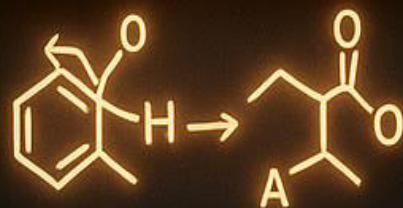
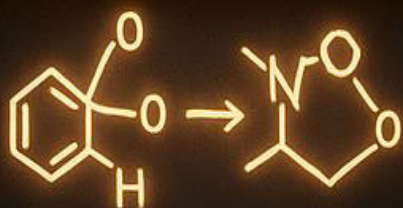
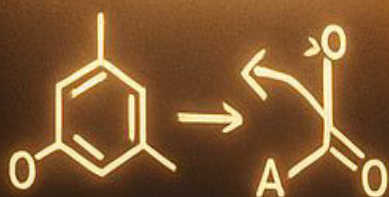


Computational Mechanistic Assessment in the Unexpected Synthesis of Indolizines Using Lawesson and Woollins Reagents

INDOLIZINE



Tesis

que para obtener el grado de
Maestro en Ciencias Químicas

Presenta

José Antonio Sandoval Mendoza

Director de Tesis:

Dr. José Oscar Carlos Jiménez Halla

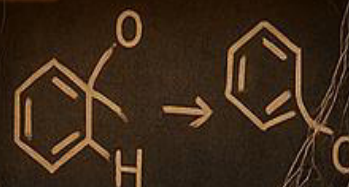
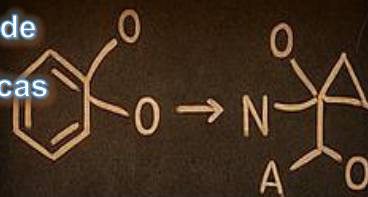
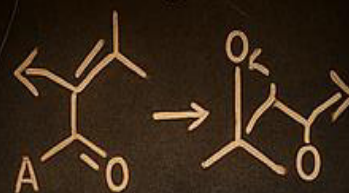
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To my family. Thanks to my parents for all the support and encouragement to keep studying and growing. My brother for the support and being there for me when I needed it. And my grandmother, for always believes in me.

Thanks to Dr. Óscar Halla for giving me the chance to work in the group and on the project.

And finally, thanks to all my friends for making my time in the master enjoyable.

UNIVERSIDAD DE GUANAJUATO
DEPARTAMENTO DE QUIMICA
DIVISION DE CIENCIAS NATURALES Y EXACTAS

The undersigned hereby certifies that the research work reported in this thesis, entitled ***Computational Mechanistic Assessment in the Unexpected Synthesis of Indolizines Using Lawesson and Woollins Reagents***, submitted in fulfillment of the requirements for the degree of Master of Science in Chemistry, has been carried out under my supervision and that of Dr. Diego Marcelo Andrada from the Department of General and Inorganic Chemistry at Saarland University, Germany. We are especially grateful to *Dr. Crispín Silviano Cristóbal Gasga* for his technical contributions and for providing the experimental data, which originated from his research group. This work is original and is being presented for the first time for the purpose of obtaining an academic degree.

A handwritten signature in blue ink, appearing to read 'JOCM', with a stylized flourish at the end.

Dr. José Oscar Carlos Jiménez Halla
Supervisor of Thesis

Publications and Conferences During this Thesis

Publications

1.- Leonardo I. Lugo-Fuentes, Victor A. Lucas-Rosales, J. Antonio Sandoval-Mendoza, Dr. Rong Shang, Dr. Juan Pablo Martínez, Prof. Dr. J. Oscar C. Jiménez-Halla "Different Reaction Modes Operating in ansa-Half-Sandwich Magnesium Catalysts". Chemistry a European Journal. 2024 Volume 30, Issue 23.

2.- [On List]

Attended Conferences

1.- LatinXChem 2024. "Lawesson and Woollins reagent: Elimination instead of substitution". Poster presentation. Online. October 2024.

2.- Aromaticity 2025. "Use of Lawesson and Woollins reagent to synthesize indolizines". Poster presentation. Mérida, Yucatán. January 2025.

3.- Jacobo Gómez Lara Symposium. Poster June 2024. Oral Presentation December 2024. Poster June 2025

Abstract

In this work, a computational study was carried out to explore the synthesis of indolizines through two different pathways employing Lawesson's reagent. Both routes have been experimentally implemented, and the aim is to understand why a substitution reaction (typically expected with this reagent) does not occur, while an anomalous elimination reaction is observed instead. The goal is to identify a synthetic route that yields indolizines efficiently at room temperature, which is also uncommon. Additionally, the specific reaction mechanism is proposed for each route, along with a theoretical alternative using Woollins' reagent to obtain the same products.

In the first mechanism, the substrate 3-(pyridin-2-ylmethylene)pentane-2,4-dione presents only two reactive sites: a carbonyl group and an adjacent unsaturated carbon. To obtain the final product, the compound must undergo cyclization and oxygen elimination. Cyclization occurs readily through the attack of the carbonyl on a phosphorus atom. For oxygen elimination, the only viable pathway involves the formation of a P–O bond and a C–S bond, with the oxygen being expelled from the bicyclic system via an attack on another fragment of Lawesson's reagent, followed by a migration and cleavage of the C–S bond. In any other scenario, the oxygen atom would be forced to donate electron density, significantly increasing the energy barriers.

In the second mechanism, the formation of the indolizine also requires cyclization, as well as the elimination of oxygen and two hydrogen atoms. In this case, the only initial reactive site in (Z)-4-(phenylamino)-3-(pyridin-2-ylmethyl)pent-3-en-2-one involves the phosphorus and the oxygen atoms. Cyclization again takes place through the attack of a carbonyl group on phosphorus. A sulfur atom induces dehydrogenation, while the oxygen is expelled from the ring, stabilized by an additional sulfur–hydrogen interaction. Hydrogen sulfide is formed as a byproduct, and the substituted fragment of Lawesson's reagent subsequently reacts to yield the indolizine and stable side products.

The results show energy barriers in the range of 20–25 kcal/mol, consistent with the experimental conditions. In contrast, calculations for substitution mechanisms in both pathways reveal significantly higher barriers, above 30 kcal/mol, making them unfeasible under the observed conditions and explaining why such reactions do not occur.

Resumen

En este trabajo se llevó a cabo un estudio computacional para explorar la síntesis de indolizinas mediante dos rutas diferentes que emplean el reactivo de Lawesson. Ambas rutas han sido realizadas experimentalmente, y el objetivo es comprender por qué no ocurre una reacción de sustitución (como cabría esperar convencionalmente con este reactivo) mientras que sí tiene lugar una reacción anómala de eliminación. Se busca así identificar una vía sintética para obtener indolizinas con buenos rendimientos a temperatura ambiente, lo cual resulta igualmente poco común. Además, se propone el mecanismo específico de reacción para cada ruta, así como una alternativa teórica que utiliza el reactivo de Woollins para alcanzar los mismos productos.

En el primer mecanismo, el sustrato 3-(piridin-2-ilmetileno)pentano-2,4-diona presenta únicamente dos sitios reactivos: un grupo carbonilo y un carbono insaturado adyacente. Para formar el producto final, el compuesto debe sufrir una ciclación y una eliminación de oxígeno. La ciclación se produce fácilmente mediante el ataque del carbonilo a un átomo de fósforo. Para la eliminación del oxígeno, se demuestra que la única vía viable implica la formación de un enlace P–O y un enlace C–S, con la expulsión del oxígeno del sistema bicíclico mediante su ataque a otro fragmento del reactivo de Lawesson, seguido por una migración y ruptura del enlace C–S. Esto se debe a que, en otros escenarios posibles, el átomo de oxígeno se vería forzado a donar densidad electrónica, lo que incrementaría considerablemente las barreras energéticas.

En el segundo mecanismo, la formación de la indolizina también requiere una ciclación, así como la eliminación de oxígeno y de dos átomos de hidrógeno. En este caso, el único sitio reactivo inicial del (Z)-4-(fenilamino)-3-(piridin-2-ilmetil)pent-3-en-2-ona involucra al oxígeno y al fósforo. La ciclación vuelve a producirse mediante el ataque de un carbonilo al fósforo. Un átomo de azufre induce la deshidrogenación, mientras que el oxígeno es eliminado del anillo, estabilizado por una interacción azufre–hidrógeno adicional. Como subproducto se forma sulfuro de hidrógeno, y el fragmento sustituido del reactivo de Lawesson reacciona posteriormente para dar lugar a la indolizina y subproductos estables.

Los resultados obtenidos muestran barreras energéticas en el rango de 20–25 kcal/mol, en consonancia con las condiciones experimentales. En contraste, los cálculos para mecanismos de sustitución en ambas rutas revelan barreras significativamente más altas, superiores a 30 kcal/mol, lo que las hace inviables bajo las condiciones observadas y explica por qué dicha reacción no se presenta.

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Abbreviation Table

Lawesson Reagent	LR
Woollins Reagent	WR
Transition state	TS
Dichloromethane	DCM
Nuclear Magnetic Resonance	NMR
Natural Bond Orbital	NBO
Nucleus Independent Chemical Shifts	NICS
Density Functional Theory	DFT
Kohn-Sham	KS
Hartree-Fock	HF

Prolog

The present thesis provides a detailed computational analysis aimed at elucidating the mechanistic pathways underlying the unexpected synthesis of indolizines using Lawesson's reagent, a reaction of considerable chemical interest. Employing state-of-the-art computational methods grounded in Density Functional Theory (DFT), this study systematically investigates two experimentally established synthetic routes, offering insights into the unique mechanistic aspects responsible for the atypical elimination reactions observed, as opposed to the anticipated substitution processes.

The document opens with a comprehensive overview of the historical context, chemical significance, and practical applications of indolizines and Lawesson's reagent in Chapter 1. This introduction serves to contextualize the research objectives, clearly highlighting the relevance and necessity of a thorough mechanistic understanding. Additionally, the potential for extending these theoretical insights to related reagents, such as Woollins' reagent, is briefly discussed to underscore broader chemical applicability.

Following the introductory framework, the thesis outlines the computational methodology employed, presenting the theoretical foundations and justifying the chosen techniques and parameters as described in Chapter 2. The core of the work subsequently details each identified reaction mechanism, elucidating critical intermediates, transition states, and energy profiles in Chapters 3 and 4. These findings are thoroughly analyzed in the context of experimental data, providing clarity on why certain pathways are energetically favored.

In the concluding discussion, the thesis synthesizes these mechanistic insights, offering interpretations that advance the fundamental understanding of reactions involving Lawesson's reagent and highlighting the implications for future synthetic and theoretical investigations. Some perspectives are exposed at the end of the document as well as previous reaction pathways initially explored in Appendix 1 and the Cartesian coordinates of the optimized structures in Appendix 2.

Thanks to Dr. Crispín Silviano Cristóbal Gasga and Dr. Christopher Emmanuel Rivas Lopez, as all experimental information corresponds to them and their work.

For all information, see Dr. Rivas's thesis in the University of Guanajuato repository:

<http://repositorio.ugto.mx/handle/20.500.12059/4489>

<http://repositorio.ugto.mx/handle/20.500.12059/8702>

Chapter 1

Lawesson and Woollins Reagents in Organic Chemistry

This chapter will cover several topics, beginning with an explanation of Lawesson reagent (LR) and Woollins' reagent (WR), their origins, and their chemistry.

Next, the cyclization process and indolizines, structural isomers of indole, with highly distinctive chemical properties will be discussed. Their stability and their synthesis have long been of interest due to the high-temperature conditions for expensive catalysts typically required.

Finally, I will relate these concepts to the synthesis under investigation an unreported reaction in which LR atypical reactivity, leading to the formation of an indolizine. WR is also considered a promising candidate for theoretical prediction.

Importance of Organophosphorus Reagents

Organophosphorus reagents play a vital role in organic synthesis, organometallic chemistry, and polymeric production due to their wide range of reactivity and functional group compatibility.¹ Throughout history, different compounds have been developed that remain in use to this day. For instance, the Wittig reaction (**Figure 1**) is a chemical reaction of a carbonyl group (often acetone or aldehyde) with a phosphorus ylide to form an alkene.²

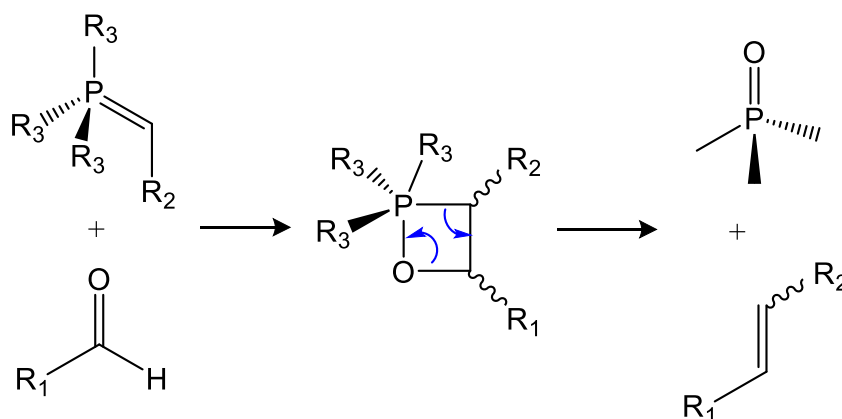


Figure 1. Overview of Wittig reaction mechanism.

Other reaction where organophosphorus compounds are involved is the Horner–Wadsworth–Emmons reaction (**Figure 2**) used in organic chemistry of stabilized

phosphonate carbanions with aldehydes (or ketones) to produce predominantly E-alkenes.³

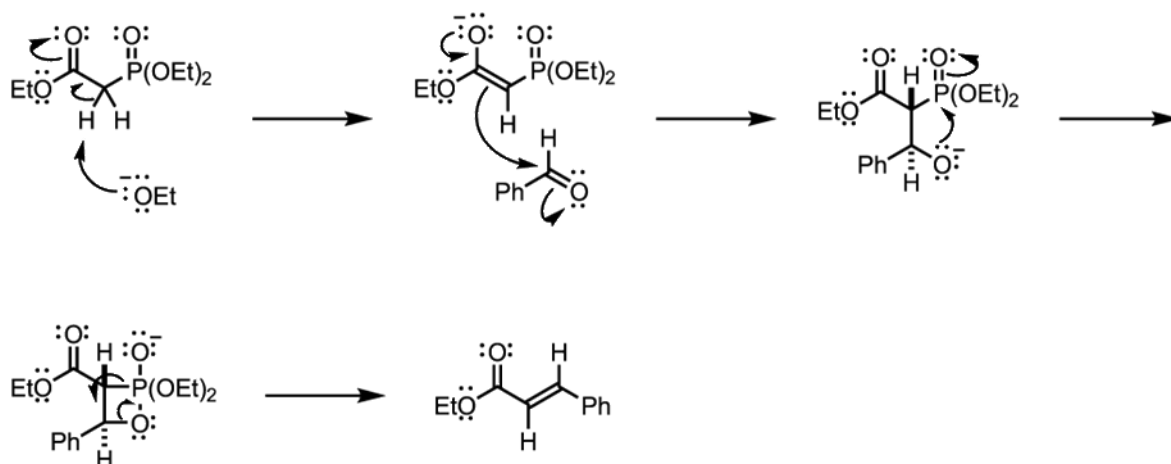


Figure 2. Overview of the Horner-Wadsworth-Emmons reaction mechanism.

Some organophosphorus compounds are used to reduce or react with oxygen, mainly carbonyls due to their affinity.⁶ Among them, Lawesson and Woollins reagents are used to replace carbonyl oxygens or alcohols with other alkyl oxygens: sulfur and selenium, respectively.^{4,5} I will delve deeper into these for the present project.

Lawesson Reagent

Lawesson reagent (**Figure 3**) is a widely used organophosphorus compound known for converting carbonyl compounds to thiocarbonyl derivatives (thionation reaction).⁷ Due to its versatility and efficiency, it has become a stable reagent in modern synthetic organic chemistry. The history of LR dates to 1956 when a group of researchers studying the reaction of arenes and aryls with various phosphorus sulfides identified this chemical species among their synthesized products (**Figure 4**).⁸

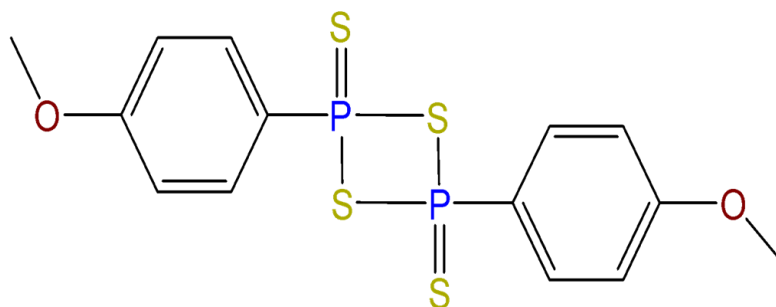


Figure 3 Lawesson Reagent

However, it was not until the 1970s that Dr. Sven-Olov Lawesson employed this reagent to replace carbonyl groups with sulfur,⁹ leading to its name in his honor.

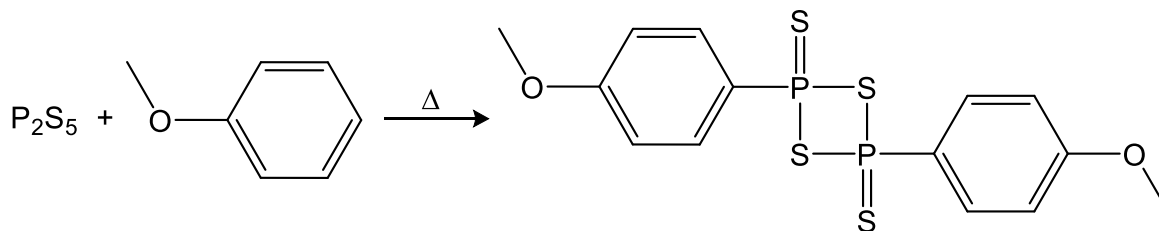


Figure 4 Synthesis of Lawesson Reagent.

In subsequent years, LR found applications in substitution reactions, metal complex formation, macrocycles, heterocycles, nucleophilic adducts, and twisted motifs, among others (**Figure 5**). However, it is worth noting that no simple elimination reactions have been reported.^{10,11}

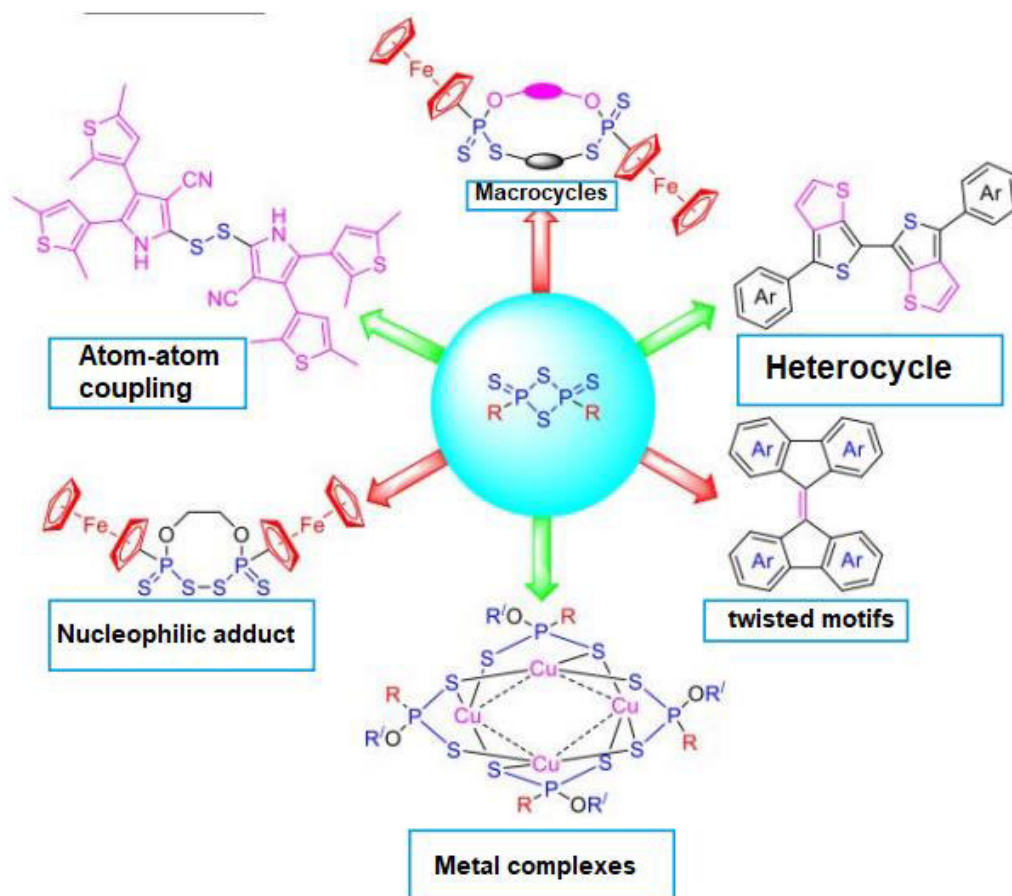


Figure 5. Reported reactivity of Lawesson Reagent.

Woollins Reagent

Woollins Reagent (**Figure 6**), on the other hand, is a chemical species synthesized and discovered by Dr. Derek Woollins in the 1990s (**Figure 7**).¹² Following the same principle as Lawesson reagent, WR was designed to generate selenones by substituting carbonyl groups.^{13,14}

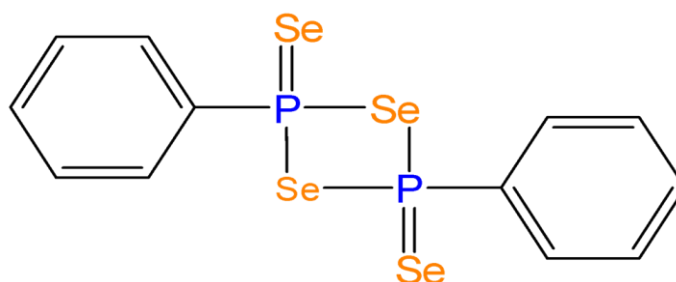


Figure 6 Woollins Reagent

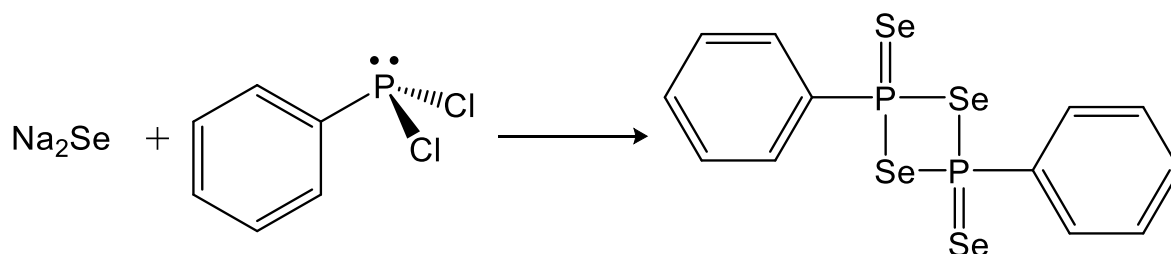


Figure 7 Synthesis of Woollins Reagent

However, due to its high lability, this reagent can also form various adducts and complexes.¹⁵ Like LR, it exhibits a broad range of reactivity, yet no reports of a simple elimination reaction exist for this reagent either (**Figure 8**).

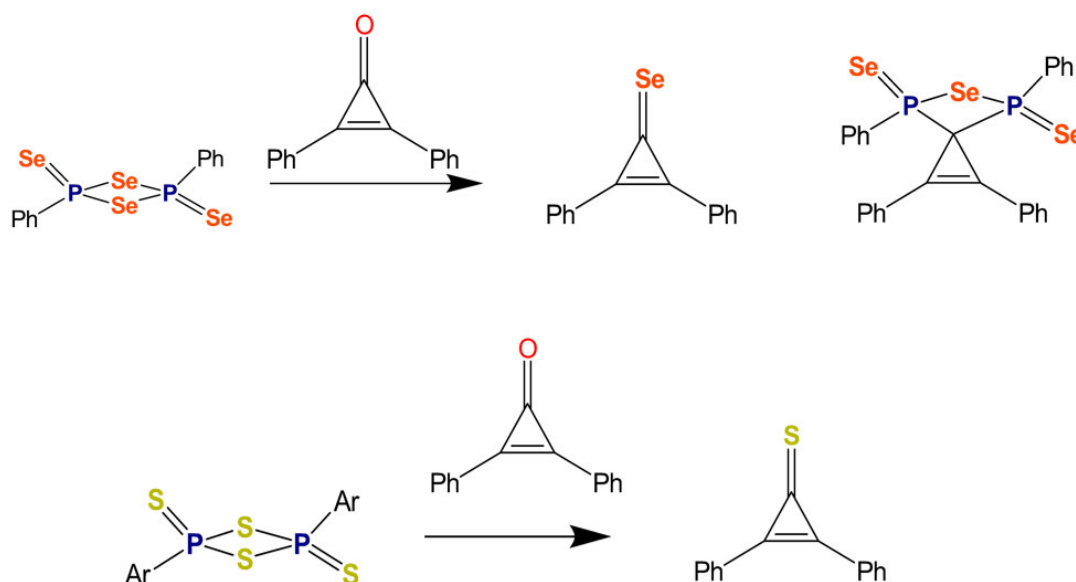


Figure 8. Lability of Woollins Reagent compared to Lawesson Reagent.

Substitution Reaction

The reaction mechanism of LR and WR, as previously mentioned, involves the substitution of a carbonyl group by the respective chalcogen of the reagent used.¹⁶

As it is appreciated in the image (**Figure 9**) in the first step, the reagent dissociates into two fragments; in the literature, this is described as an equilibrium.

These fragments are then attacked by the carbonyl oxygen through a first transition state (TS), forming a four-membered cyclic intermediate.

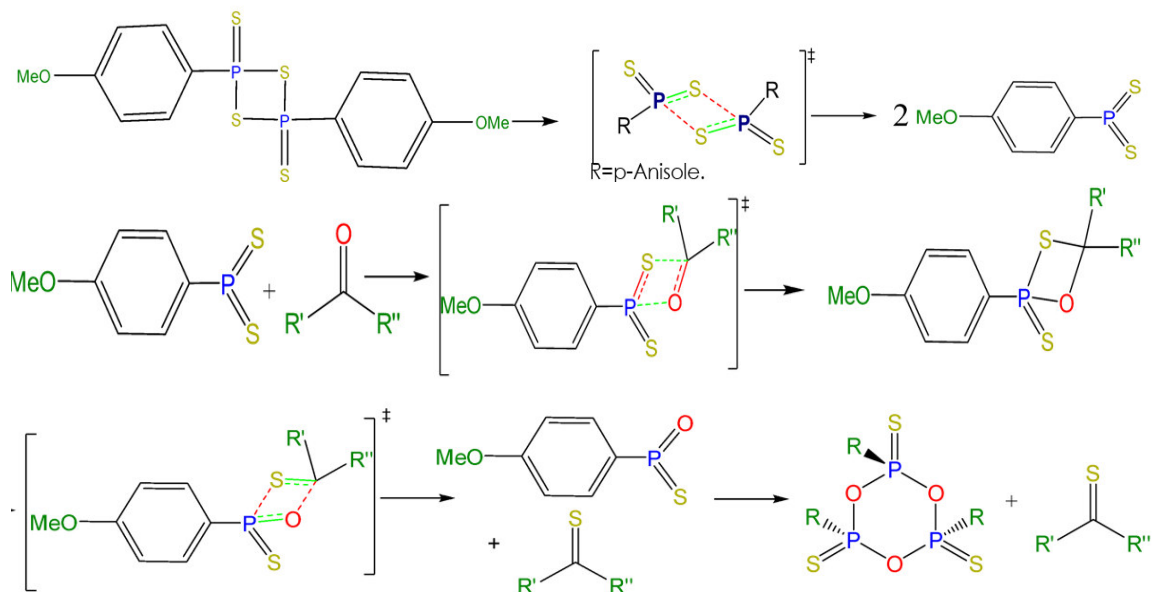


Figure 9. Lawesson Reagent Mechanism

This intermediate subsequently undergoes cleavage via another TS, leading to the expected substitution. Some reports consider this to be the final step of the reaction; however, characterization studies have shown that, in addition to the substituted molecule, the final product also includes a six-membered ring formed by three substituted fragments in the case of Lawesson reagent.¹⁷

For Woollins' reagent, the mechanism (**Figure 10**) follows the same pattern of reactivity with carbonyl.^{18,19} However, there are no reports of the formation of a six-membered ring, as the substituted fragment itself is highly stable.

