	H65	0.1034	H89	0.1534	C113	-0.1065	C137	0.1184	C161	-0.1443	H185	0.1871
H18	0.1403	C42	0.0536	066	-0.5123	C90	-0.0924	H114	0.1666	C138	-0.1446	H162	0.1621	H186	0.1530
н19 Н20	0.1357	043	-0.5148	C68	0.0160	л91 С92	-0.1429	C115 C116	-0.1073	H140	0.1606	d163 C164	-0.1929	H187	0.1533
H21	0.1322	C45	0.0583	069	-0.4955	H93	0.1329	H117	0.1679	H141	0.1461	C165	0.0786	H189	0.1919
H22 H23	0.1328	C46	0.0507	C70	0.0594	C94 C95	0.3248	C118 H119	-0.0863	H142 H143	0.1765	C166 C167	-0.1202	H190 H191	0.1884
H24	0.1536	C48	0.3445	072	-0.4682	H96	0.1291	C120	0.1624	H144	0.1957	C168	0.0884	Total	6.0000
z = -	44.83 Å		-0.2050		-0.0005		0 1001		-0.0011		-0 1071	D4.45	0 1010	0100	-0.0007
U1 C2	-0.4013	526 S26	-0.3058 0.4296	C50	-0.2005	н/З Н74	0.1234	U97 H98	-0.0914 0.1417	C121 C122	-0.1271 0.1194	н145 H146	0.1942	C169 C170	-0.0987
C3	0.0300	C27	-0.2430	C51	-0.1217	H75	0.0672	C99	0.0338	C123	-0.1455	H147	0.1234	H171	0.1354
U4 C5	-0.3817 0.0182	C28 S29	-U.1404 0.4136	C52 C53	-0.0845 -0.0794	H76 H77	0.0757	C100 C101	0.0618 -0.0997	0124 N125	0.1663 -0.4130	H148 H149	0.1467 0.1456	H172 C173	0.1357 -0.1737
C6	0.0434	C30	0.0761	C54	-0.1246	H78	0.1033	H102	0.1455	C126	-0.1702	H150	0.1871	N174	-0.4134
07	-0.5101	031	-0.5160	C55	-0.0919	H79	0.1058	C103	-0.0943	C127	0.0881	H151	0.1926	C175	0.1774
C9	-0.1407	C32	0.0518	C57	0.3642	H81	0.3356	C105	0.1535	C128	-0.1056	H152 H153	0.1764	C177	0.1240
C10	-0.2406	034	-0.5105	H58	0.1219	H82	0.2103	C106	-0.0945	C130	0.0849	H154	0.1697	C178	-0.1467
S11 C12	0.4336 -0.3053	H35 H36	0.1474 0.1451	H59 H60	0.1233 0.1116	н83 H84	0.2033	H107 C108	0.1521 -0.0993	C131 C132	-0.1141 -0.0994	H155 C156	0.1936 0.1171	0179 H180	0.1666 0.1945
S13	0.4126	H37	0.1258	H61	0.1113	H85	0.0982	H109	0.1499	C133	-0.1715	C157	-0.1226	H181	0.1639
H14	0.3707	H38 H30	0.1269	H62	0.0834	H86	0.1232	C110	0.0395	N134	-0.4017	C158	0.1689	H182	0.1493
H16	0.1623	H40	0.1277	H64	0.1230	H88	0.0963	H112	0.1463	C136	-0.1224	C160	0.1611	H184	0.2012
H17	0.1619	041	-0.5241	H65	0.1355	H89	0.1414	C113	-0.1093	C137	0.1208	C161	-0.1314	H185	0.1849
H18 H19	0.1624 0.1620	C42 C43	0.0437 0.0507	066 C67	-0.5287 0.0149	C90 H91	-0.0912 0.1429	H114 C115	0.1595 0.3468	C138 C139	-0.1332 0.1545	H162 H163	0.1647 0.1994	H186 H187	0.1437 0.1414
H20	0.1621	044	-0.5030	C68	0.0923	C92	-0.1164	C116	-0.1101	H140	0.1718	C164	-0.1737	H188	0.1904
H21	0.1364	C45	0.0797	069	-0.4980	H93	0.1415	H117	0.1609	H141	0.1451	C165	0.0776	H189	0.1977
п22 Н23	0.1570	040	-0.5312	C71	0.0531	C94 C95	-0.1161	H119	0.1466	H142 H143	0.2023	C165	-0.1058	H190	0.1904
H24	0.1514	C48	0.3563	072	-0.5348	H96	0.1397	C120	0.1799	H144	0.1877	C168	0.0839	Total	6.0000

Appendix F

Consideration of Metric Effect on the Bistable [2]Rotaxane Molecule during the Constant MD Simulations using Fixman's Theorem