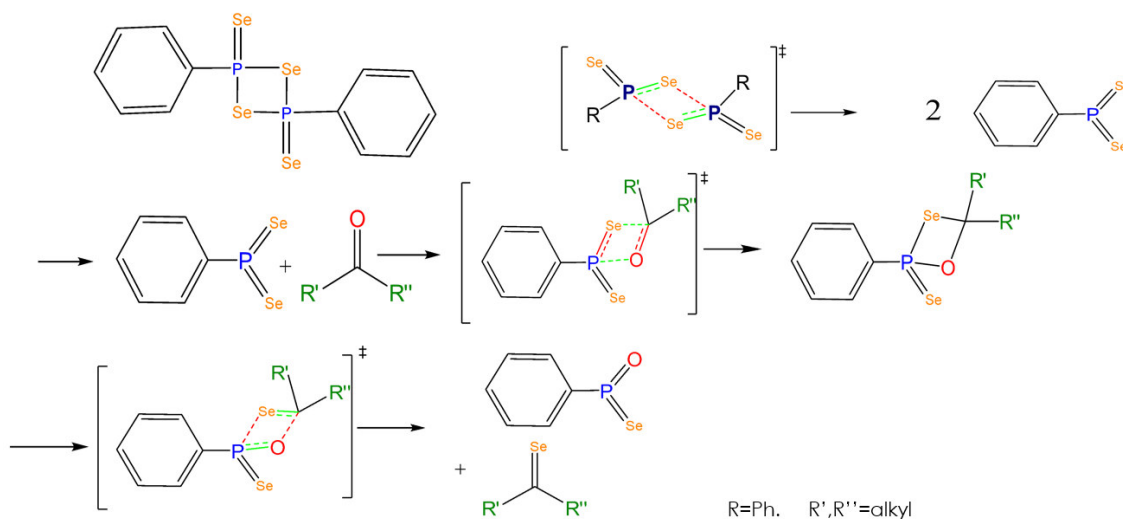


Figure 10. Woollins Reagent Mechanism

Cyclization and the importance of Indolizines

Chemical cyclization is a chemical reaction that forms rings from linear chains.²⁰ Cyclization is a fundamental type of intramolecular reaction in organic chemistry, involves the formation of new bonds that connect the ends of a molecular chain, closing it into a ring.^{21,22}

This process typically involves the formation of a new covalent bond between two non-adjacent atoms within the same molecule, often accompanied by the elimination of small molecules such as water, hydrogen halides, or alcohols.^{23,24,25}

The importance of cyclization lies in its central role in the synthesis of cyclic compounds, which are prevalent in both natural products and synthetic molecules.²⁶ Many biologically active compounds, including hormones, alkaloids, and antibiotics, possess cyclic frameworks that are crucial to their function.^{27,28,29,30} Moreover, cyclization reactions are widely employed in the design and construction of complex molecular architectures in medicinal chemistry, materials science, and supramolecular chemistry.^{31,32}

From a mechanistic standpoint, cyclization can proceed through various pathways such as nucleophilic substitution, electrophilic addition, pericyclic reactions, or radical mechanisms.^{33,34,35} The efficiency and selectivity of cyclization reactions are influenced by several factors, including ring size, conformational flexibility, electronic effects, and the presence of directing groups or catalysts.³⁶

Indolizine is a heterocyclic compound with the molecular formula C_8H_7N .³⁷ It is an uncommon isomer of indole, with the nitrogen positioned at the ring fusion site consists of a 10π conjugated planar electronic structure.³⁸ It is primarily used (**Figure 11**) in the pharmaceutical industry and in the synthesis of natural products.^{39,40} However, it also has applications in heterocyclic synthesis, photophysical studies, and the development of materials such as semiconductor polymers.^{41,42}

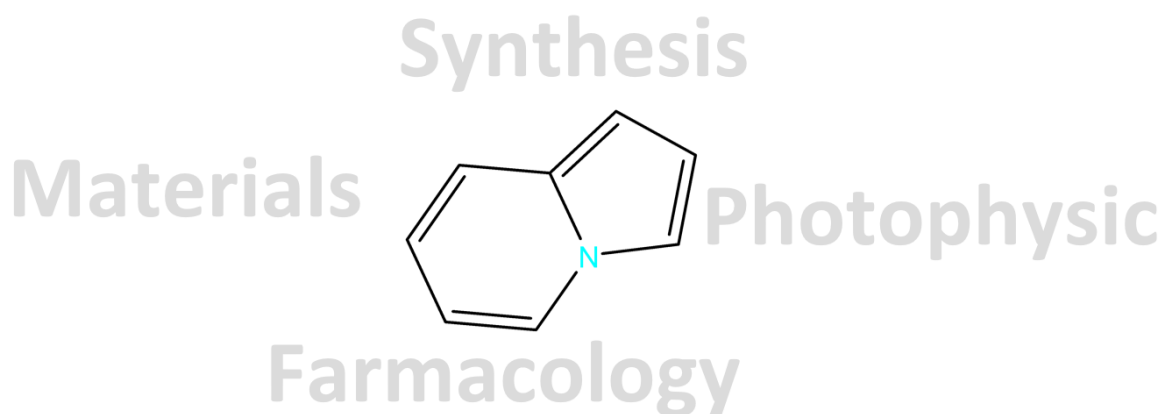


Figure 11 Uses of indolizines

Since the late 19th century, various synthetic approaches have been reported for this compound, including the Scholtz (**Figure 12**) and Tchitchibabine (**Figure 13**) reactions.^{43,44}

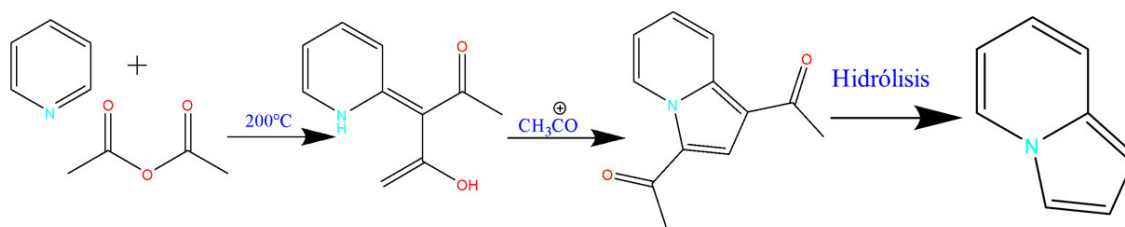


Figure 12 Scholtz Reaction for indolizines

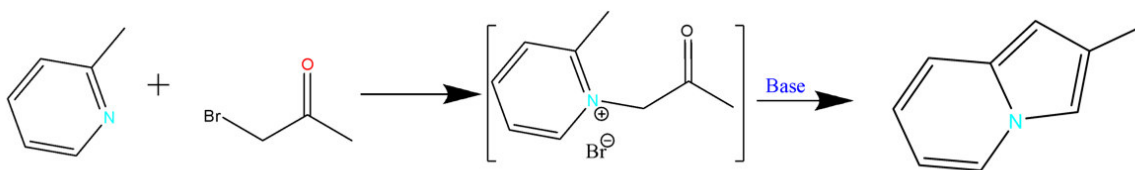
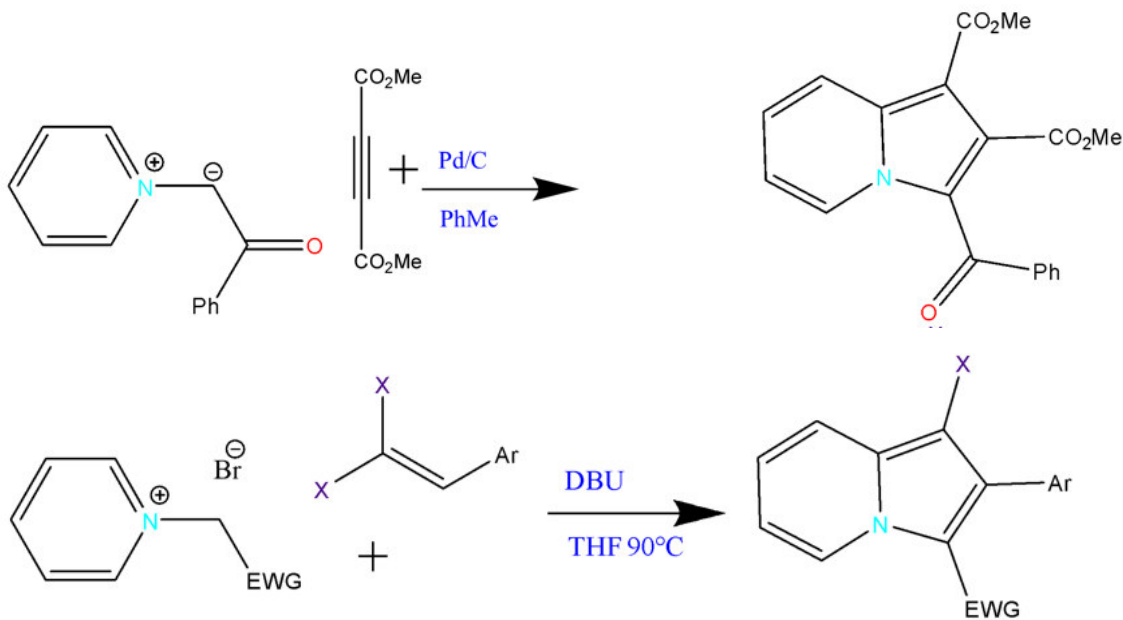


Figure 13 Tchitchibabine Reaction for indolizines

As well as different transition-metal-catalyzed cycloadditions(**Figure 14**).^{45,46,47}



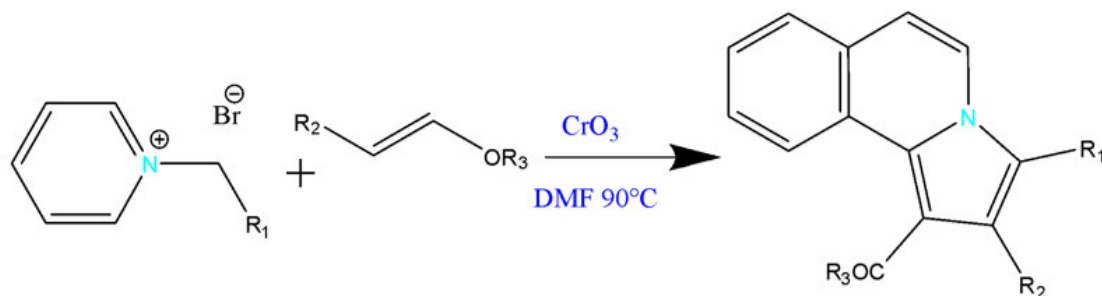


Figure 14 Cycloadditions to synthesize indolizines

As observed, these methods typically require high temperatures, expensive metals, and considerable reaction times. Moreover, only the most efficient of these reactions achieve yields over 60%. Except for the electrocyclic reactions, but these reactions are entirely dependent on a single type of substituent so that the frontier orbitals match. Otherwise, the reaction would not proceed, and this is a major constraint.⁴⁸

Unique synthesis reactions

The reaction systems studied in this work are unique. They were initially reported during ligand synthesis attempts, but the products obtained included 1-(3-methylindolizin-2-yl)ethan-1-one, from now on called O,O-Ligand (**Figure 15**).

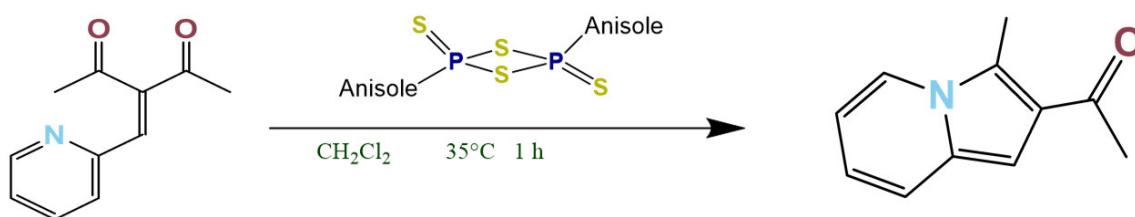


Figure 15 Indolizine Synthesis With O,O-Ligand

and (E)-1-(3-methylindolizin-2-yl)-N-phenylethan-1-imine from now on called N,O-Ligand (**Figure 16**)

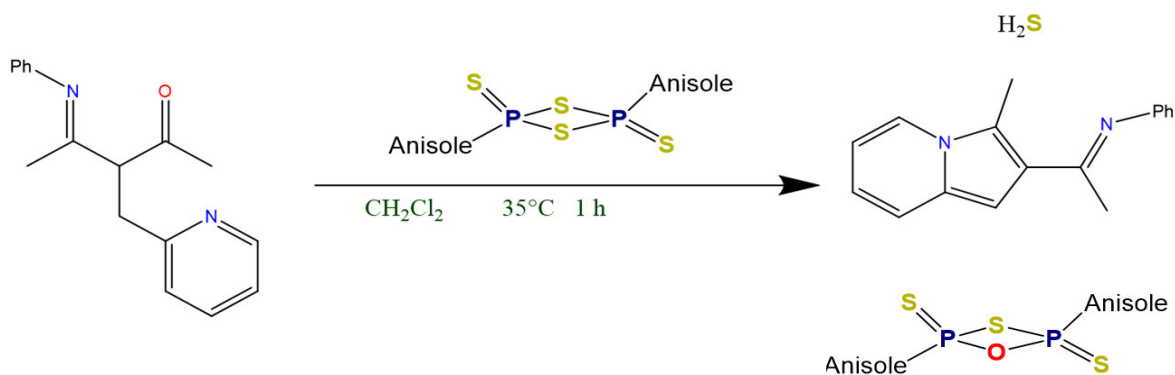


Figure 16 Indolizine Synthesis With N,O-Ligand

The reactions conditions are simple: 35°C for 1 hour in dichloromethane (DCM), yielding $\approx 70\%$ conversion and resulting in simple elimination reactions. Well characterized by X-ray and Nuclear Magnetic Resonance (NMR).

And of course I will explore the respective analogues for WR.

Chapter 2

Conceptual Framework of Quantum Mechanics

Density Functional Theory (DFT) has emerged as a powerful quantum mechanical framework for investigating chemical systems.⁴⁹

This method enables the prediction of molecular geometries, transition states, harmonic vibrational frequencies, and various spectroscopic properties, including Raman, UV/Vis, circular dichroism, magnetic circular dichroism, X-ray absorption,

electron paramagnetic resonance (EPR), and nuclear magnetic resonance (NMR) spectroscopy, among others.^{50,51}

Schrödinger Equation

The Schrödinger equation is the fundamental equation of quantum mechanics, describing how the quantum state of a physical system evolves over time. Proposed by Erwin Schrödinger in 1926, it plays a role in quantum theory analogous to Newton's laws in classical mechanics.⁵²

Under the assumption that the wavefunction can be separated into spatial and temporal components, the **time-independent Schrödinger equation** can be derived.⁵³ The corresponding Hamiltonian operator encapsulates both kinetic and potential energy contributions. For many-particle systems (electrons and nuclei), the Hamiltonian becomes more complex, incorporating interparticle Coulomb interactions.⁵⁴ This general formulation underlies the approximations commonly used in practical computations:

$$i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \hat{H} \Psi(r, t) \quad (1)$$

This equation describes how the wavefunction evolves with time. The Hamiltonian operator $\hat{H}$ represents the total energy (kinetic + potential) of the system.

$$\hat{H} \psi(r) = E \psi(r) \quad (2)$$

This form is used when the Hamiltonian is time-independent. It allows us to determine stationary states and their corresponding energy levels. For a system composed of N electrons and M nuclei, the Hamiltonian is written as:

$$\hat{H} = -\sum_{i=1}^N \frac{1}{2} \nabla_i^2 - \sum_{A=1}^M \frac{1}{2M_A} \nabla_A^2 - \sum_{i=1}^N \sum_{A=1}^M \frac{Z_A}{r_{iA}} + \sum_{i=1}^N \sum_{j>i}^N \frac{1}{r_{ij}} + \sum_{A=1}^M \sum_{B>A}^M \frac{Z_A Z_B}{R_{AB}} \quad (3)$$

Born-Oppenheimer Approximation

The Born–Oppenheimer approximation simplifies the Schrödinger equation by exploiting the large mass difference between electrons and nuclei.⁵⁵ Since nuclei move much more slowly, we can treat them as stationary while solving the electronic problem.⁵⁶ This separation leads to the **electronic Schrödinger equation**, in which the nuclear positions are treated as fixed parameters. Once solved, the total molecular energy is obtained by adding the nuclear repulsion energy and solving the nuclear part of the Schrödinger equation.⁵⁷

As an example, for a diatomic molecule, the Hamiltonian can be expressed as:

$$\hat{H}(r, R) = \hat{T}_{nuc}(R) + \frac{e^2}{4\pi\epsilon_0} \frac{Z_A Z_B}{R} + \hat{H}_{elec}(r, R) \quad (4)$$

with the nuclear kinetic energy operator:

$$\hat{T}_{nuc}(R) = -\frac{\hbar^2}{2m_A} \nabla_A^2 - \frac{\hbar^2}{2m_B} \nabla_B^2 \quad (5)$$

The electronic Hamiltonian becomes:

$$\hat{H}_{elec}(\vec{r}, \vec{R}) = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \frac{e^2}{4\pi\epsilon_0} \left(-\sum_i \frac{Z_A}{r_{Ai}} - \sum_i \frac{Z_B}{r_{Bi}} + \frac{1}{2} \sum_i \sum_{j \neq i} \frac{1}{r_{ij}} \right) \quad (6)$$

This approach allows us to represent the total molecular wavefunction as a product of electronic, vibrational, rotational, and translational wavefunctions.⁵⁸

Hartree-Fock equations

The **Hartree-Fock (HF)** method provides an approximate solution to the many-electron Schrödinger equation by assuming that the total wavefunction can be expressed as a single **Slater determinant** of spin orbitals.⁵⁹ This leads to a set of coupled one-electron equations in which each electron moves in an average field generated by the others.⁶⁰ These equations are solved iteratively using the **Self-Consistent Field (SCF)** method until convergence is achieved.⁶¹

Although the HF method neglects dynamic electron correlation, it establishes a foundation for more sophisticated post-HF methods.⁶²

To describe the ground state of an N-electron system while obeying the Pauli exclusion principle,⁶³ we construct a Slater determinant:

$$|\Psi_0\rangle = |\chi_1 \chi_2 \dots \chi_N| \quad (7)$$

where each χ_i is a spin orbital.

We then introduce the **Fock operator** by minimizing the total energy E_0 with respect to the spin orbitals, obtaining:

$$\hat{f}(i) = -\frac{1}{2} \nabla_i^2 - \sum_{A=1}^M \frac{Z_A}{r_{iA}} + v^{HF}(i) \quad (8)$$

This leads to the **Hartree–Fock equation**:

$$\hat{f}(r_1)\psi_i(r_1) = E_i\psi_i(r_1) \quad (9)$$

Each molecular orbital ψ_i is expressed as a linear combination of atomic basis functions:

$$\psi_i = \sum_{\mu=1}^K c_{\mu i} \phi_{\mu} \quad (10)$$

Substituting this expansion into the Fock equation and integrating yields:

$$\sum_{\nu} F_{\mu\nu} C_{\nu i} = \epsilon_i \sum_{\nu} S_{\mu\nu} C_{\nu i} \quad (11)$$

where $F_{\mu\nu}$ are the elements of the **Fock matrix**, and $S_{\mu\nu}$ are elements of the **overlap matrix**:

$$F_{\mu\nu} = \int dr_1 \phi_{\mu}^*(1) \hat{f}(1) \phi_{\nu}(1) \quad (12)$$

$$S_{\mu\nu} = \int dr_1 \phi_{\mu}^*(1) \phi_{\nu}(1) \quad (13)$$

For closed-shell systems, the Fock matrix is written as:

$$F_{\mu\nu} = \int dr_1 \phi_{\mu}^*(1) \hat{h}(1) \phi_{\nu}(1) + \sum_a \sum_{\lambda\sigma}^{N/2} C_{\lambda a} C_{\sigma a}^* [2(\mu\nu|\sigma\lambda) - (\mu\lambda|\sigma\lambda)] \quad (14)$$

The **core Hamiltonian** is given by:

$$H_{\mu\nu}^{\text{core}} = \int dr_1 \phi_{\mu}^*(1) \hat{h}(1) \phi_{\nu}(1) \quad (15)$$

The **density matrix** is defined as:

$$P_{\mu\nu} = 2 \sum_a^{N/2} C_{\mu a} C_{\nu a}^* \quad (16)$$

Substituting into the Fock matrix expression gives:

$$F_{\mu\nu} = H_{\mu\nu}^{\text{core}} + \sum_{\lambda\sigma} P_{\lambda\sigma} \left[(\mu\nu|\sigma\lambda) - \frac{1}{2} (\mu\lambda|\sigma\lambda) \right] \quad (17)$$

This is commonly summarized as:

$$F_{\mu\nu} = H_{\mu\nu}^{\text{core}} + G_{\mu\nu} \quad (18)$$

Since the Fock matrix depends on the density matrix (or the orbital coefficients), the **Roothaan equations** are **nonlinear**.⁶⁴ As a result, they must be solved iteratively using the SCF procedure. However, we note that this iterative solution process will not be employed in the present thesis work.

Density Functional Theory

The foundations of Density Functional Theory (DFT) trace back to the work of Thomas and Fermi in the 1920s.⁶⁵ They considered a uniform electron distribution, where electrons fill states at a rate of two per volume element. Using an effective potential to account for interactions between the nucleus and the electron cloud, they proposed an expression for the total energy of an atom as a functional of the electron density.⁶⁶

The energy functional of the **Thomas–Fermi model** is given by:

$$E_{TF}[\rho(r)] = C_F \int \rho^{5/3}(r) dr - Z \int \frac{\rho(r)}{r} dr + \frac{1}{2} \iint \frac{\rho(r_1)\rho(r_2)}{|r_1 - r_2|} dr_1 dr_2 \quad (19)$$

It is assumed that in the ground state, this functional is minimized by the correct electron density.

DFT reinterprets quantum mechanics in terms of **electron density** rather than wavefunctions. According to the **Hohenberg–Kohn (HK) theorems**, all ground-state properties of a system are uniquely determined by its electron density. The total energy is expressed as a functional of the electron density, consisting of kinetic, Coulomb, and exchange-correlation contributions.⁶⁷ These results are established through two theorems:

1. The external potential V_{ext} , and hence the total Hamiltonian, is uniquely determined (up to a constant) by the ground-state electron density ρ_0 .
2. There exists a universal functional such that the total energy is:

$$E[\rho] = F[\rho] + \int V_{\text{ext}}(r) \rho(r) dr \quad (20)$$

This formulation establishes a **variational principle** for the electron density: the correct ground-state density minimizes the total energy functional. Applying this principle, the ground state must satisfy the stationarity condition:

$$\delta \left\{ E_v[\rho] - \mu \left[\int \rho(r) dr - N \right] \right\} = 0 \quad (21)$$

By applying the Euler–Lagrange equation, we obtain:

$$\mu = \frac{\delta E_v[\rho]}{\delta \rho(r)} = v(r) + \frac{\delta F_{HK}[\rho]}{\delta \rho(r)} \quad (22)$$

This defines the **chemical potential**. Under the HK formalism, Equation (22) becomes the key expression for minimizing the energy and obtaining the ground-state density.

Since the exact form of the exchange-correlation functional $E_{xc}[\rho]$ is unknown, it must be approximated; an approximation that determines the method's accuracy.

The **Kohn–Sham (KS)** formalism introduces a system of non-interacting electrons that reproduce the same ground-state density as the interacting system.⁶⁸ The KS method closely resembles the Hartree–Fock approach, as it also uses a mono-electronic operator and Slater determinants. The KS Hamiltonian is:

$$\widehat{H}_s = \sum_{i=1}^N \widehat{h}(i) = \sum_{i=1}^N \left(-\frac{1}{2} \nabla^2(i) \right) + \sum_{i=1}^N \widehat{v}_s(i) \quad (23)$$

The electron density is obtained from the Kohn–Sham orbitals:

$$\rho(\vec{r}) = \sum_{i=1}^{N_{\text{occ}}} |\chi_i(\vec{r})|^2 \quad (24)$$

The associated non-interacting kinetic energy functional is:

$$T_s[\rho] = \sum_{i=1}^{N_{\text{occ}}} \left\langle \chi_i \left| -\frac{1}{2} \nabla^2 \right| \chi_i \right\rangle \quad (25)$$

Solving Equation (22) together with the Kohn–Sham system leads to the exact non-interacting electron density. The total energy in the KS framework is:

$$E_v[\rho] = \sum_{i=1}^{N_{\text{occ}}} \varepsilon_i = T_s[\rho] + \int \rho(\vec{r}) v_s(\vec{r}) d\vec{r} \quad (26)$$

For a fully interacting system, we must include the electron–electron interaction term $V_{ee}[\rho]$. We define two important quantities:

$$T[\rho] - T_s[\rho] = T_c[\rho] \quad (27)$$

$$V_{ee}[\rho] - J[\rho] = W_{xc}[\rho] \quad (28)$$

which give the total exchange-correlation energy:

$$E_{xc}[\rho] = T_c[\rho] + W_{xc}[\rho] \quad (29)$$

We can now summarize the total energy as:

$$E_v[\rho] = \sum_{i=1}^{N_{\text{occ}}} \varepsilon_i = T_s[\rho] + \int \rho(\vec{r}) v_s(\vec{r}) d\vec{r} + J[\rho] + (T[\rho] - T_s[\rho]) + (V_{ee}[\rho] - J[\rho]) \quad (30)$$

Substituting the Coulomb repulsion term:

$$\frac{1}{2} \iint \frac{\rho(\vec{r}_1) \rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 \quad (31)$$

and the exchange-correlation functional (29), we finally express the total Kohn–Sham energy as:

$$E_v[\rho] = T_s[\rho] + \int \rho(\vec{r}) v_n(\vec{r}) d\vec{r} + \frac{1}{2} \iint \frac{\rho(\vec{r}_1) \rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_1 d\vec{r}_2 + E_{xc}[\rho] \quad (32)$$

If we express this in terms of the **chemical potential**, for physical interpretation, we obtain:

$$\mu = \frac{\delta E_v[\rho]}{\delta \rho(\vec{r})} = \frac{\delta T_s[\rho]}{\delta \rho(\vec{r})} + \left[v_n(\vec{r}) + \int \frac{\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} d\vec{r}_2 \right] + \frac{\delta E_{xc}[\rho]}{\delta \rho(\vec{r})} \quad (33)$$

Transition State Theory

Transition State Theory (TST) provides a framework to estimate the rate of a chemical reaction by assuming a quasi-equilibrium between the Reagents and an activated complex (or transition state).⁶⁹ The rate depends on the number of molecules that possess sufficient energy to overcome the activation barrier. Introduced in 1935 by **Henry Eyring** and **Michael Polanyi**,⁷⁰ TST has become a cornerstone of chemical kinetics and theoretical chemistry. This framework offers a rigorous approach to understanding and quantifying molecular transformations, particularly through the analysis of how a system evolves along its **potential energy surface (PES)**.⁷¹

TST offers insight into how chemical reactions proceed by examining the **energetic landscape** that governs molecular motion. The PES (Figure 17) is a multidimensional surface representing the energy of a system as a function of the positions of all its nuclei.⁷² Within this surface, two fundamental regions are distinguished: the **Reagent and product basins**, which correspond to stable molecular configurations, and the **reaction pathway**, which connects these regions through a critical energy point known as the **transition state** or **activated complex**.⁷³

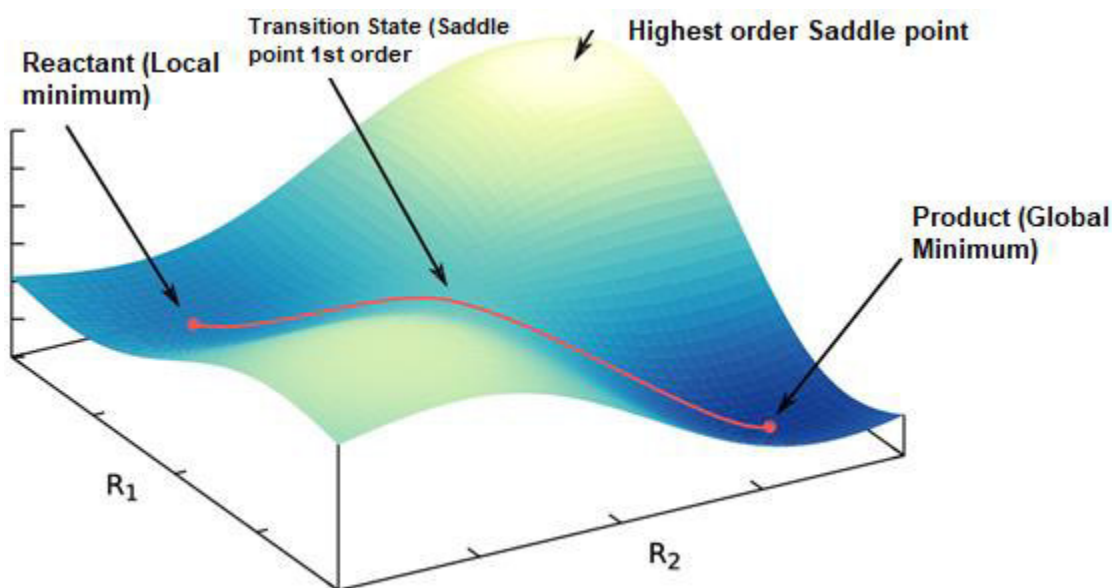


Figure 17. Representation of a potential energy surface (PES).