When we consider a system with N generalized coordinates q_i , associated conjugated momenta p_i , and masses m_i , the Hamiltonian of this system H is given by

$$H(p,q) = \frac{1}{2}\mathbf{p}^{T}\mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q}), \qquad (F.1)$$

where \mathbf{M} is the "symmetric metric tensor" or "mass-metric tensor" that is defined as

$$M_{kl} = \sum_{i}^{N} m_i \frac{\partial \mathbf{r}_i}{\partial q_k} \cdot \frac{\partial \mathbf{r}_i}{\partial q_l}.$$
 (F.2)

Among N generalized coordinates, we consider that ν generalized coordinates q''_i are constrained, and rests of them q'_i are not. Then, according to the Fixman's theorem [3], the ratio of the original partition function Q and the partition function from the constraint dynamics Q_c is

$$\frac{Q}{Q_c} = \left(\det \mathbf{Z}\right)^{-1/2},\tag{F.3}$$

where

$$Z_{kl} = \sum_{i}^{\nu} \frac{1}{m_i} \frac{\partial q_k''}{\partial \mathbf{r}_i} \cdot \frac{\partial q_l''}{\partial \mathbf{r}_i}.$$
 (F.4)

In our simulation, the (det **Z**) is determined as the inverse of the CBPQT⁴⁺ ring's mass, $1/M_{\text{ring}}$. From Equation F.3, the difference between the original free energy $F = -k_BT \ln Q$ and the free energy from the constraint dynamics $F_c = -k_BT\ln Q$ is determined by

$$F - F_c = -k_B T \ln \left(\det \mathbf{Z}\right)^{-1/2} = -\frac{1}{2} k_B T \ln M_{\text{ring}} = \text{const.}$$
 (F.5)

Therefore, the metric effect only adds a constant scalar value to the absolute free energy values, which has no influence on the relative energetics.

Appendix G Time for Consumption of POPG

The formation of primary ozonide (POZ), which is the first step in the ozonolysis of 1-palmitoyl-2oleoyl-*sn*-phosphatidylglycerol (POPG) at the air-liquid interface, is described as

$$O_3 + POPG \xrightarrow{k_1} POZ.$$
 (G.1)

The ozone concentration is assumed to be constant during the reaction, which allows calculating the reaction rate using the pseudo-first order rate constant $k_2 = k_1 [O_3]$, where $k_1 = 4.5 \times 10^{-16}$ cm³ molecule⁻¹ s⁻¹ adopted from the OPPC ozonolysis on NaCl [4]. The ozone concentration, measured spectrophotometrically using an absorption cell with 10 cm path length, is determined to be $\sim 5 \times 10^{14}$ molecule cm⁻³ (20 ppm). The reaction rate is expressed as

$$-\frac{d\left[\text{POPG}\right]_{surf}}{dt} = k_2 \left[\text{POPG}\right]_{surf,0}.$$
(G.2)

Solving Equation G.2 gives

$$\frac{[\text{POPG}]_{surf}}{[\text{POPG}]_{surf,0}} = e^{-k_2 t}.$$
(G.3)

For 90 % and 99 % depletion of POPG at the air-liquid interface, it takes \sim 10 s and \sim 20 s, respectively.

Appendix H Bulk-phase Ozonolysis

H.1 Methods

H.1.1 Chemicals and Reagents

Ammonium bicarbonate (NH_4HCO_3), iron (II) dichloride ($FeCl_2$), sodium ethylenediaminetetraacetic acid (EDTA), trypsin from porcine pancreas were purchased from Sigma-Aldrich (St. Louis, MO). SP-B₁₋₂₅ was purchased from Biomer Technology (Hayward, CA).

H.1.2 Bulk-phase O₃ Reaction

A continuous flow of ~ 20 ppm O₃ in air was applied to the 100 μ M SP-B₁₋₂₅ solution in 1:1 (by volume) water and methanol solvent for 30 s, 1, 1.5, 2, 3, 4, and 5 min. The SP-B₁₋₂₅ solution was diluted to 50 μ M for ESI with 1:1 water/methanol and 1 % acetic acid by volume. Trypsin digests of SP-B₁₋₂₅ and O₃ treated SP-B₁₋₂₅ were prepared by incubating 200 μ M of SP-B₁₋₂₅ with 6 μ g of trypsin from porcine pancreas in 1 mL of water containing 25 mM ammonium bicarbonate (NH₄HCO₃) at 37°C for 4 hours. The trypsin was then removed using a Millipore Microcon centrifugal filter fitted with an Ultracel YM-10 membrane. The sample solution was diluted to an appropriate concentration for ESI with 1:1 water/methanol and 1 % acetic acid by volume. Product analysis was performed on a Thermo Finnigan LCQ Deca XP ion trap mass spectrometer (ITMS) in positive and negative modes. The nomenclature proposed by Roepstorff and Fohlman [5] was used for the parent and fragment ions.