The **Eyring equation** describes the variation in the rate of a chemical reaction with temperature. It is derived from Transition State Theory (also called **Activated Complex Theory**). Assuming constant enthalpy and entropy of activation, the Eyring equation bears a strong resemblance to the empirical **Arrhenius equation**.⁷⁴

$$k = \frac{\kappa k_B T}{h} e^{-\frac{\Delta G^\ddagger}{RT}} \quad (34)$$

The **statistical mechanical form** of the rate constant and the equilibrium constant for the formation of the activated complex are given as:⁷⁵

$$k = \kappa \frac{kT}{h} \frac{Q^\ddagger}{Q_X Q_{YZ}} e^{-\frac{E_0}{RT}} \quad (35)$$

$$K^{\ddagger*} = \frac{Q^{\ddagger*}}{Q_X Q_{YZ}} e^{-\frac{E_0}{RT}} \quad (36)$$

These expressions can be reformulated in **thermodynamic terms**, where $\Delta G^{\ddagger*}$, $\Delta H^{\ddagger*}$ and $\Delta S^{\ddagger*}$ denote the **Gibbs free energy**, **enthalpy**, and **entropy of activation**, respectively:

$$k = \frac{\kappa kT}{h} e^{-\frac{\Delta G^{\ddagger*}}{RT}} = \frac{\kappa kT}{h} e^{\left(-\frac{\Delta H^{\ddagger*}}{RT}\right)} e^{\left(\frac{\Delta S^{\ddagger*}}{R}\right)} \quad (37)$$

Chapter 3

Mechanistic Exploration of O,O-Ligand Activation by Lawesson and Woollins Reagents

In this chapter, we discuss the results obtained from the mechanistic analysis and design concerning the possible interactions involving the oxygen–phosphorus bond.

It is important to note that only the most energetically favorable mechanisms are presented here; additional pathways are discussed in **Appendix 1**.

We begin with the compound 3-(pyridin-2-ylmethylene)pentane-2,4-dione, an O,O-ligand, which, under the conditions previously described and in the presence of the Lawesson reagent (LR), leads to the formation of the corresponding indolizine (**Figure 18**). In this transformation, the stoichiometry suggests the elimination of one oxygen atom from the ligand. This observation needs consideration of viable alternative byproducts.

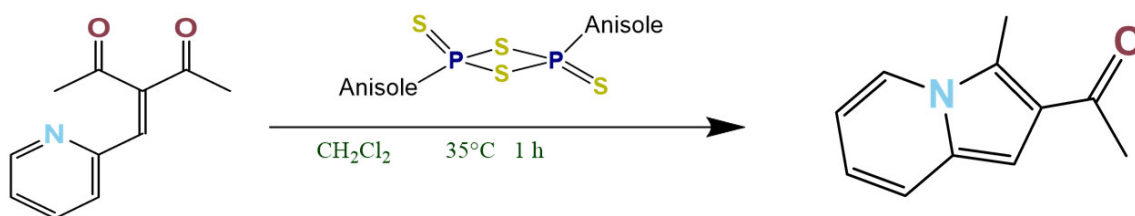


Figure 18. Synthesis of indolizine with O,O-Ligand.

Theoretical Mechanistic Proposals with Lawesson Reagent

Given the known reactivity of the oxygen atom, several plausible mechanistic scenarios were evaluated (**Figure 19**). In all cases examined, the cyclized structures in which the oxygen atom remains bonded to the Lawesson reagent were found to be energetically accessible. Therefore, mechanistic pathways leading to these potential side products were explored in detail.

However, we found that only those mechanisms in which the resulting cyclic intermediate features the oxygen atom positioned between the two phosphorus atoms provided energetically viable pathways under the reported conditions.

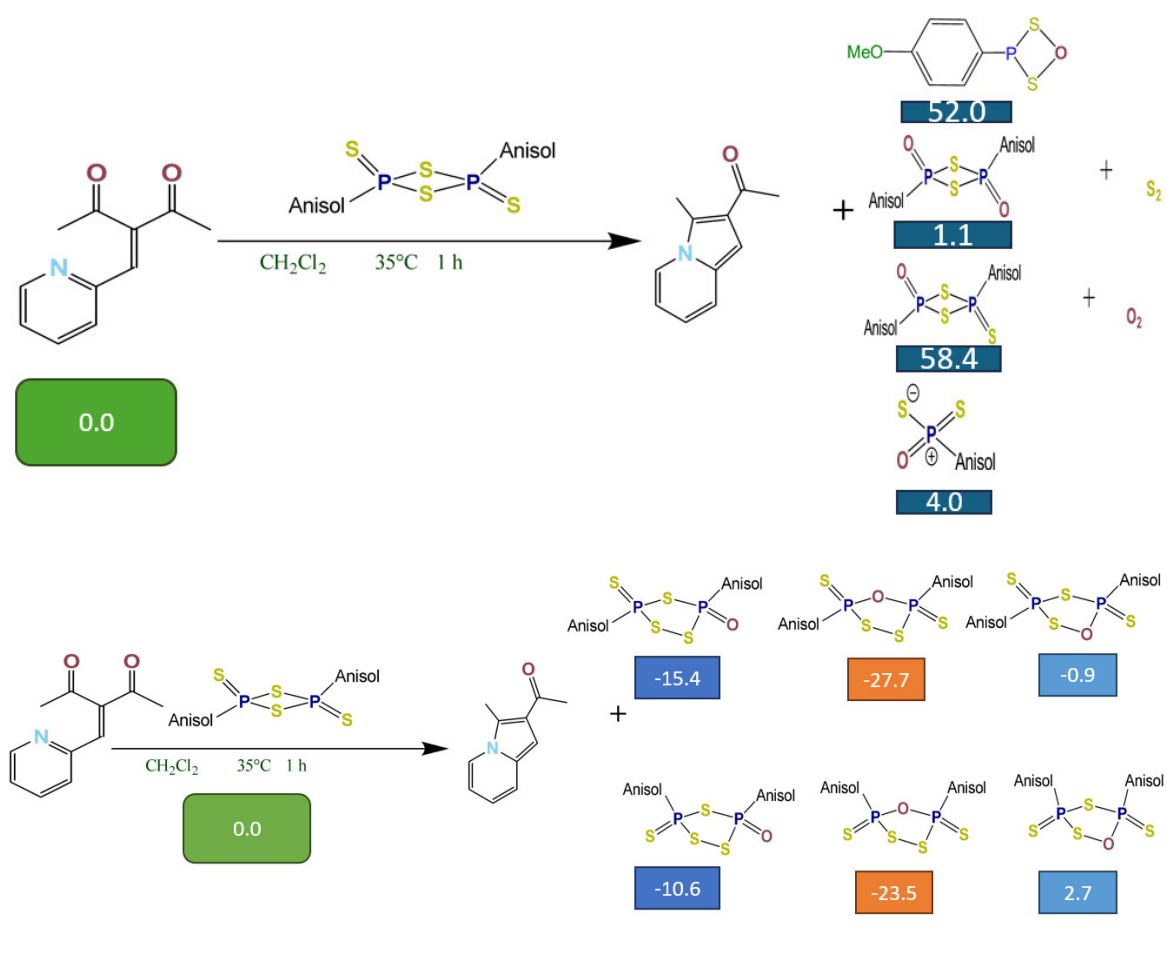


Figure 19. a) Proposed byproducts explored for the O,O-Ligand Activation by **Lawesson Reagent** calculated in gas phase. b) Conformational study of the O-insertion to the **Lawesson Reagent** generating five-membered rings as other byproduct formation. Gibbs free energy values are in kcal/mol.

The proposed reaction mechanisms and their corresponding energetic profiles were investigated using density functional theory (DFT) as implemented in the Gaussian 09 software package. All geometry optimizations and harmonic vibrational frequency calculations were performed at the $\omega\text{B97X-D/def2-SVP}$ level of theory. No geometrical constraints were applied during the optimization processes. Single-point energy corrections were subsequently computed at the $\omega\text{B97X-D/6-311+G(d)}$ level using the gas-phase optimized geometries. Solvent effects were modeled using the SMD continuum solvation model with dichloromethane (CH_2Cl_2) as the solvent. Solvation corrections were evaluated at the $\omega\text{B97X-D/def2-SVP}$ level. All thermochemical corrections were obtained from the frequency calculations and correspond to a temperature of 298.15 K and a pressure of 1 atm. The final reported energies are Gibbs free energies (ΔG) and are expressed in kcal/mol. To enhance the mechanistic discussion, both gas-phase and solvent-corrected energies are presented where relevant.

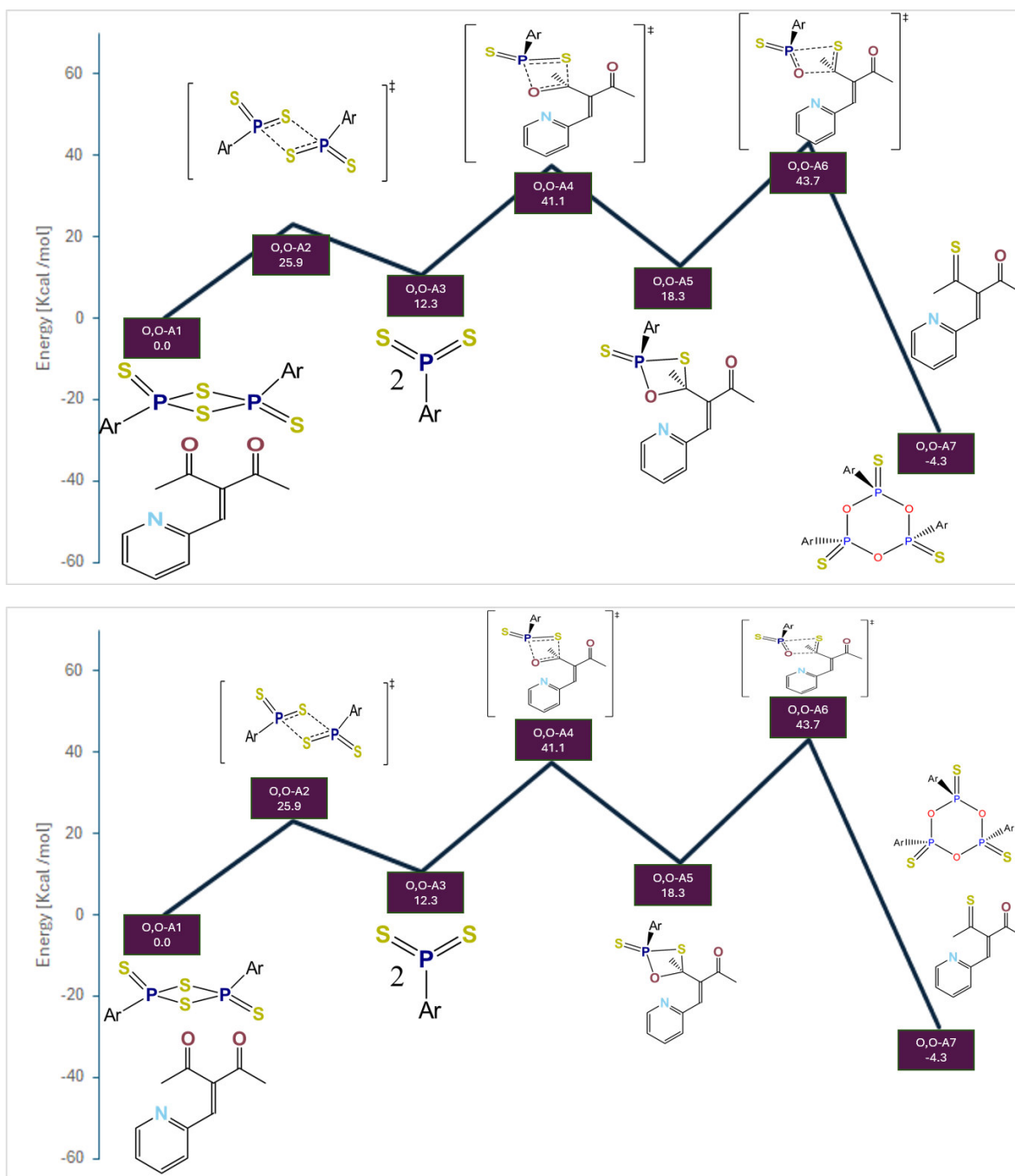


Figure 20. Energy profile of the substitution mechanism ($C4$ carbonyl or $C=O^\beta$), Lawesson Reagent, as it is described in the literature. a) Gas-phase calculations; b) solvent-included calculations.

First, substitution mechanisms involving both carbonyl groups ($C=O^\alpha$ at position 2 near to the methyl group, and $C=O^\beta$ at position 4 conjugated with the pyridine ring) are proposed (see **Figure 20** and **Figure 21**) to demonstrate that the pathways reported in the literature are both energetically and synthetically unfeasible. Although the free energy differences between Reagents and products

appear favorable, the calculated total energy barriers (43.1 and 46.2 kcal/mol, respectively) indicate that these reactions are unlikely to proceed under the conditions employed.

It is important to note that, for the products, we considered both the simple substituted species and a hexacyclic structure incorporating three substituted fragments of LR, as such structures have been experimentally characterized in related systems. Even after including solvent effects and thermodynamic corrections, the results remain consistent: the substitution mechanisms are inaccessible under the studied conditions.

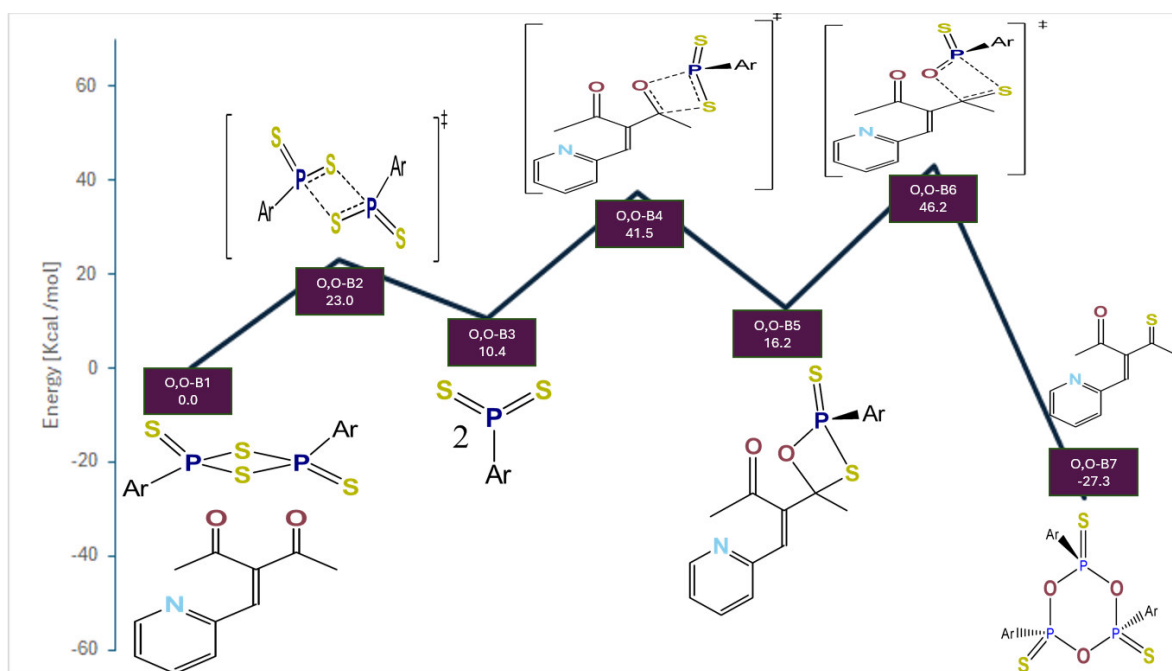


Figure 21. Gas-phase calculated energy profile of the substitution mechanism via C2 carbonyl ($C=O^\alpha$), Lawesson Reagent.

Additionally, we also considered the reaction with the full LR (no previous dissociation step occurs initially) to rule out this possibility in the substitution mechanism (**Figure 22**). In this case, a total energy barrier of 43.1 kcal/mol demonstrates that there is no difference between using the full LR or just a monomer to react with the diketone (O,O-ligand).

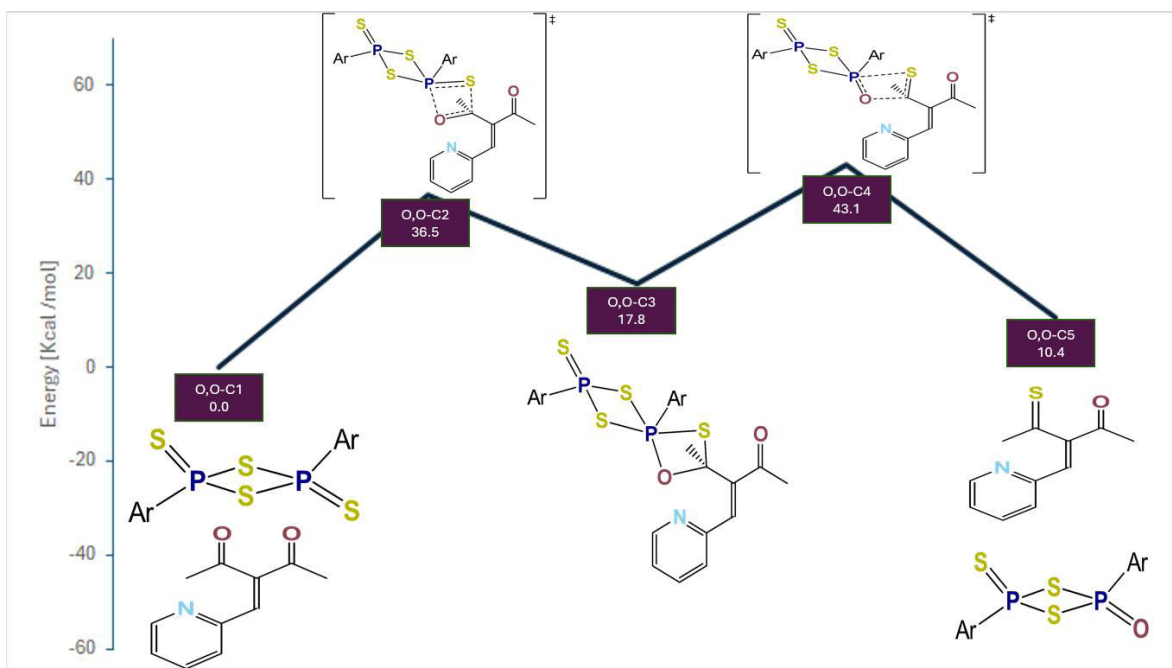


Figure 22. Gas-phase calculated energy profile of other reaction pathway considered for the substitution mechanism (*C4 carbonyl or C=O β*) using the full **Lawesson Reagent**.

The first viable mechanism (**Figure 23**) begins with the fragmentation of the Lawesson reagent, followed by cyclization that forms the indolizine ring. This process is initiated by nucleophilic attack of the nitrogen atom on a carbon center, while the carbonyl oxygen coordinates to the phosphorus atom of the fragment. The sulfur atom closest to the forming ring bonds to the sp^2 -hybridized carbon, where the resulting positive charge can be delocalized.

Subsequently, the carbonyl oxygen is attacked by the second fragment of the Lawesson reagent, leading to its detachment from the ring. This step is particularly significant, as alternative pathways in which the oxygen atom departs without stabilizing interactions are associated with prohibitively high transition state energies (see **Appendix 1**).

The resulting intermediate undergoes a sulfur migration toward the adjacent carbon atom, which is electron-deficient due to the presence of a neighboring nitrogen atom. From this point, rotation around the distal P–O bond (with respect to the ring) enables the system to access a final transition state. This leads to the formation of the indolizine product and a substituted Lawesson reagent, in which the oxygen atom is trapped between two phosphorus centers and both anisole groups adopt a cisoid configuration.

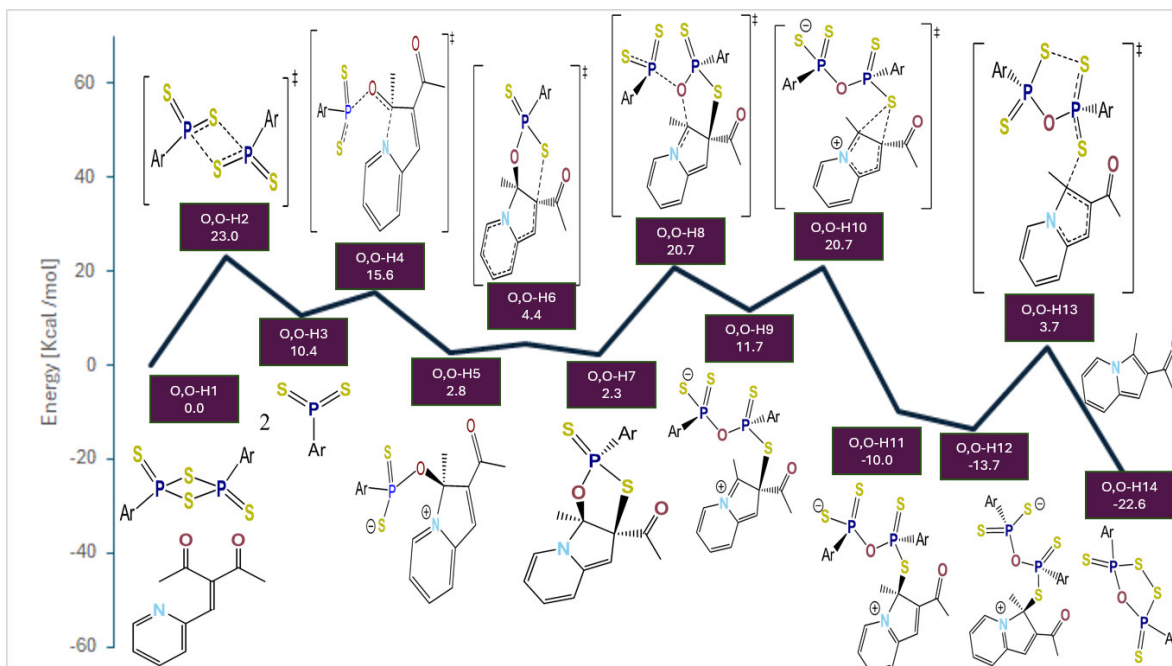


Figure 23. Gas-phase calculated energy profile of the oxygen elimination mechanism where migration and rotation of the $(S_2PAR)_2O$ moiety occurs (**Lawesson Reagent**).

The alternative mechanistic proposal (**Figure 24**) follows an identical sequence of steps up to sulfur migration. However, in this pathway, no rotation occurs; instead, a conformer of the substituted Lawesson reagent is formed directly.

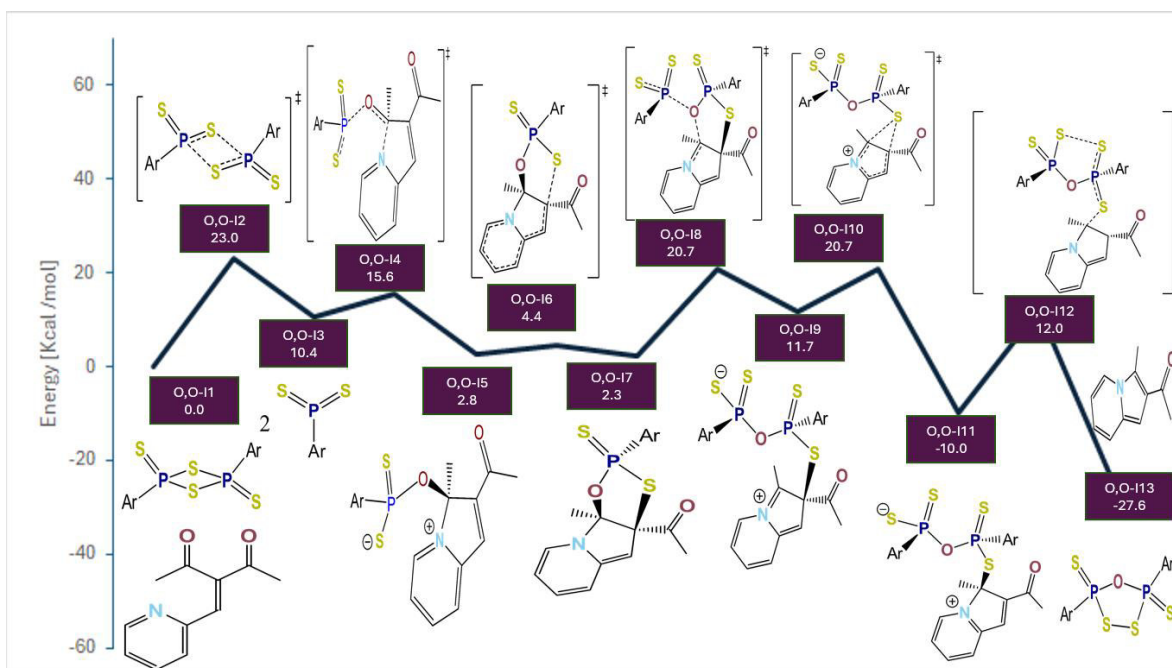


Figure 24. Gas-phase calculated energy profile of the oxygen elimination mechanism where only migration of the $(S_2PAR)_2O$ moiety occurs (**Lawesson Reagent**).

This conformer is more stable due to the transoid arrangement of the anisole groups, and the simultaneous formation of the indolizine ring. This mechanism is also considered viable based on the calculated energy barriers. Although it involves a greater overall energy difference between the Reagents and products, the final transition state displays only a slightly higher barrier. Nevertheless, it remains an energetically accessible and plausible reaction pathway.

The final viable mechanism (**Figure 25**) begins with a direct attack of the carbonyl oxygen atom on the intact Lawesson reagent, followed by cyclization to form the indolizine ring and establishment of a bond at the α -carbon relative to the second carbonyl group. A fragment of the Lawesson reagent then dissociates from the intermediate and is promptly attacked by the oxygen atom, resulting in its detachment from the ring, as observed in previous mechanisms. This is followed by sulfur migration, rotation, and the formation of the indolizine product along with the substituted Lawesson reagent, in which the anisole groups adopt a cisoid configuration.

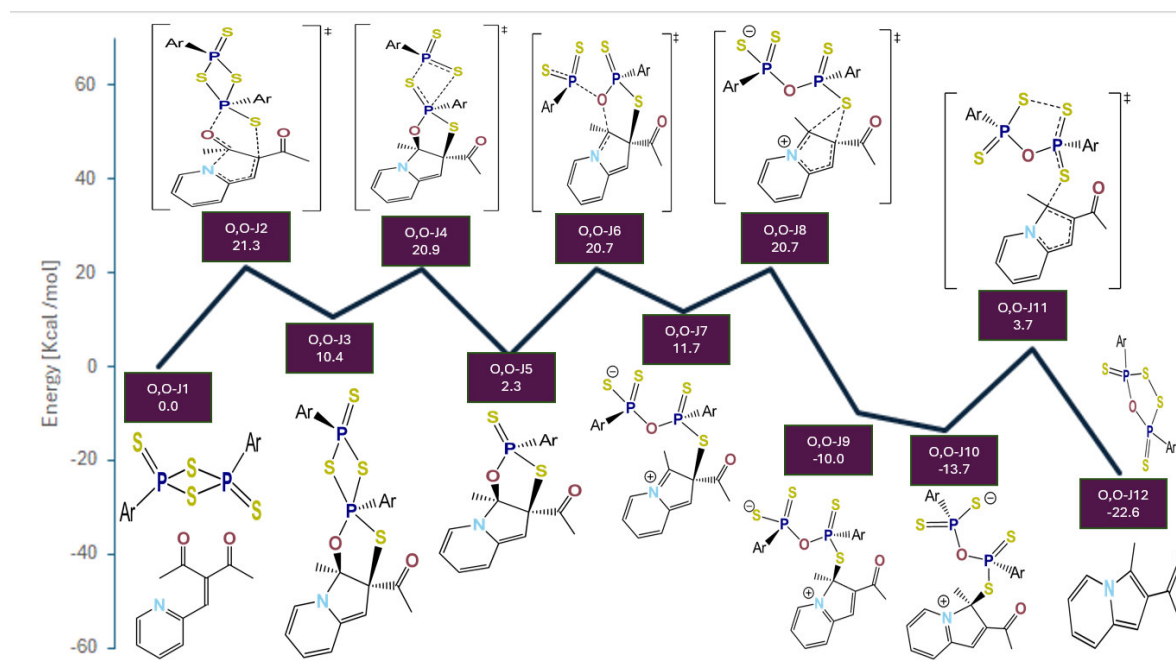


Figure 25. Gas-phase calculated energy profile of the oxygen elimination mechanism, without initial Lawesson Reagent dissociation, where migration and rotation of the $(S_2PAR)_2O$ moiety occurs.

We also evaluated the effect of using solvent effects and a bigger basis set, as described above, in the previously proposed, calculated mechanisms (**Figure 26**). They maintain all energy barriers below the established threshold for synthetic feasibility. Therefore, we consider them viable pathways to explain the observed formation of indolizines using Lawesson reagent.

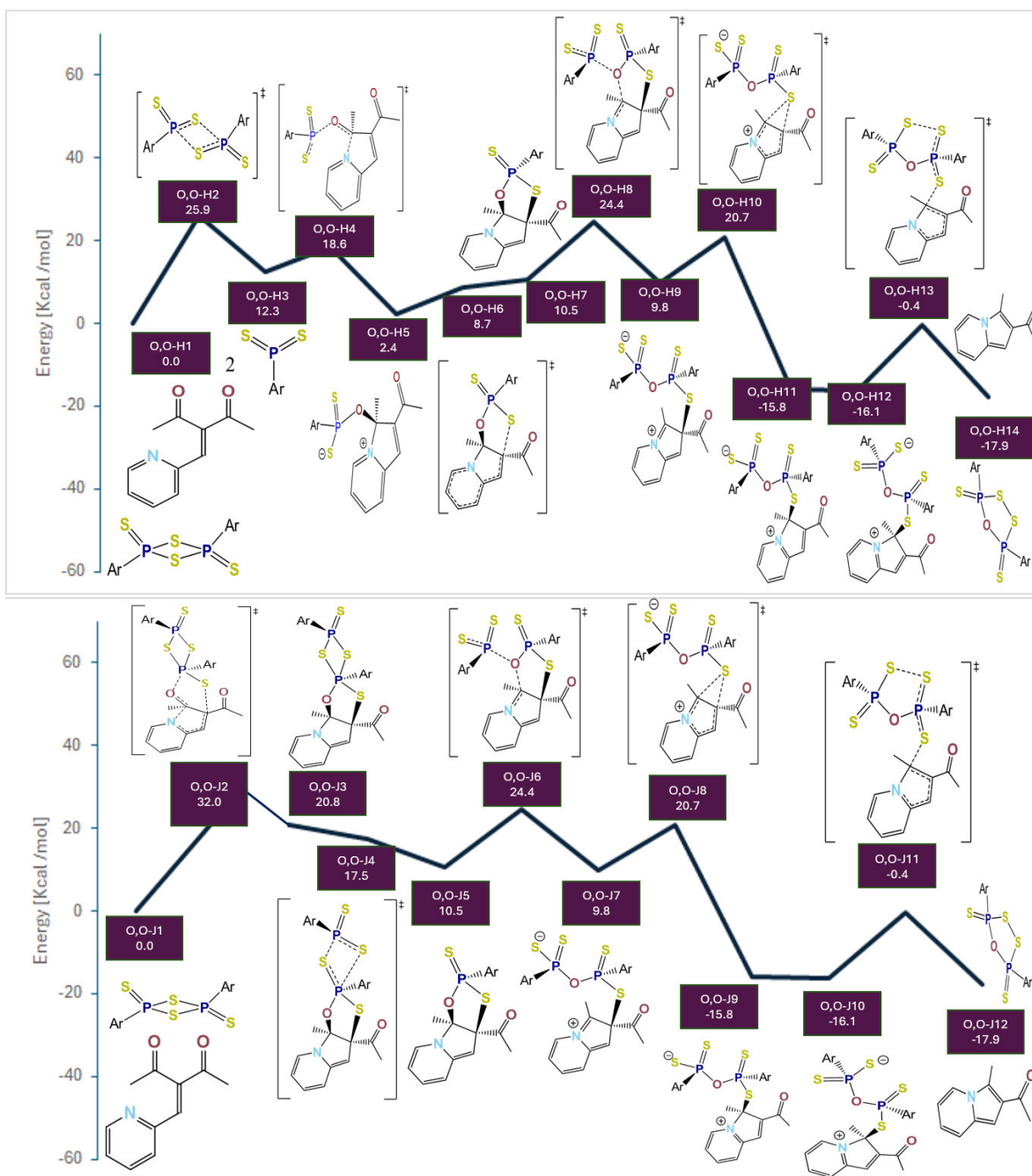


Figure 26. Energy profiles of the same reaction mechanisms shown in **Figures 23** and **25** but both incorporating the energy corrections and solvent effects (calculated at the SMD:(CH₂Cl₂) ωB97X-D/6-311+G(d)// ωB97X-D/def2-SVP level) using the **Lawesson Reagent**.

Theoretical Mechanistic Proposals with Woollins Reagent

In the case of Woollins reagent, potential side-product formation must also be considered. As shown in **Figure 27**, the general reactivity trend mirrors that observed with Lawesson reagent. We replicated the mechanisms previously proposed for Lawesson reagent to evaluate energetic correlations and identify viable pathways.

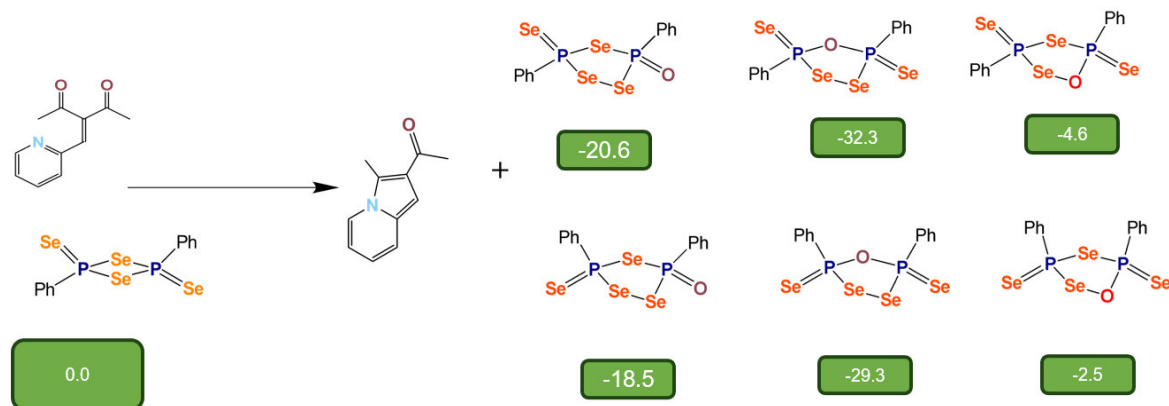


Figure 27. Conformational analysis of feasible byproducts in the cyclization reaction using the **Woollins Reagent**. Energy values from our gas-phase calculations are expressed in kcal/mol.

We first re-examined the substitution mechanism, in which the intact WR approaches the substrate without fragmentation.

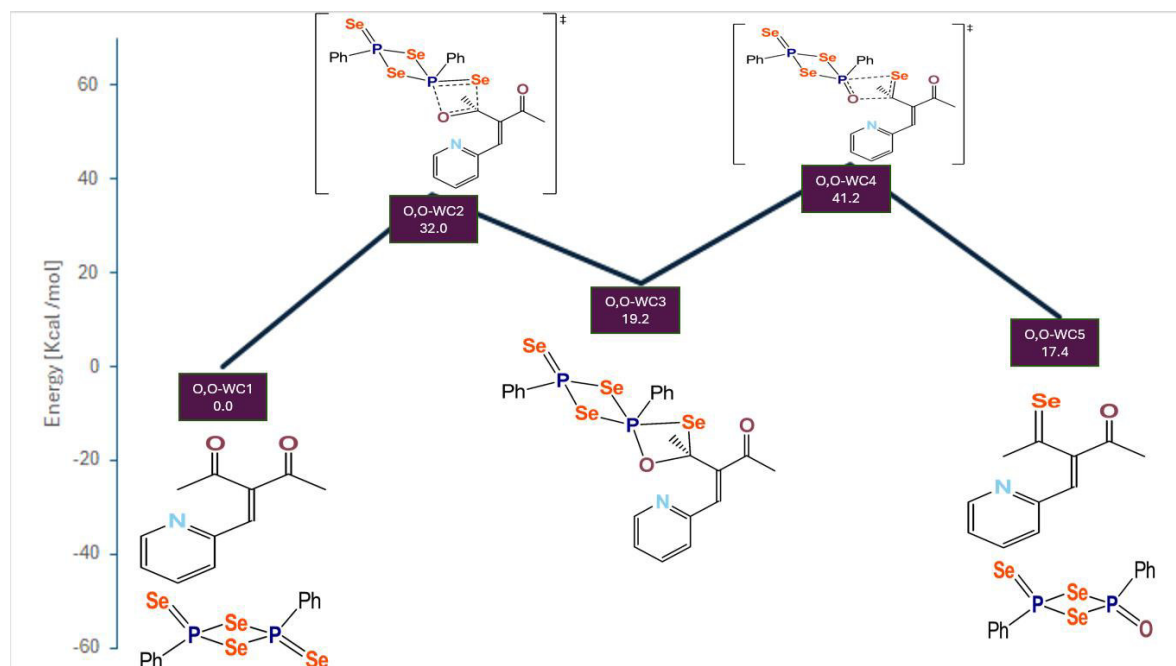


Figure 28. Gas-phase calculated energy profile for the substitution mechanism using the full **Woollins Reagent**.

This pathway results in prohibitively high-energy transition states, and the resulting products are synthetically inaccessible based on Gibbs free energy calculations. Specifically, the product lies 17.4 kcal/mol above the Reagents (**Figure 28**), confirming that this route is not viable under the conditions studied.

Next, we considered a mechanism for Woollins reagent that aligns more closely with literature reports (**Figure 29**). In this scenario, fragmentation of the reagent leads to extremely high-energy transition states, and the final product is only marginally more stable than the starting materials. These findings further reinforce the notion that substitution pathways, whether involving intact or fragmented reagents, are energetically disfavored.

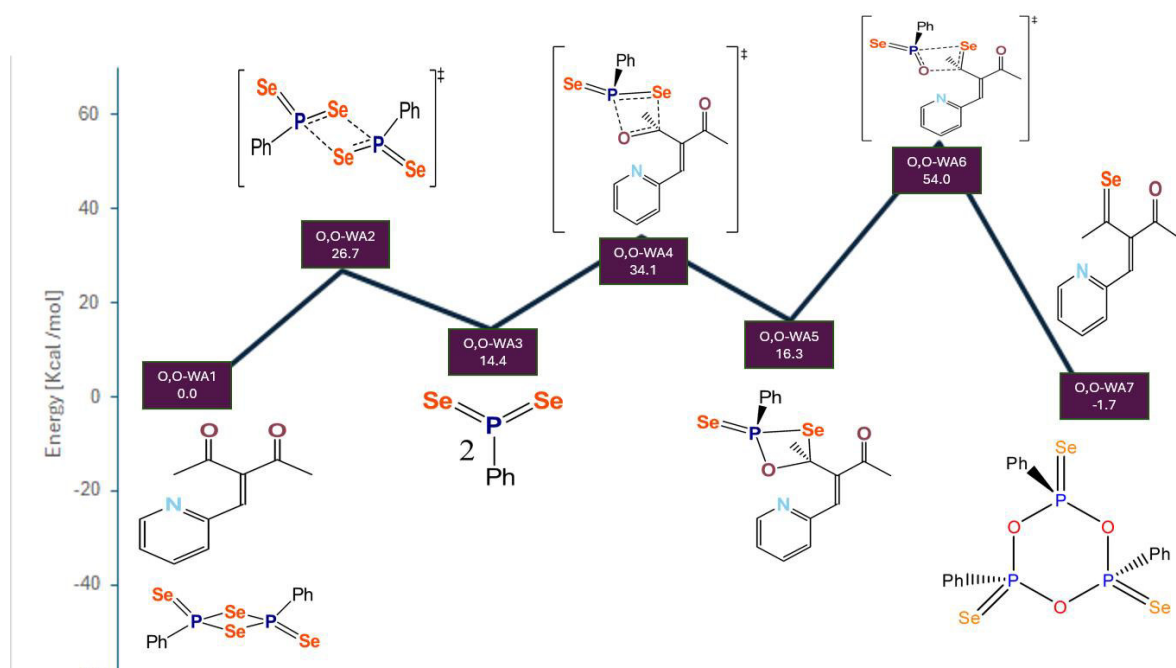


Figure 29. Gas-phase calculated energy profile for the substitution mechanism considering an initial fragmentation of the **Woollins Reagent** in two Se_2PPh fragments.

The first viable mechanism (**Figure 30**) for oxygen elimination begins with nucleophilic attack by the carbonyl group on the intact Woollins reagent, followed by adjacent cyclization to form an intermediate. From this intermediate, a fragment of the reagent is expelled and rearranges into a pentacyclic structure, producing both the desired indolizine and a modified Woollins reagent in which the oxygen is retained as a carbonyl group. This same mechanism was evaluated with Lawesson reagent but proved unfeasible (see **Appendix 1**). In contrast, with Woollins reagent, the energy barriers are significantly lower, supporting the viability of this pathway.

The second mechanism (**Figure 31**), which was also unsuccessful with Lawesson reagent, involves fragmentation of Woollins reagent followed by nucleophilic attack and cyclization. The remaining fragment associates via Se–Se

bonds and P–C interactions with the ring. In a subsequent single step, the oxygen atom coordinates to phosphorus and detaches from the ring.

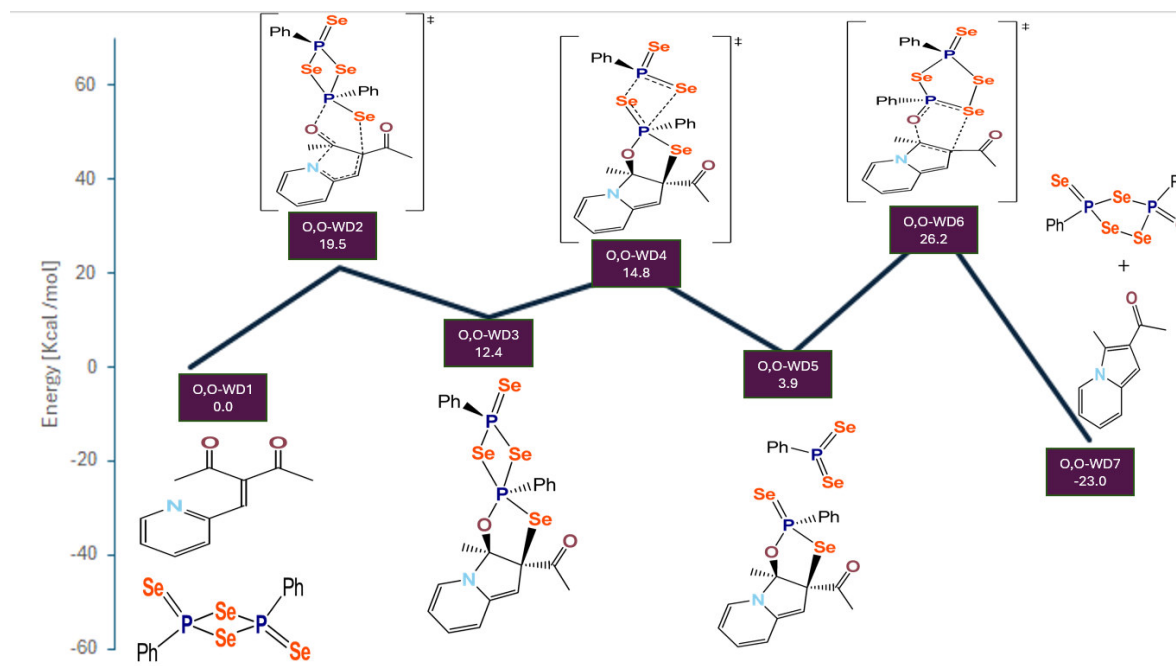


Figure 30. Gas-phase calculated energy profile of the oxygen elimination mechanism considering an initial cycloaddition where selenium attacks on the alpha carbon of the O,O-ligand (**Woollins Reagent**).

This results in a Woollins reagent derivative in which the oxygen bridges two phosphorus atoms and the phenyl groups adopt a cisoid arrangement. All steps in this pathway proceed with energy barriers of mechanistic relevance and are within synthetically accessible ranges.

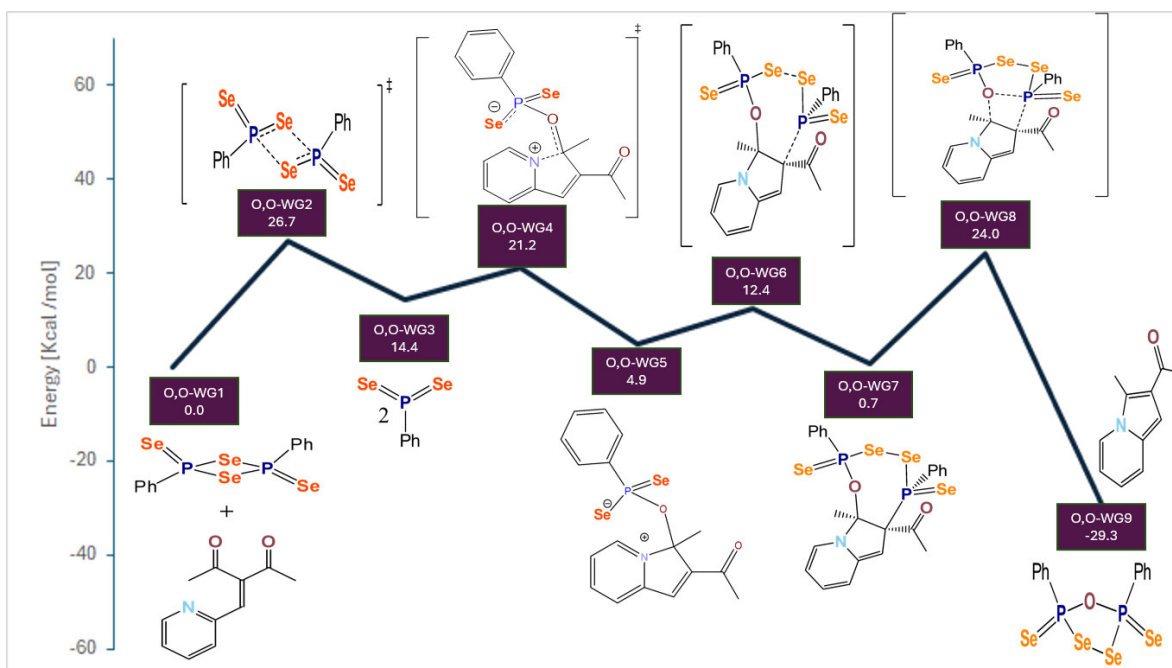


Figure 31. Gas-phase calculated energy profile of the elimination mechanism where the second Se_2PPh moiety attacks on the O,O-WG5 intermediate to form a $\text{P}-\text{C}(\alpha)$ bond (**Woollins Reagent**).

We also explored a third viable mechanism (**Figure 32**) by replicating the migration–rotation pathway observed with Lawesson reagent. The steps include fragmentation, nucleophilic attack and cyclization, $\text{Se}-\text{C}$ bond formation at an electrophilic carbon (facilitated by resonance), separation of the oxygen atom with the other Woollins fragment, selenium migration to the most electrophilic carbon, rotation, and final release of the Woollins reagent bearing the oxygen atom and phenyl groups in a cisoid configuration. All steps occur with manageable energy barriers, although in this case, the initial fragmentation of the reagent represents the highest energy barrier. However, this is consistent with literature descriptions of Lawesson and Woollins reagent fragmentation as reversible equilibria, supporting the feasibility of this mechanism under practical conditions.

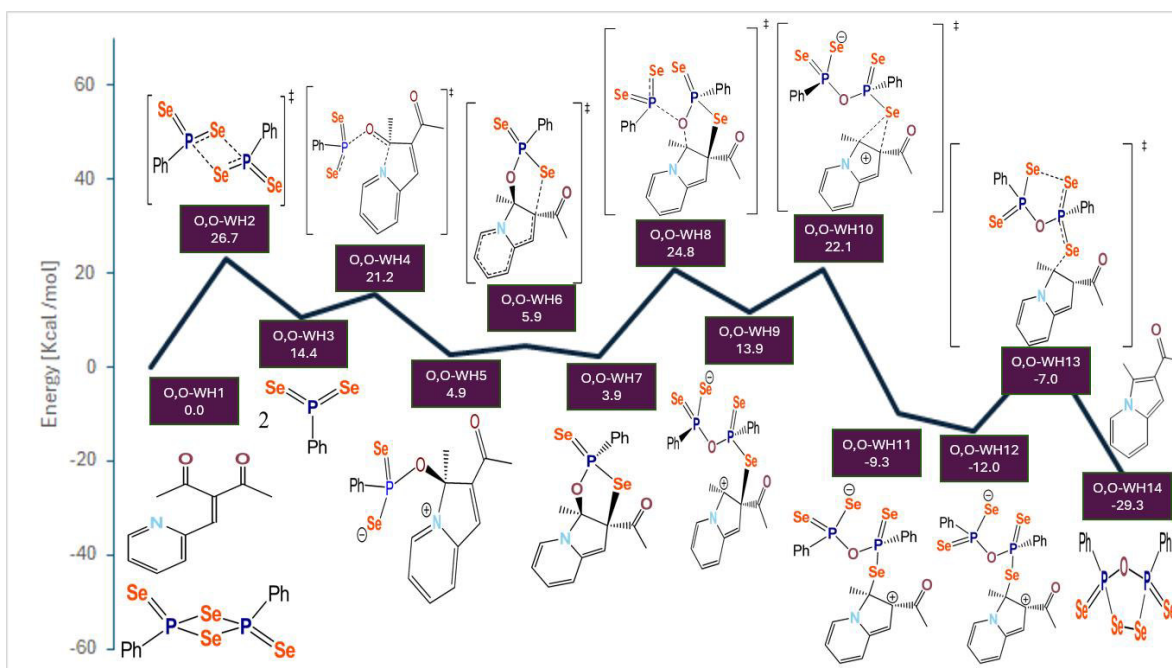


Figure 32. Gas-phase calculated energy profile of the oxygen elimination mechanism where migration and rotation of the $(\text{Se}_2\text{PPh})_2\text{O}$ moiety occurs (**Woollins Reagent**).

Finally, we identified what we consider the most viable mechanism for the synthesis of indolizines using Woollins reagent (**Figure 33**). This mechanism begins with nucleophilic attack of the carbonyl group on the intact reagent, leading to cyclization. A reagent fragment is then released and later reattaches to the intermediate to facilitate oxygen detachment from the ring. This is followed by selenium migration and a conformational rotation, passing through a final transition state that leads to the formation of the indolizine and a Woollins reagent derivative in which the oxygen is trapped between two phosphorus atoms.

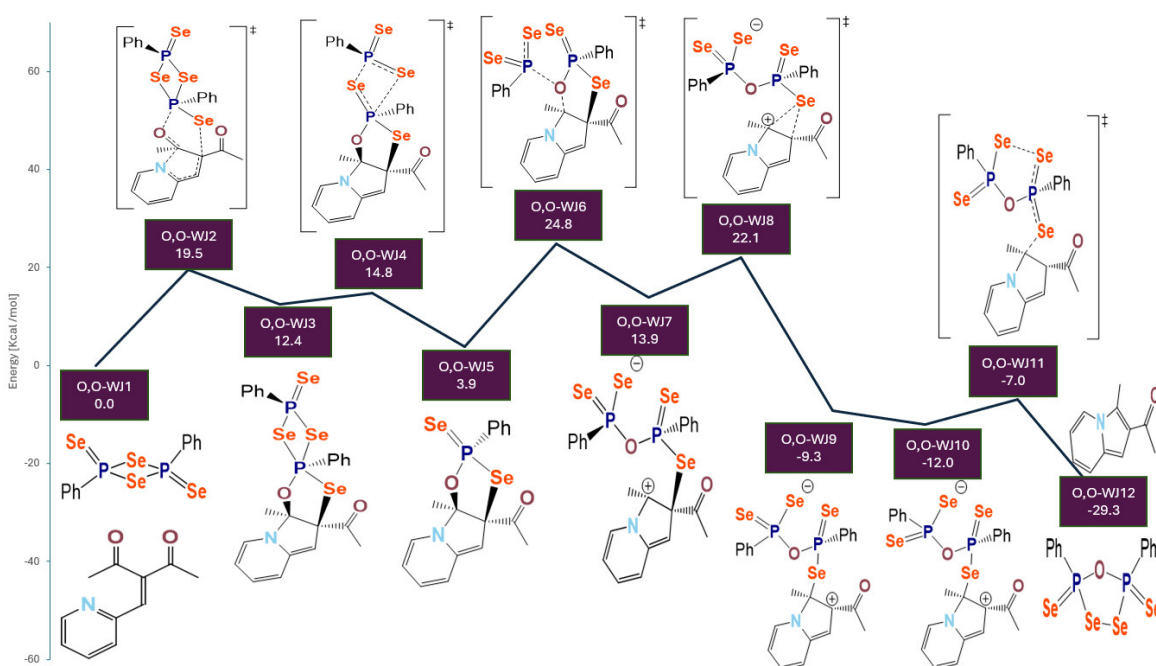


Figure 33. Gas-phase calculated energy profile of the oxygen elimination mechanism where migration and rotation of the $(\text{Se}_2\text{PPh})_2\text{O}$ using the full **Woollins Reagent**.