H.1.3 Fenton Reaction

SP-B₁₋₂₅ (500 μ M) was incubated with 600 μ M FeCl₂, 600 μ M sodium EDTA, and 30 mM H₂O₂ in 1 mL water at 37°C for 12, 18, and 24 h. The peptide was purified using a Varian C18 OMIX 100 μ L pipette tip. The sample solution was diluted to an appropriate concentration with 1:1



Figure H.1: (a) Quadruply charged SP- B_{1-25} and oxidized products from (b) the bulk-phase O_3 reaction and (c) the Fenton reaction with intact SP- B_{1-25} . (d) Triply charged SP- B_{1-25} and oxidized products from (e) the bulk-phase O_3 reaction and (f) the Fenton reaction are also shown.

water/methanol and 1 % acetic acid by volume. Product analysis was performed on a Micromass QTof2 quadrupole time of flight mass spectrometer in the positive ion mode.

H.2 Results and Discussion

Triply and quadruply protonated SP-B₁₋₂₅ are observed as dominating ions in the ESI-MS spectrum with a small amount of doubly protonated peptides (Figures H.1a and H.1d). Figure H.1 shows oxidized products of triply and quadruply charged SP-B₁₋₂₅ from the bulk-phase O₃ reaction and the Fenton reaction with intact SP-B₁₋₂₅. As seen in Figures H.1b and H.1e, incorporation of three and nine oxygens in SP-B₁₋₂₅ are observed as major products from the bulk-phase O₃ reaction with the peptide. Other oxygenated peptides (+ 4O and + 5O) are also observed as minor products in the spectrum. The Fenton reaction yields a series of oxidized SP-B₁₋₂₅ products with up to 10 oxygen atoms (Figures H.1c and H.1f). It is notable that the bulk-phase O₃ reaction yields dominating products of 3- and 9-oxygenated SP-B₁₋₂₅. This suggests the high stability of SP-B₁₋₂₅ incorporating 3 and 9 oxygen atoms. In order to determine structures of the oxidized SP-B₁₋₂₅ by the bulk-phase O₃ reaction, trypsin digest was performed after applying O₃ for 3 min to the SP-B₁₋₂₅ solution.



 $SP-B_{1\cdot 25}:\ F_1P_2I_3P_4L_5P_6Y_7C_8W_9L_{10}C_{11}R_{12}A_{13}L_{14}I_{15}K_{16}R_{17}I_{18}Q_{19}A_{20}M_{21}I_{22}P_{23}K_{24}G_{25}$

Figure H.2: (a) The ESI mass spectrum of the trypsin digests of SP-B₁₋₂₅ in positive mode. (b) The ESI mass spectrum of the trypsin digests of the oxidized SP-B₁₋₂₅ from the bulk-phase O₃ reaction in positive mode. (c) The negative mode ESI mass spectrum of the trypsin digests of the oxidized SP-B₁₋₂₅ from the bulk-phase O₃ reaction.



Figure H.3: (a) The CID spectrum of cationic IQAMIPK + 3O at m/z 817 from the tryptic digest of the oxidized SP-B₁₋₂₅. (b) The CID of cationic FPIPLPYCWLCR + 8O at m/z 1636 from the tryptic digest of the oxidized SP-B₁₋₂₅. (c) The CID of anionic FPIPLPYCWLCR + 8O at m/z 1634 from the tryptic digest of the oxidized SP-B₁₋₂₅.

The ESI mass spectrum of a trypsin digest of SP-B_{1-25} exhibits 7 major ion peaks. The masses and segments of the observed tryptic digest ions of SP-B_{1-25} are indicated in Figure H.2a. The ESI mass spectrum of a trypsin digest of SP-B_{1-25} oxidized by reaction with bulk-phase O₃ exhibits segments with MetSO (m/z 817, m/z 874, and m/z 1030) and the less abundant N-terminal segment of FPIPLPYCWLCR + 8O at m/z 1636 in positive ion mode (Figure H.2b). The negative ion mode ESI mass spectrum also exhibits corresponding deprotonated segment ion peaks (Figure H.2c).