To evaluate the accuracy of the predicted profiles, we further analyzed the two most viable mechanisms at the full theoretical level, including energy corrections and solvent effects. This analysis was performed to address potential overestimation errors commonly observed in DFT-based calculations. As shown, although we identified only one pathway in which the oxygen atom becomes trapped between two phosphorus centers, an unexpected trend emerged: in the first mechanism, an early-stage intermediate appears slightly higher in energy than its corresponding transition state once solvation energy is included. This behavior persists even in gas-phase calculations with thermal corrections. While counterintuitive, this result is important to report and serves to illustrate the sensitivity of such calculations to solvation effects.

A similar phenomenon is observed in the second mechanism. Although the overall energy profile remains consistent with the expected trend, one intermediate is again calculated to lie marginally higher in energy than its associated transition state. These discrepancies, though small, warrant mention as they highlight limitations in the precision of energy ordering within current computational models, especially for transition states and shallow potential energy surfaces.

Chapter 4

Mechanistic Exploration of N,O-Ligand Activation by Lawesson and Woollins Reagents

The reaction of (Z)-4-(phenylamino)-3-(pyridin-2-ylmethyl)pent-3-en-2-one, an N,O-type ligand, with Lawesson reagent reveals a notable and unexpected transformation (**Figure 34**). Based on the known reactivity of Lawesson reagent, the anticipated outcome would be the substitution of the carbonyl oxygen atom, yielding a thiocarbonyl derivative. However, the experimental reaction instead proceeds to form an indolizine, indicating a mechanistic pathway beyond simple oxygen substitution.

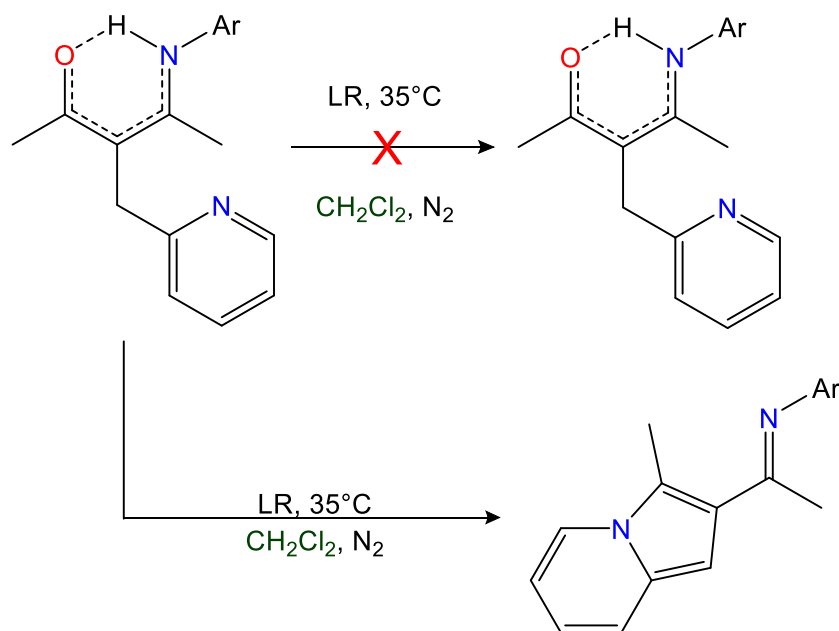


Figure 34. Unexpected synthesis of indolizine conducted in the lab of Dr. Crispin when using the Lawesson Reagent.

To gain insight into the origin of this reactivity, we first analyzed the electronic structure of the ligand. The molecule can be described by three resonance forms (**Figure 35**) arising from π -conjugation and tautomeric proton transfer. We evaluated the relative gas-phase energies of these forms to identify the lowest-energy structure for further mechanistic investigation. The most stable conformer corresponds to the neutral molecule bearing both a carbonyl and an amino group, which is also chemically reasonable as it presents a nucleophilic and electrophilic site capable of engaging Lawesson reagent.

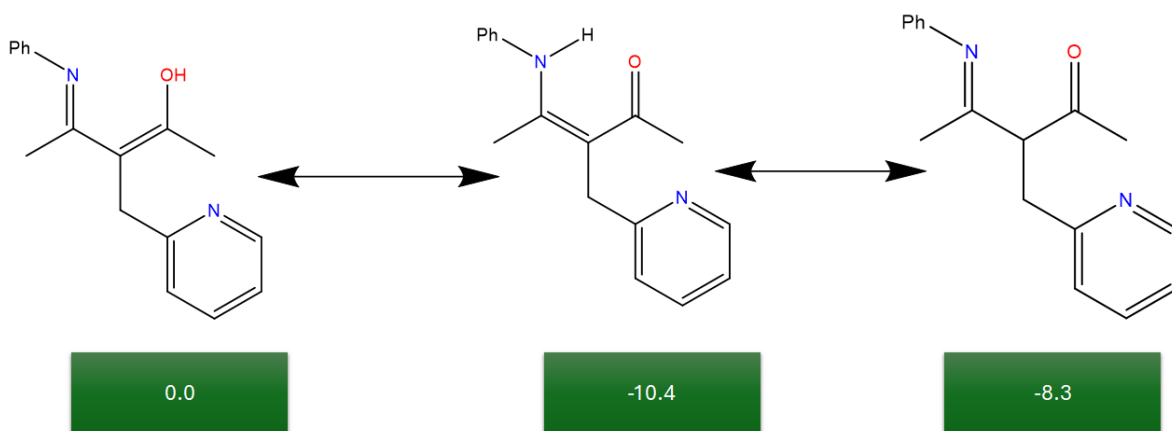


Figure 35. Calculated resonance structure of the N,O-ligand as the Reagent of reaction. Energy values are in kcal/mol.

Having defined the relevant starting structure, we confirmed the formation of the indolizine product via NMR spectroscopy and single-crystal X-ray diffraction. While the product structure is clearly established, it is also essential to understand the identity of the byproducts to fully account for the observed stoichiometry. The overall transformation results in the loss of two hydrogen atoms and one oxygen atom, suggesting three possible mechanistic scenarios.

In the first proposed mechanism (**Figure 36**), the reaction proceeds via elimination of water, resulting in the formation of the indolizine and implying that Lawesson reagent acts merely as a catalyst. This interpretation is attractive due to its simplicity; however, gas-phase Gibbs free energy calculations yield a reaction energy of only 3.5 kcal/mol, which appears inconsistent with the observed high yield and rapid reaction rate. Although this pathway is thermodynamically feasible, it is unlikely to be the dominant mechanism.

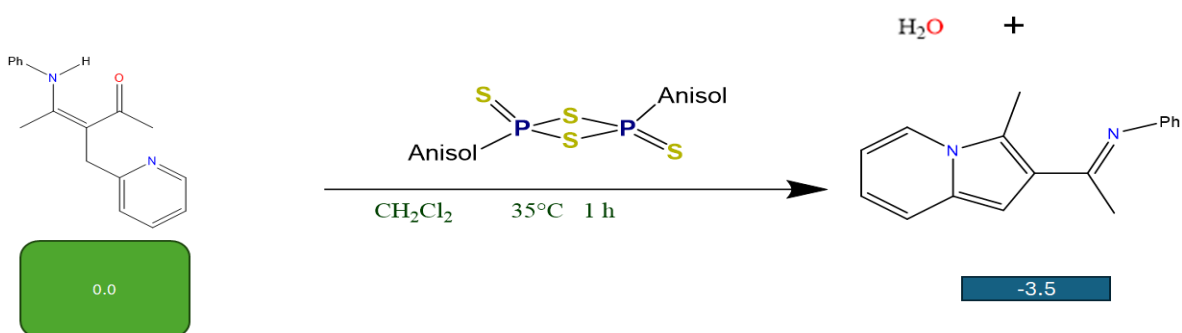


Figure 36. Cyclization reaction of the N,O-ligand using the **Lawesson Reagent** and proposing water as the reaction byproduct. Calculated energy values are in kcal/mol.

In a second hypothetical pathway (**Figure 37**), the reaction generates molecular hydrogen and a Lawesson reagent derivative bearing an oxygen bridge between the two phosphorus atoms, analogous to the mechanism observed for the O,O-ligand. However, this mechanism is thermodynamically unfavorable, and there

is no experimental evidence (e.g., gas evolution) supporting the release of hydrogen gas. Therefore, this scenario can be ruled out as implausible.

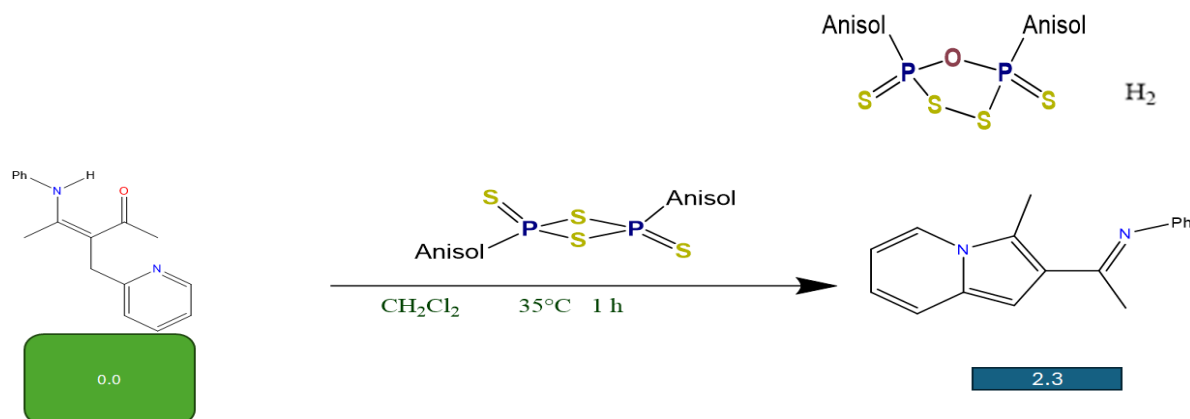


Figure 37. Cyclization reaction of the N,O-ligand using the **Lawesson Reagent** and proposing hydrogen and the five-membered ring are the reaction byproducts. Calculated energy values are in kcal/mol.

A third possibility involves the formation of hydrogen sulfide as a byproduct, along with a substituted Lawesson reagent. This pathway is thermodynamically viable and aligns with known reactivity patterns of Lawesson reagent. Within this context, we explored two configurations for the resulting Lawesson derivative: one in which the oxygen remains as a carbonyl group (**Figure 38**), and another in which the oxygen bridges the two phosphorus atoms (**Figure 39**). Our calculations indicate that the latter configuration is energetically more favorable and more consistent with known structural preferences of Lawesson-derived products.

Based on this analysis, we selected this final pathway (featuring oxygen transfer to Lawesson reagent and formation of hydrogen sulfide) as the most plausible mechanism for the reaction. The remainder of our mechanistic study focuses on this scenario, examining its feasibility across all critical steps and comparing it with the behavior of structurally analogous systems.

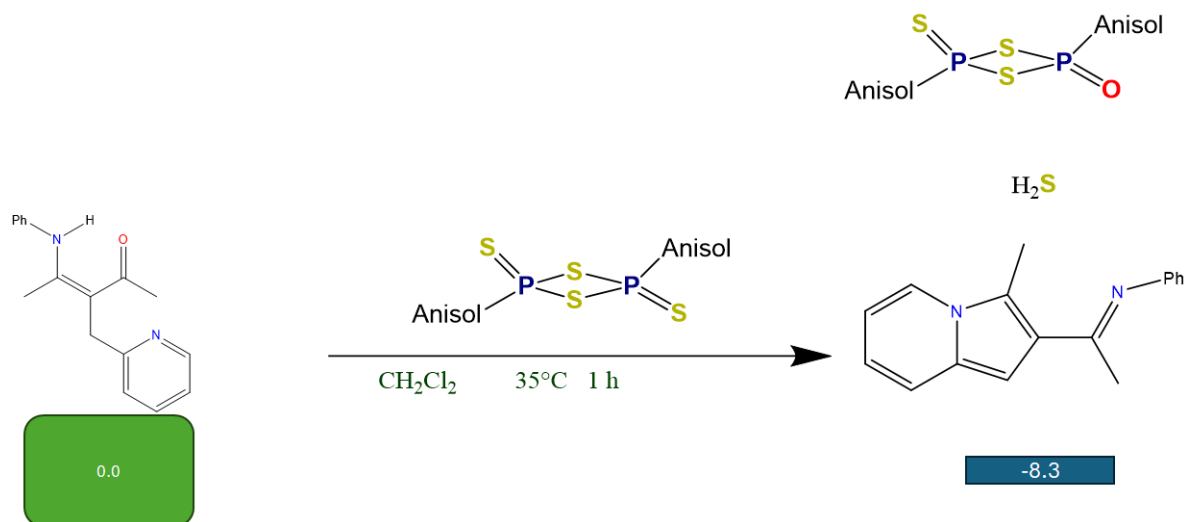


Figure 38. Cyclization reaction of the N,O-ligand using the **Lawesson Reagent** and proposing H_2S and first conformer of O-exchange Lawesson are the reaction byproducts. Calculated energy values are in kcal/mol.

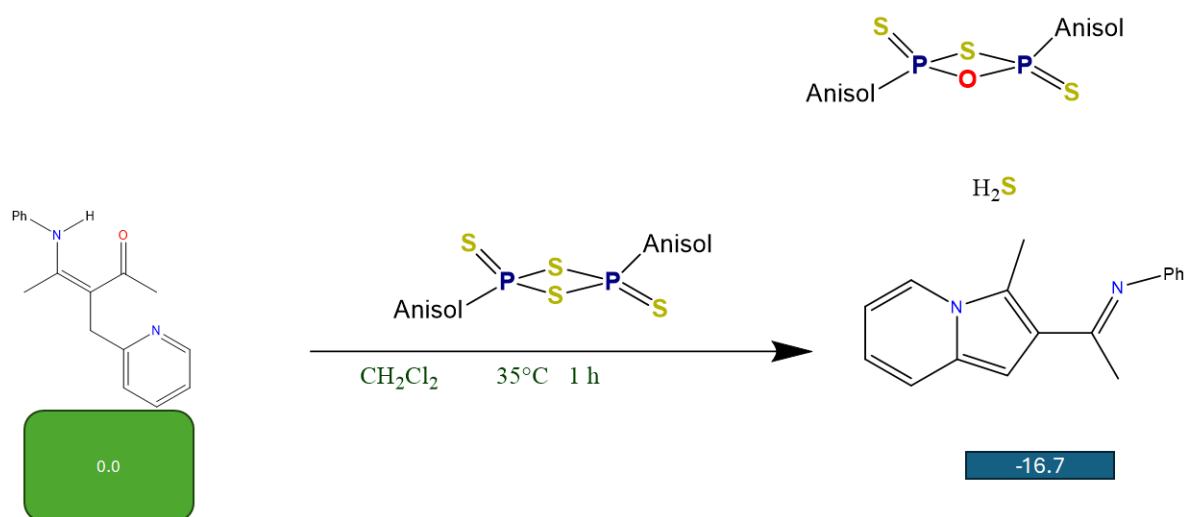


Figure 39. Cyclization reaction of the N,O-ligand using the **Lawesson Reagent** and proposing H_2S and second conformer of O-exchange Lawesson are the reaction byproducts. Calculated energy values are in kcal/mol.

All calculations were performed using density functional theory (DFT) as implemented in the Gaussian09 software package. Geometry optimizations and harmonic frequency analyses were conducted at the $\omega\text{B97X-D/def2-SVP}$ level of theory. No constraints were applied during the optimization procedures.

To refine the electronic energies, single-point energy calculations were performed using the $\omega\text{B97X-D/6-311+G(d)}$ basis set on the previously optimized geometries. Solvent effects were included through the SMD continuum solvation model, using dichloromethane (CH_2Cl_2) as the implicit solvent, also at the $\omega\text{B97X-D/def2-SVP}$ level.

When calculations are labeled as gas phase, they refer exclusively to the geometry optimization and frequency calculations performed at the ω B97X-D/def2-SVP level, with no solvent corrections applied.

All thermodynamic corrections were obtained from frequency calculations and correspond to standard conditions (298.15 K and 1 atm). Final energies are reported as Gibbs free energies (ΔG) and are given in kcal/mol.

This section presents the viable and mechanistically relevant pathways identified through computational analysis. Additional mechanisms that were assessed but found to be unfeasible are provided and discussed in **Appendix 1**.

The first viable mechanism (**Figure 40**) begins with the fragmentation of Lawesson reagent, generating a reactive monomeric species. One of these fragments engages with the carbonyl group of the N,O-ligand via a nucleophilic attack, establishing the expected P–O interaction. Simultaneously, cyclization occurs, resulting in the closure of the indolizine ring and formation of an intermediate exhibiting a dipolar character.

In this dipolar intermediate, the negatively charged sulfur atom deprotonates the only sp^3 -hybridized carbon bearing hydrogens, yielding a high-energy intermediate that rapidly undergoes elimination. This step leads to the simultaneous release of the Lawesson fragment and the oxygen atom, forming a new intermediate along the reaction coordinate.

This finding is particularly noteworthy in comparison to the behavior observed for the O,O-ligand, where elimination of the oxygen atom was only feasible following a substantial redistribution of electron density and stabilization through additional interactions. In contrast, the N,O-ligand exhibits enhanced reactivity in this regard. Here, the elimination step is facilitated by an intramolecular hydrogen bond, where sulfur interacts with the N–H proton of the aniline moiety, stabilizing the transition state and enabling oxygen departure under mild conditions.

As the reaction progresses, a transition state is reached in which the Coulombic stabilization shifts: the nitrogen atom assumes a more prominent role in interacting with the departing proton. This culminates in the formation of a stable N–H bond, completing the indolizine ring construction.

The remaining fragment of Lawesson reagent then dissociates, resulting in the formation of a substituted Lawesson fragment and hydrogen sulfide (H_2S). Notably, this substituted intermediate is not inert. It subsequently reacts with a second, unmodified molecule of Lawesson reagent to form the three final products observed. The calculated energy barriers for each step are consistent with the thermodynamic conditions under which the reaction is known to proceed.

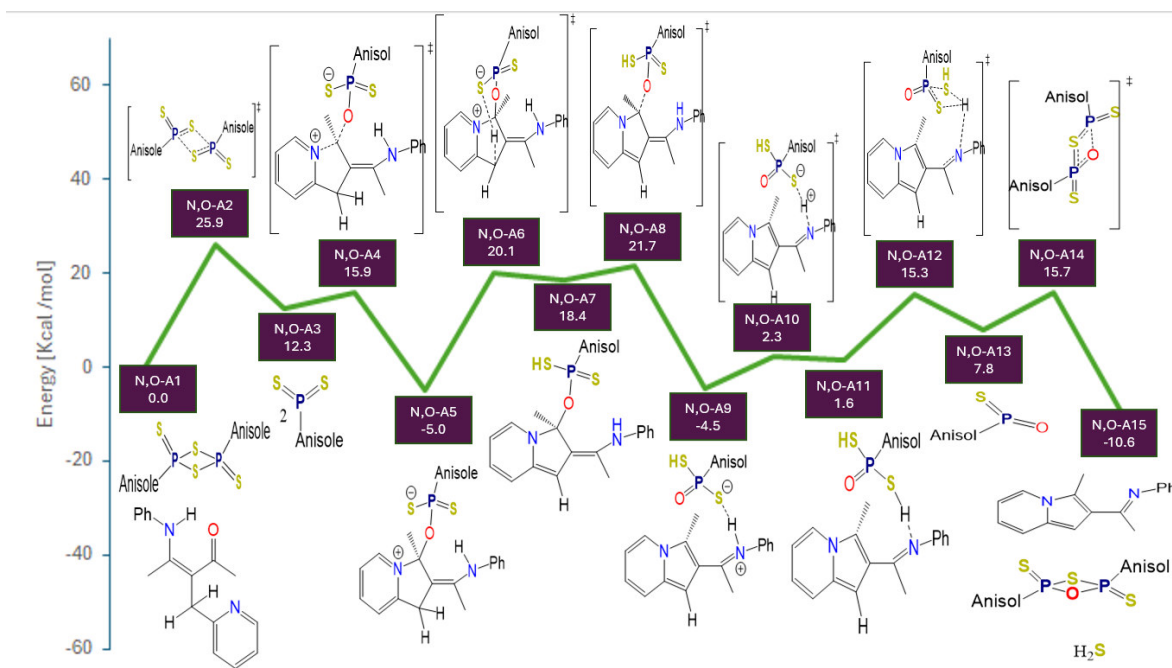


Figure 40. Gas-phase calculated energy profile of the N,O-ligand cyclization mechanism where a double proton migration occurs with the formation of H₂S using the **Lawesson Reagent**.

An alternative mechanistic pathway (**Figure 41**) was identified is energetically viable and leads to similarly favorable products. This mechanism begins with the fragmentation of Lawesson reagent, followed by cyclization via the interaction between the carbonyl oxygen of the N,O-ligand and the phosphorus atom of the reactive fragment. This process is accompanied by deprotonation of the adjacent sp³-hybridized carbon, analogous to the first mechanism.

Following oxygen elimination, the system evolves into a distinct intermediate in which both sulfur atoms (one forming part of a thiocarbonyl group and the other present as a thiol) engage in hydrogen bonding with the N–H proton of the amino group. This dual sulfur–hydrogen interaction contributes significant stabilization to the intermediate.

From this point, an energetically accessible transition state leads directly to the formation of the indolizine and hydrogen sulfide (H₂S), leaving behind only the substituted Lawesson fragment. As observed in the previous mechanism, this fragment subsequently reacts with a molecule of unmodified Lawesson reagent, completing the reaction and forming the final product distribution.

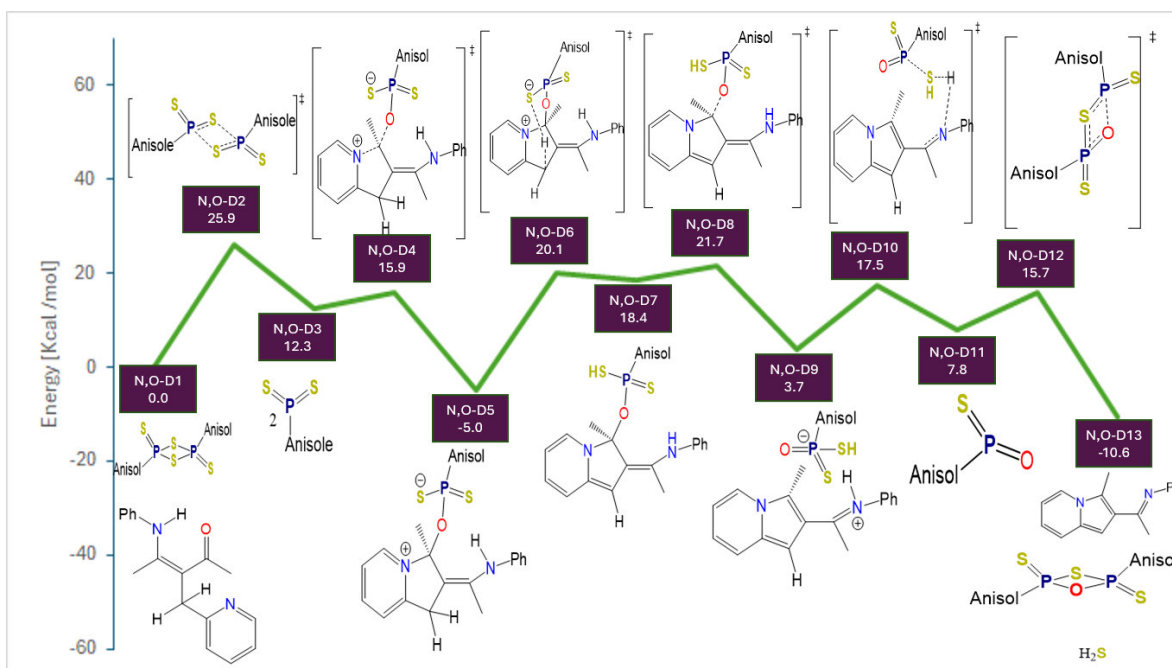


Figure 41. Gas-phase calculated energy profile of the N,O-ligand cyclization mechanism where a proton migration and double interaction takes place with the formation of H₂S using the **Lawesson Reagent**.

A mechanistic pathway involving WR was also investigated (**Figure 42**), despite the modest overall reaction energy difference between Reagents and products, calculated to be only 2 kcal/mol, and the well-known toxicity of hydrogen selenide (H₂Se), one of the most hazardous selenium-containing compounds.

The mechanism is theoretically viable and begins with the fragmentation of the Woollins reagent into reactive monomeric species. One fragment engages with the carbonyl group of the N,O-ligand, forming a P–O bond, while the adjacent nucleophilic nitrogen forms a C–N bond that completes the cyclization into the indolizine core. Simultaneously, deprotonation of the sp³-hybridized carbon occurs, facilitating the elimination of the carbonyl oxygen atom. A Se stabilizes this elimination step–H interaction, analogous to the S–H interaction observed in the corresponding mechanism with LR.

The reaction proceeds directly to the formation of hydrogen selenide (H₂Se) and the indolizine product, while the remaining substituted Woollins fragment is generated. This intermediate subsequently reacts with an unmodified Woollins reagent, completing the stoichiometry and affording the predicted three-product distribution under energetically accessible conditions.

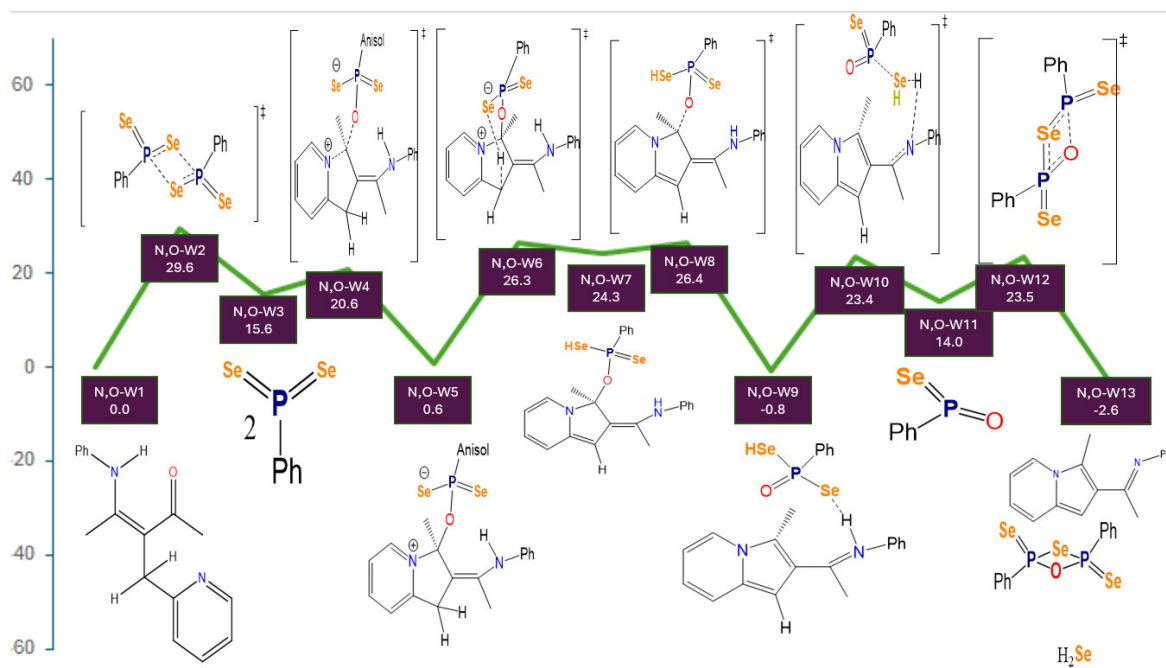


Figure 42. Gas-phase calculated energy profile of the N,O-ligand cyclization mechanism using the **Woollins Reagent**.

Conclusions

This Thesis presents a detailed computational investigation into the reactivity of O,O- and N,O-type ligands with Lawesson and Woollins reagents, two widely used organophosphorus-based thionation agents. Through a combination of density functional theory (DFT) calculations and mechanistic exploration, we have uncovered key structural and energetic factors that govern the observed chemoselectivity and product formation in these systems. We can conclude the following points:

- 1) Our study confirms that Lawesson reagent and Woollins reagent, though structurally analogous, exhibit subtle yet significant differences in their reactivity profiles. Both reagents were shown to undergo fragmentation into reactive intermediates, which initiate nucleophilic attack and ring closure in ligands bearing carbonyl and amino functionalities. In particular, the formation of indolizines—rather than the expected thiocarbonyl products—was explained by favorable reaction pathways featuring oxygen elimination, sulfur or selenium migration, and intramolecular hydrogen bonding that stabilizes critical intermediates and transition states.
- 2) For the O,O-type ligand, oxygen elimination proved challenging without significant stabilization, requiring rearrangement and Coulombic interaction with neighboring phosphorus atoms. In contrast, for the N,O-type ligand, multiple mechanisms were found to be energetically viable under mild conditions. The presence of an amino group facilitated the elimination step via S–H or Se–H interactions, depending on the reagent, and enabled smoother formation of the indolizine core.
- 3) Among the tested mechanisms, those leading to oxygen bridging between two phosphorus atoms—as observed in the final Lawesson or Woollins fragments—were consistently more stable and synthetically plausible. Moreover, the formation of hydrogen sulfide or hydrogen selenide as byproducts provided a rational basis for the reaction stoichiometry and accounted for the overall redox balance in the systems studied.
- 4) Solvent effects and thermodynamic corrections were found to influence the ordering of intermediates and transition states. In some cases, solvation led to unexpected energy inversions, with intermediates appearing slightly higher in energy than their corresponding transition states. These findings underscore the limitations of gas-phase-only models and the importance of including solvent environments in mechanistic studies.

Perspectives

The perspectives of this thesis revolve primarily around the exploration of substituents capable of imparting desired chemical and functional properties to the indolizine core structure. Consequently, comprehensive reactivity studies are essential to identify suitable precursors that yield targeted indolizine derivatives efficiently. Given the antisymmetric aromatic nature of indolizines, their susceptibility to various reaction types is significantly influenced by substituent positions within their bicyclic ring system. Thus, evaluating the stability and synthetic viability of indolizines as potential precursors forms a critical component of future research directions.

A secondary yet noteworthy consideration pertains to the optical properties of indolizines. These molecules demonstrate intriguing optical characteristics, notably fluorescence. With suitable substituents strategically positioned along their extensively delocalized π -system, indolizines have the potential to exhibit enhanced optical behaviors, including phosphorescence and nonlinear optical phenomena such as second-harmonic generation, third-harmonic generation, and Raman amplification.

Lastly, exploring the possibility of forming doubly linked indolizine structures through mechanisms involving N,O-ligands warrants consideration. Although preliminary attempts utilizing O,O-ligands yielded negative results and were not aligned closely with the principal objectives of this thesis, future work may benefit from further systematic investigation of alternative ligand frameworks.

Appendix 1

Exploration of Alternative Mechanisms

This appendix presents alternative mechanistic pathways for the synthesis of both indolizine derivatives. Although these routes do not coincide thermodynamically with the most favorable pathways previously discussed, they serve to demonstrate that a comprehensive mechanistic exploration was undertaken.

All calculations were performed at the ω B97X-D/def2-SVP level of theory for both geometry optimizations and harmonic frequency analyses. Thermochemical corrections were computed at 298.15 K and 1 atm, and all reported energies correspond to Gibbs free energies (ΔG), expressed in kcal/mol.

Alternative Pathway for 3-(pyridin-2-ylmethylene)pentane-2,4-dione (O,O-ligand)

In this proposed mechanism (**Figure 43**), previously shown to be viable with Woollins reagent, we evaluated its feasibility using Lawesson reagent under the same theoretical conditions. The pathway begins with a nucleophilic attack of the carbonyl oxygen on a phosphorus atom of the fragmented Lawesson reagent, followed by cyclization to form the indolizine ring.

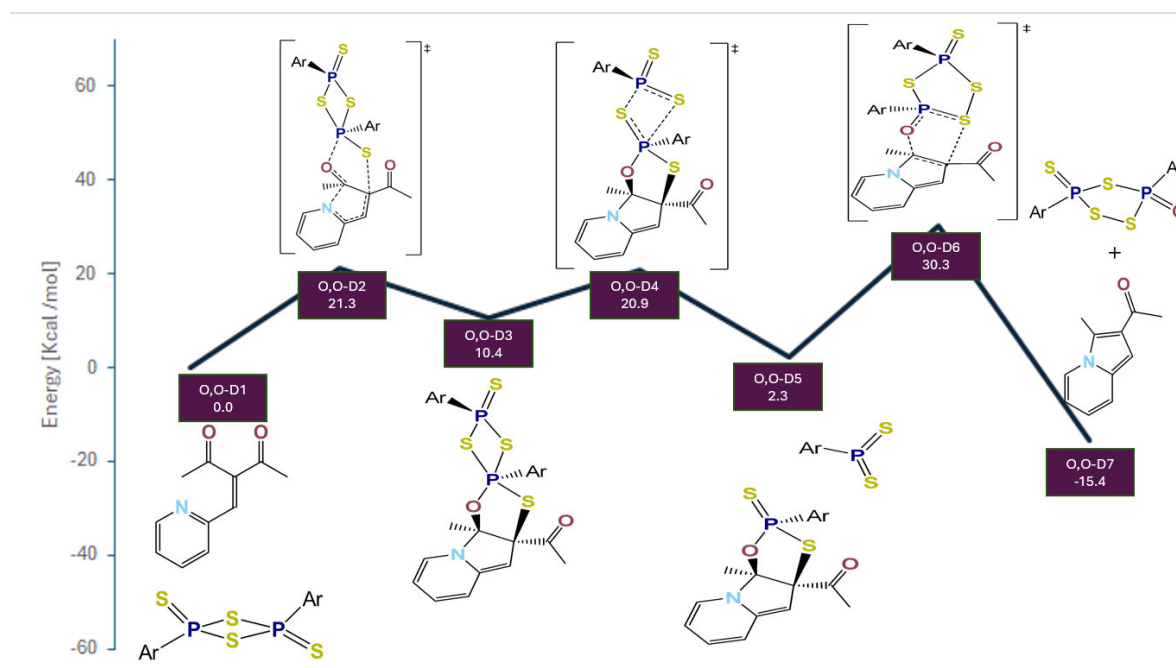


Figure 43. Gas phase.Elimination Mechanism, alpha carbon

Subsequently, a fragment of the reagent undergoes separation and rearrangement, capturing the oxygen atom as a carbonyl group attached to Lawesson reagent and completing the formation of the indolizine core. While the mechanistic sequence is chemically sound and consistent with prior findings, the calculated activation barrier of 30.3 kcal/mol places this pathway well outside the range of feasibility under the reaction conditions studied. As such, it is excluded from the set of mechanisms considered synthetically accessible in this work.

The pathway involving the direct elimination of the oxygen atom (**Figure 44**) clearly demonstrates that oxygen is not readily disposed to relinquish electron density. Achieving the required bond cleavage would necessitate a significant increase in thermal energy, to enhance vibrational motion and distort the geometry toward a reactive conformation. The calculated activation barrier of 42.8 kcal/mol places this mechanism far above the 25 kcal/mol threshold targeted in this investigation. Barriers exceeding 40 kcal/mol are only accessible through non-conventional activation techniques, such as microwave irradiation. Therefore, this mechanism was justifiably excluded from further consideration.

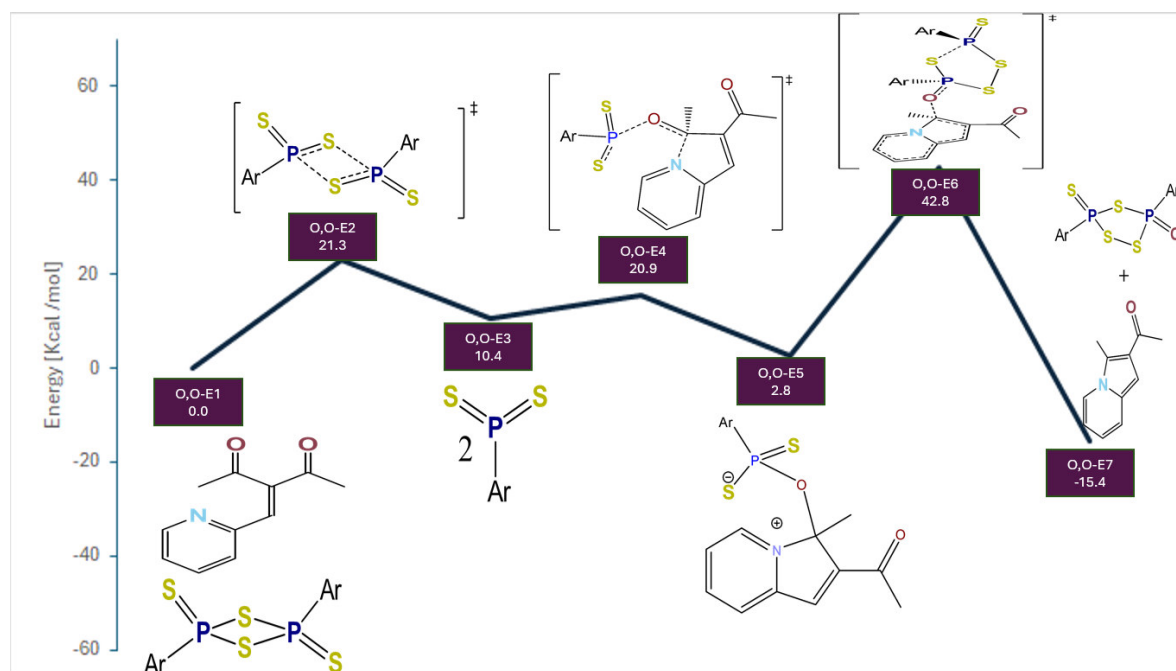


Figure 44. Gas phase. Elimination Mechanism, oxygen departure

Similarly, the pathway involving sulfur bonding to the β -carbon atom (**Figure 45**) consistently produced transition states ranging between 30 and 40 kcal/mol, further reinforcing its synthetic infeasibility. These values exceed the limits for plausible reaction conditions and, as such, this pathway was also discarded.

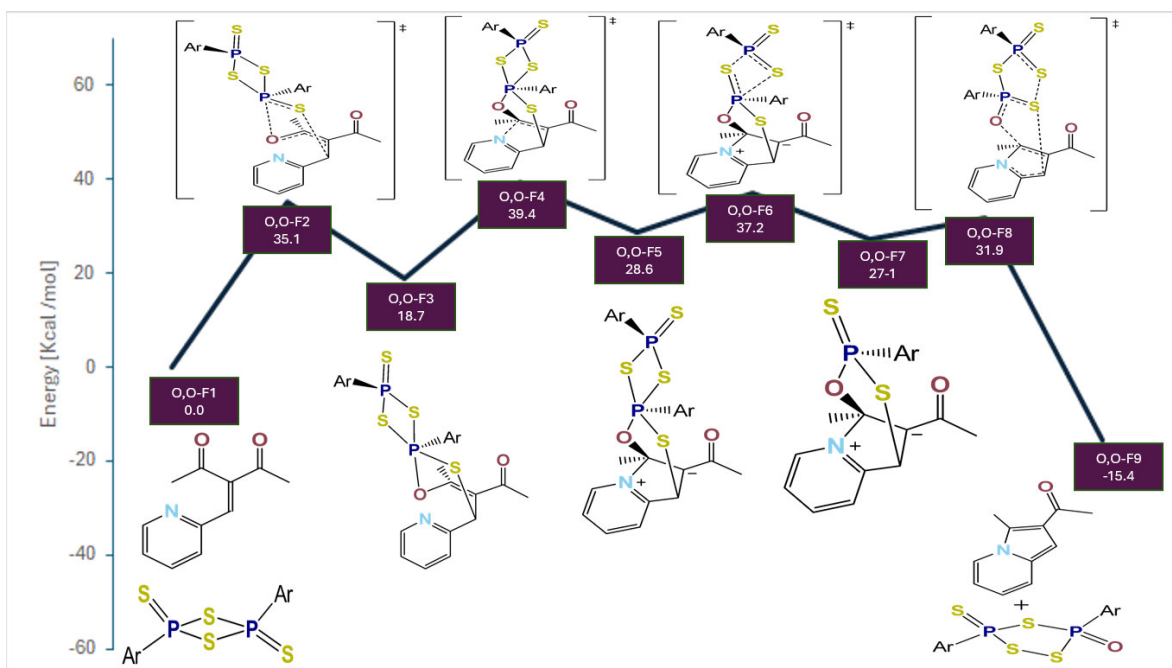


Figure 45. Gas phase. Elimination Mechanism, Beta Carbon

The mechanism featuring C–P bond formation (**Figure 46**), while previously identified as a viable route for Woollins reagent, reaches a final energy barrier of 32.6 kcal/mol when applied to Lawesson reagent. This result places it beyond the practical energy window and thus renders it unfeasible in this system. Nonetheless, its conceptual appeal makes it worth noting, as systematically ruling out mechanistic alternatives is essential to avoid incomplete or misleading conclusions.

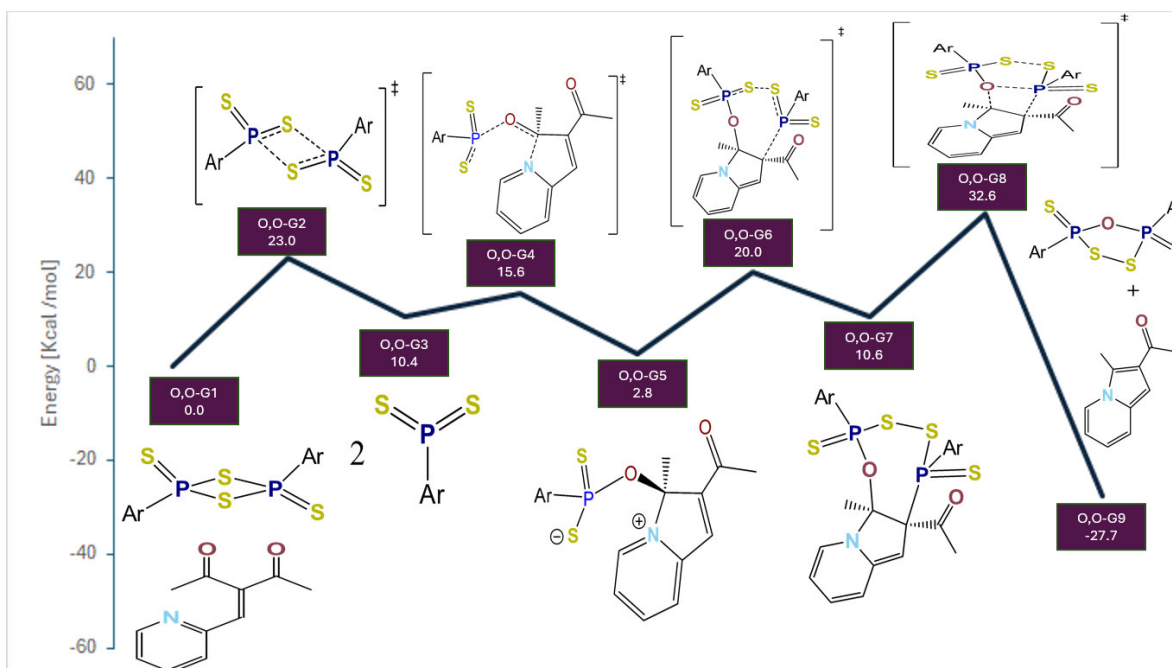


Figure 46. Gas phase Elimination Mechanism, P-C Bond.

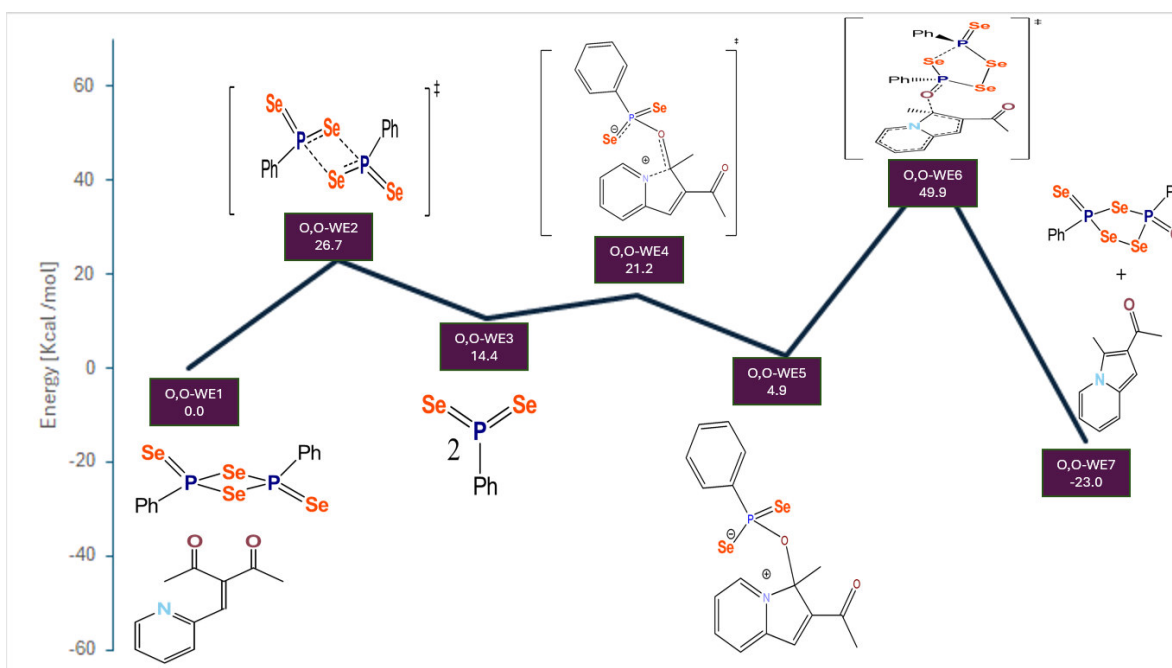


Figure 47. Gas phase. Elimination Mechanism, Oxygen Departure Woollins

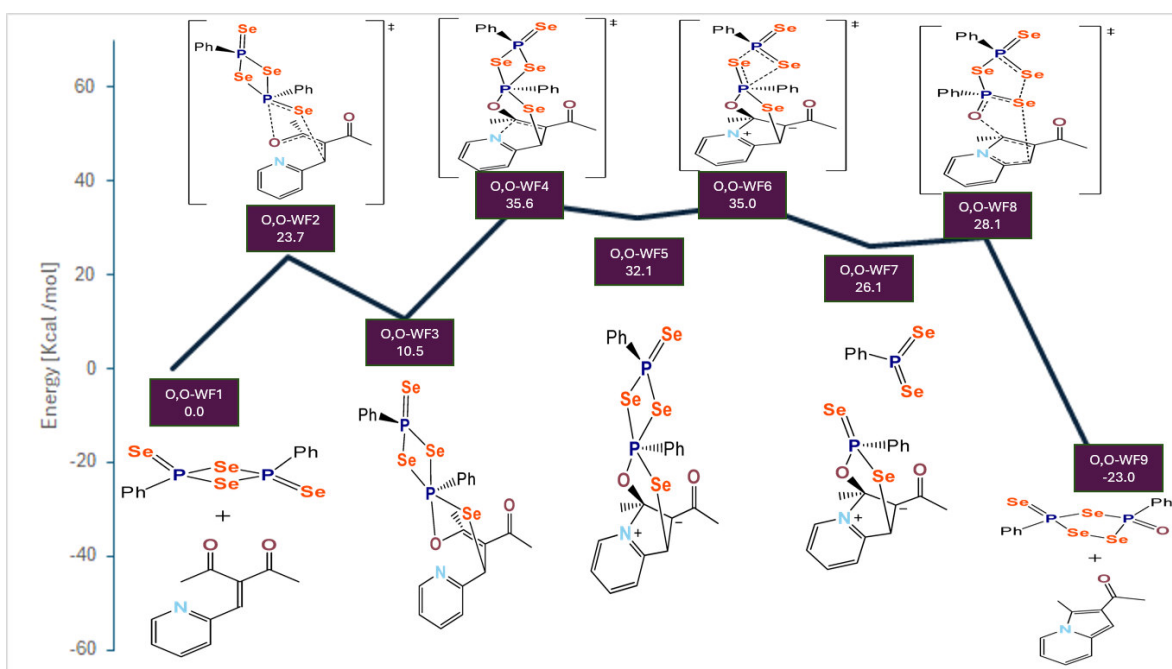


Figure 48. Gas phase. Elimination Mechanism, Beta Carbon Woollins

Returning to Woollins reagent, the oxygen elimination pathway (**Figure 47**) exhibits behavior analogous to that observed with Lawesson reagent. Here too, the oxygen atom resists electron withdrawal, and the energetic cost of elimination

approaches 50 kcal/mol. This makes the process not only unfavorable under standard conditions but synthetically unachievable altogether.

Finally, the β -carbon pathway for Woollins reagent (**Figure 48**) mirrors the behavior found in the Lawesson case. All associated transition states exhibit barriers of approximately 30 kcal/mol or higher, leading us to confidently exclude this pathway as well.

Alternative Pathway for (Z)-4-(phenylamino)-3-(pyridin-2-ylmethyl)pent-3-en-2-one (N,O-Ligand)

In the first alternative mechanism (**Figure 49**), the reaction begins once again with the fragmentation of Lawesson reagent, followed by cyclization, during which a P–O bond is formed and deprotonation of the sp^3 -hybridized carbon occurs. As observed in the first viable mechanism described earlier, the intermediate is stabilized via an S–H interaction, where proton migration toward sulfur facilitates a shift in the Coulombic interaction to nitrogen, leading to formation of the indolizine ring.

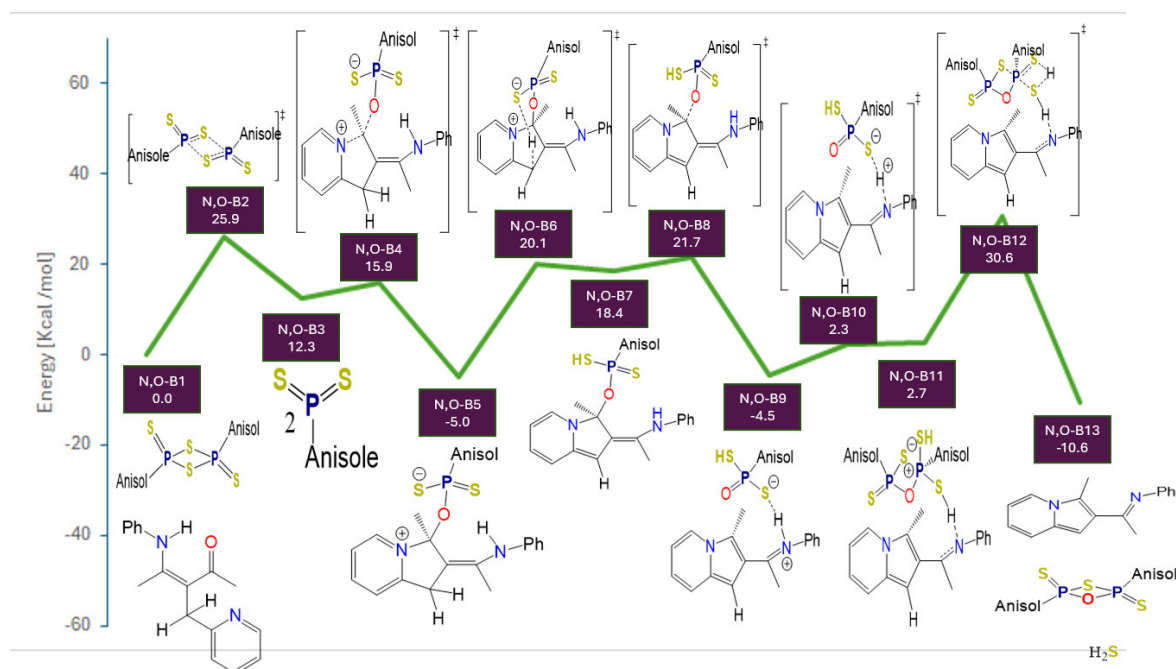


Figure 49. Three Side-products generation in one step.

From this intermediate, association with a Lawesson fragment is proposed to occur via a barrierless step. The mechanism then proceeds through a single concerted event that results in the formation of a substituted Lawesson reagent, hydrogen sulfide, and the dissociation of the Coulombic interaction, thereby releasing the final indolizine product. However, this last step requires an activation

energy of 30.6 kcal/mol, which is significantly high relative to the experimental temperatures employed. Consequently, while mechanistically consistent, this pathway was ruled out due to its energetic cost.

The next proposed mechanism for the N,O-ligand (**Figure 50**), although unfeasible, is included here for completeness. It follows the same sequence of steps as the previous mechanism: fragmentation, ring closure, deprotonation, exchange of Coulombic interactions, and barrierless association of a Lawesson fragment. The key difference lies in the final stage, where the indolizine is proposed to form via disruption of the nitrogen-based Coulombic interaction, while the remaining intermediate evolves into a substituted Lawesson fragment bearing two thiol groups, which then separate to yield hydrogen sulfide. However, this last transformation exhibits a calculated activation barrier exceeding 31 kcal/mol, rendering the mechanism thermodynamically inaccessible under the experimental conditions.

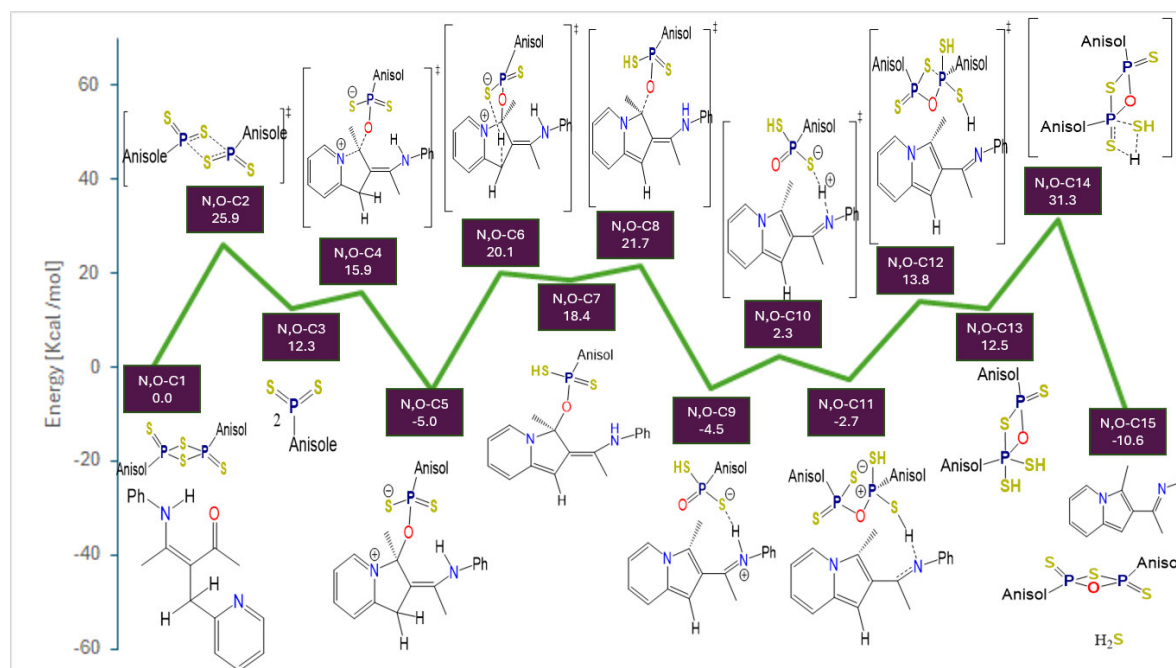


Figure 50. Doble Group-Thiol Generation.

The substitution mechanism (**Figure 51**) is included solely to illustrate that the associated energy barriers are significantly higher than those of the viable mechanisms, thereby justifying its exclusion. This analysis confirms that a structure commonly reported in Lawesson reagent-based reactions (namely the hexacyclic system formed from the association of three substituted fragments) is less stable than the alternative in which the reagent forms a four-membered ring. Nonetheless, experimental data from ^{31}P NMR suggest the presence of multiple phosphorus-containing species, implying that a variety of byproducts may form alongside the substituted Lawesson fragment (**Figure 52**).