The structures of segments are confirmed by CID spectra. As seen in Figure H.3a, the CID of the ion at m/z 817 exhibits the elimination of hydrosulfinylmethane (CH₄SO, 64 mass unit), which is the characteristic dissociation pathway of methionine sulfoxide (MetSO) [6, 7]. The structure of the segment FPIPLPYCWLCR + 80 is also investigated using CID. Fragments from the CID of



Figure H.4: ESI-MS² of triply oxygenated products of quadruply protonated SP-B₁₋₂₅ from (a) bulk-phase O_3 application, and from (b) the Fenton reaction. M denotes a parent ion, which is triply oxygenated SP-B₁₋₂₅.

the cationic FPIPLPYCWLCR + 80 at m/z 1636 yields y-type fragments (y_7 and y_9) with all eight oxygen atoms as dominant products (Figure H.3b). The fragment PLPYCW with six oxygen atoms indicates that Cys₈ and Trp₉ are oxidized to sulfonic acid (+ 30) and hydroxy-Nformylkynurenine (HNFKyn, + 30), respectively. Thus, we can assume that Cys₁₁ is oxidized to sulfenic acid (+ 20). The structures are further confirmed by the fragments of c_8 + 30 and PLPYC + 30 resulting from the CID of FPIPLPYCWLCR + 80 in negative ion mode (Figure H.3c). It is notable that Cys₈ and Cys₁₁ are located next to each other in the helical structure [8]. Asymmetric oxidation of closely located Cys residues is caused by the possible formation of sulfonic anhydride (R₁-O₂SOSO₂-R₂). No segment peak is observed from the triply oxygenated SP-B₁₋₂₅ after tryptic digest of the products from the bulk-phase O₃ reaction.

The observed high abundance of SP-B₁₋₂₅ where 3 and 9 oxygen atoms have been added can be explained by the distinct oxidation mechanisms of O₃ in aqueous solution. Cys easily undergoes oxidation by O₃ to form sulfonic acid in aqueous solution primarily by reactions with secondary oxidants [9]. Cys₈ and Cys₁₁, which are located near the hydrophobic N-terminal site in SP-B₁₋₂₅, are hardly oxidized by reactive oxygen species (ROS) at the air-liquid interface. Trp₉ and Met₂₁ are oxidized to form NFKyn and MetSO by ozonolysis and ROS, respectively, by interfacial reactions. This induces a change in peptide orientation in the interface that results in NFKyn, Cys₈, and Cys₁₁ being exposed to ROS for further oxidation. As a result, NFKyn occurs to form HNFKyn and, simultaneously, Cys₈ and Cys₁₁ are also oxidized by ROS to form sulfonic anhydride.

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The $SP-B_{1-25}$ products with three additional oxygen atoms from both reactions are analyzed using CID. Figure H.4 shows CID spectra ($ESI-MS^2$) of triply oxygenated products of quadruply protonated SP-B₁₋₂₅ from bulk-phase O_3 application and from the Fenton reaction. The ESI-MS² spectrum of the triply oxygenated SP-B₁₋₂₅ by bulk-phase O_3 application implies the presence of two products, one with NFKyn (+20) and MetSO (+10), and the other with HNFKyn (+30). Evidence of the MetSO in the oxidized SP- B_{1-25} is found from the CID experiment involving the quadruply charged SP- B_{1-25} product from the bulk-phase O_3 reaction (Figure H.4a). For example, the paired fragments of y_{20} -CH₄SO and y_{20} fragments, which are observed at m/z 782 and m/z 803 (triply charged) and at m/z 1172 and m/z 1204 (doubly charged), confirm the presence of MetSO (Figure H.4a). Interesting CID fragments are also observed in the $ESI-MS^2$ spectrum. The singly charged fragment at m/z 680, m/z 832, and m/z 938 are WLCRA + 30, LPYCWLCRALIKR + 30 and PLPYCWLCRALIKRI + 30, respectively. These fragments are evidence of the formation of HNFKyn through the oxidation of Trp_9 from the bulk-phase O_3 reaction. This is further supported by the singly charged fragment at m/z 652, QAMIPK-NH₃, which indicates that no oxidation has occurred at Met₂₁. The ESI-MS² spectrum of the triply oxygenated SP-B₁₋₂₅ by bulk-phase O_3 reaction implies the presence of two products, one with NFKyn (+20) and MetSO (+10), and the other with HNFKyn (+ 3O). The CID fragment abundance implies that the bulk-phase O₃ reaction with $SP-B_{1-25}$ yields more product peptides with HNFKyn compared to product peptides with NFKyn and MetSO. The ESI-MS² spectrum of $SP-B_{1-25}$ product from the Fenton reaction is shown in Figure H.4b. The CID of the Fenton product exhibits the presence of HNFKyn at m/z 652, m/z 680, and m/z 938, which corresponds to the singly charged fragments QAMIPK-NH₃, WLCRA + 3O, and PLPYCWLCRALIKRI + 3O, respectively. However, evidence for the formation of the product with NFKyn and MetSO is not found in the spectrum.

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