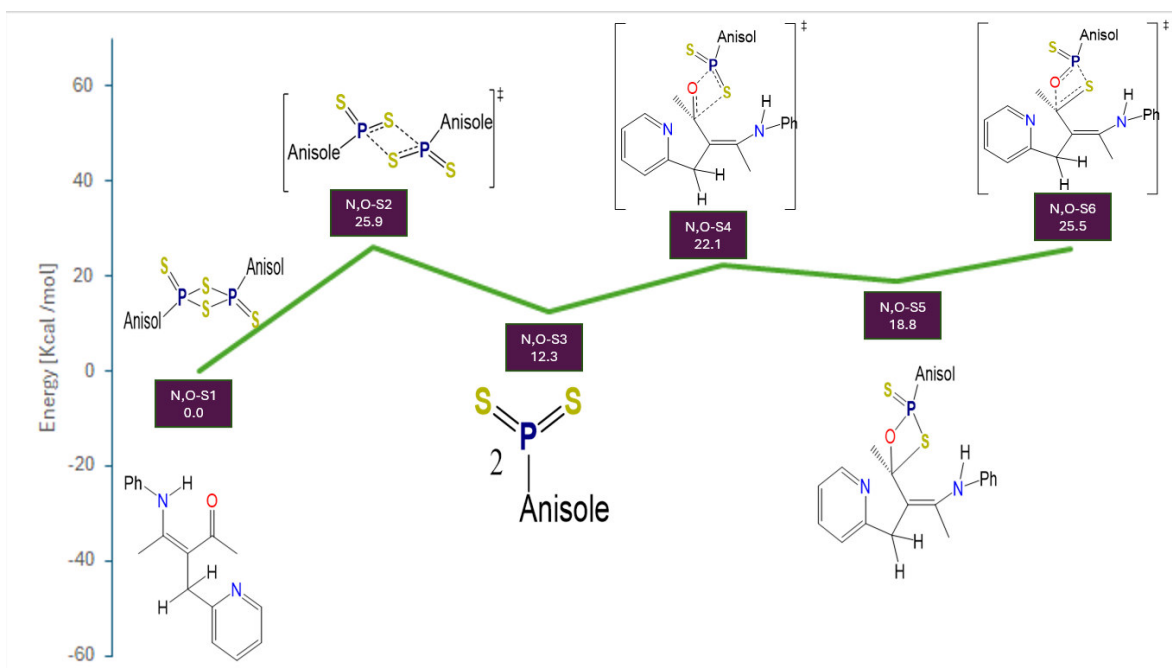


Figure 51. Substitution Approach Mechanism.

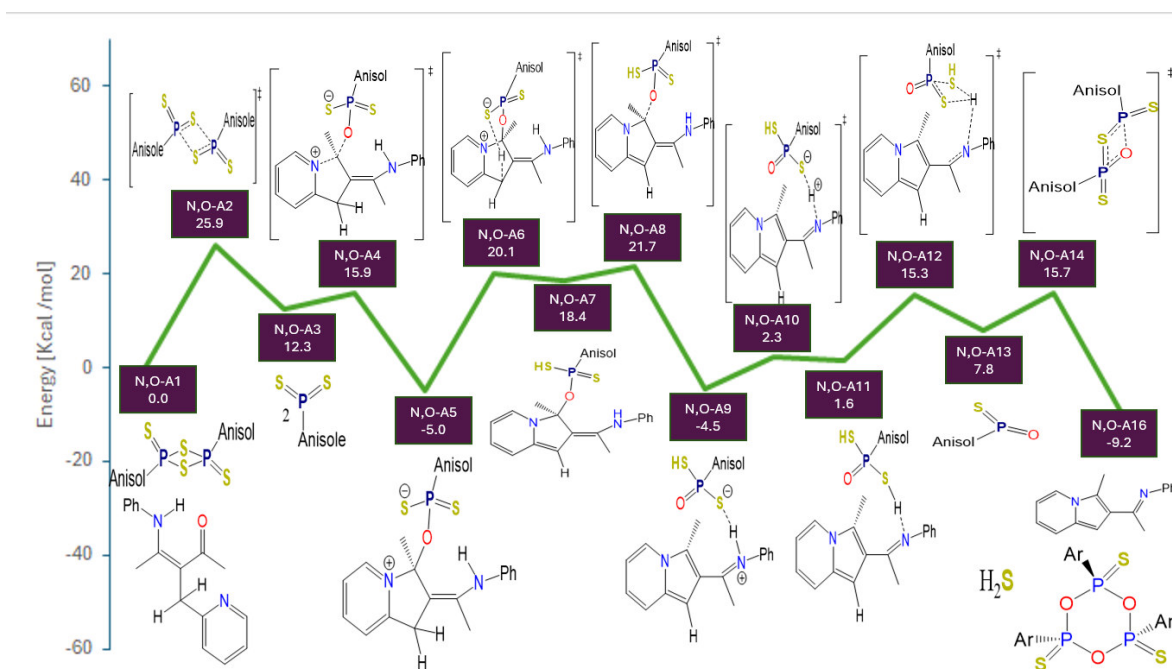


Figure 52. Hexacycle Generation as product instead of Substituted Lawesson Reagent.

Finally, it is important to note that these represent the only viable interactions from which a mechanistic pathway could be derived. Additional possibilities were examined, including mechanisms beginning with initial deprotonation of the amino

group or those involving octet rule violations; however, no energy minimum or convergent structures were in these cases (**Figure 53**). Accordingly, we report only four mechanisms as the viable pathways supported by computational analysis.

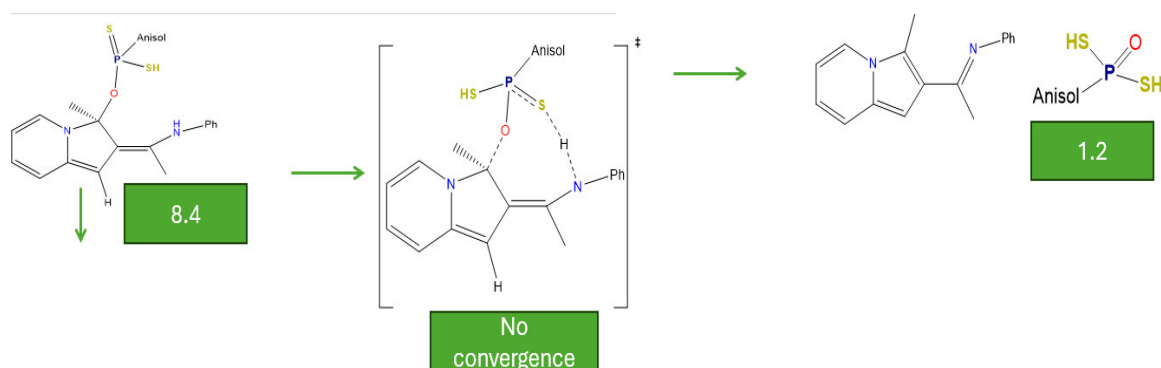


Figure 53. Discarded reactions Gas phase (Compared to reagents). Calculated energy values are in kcal/mol.

Appendix 2

Cartesian Coordinates of calculated mechanisms

Figure 20				1	-2.307453	1.395396	0.536
O,O-A1				6	-4.970864	-1.427866	-0.432
LR				1	-3.315267	-2.803163	-0.809
6	4.399900	-0.931020	0.078	6	-5.371350	-0.082808	0.013
6	3.051574	-0.594451	0.074	1	-4.679935	1.983600	0.725
6	2.652608	0.746089	0.098	1	-5.741489	-2.199662	-0.707
6	3.625607	1.755391	0.006	8	-6.693755	0.139912	0.103
6	4.971010	1.427326	0.027	6	-7.175115	1.459861	0.447
6	5.371218	0.082184	0.079	1	-6.850662	2.011249	-0.898237
1	4.679398	-1.984067	0.068	1	-8.269204	1.391129	0.340
1	2.307030	-1.395415	0.071	1	-6.850803	2.010720	0.899507
1	3.315697	2.802948	-0.108				
1	5.741782	2.198979	-0.020	Preindolizine			
8	6.693580	-0.140809	0.086	6	0.178997	-1.007094	-0.061471
6	7.174688	-1.460847	0.183	1	0.344103	-2.083841	-0.158607
1	8.268794	-1.392340	0.326	6	1.241723	-0.189608	0.035834
1	6.850105	-2.011894	0.899028	6	1.157013	1.312645	0.278992
1	6.850302	-2.011911	-0.898728	6	2.649285	-0.701640	-0.049454
15	0.901258	1.184195	-0.247	6	2.902049	-2.193470	-0.049733
15	-0.901144	-1.183693	-0.071	1	2.462099	-2.668778	0.839244
16	-0.184	0.609	-1.552090	1	2.458138	-2.665040	-0.939439
16	-0.116	0.185	1.553327	1	3.985338	-2.360717	-0.058901
16	0.492940	3.068803	-0.771	8	1.125	1.721883	1.410299
16	-0.492242	-3.068189	-0.603	8	3.564577	0.088276	-0.125556
6	-2.652613	-0.746168	-0.150	6	-1.233616	-0.593404	-0.052625
6	-3.051857	0.594301	0.287	6	-2.248065	-1.556404	0.038139
6	-3.625394	-1.755670	-0.493	7	-1.504383	0.713443	-0.139051
6	-4.400241	0.930604	0.362	6	-3.574545	-1.136383	0.056104

1	-1.995603	-2.616824	0.099871	6	2.490809	-0.781376	0.315290
6	-2.769395	1.109466	-0.122320	6	3.153407	0.389017	0.699605
6	-3.846604	0.226048	-0.023242	6	3.216076	-1.815551	-0.301885
1	-4.384517	-1.864961	0.130790	6	4.518843	0.533126	0.484738
1	-2.942230	2.188329	-0.193797	1	2.590010	1.198244	1.169247
1	-4.870163	0.603990	-0.011555	6	4.574104	-1.679850	-0.516320
6	1.239675	2.194562	-0.935888	1	2.700275	-2.728593	-0.606940
1	1.074718	3.239890	-0.646013	6	5.239282	-0.503636	-0.127213
1	2.245811	2.082825	-1.369636	1	5.008365	1.456113	0.793375
1	0.497232	1.881452	-1.682557	1	5.155828	-2.472745	-0.988319
O,O-A2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	O,O-A3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410

1	-4.625439	1.226573	0.899941	6	-3.760029	-0.449782	-0.052835
1	-4.622697	1.228758	-0.898633	6	-4.440744	-0.749808	-1.240515
O,O-A4				7	-3.623973	-1.342453	0.932753
15	0.602125	0.221886	-0.632331	6	-4.952239	-2.029878	-1.417847
16	0.351230	1.682449	-1.883052	1	-4.541484	0.007447	-2.020053
16	-0.650496	-1.353888	-0.532222	6	-4.127766	-2.559300	0.763298
6	2.329525	-0.221552	-0.354969	6	-4.793067	-2.959983	-0.395276
6	3.356859	0.627465	-0.769392	1	-5.468253	-2.296779	-2.342245
6	2.654154	-1.416464	0.307549	1	-3.995129	-3.260520	1.593574
6	4.690193	0.306650	-0.526824	1	-5.180185	-3.976034	-0.485934
1	3.106240	1.552789	-1.293383	6	-1.288147	-0.128959	2.644854
6	3.975646	-1.744607	0.552738	1	-0.453047	-0.758495	2.971592
1	1.852203	-2.090458	0.617814	1	-1.419044	0.712075	3.350574
6	5.006288	-0.883404	0.141462	1	-2.236345	-0.677934	2.567683
1	5.469281	0.990119	-0.863571	O,O-A5			
1	4.245952	-2.670037	1.063436	15	-0.826196	0.665689	0.704381
8	6.258027	-1.281595	0.425830	16	-0.791873	1.961222	2.132226
6	7.339127	-0.464996	0.060504	16	0.637086	-0.868772	0.580693
1	7.282141	0.525434	0.543626	6	-2.460122	0.006535	0.322408
1	8.246966	-0.975674	0.402900	6	-3.594780	0.527986	0.944925
1	7.397175	-0.327843	-1.032923	6	-2.614890	-1.020129	-0.624759
6	-3.192800	0.902224	0.097163	6	-4.866074	0.049069	0.635456
1	-3.785387	1.680067	-0.392831	1	-3.478882	1.322139	1.686219
6	-2.035276	1.310671	0.647629	6	-3.871063	-1.501305	-0.941769
6	-0.986385	0.497899	1.344872	1	-1.735311	-1.456847	-1.101504
6	-1.731111	2.795874	0.733378	6	-5.011358	-0.968315	-0.315580
6	-2.307242	3.720143	-0.311360	1	-5.731008	0.478957	1.139769
1	-2.142886	3.315521	-1.319379	1	-4.006133	-2.298210	-1.674384
1	-3.387909	3.857842	-0.150528	8	-6.188022	-1.497221	-0.686170
1	-1.816385	4.694967	-0.209619	6	-7.372471	-1.021799	-0.100786
8	0.252588	0.729538	1.071809	1	-7.524657	0.052034	-0.302939
8	-1.069567	3.201590	1.658960	1	-8.194454	-1.588302	-0.553957

1	-7.382205	-1.187299	0.990045	6	2.952238	0.652955	0.916698
6	3.450980	0.748595	-0.275271	6	4.426795	-0.959480	-0.827951
1	4.197993	1.544348	-0.184181	1	2.682431	-0.912644	-2.095734
6	2.222141	1.116302	-0.671147	6	4.247756	0.293918	1.242899
6	0.987217	0.260146	-0.871775	1	2.370201	1.291879	1.583978
6	2.021731	2.557440	-1.114798	6	4.995502	-0.519552	0.375258
6	2.095859	3.616521	-0.052237	1	4.988425	-1.584153	-1.522077
1	1.280886	3.431189	0.667513	1	4.716888	0.632013	2.168097
1	3.039146	3.548791	0.509935	8	6.242740	-0.820873	0.776235
1	1.987723	4.609883	-0.504659	6	7.050523	-1.628707	-0.038489
8	-0.166767	1.117882	-0.745589	1	7.231694	-1.163021	-1.022377
8	1.799927	2.788558	-2.277892	1	8.008550	-1.741809	0.482654
6	3.962807	-0.593687	0.040195	1	6.605911	-2.627272	-0.190638
6	5.220550	-0.727411	0.649511	6	-3.229996	0.543635	-0.371409
7	3.222489	-1.663054	-0.275456	1	-3.843247	1.112628	-1.076590
6	5.700804	-1.998449	0.939843	6	-2.267430	1.198835	0.303704
1	5.805631	0.161395	0.893412	6	-1.296957	0.539900	1.189937
6	3.683171	-2.876201	0.008304	6	-2.218529	2.722651	0.228892
6	4.917600	-3.103447	0.613926	6	-2.186814	3.334883	-1.143880
1	6.675355	-2.126371	1.415752	1	-2.018031	4.413232	-1.041905
1	3.034594	-3.715684	-0.263279	1	-1.392196	2.866238	-1.742020
1	5.253421	-4.120870	0.819815	1	-3.144298	3.170040	-1.661838
6	0.967251	-0.414551	-2.226369	8	0.251002	1.859284	0.255737
1	0.009618	-0.929090	-2.382136	8	-2.244494	3.372155	1.243572
1	1.089816	0.365606	-2.991670	6	-3.619054	-0.862195	-0.167790
1	1.793336	-1.132373	-2.291221	6	-4.152780	-1.605123	-1.227503
O,O-A6				7	-3.459511	-1.375147	1.058469
15	0.689005	0.710468	-0.661748	6	-4.487306	-2.936865	-1.007313
16	0.204910	0.626763	-2.533172	1	-4.277396	-1.146535	-2.210068
16	-0.411128	-0.854379	0.642354	6	-3.785740	-2.645583	1.261836
6	2.376032	0.213973	-0.286981	6	-4.298354	-3.474320	0.262924
6	3.124390	-0.586069	-1.151154	1	-4.889232	-3.548084	-1.817974

1	-3.635951	-3.030685	2.275787	16	1.214097	-1.905937	-1.307786
1	-4.548324	-4.513367	0.482845	LR-Six Member Ring			
6	-1.258773	0.910452	2.616858	15	0.131650	-1.506650	1.034386
1	-0.335054	0.575747	3.100187	15	0.024047	1.455891	1.224303
1	-1.439325	1.988385	2.731565	15	-1.276146	0.068876	-1.151524
1	-2.123043	0.383890	3.062565	8	0.790605	-0.003596	1.185630
O,O-A7				8	-0.798727	-1.244941	-0.296037
Thiocarbonyl				8	-0.904988	1.288400	-0.123373
6	0.027046	1.150957	0.040778	16	-0.820322	-2.188495	2.543900
1	0.142126	2.234794	-0.038112	16	-0.458706	0.219246	-2.883826
6	1.136939	0.389817	0.088947	16	-0.956048	1.879185	2.807476
6	1.153629	-1.107757	0.106387	6	1.510042	-2.442884	0.392144
6	2.507510	1.016691	0.144282	6	2.075731	-3.461060	1.158858
6	2.660732	2.489780	-0.166894	6	2.044201	-2.151160	-0.875343
1	2.217180	2.738523	-1.141804	6	3.169379	-4.183565	0.687410
1	2.165266	3.105080	0.599202	1	1.650880	-3.694915	2.137918
1	3.730934	2.727174	-0.174608	6	3.127568	-2.865141	-1.350467
8	3.464210	0.339697	0.443517	1	1.594072	-1.376726	-1.502342
6	-1.365083	0.676180	0.062955	6	3.702479	-3.886413	-0.573058
6	-2.406224	1.551268	-0.280335	1	3.591128	-4.973705	1.307841
7	-1.597523	-0.591786	0.418995	1	3.552637	-2.662006	-2.334273
6	-3.714190	1.077741	-0.273171	6	1.326414	2.559475	0.697897
1	-2.186871	2.585240	-0.554025	6	1.816436	3.537414	1.575236
6	-2.846048	-1.038195	0.425838	6	1.878601	2.442085	-0.581111
6	-3.944856	-0.247747	0.083317	6	2.846656	4.373889	1.181924
1	-4.542356	1.736249	-0.543578	1	1.375723	3.638210	2.569718
1	-2.987250	-2.083429	0.720524	6	2.913479	3.279251	-0.983534
1	-4.952627	-0.665549	0.102903	1	1.489593	1.705261	-1.289099
6	1.234622	-1.753238	1.452132	6	3.406480	4.250649	-0.099700
1	1.188711	-2.845624	1.365995	1	3.240363	5.141010	1.849968
1	2.190401	-1.458446	1.915555	1	3.321511	3.169153	-1.987765
1	0.413458	-1.387081	2.086001	6	-3.053876	-0.014215	-1.043749

6	-3.853995	0.044008	-2.192383	6	4.971010	1.427326	0.027
6	-3.653510	-0.140169	0.213925	6	5.371218	0.082184	0.079
6	-5.232593	-0.022136	-2.082678	1	4.679398	-1.984067	0.068
1	-3.383915	0.142661	-3.173600	1	2.307030	-1.395415	0.071
6	-5.036296	-0.207730	0.330997	1	3.315697	2.802948	-0.108
1	-3.043083	-0.187879	1.120391	1	5.741782	2.198979	-0.020
6	-5.835689	-0.148469	-0.821226	8	6.693580	-0.140809	0.086
1	-5.875133	0.021152	-2.963074	6	7.174688	-1.460847	0.183
1	-5.477454	-0.307584	1.321965	1	8.268794	-1.392340	0.326
8	4.748493	-4.523314	-1.121040	1	6.850105	-2.011894	0.899028
8	-7.175928	-0.204808	-0.810455	1	6.850302	-2.011911	-0.898728
8	4.399020	5.103817	-0.395352	15	0.901258	1.184195	-0.247
6	5.004809	5.046620	-1.661283	15	-0.901144	-1.183693	-0.071
1	4.279707	5.247852	-2.467989	16	-0.184	0.609	-1.552090
1	5.776051	5.825462	-1.673243	16	-0.116	0.185	1.553327
1	5.481419	4.067803	-1.839983	16	0.492940	3.068803	-0.771
6	-7.852984	-0.327003	0.414434	16	-0.492242	-3.068189	-0.603
1	-7.586552	-1.262400	0.934978	6	-2.652613	-0.746168	-0.150
1	-7.646464	0.527685	1.080576	6	-3.051857	0.594301	0.287
1	-8.923587	-0.344077	0.179067	6	-3.625394	-1.755670	-0.493
6	5.369606	-5.565623	-0.413690	6	-4.400241	0.930604	0.362
1	5.798888	-5.210752	0.538767	1	-2.307453	1.395396	0.536
1	4.667621	-6.391428	-0.207750	6	-4.970864	-1.427866	-0.432
1	6.179094	-5.936902	-1.052952	1	-3.315267	-2.803163	-0.809
Figure 21				6	-5.371350	-0.082808	0.013
O,O-B1				1	-4.679935	1.983600	0.725
LR				1	-5.741489	-2.199662	-0.707
6	4.399900	-0.931020	0.078	8	-6.693755	0.139912	0.103
6	3.051574	-0.594451	0.074	6	-7.175115	1.459861	0.447
6	2.652608	0.746089	0.098	1	-6.850662	2.011249	-0.898237
6	3.625607	1.755391	0.006	1	-8.269204	1.391129	0.340
				1	-6.850803	2.010720	0.899507

				6	-4.758656	0.886153	0.643939
Preindolizine				6	-5.024024	-0.367057	0.059747
6	0.178997	-1.007094	-0.061471	1	-4.217340	-1.963686	-1.181138
1	0.344103	-2.083841	-0.158607	1	-2.040794	-0.873401	-1.495921
6	1.241723	-0.189608	0.035834	1	-3.326587	2.460132	0.924601
6	1.157013	1.312645	0.278992	1	-5.542149	1.356584	1.239391
6	2.649285	-0.701640	-0.049454	8	-6.239018	-0.877646	0.295638
6	2.902049	-2.193470	-0.049733	6	-6.575757	-2.137635	-0.229085
1	2.462099	-2.668778	0.839244	1	-7.598145	-2.349814	0.104217
1	2.458138	-2.665040	-0.939439	1	-6.550899	-2.137520	-1.331831
1	3.985338	-2.360717	-0.058901	1	-5.902560	-2.925468	0.148168
8	1.125	1.721883	1.410299	15	-0.937468	1.631443	-0.512316
8	3.564577	0.088276	-0.125556	15	0.725823	-0.944103	0.573580
6	-1.233616	-0.593404	-0.052625	16	-0.037424	0.374100	1.823646
6	-2.248065	-1.556404	0.038139	16	0.299548	0.620838	-1.668058
7	-1.504383	0.713443	-0.139051	16	-0.803876	3.498794	-0.124871
6	-3.574545	-1.136383	0.056104	16	-0.045896	-2.658290	0.185837
1	-1.995603	-2.616824	0.099871	6	2.490809	-0.781376	0.315290
6	-2.769395	1.109466	-0.122320	6	3.153407	0.389017	0.699605
6	-3.846604	0.226048	-0.023242	6	3.216076	-1.815551	-0.301885
1	-4.384517	-1.864961	0.130790	6	4.518843	0.533126	0.484738
1	-2.942230	2.188329	-0.193797	1	2.590010	1.198244	1.169247
1	-4.870163	0.603990	-0.011555	6	4.574104	-1.679850	-0.516320
6	1.239675	2.194562	-0.935888	1	2.700275	-2.728593	-0.606940
1	1.074718	3.239890	-0.646013	6	5.239282	-0.503636	-0.127213
1	2.245811	2.082825	-1.369636	1	5.008365	1.456113	0.793375
1	0.497232	1.881452	-1.682557	1	5.155828	-2.472745	-0.988319
O,O-B2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917

O,O-B3				6	5.078616	-2.218799	-0.258748
6	-2.563014	-0.295727	0.078	7	4.828457	0.047223	0.475889
6	-1.761443	-1.451863	-0.463	6	6.461676	-2.073118	-0.286165
6	-0.384385	-1.344393	-0.361	1	4.608495	-3.165062	-0.533562
6	0.230510	-0.078248	0.234	6	6.146860	0.180897	0.450477
6	-0.571133	1.069674	0.902	6	7.013633	-0.846764	0.072285
6	-1.957541	0.970024	0.948	1	7.100753	-2.906861	-0.584755
8	-3.885436	-0.498129	-0.230	1	6.542640	1.157891	0.747083
6	-4.759250	0.603778	-0.315	1	8.092563	-0.684280	0.064238
15	2.021612	0.066269	-0.039	6	2.467578	1.804189	1.752212
16	2.707743	1.856016	-0.605	1	2.878286	2.819884	1.693313
16	2.982996	-1.591296	0.363	1	1.461488	1.826756	2.197284
1	-2.254777	-2.424604	-0.001081	1	3.112430	1.165299	2.371281
1	0.236002	-2.243390	-0.730	6	-5.321555	-0.759567	0.424167
1	-0.098402	2.054262	0.001405	6	-4.926146	0.422958	1.075990
1	-2.554405	1.881627	0.001668	6	-3.723836	1.025127	0.760376
1	-5.775254	0.192793	-0.002410	6	-2.877713	0.453992	-0.206960
1	-4.625439	1.226573	0.899941	6	-3.274567	-0.717593	-0.855147
1	-4.622697	1.228758	-0.898633	6	-4.490255	-1.325660	-0.550699
O,O-B4				8	-6.504817	-1.268276	0.797307
6	2.823614	-1.246353	0.136025	6	-6.974510	-2.444238	0.189512
1	2.445674	-2.265197	0.018459	15	-1.314538	1.236848	-0.616616
6	1.943185	-0.236528	0.269069	16	-0.165741	0.142046	-1.832015
6	2.349610	1.233621	0.365733	16	-1.256836	3.132270	-0.434494
6	0.477381	-0.489317	0.359942	1	-5.593820	0.846584	1.827570
6	-0.036779	-1.908264	0.381627	1	-3.427029	1.950577	1.258581
1	0.369264	-2.537892	-0.418269	1	-2.623583	-1.153442	-1.616709
1	0.240215	-2.337714	1.359302	1	-4.777491	-2.233822	-1.079991
1	-1.130799	-1.895200	0.319972	1	-7.942474	-2.668384	0.652515
8	2.488468	1.877062	-0.640416	1	-7.118725	-2.310415	-0.895949
8	-0.211190	0.394121	0.998727	1	-6.289558	-3.291829	0.361550
6	4.288555	-1.123330	0.119519	O,O-B5			

6	-2.920234	-1.264372	-0.066863	6	7.208293	-2.191642	-0.171010
1	-2.616018	-2.313387	-0.044257	15	1.226968	1.068500	0.287522
6	-1.984424	-0.304841	0.011048	16	0.211277	-0.087821	1.756573
6	-2.329836	1.183718	0.061387	16	1.116297	2.980304	0.213443
6	-0.510422	-0.638437	0.104165	1	5.782927	1.180109	-1.602374
6	-0.140312	-2.074832	-0.213172	1	3.502083	2.085149	-1.166510
1	-0.555917	-2.773696	0.525158	1	2.629502	-1.357133	1.272081
1	-0.511868	-2.339199	-1.213903	1	4.881741	-2.241895	0.862401
1	0.951822	-2.176321	-0.211297	1	8.232021	-2.313286	-0.543948
8	-2.440268	1.720508	1.133142	1	7.229390	-2.167973	0.931935
8	0.230464	0.239983	-0.755219	1	6.603368	-3.053408	-0.501471
6	-4.373507	-1.052749	-0.171816	O,O-B6			
6	-5.247838	-2.148018	-0.109460	6	3.027482	-1.270077	0.125546
7	-4.822355	0.195524	-0.334683	1	2.794315	-2.335900	0.184902
6	-6.616746	-1.924041	-0.209201	6	2.023427	-0.386090	-0.022676
1	-4.852603	-3.157731	0.018811	6	2.253325	1.122212	-0.142785
6	-6.128168	0.405496	-0.430280	6	0.620012	-0.881934	-0.165979
6	-7.074031	-0.618949	-0.371682	6	0.297493	-2.204920	0.473291
1	-7.319569	-2.758585	-0.160852	1	0.701212	-3.011181	-0.157809
1	-6.443960	1.445878	-0.561252	1	0.723635	-2.280026	1.482631
1	-8.138654	-0.395182	-0.454890	1	-0.787956	-2.339474	0.527419
6	-2.399368	1.916715	-1.250488	8	2.205628	1.657008	-1.217536
1	-2.930426	2.865428	-1.104756	8	-0.292482	0.233804	0.895428
1	-1.367431	2.126786	-1.571891	6	4.465021	-0.960446	0.169700
1	-2.892361	1.309437	-2.020502	6	5.400391	-1.999483	0.290469
6	5.478523	-0.588595	-0.418929	7	4.843682	0.319042	0.091918
6	5.072248	0.632321	-0.981922	6	6.754806	-1.686593	0.325945
6	3.802618	1.124980	-0.741707	1	5.063177	-3.036074	0.353603
6	2.894588	0.406352	0.055889	6	6.135917	0.614279	0.127598
6	3.309129	-0.800910	0.622697	6	7.137842	-0.350546	0.241811
6	4.589401	-1.302036	0.394683	1	7.503353	-2.476693	0.416178
8	6.728212	-0.985724	-0.705775	1	6.392502	1.676620	0.057706

1	8.188727	-0.057553	0.262197	1	-1.994535	2.732771	-0.954528
6	2.420662	1.866543	1.156899	1	-3.520100	2.585572	-0.041563
1	2.859836	2.850943	0.953758	8	-0.846033	-1.700968	1.383131
1	1.421890	1.996110	1.600164	16	-3.644505	-0.145243	-0.054049
1	3.044854	1.303644	1.862552	6	1.538765	0.579489	-0.049506
6	-5.597253	-0.463311	0.276443	6	2.565787	1.533303	0.011424
6	-5.295779	0.883236	0.538613	7	1.796927	-0.732020	-0.099647
6	-3.996731	1.343195	0.422097	6	3.887265	1.099425	0.036426
6	-2.961220	0.465886	0.052811	1	2.325889	2.597911	0.044407
6	-3.269368	-0.869871	-0.221875	6	3.057194	-1.141407	-0.076916
6	-4.573539	-1.339483	-0.113247	6	4.144528	-0.267710	-0.005963
8	-6.882281	-0.818445	0.413580	1	4.705207	1.821	0.088413
6	-7.265240	-2.144156	0.148942	1	3.217789	-2.223782	-0.118359
15	-1.273703	1.071199	-0.028397	1	5.163901	-0.656426	0.013508
16	-0.137429	-0.590897	-1.782027	6	-0.865404	-2.155440	-0.969796
16	-1.057044	2.956815	-0.178712	1	-0.664043	-3.193297	-0.676123
1	-6.107719	1.550589	0.830512	1	-1.856172	-2.092351	-1.445039
1	-3.772526	2.393749	0.617395	1	-0.107609	-1.807779	-1.684772
1	-2.481236	-1.538645	-0.573564	LR Six Members Ring			
1	-4.782029	-2.383510	-0.345187	15	0.131650	-1.506650	1.034386
1	-8.345395	-2.198909	0.327328	15	0.024047	1.455891	1.224303
1	-7.060573	-2.423204	-0.898515	15	-1.276146	0.068876	-1.151524
1	-6.755139	-2.856023	0.819686	8	0.790605	-0.003596	1.185630
O,O-B7				8	-0.798727	-1.244941	-0.296037
Thiocarbonyl 2				8	-0.904988	1.288400	-0.123373
6	0.136309	1.017249	-0.061481	16	-0.820322	-2.188495	2.543900
1	0.001966	2.098003	-0.147955	16	-0.458706	0.219246	-2.883826
6	-0.958587	0.229830	0.028802	16	-0.956048	1.879185	2.807476
6	-0.864281	-1.280955	0.255924	6	1.510042	-2.442884	0.392144
6	-2.316564	0.811697	-0.020976	6	2.075731	-3.461060	1.158858
6	-2.459249	2.311987	-0.048546	6	2.044201	-2.151160	-0.875343
1	-1.965007	2.769341	0.822925	6	3.169379	-4.183565	0.687410

1	1.650880	-3.694915	2.137918
6	3.127568	-2.865141	-1.350467
1	1.594072	-1.376726	-1.502342
6	3.702479	-3.886413	-0.573058
1	3.591128	-4.973705	1.307841
1	3.552637	-2.662006	-2.334273
6	1.326414	2.559475	0.697897
6	1.816436	3.537414	1.575236
6	1.878601	2.442085	-0.581111
6	2.846656	4.373889	1.181924
1	1.375723	3.638210	2.569718
6	2.913479	3.279251	-0.983534
1	1.489593	1.705261	-1.289099
6	3.406480	4.250649	-0.099700
1	3.240363	5.141010	1.849968
1	3.321511	3.169153	-1.987765
6	-3.053876	-0.014215	-1.043749
6	-3.853995	0.044008	-2.192383
6	-3.653510	-0.140169	0.213925
6	-5.232593	-0.022136	-2.082678
1	-3.383915	0.142661	-3.173600
6	-5.036296	-0.207730	0.330997
1	-3.043083	-0.187879	1.120391
6	-5.835689	-0.148469	-0.821226
1	-5.875133	0.021152	-2.963074
1	-5.477454	-0.307584	1.321965
8	4.748493	-4.523314	-1.121040
8	-7.175928	-0.204808	-0.810455
8	4.399020	5.103817	-0.395352
6	5.004809	5.046620	-1.661283
1	4.279707	5.247852	-2.467989
1	5.776051	5.825462	-1.673243

1	5.481419	4.067803	-1.839983
6	-7.852984	-0.327003	0.414434
1	-7.586552	-1.262400	0.934978
1	-7.646464	0.527685	1.080576
1	-8.923587	-0.344077	0.179067
6	5.369606	-5.565623	-0.413690
1	5.798888	-5.210752	0.538767
1	4.667621	-6.391428	-0.207750
1	6.179094	-5.936902	-1.052952

Figure 22

O,O-C1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327

16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139

7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-C2

6	-3.640736	1.233283	-0.679088
6	-2.255170	1.337839	-0.617045
6	-1.648260	2.530683	-0.212921
6	-2.451053	3.626591	0.132409
6	-3.832639	3.527430	0.079437
6	-4.439618	2.330295	-0.327177
1	-4.078239	0.293496	-1.014123
1	-1.652736	0.468899	-0.898119
1	-1.977937	4.561778	0.441058
1	-4.471296	4.371144	0.344954
8	-5.784145	2.321605	-0.352698
6	-6.454076	1.161716	-0.767110
1	-7.526937	1.378003	-0.701863
1	-6.204428	0.895047	-1.808564
1	-6.224591	0.302294	-0.112891
15	0.158318	2.662699	-0.100748
15	1.346246	-0.086025	-0.338316
16	0.728726	1.107793	1.286441
16	0.974366	1.576007	-1.733894

16	0.843489	4.429158	0.264929	1	-4.615714	-1.755075	0.424516
16	0.185047	-1.528059	-1.168337	6	-2.504988	-3.964454	-1.844091
6	3.141568	-0.205977	-0.441283	6	-3.824348	-3.720820	-2.224388
6	3.938831	0.908073	-0.183003	1	-5.649713	-2.709957	-1.645526
6	3.737247	-1.424963	-0.787493	1	-1.862248	-4.603983	-2.457875
6	5.325826	0.814185	-0.258829	1	-4.227299	-4.162323	-3.137076
1	3.482125	1.866004	0.078985	6	0.753468	-3.765798	0.950546
6	5.114725	-1.522957	-0.873831	1	1.706849	-3.939308	0.436682
1	3.110778	-2.294841	-0.993269	1	0.840392	-4.125254	1.990179
6	5.921834	-0.406022	-0.604019	1	-0.074490	-4.280768	0.450449
1	5.926272	1.698637	-0.048351	O,O-C3			
1	5.600752	-2.461386	-1.143795	6	3.657488	-1.430890	-0.291552
8	7.247799	-0.598130	-0.703206	6	2.268028	-1.446565	-0.242845
6	8.119785	0.472197	-0.449296	6	1.574339	-2.621213	0.059518
1	8.009147	0.853847	0.580030	6	2.296448	-3.793487	0.316794
1	9.136599	0.082440	-0.577090	6	3.682584	-3.787907	0.270683
1	7.962593	1.302148	-1.159374	6	4.374832	-2.607596	-0.035006
6	-2.106526	-2.054819	1.248054	1	4.161926	-0.496661	-0.537188
1	-2.877420	-1.642951	1.906007	1	1.727059	-0.520440	-0.449516
6	-0.838789	-1.884756	1.672857	1	1.756136	-4.713822	0.551413
6	0.491644	-2.294319	1.055562	1	4.257827	-4.694057	0.466122
6	-0.667234	-1.333414	3.077598	8	5.717804	-2.691516	-0.062592
6	-1.628013	-0.272624	3.576271	6	6.467885	-1.546621	-0.363649
1	-1.922838	0.430645	2.785998	1	7.522785	-1.844921	-0.335033
1	-2.535177	-0.751081	3.978776	1	6.233895	-1.154794	-1.368844
1	-1.142323	0.262945	4.401414	1	6.304722	-0.745010	0.378298
8	1.479814	-1.512460	1.243595	15	-0.243026	-2.633888	0.112700
8	0.192266	-1.788334	3.791706	15	-1.381812	0.225305	-0.062191
6	-2.685139	-2.661332	0.039647	16	-0.716516	-1.034381	1.503260
6	-4.032893	-2.385300	-0.250273	16	-0.962083	-1.553789	-1.527280
7	-1.953103	-3.457550	-0.747692	16	-1.032433	-4.352779	0.516012
6	-4.605577	-2.915982	-1.399658	16	-0.014083	1.379215	-1.148536

6	-3.178691	0.215950	-0.296368	6	4.182620	2.873851	-2.614139
6	-3.899406	-0.979111	-0.361882	1	5.977434	2.211944	-1.602026
6	-3.872930	1.434124	-0.360096	1	2.218751	3.503091	-3.275174
6	-5.283888	-0.969987	-0.497300	1	4.649214	3.734	-3.592006
1	-3.382806	-1.939115	-0.301944	6	-0.747876	3.832182	0.064573
6	-5.247143	1.451919	-0.524612	1	-1.606023	3.812120	-0.621763
1	-3.331819	2.374943	-0.265973	1	-1.030374	4.319872	1.007203
6	-5.967250	0.249681	-0.593471	1	0.075666	4.384381	-0.406717
1	-5.814042	-1.921156	-0.531754	O,O-C4			
1	-5.795847	2.392490	-0.588146	6	4.409436	-1.158614	-0.084085
8	-7.296297	0.362381	-0.745749	6	3.026703	-1.177881	-0.247446
6	-8.084203	-0.798691	-0.802061	6	2.344152	-2.380725	-0.438830
1	-8.008856	-1.386409	0.128622	6	3.073820	-3.580989	-0.479274
1	-9.121100	-0.466330	-0.930238	6	4.446300	-3.571826	-0.310195
1	-7.805776	-1.439335	-1.656103	6	5.128844	-2.360613	-0.106672
6	2.200279	2.437704	1.081818	1	4.912325	-0.201991	0.056221
1	2.878658	2.374737	1.938158	1	2.478323	-0.233766	-0.234452
6	0.882892	2.394202	1.344646	1	2.552485	-4.524646	-0.655369
6	-0.290900	2.419635	0.375446	1	5.025389	-4.495972	-0.335460
6	0.458462	2.465010	2.802537	8	6.457663	-2.450171	0.047480
6	1.016286	1.447442	3.763167	6	7.207830	-1.284701	0.275021
1	0.537465	0.481352	3.539269	1	8.251415	-1.601434	0.385276
1	2.098175	1.298867	3.645207	1	7.135585	-0.581039	-0.571713
1	0.779093	1.746505	4.791286	1	6.890383	-0.771764	1.198786
8	-1.340013	1.638096	0.924636	15	0.546831	-2.433314	-0.635460
8	-0.315362	3.323481	3.150665	15	-1.184021	-0.424038	0.653664
6	2.892531	2.591863	-0.206884	16	-0.309098	-2.219494	1.358389
6	4.263180	2.297646	-0.289883	16	-0.087484	-0.396240	-1.135270
7	2.205218	3.026275	-1.269732	16	-0.110707	-3.924391	-1.675397
6	4.912447	2.436864	-1.510990	16	-1.380619	2.150278	-0.567712
1	4.802073	1.960177	0.597784	6	-2.918587	-0.723921	0.374676
6	2.829421	3.156309	-2.435348	6	-3.342104	-1.731409	-0.494422

6	-3.863455	0.046007	1.068058	1	-0.593452	6.423155	-1.350874
6	-4.698776	-1.966984	-0.687045	1	0.372772	6.115506	-3.633697
1	-2.615019	-2.347874	-1.031243	6	-1.553701	3.127614	2.006122
6	-5.213587	-0.190284	0.886580	1	-2.624704	2.938668	1.863657
1	-3.529442	0.830900	1.747568	1	-1.242801	2.966274	3.045088
6	-5.644203	-1.194725	0.004239	1	-1.344725	4.174930	1.734538
1	-5.004774	-2.754055	-1.375233	O,O-C5			
1	-5.967282	0.395617	1.414055	LR sub			
8	-6.971342	-1.346652	-0.112136	6	-4.591026	0.652266	-0.099
6	-7.484012	-2.324546	-0.980633	6	-3.210603	0.490969	-0.083
1	-7.164886	-3.338757	-0.686219	6	-2.647248	-0.787501	0.112
1	-8.576091	-2.260583	-0.909747	6	-3.479101	-1.917019	0.287
1	-7.181425	-2.139698	-2.025214	6	-4.855215	-1.763079	0.271
6	1.622678	2.998261	0.471240	6	-5.423032	-0.478913	0.083
1	2.686536	2.944416	0.734717	1	-5.007941	1.658813	-0.257
6	0.748641	2.375817	1.274975	1	-2.565544	1.374219	-0.219
6	-0.741510	2.303603	1.046027	1	-3.029906	-2.912355	0.439
6	1.269504	1.821904	2.590583	1	-5.523903	-2.625051	0.404
6	2.314631	0.738247	2.531187	8	-6.763130	-0.426053	0.093
1	1.823827	-0.182564	2.178295	6	-7.407459	0.822373	-0.052
1	3.121087	0.975360	1.823923	1	-8.484358	0.617490	0.042
1	2.724568	0.567204	3.533980	1	-7.155374	1.410215	0.898862
8	-0.918407	0.640994	1.741678	1	-7.155479	1.409951	-0.899169
8	0.846156	2.241303	3.639719	15	-0.874922	-1.044572	0.155
6	1.303480	3.850430	-0.700629	15	0.969749	1.249343	-0.180
6	1.930324	3.623815	-1.930944	16	-0.054899	0.170519	-1.555593
7	0.436885	4.848438	-0.508264	16	-0.054915	0.170994	1.555543
6	1.597054	4.434575	-3.009673	16	0.756890	3.162759	-0.467
1	2.646324	2.806535	-2.039167	6	2.664637	0.623178	-0.086
6	0.128316	5.622162	-1.542910	6	2.920779	-0.752216	0.092
6	0.668922	5.454683	-2.817345	6	3.738024	1.524777	-0.195
1	2.052993	4.271162	-3.988643	6	4.226757	-1.227421	0.152

1	2.099807	-1.474844	0.183
6	5.041943	1.057548	-0.133
1	3.539589	2.598979	-0.336
6	5.298977	-0.321738	0.038
1	4.395534	-2.303752	0.292
1	5.888825	1.745064	-0.216
8	6.590596	-0.684177	0.080
6	6.925207	-2.048600	0.201
1	6.541888	-2.560931	-0.898369
1	8.020183	-2.101895	0.196
1	6.541904	-2.560771	0.898868
8	-0.464548	-2.472621	0.376

Thiocarbonyl

6	0.027046	1.150957	0.040778
1	0.142126	2.234794	-0.038112
6	1.136939	0.389817	0.088947
6	1.153629	-1.107757	0.106387
6	2.507510	1.016691	0.144282
6	2.660732	2.489780	-0.166894
1	2.217180	2.738523	-1.141804
1	2.165266	3.105080	0.599202
1	3.730934	2.727174	-0.174608
8	3.464210	0.339697	0.443517
6	-1.365083	0.676180	0.062955
6	-2.406224	1.551268	-0.280335
7	-1.597523	-0.591786	0.418995
6	-3.714190	1.077741	-0.273171
1	-2.186871	2.585240	-0.554025
6	-2.846048	-1.038195	0.425838
6	-3.944856	-0.247747	0.083317
1	-4.542356	1.736249	-0.543578
1	-2.987250	-2.083429	0.720524

1	-4.952627	-0.665549	0.102903
6	1.234622	-1.753238	1.452132
1	1.188711	-2.845624	1.365995
1	2.190401	-1.458446	1.915555
1	0.413458	-1.387081	2.086001
16	1.214097	-1.905937	-1.307786

Figure 23

O,O-H1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771

16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051

6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-H2

6	-4.040100	-0.995309	-0.715057
6	-2.806060	-0.380074	-0.894362
6	-2.537931	0.861547	-0.308140
6	-3.531311	1.490869	0.464960
6	-4.758656	0.886153	0.643939
6	-5.024024	-0.367057	0.059747
1	-4.217340	-1.963686	-1.181138
1	-2.040794	-0.873401	-1.495921
1	-3.326587	2.460132	0.924601
1	-5.542149	1.356584	1.239391
8	-6.239018	-0.877646	0.295638
6	-6.575757	-2.137635	-0.229085
1	-7.598145	-2.349814	0.104217
1	-6.550899	-2.137520	-1.331831
1	-5.902560	-2.925468	0.148168
15	-0.937468	1.631443	-0.512316
15	0.725823	-0.944103	0.573580
16	-0.037424	0.374100	1.823646
16	0.299548	0.620838	-1.668058
16	-0.803876	3.498794	-0.124871

16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	O,O-H4			
6	4.518843	0.533126	0.484738	6	-3.334661	0.397287	-0.108530
1	2.590010	1.198244	1.169247	1	-4.118597	0.841972	-0.722543
6	4.574104	-1.679850	-0.516320	6	-2.413161	1.137904	0.523965
1	2.700275	-2.728593	-0.606940	6	-1.331402	0.469811	1.339344
6	5.239282	-0.503636	-0.127213	6	-2.423406	2.642127	0.573366
1	5.008365	1.456113	0.793375	6	-3.226687	3.371879	-0.471469
1	5.155828	-2.472745	-0.988319	1	-2.942736	3.028651	-1.475901
8	6.554046	-0.461539	-0.378351	1	-4.301678	3.184930	-0.320741
6	7.292017	0.681090	-0.023996	1	-3.035202	4.446410	-0.371560
1	7.259570	0.862974	1.063412	8	-0.181966	0.303263	0.873581
1	8.328884	0.487145	-0.321802	8	-1.840026	3.212329	1.466614
1	6.928185	1.578435	-0.551917	6	-3.262443	-1.057243	0.047002
O,O-H3				6	-4.026569	-1.984634	-0.659766
6	-2.563014	-0.295727	0.078	7	-2.344662	-1.437919	0.937046
6	-1.761443	-1.451863	-0.463	6	-3.781158	-3.337644	-0.441352
6	-0.384385	-1.344393	-0.361	1	-4.772442	-1.650062	-1.381820
6	0.230510	-0.078248	0.234	6	-2.094447	-2.720682	1.142669
6	-0.571133	1.069674	0.902	6	-2.797807	-3.718820	0.469015
6	-1.957541	0.970024	0.948	1	-4.347532	-4.093322	-0.989262
8	-3.885436	-0.498129	-0.230	1	-1.306134	-2.962164	1.861521
6	-4.759250	0.603778	-0.315	1	-2.572631	-4.769972	0.652262
15	2.021612	0.066269	-0.039	6	-1.475502	0.477469	2.828198
16	2.707743	1.856016	-0.605	1	-0.772198	-0.234987	3.276436
16	2.982996	-1.591296	0.363	1	-1.221252	1.499873	3.148804
1	-2.254777	-2.424604	-0.001081	1	-2.506781	0.258154	3.129696
1	0.236002	-2.243390	-0.730	6	4.776332	-0.086964	0.264722
1	-0.098402	2.054262	0.001405	6	4.160975	1.175118	0.271815
1	-2.554405	1.881627	0.001668	6	2.839920	1.309386	-0.118334

6	2.099257	0.186979	-0.519755	6	-2.779272	-1.671388	1.127676
6	2.712662	-1.064653	-0.522233	6	-3.951747	-2.354049	0.871303
6	4.044366	-1.211129	-0.135774	1	-5.923496	-2.216349	-0.626
8	6.065983	-0.118937	0.651254	1	-1.897723	-2.106604	1.599296
6	6.750251	-1.342013	0.655008	1	-4.039900	-3.400726	1.158560
15	0.365113	0.365313	-1.020351	6	-1.536444	0.938450	2.474250
16	-0.395518	-1.250449	-1.791788	1	-1.392286	0.061315	3.119785
16	-0.068646	2.175	-1.599652	1	-0.715143	1.646720	2.632687
1	4.751288	2.038421	0.583111	1	-2.495026	1.423241	2.705257
1	2.366028	2.293570	-0.127409	6	4.722340	-0.478309	0.214403
1	2.137963	-1.937187	-0.842338	6	4.147210	-1.725998	-0.061687
1	4.497353	-2.202090	-0.158553	6	2.789598	-1.825263	-0.329545
1	7.772680	-1.129256	0.989940	6	1.981623	-0.683022	-0.334273
1	6.291452	-2.066358	1.350436	6	2.557916	0.559332	-0.060484
1	6.791949	-1.791956	-0.352023	6	3.917767	0.669611	0.217513
O,O-H5				8	6.048008	-0.475075	0.464652
6	-3.140294	1.584731	-0.280793	6	6.684189	0.737929	0.757572
1	-3.709346	2.314968	-0.851029	15	0.206411	-0.789886	-0.700188
6	-1.835213	1.665546	0.090194	16	-0.436380	-2.634319	-0.905621
6	-1.480183	0.491734	1.008572	16	-0.346921	0.608717	-2.010456
6	-0.930	2.850856	-0.038497	1	4.791428	-2.606844	-0.058579
6	-1.271552	3.857357	-1.106844	1	2.335118	-2.797119	-0.537347
1	-1.458073	3.363216	-2.069440	1	1.938599	1.459807	-0.058644
1	-2.182418	4.403799	-0.811958	1	4.336146	1.653318	0.429602
1	-0.445870	4.572077	-1.201154	1	7.743047	0.506438	0.926120
8	-0.317280	-0.179641	0.828175	1	6.605952	1.456258	-0.077134
8	-0.016499	3.007072	0.741074	1	6.272880	1.206956	1.668523
6	-3.641042	0.282075	0.068685	O,O-H6			
6	-4.848867	-0.366933	-0.195334	6	-3.043024	1.615854	-0.424540
7	-2.680203	-0.390818	0.748746	1	-3.550137	2.357962	-1.035124
6	-4.992672	-1.686546	0.211374	6	-1.693679	1.592308	-0.090715
1	-5.639784	0.157630	-0.730794	6	-1.486268	0.486157	0.957232

6	-0.777777	2.779544	-0.142998	1	4.896774	-2.516276	-0.361195
6	-1.068109	3.811276	-1.203859	1	2.433887	-2.789243	-0.747939
1	-1.280202	3.343998	-2.174774	1	1.842490	1.349510	0.287800
1	-1.953273	4.393761	-0.900663	1	4.247329	1.618022	0.679087
1	-0.211021	4.489582	-1.287191	1	7.732382	0.615912	0.860160
8	-0.349369	-0.266441	0.897599	1	6.505316	1.605167	0.011691
8	0.112	2.919999	0.669410	1	6.269772	1.160440	1.735250
6	-3.623798	0.390288	-0.023018	O,O-H7			
6	-4.890438	-0.189011	-0.242197	15	0.296444	-0.904243	-0.428162
7	-2.714320	-0.334889	0.690066	6	2.030900	-0.520070	-0.137545
6	-5.131906	-1.461224	0.232518	6	3.017294	-1.441893	-0.483827
1	-5.643177	0.367222	-0.800347	6	2.403187	0.711716	0.429052
6	-2.922611	-1.581489	1.149019	6	4.365612	-1.156383	-0.275039
6	-4.138567	-2.181494	0.931193	1	2.725651	-2.401860	-0.916517
1	-6.103297	-1.926686	0.052873	6	3.738244	0.999194	0.644011
1	-2.076555	-2.056875	1.647020	1	1.642077	1.444383	0.707914
1	-4.311228	-3.199385	1.276797	6	4.732325	0.068742	0.294007
6	-1.595970	1.044416	2.378809	1	5.114101	-1.896849	-0.555611
1	-1.571487	0.208965	3.091747	1	4.047584	1.946106	1.088737
1	-0.736349	1.700298	2.554668	6	-3.060115	1.387318	-0.672971
1	-2.528019	1.612350	2.502307	1	-3.523747	2.058146	-1.390502
6	4.731689	-0.444499	0.178297	6	-1.627126	1.389576	-0.299267
6	4.208352	-1.680602	-0.226165	6	-1.565539	0.395579	0.903921
6	2.846407	-1.824713	-0.442131	6	-0.930807	2.734875	-0.116813
6	1.981595	-0.738272	-0.264937	6	-1.346157	3.831190	-1.065139
6	2.504811	0.493408	0.136641	1	-2.325832	4.220322	-0.746455
6	3.870046	0.646163	0.361495	1	-0.606726	4.639587	-1.031161
8	6.064662	-0.396778	0.368521	1	-1.456389	3.455297	-2.092335
6	6.657464	0.810499	0.762681	8	-0.385900	-0.333136	0.973482
15	0.206803	-0.911107	-0.574946	8	-0.085370	2.911640	0.729031
16	-0.387124	-2.749520	-0.831471	6	-3.619909	0.225401	-0.214364
16	-0.440168	0.512659	-1.871444	6	-4.901874	-0.392671	-0.410305

7	-2.723987	-0.468691	0.587688	6	2.925583	-0.109628	-0.607024
6	-5.161418	-1.601271	0.164088	6	3.856924	-0.404005	-1.647
1	-5.638720	0.117596	-1.030777	6	3.293506	-0.243282	0.741448
6	-2.982541	-1.668508	1.165883	6	5.149287	-0.810617	-1.268932
6	-4.185434	-2.274728	0.968358	1	3.562374	-0.328568	-2.649612
1	-6.132445	-2.074842	0.002160	6	4.570509	-0.650217	1.080398
1	-2.164351	-2.101798	1.743542	1	2.557251	-0.059077	1.526776
1	-4.383785	-3.253846	1.400537	6	5.511952	-0.934153	0.077294
6	-1.793268	1.043678	2.264052	1	5.855023	-1.037460	-2.067619
1	-1.900362	0.251902	3.018046	1	4.867338	-0.778058	2.122275
1	-0.942153	1.681752	2.520454	6	-1.376270	2.514739	-1.029560
1	-2.712623	1.645142	2.238533	1	-1.491252	2.814405	-2.066853
8	6.119	0.438366	0.542909	6	-0.176895	2.812244	-0.166392
6	7.047297	-0.437097	0.217718	6	-0.442264	1.960804	1.054029
1	6.966977	-1.391228	0.766202	6	-0.354109	4.321080	0.236581
1	7.081005	-0.647887	-0.865011	6	-0.012731	5.336112	-0.823064
1	7.977252	0.064347	0.510775	1	1.065980	5.549154	-0.758636
16	-0.089138	-2.737366	-0.889894	1	-0.213514	4.971407	-1.838175
16	-0.557179	0.561452	-1.689995	1	-0.564913	6.261485	-0.617730
O,O-H8				8	0.332211	0.208114	0.215068
6	-3.176366	-1.962081	-1.557479	8	-0.756347	4.631041	1.326641
6	-1.920802	-1.902966	-0.961774	6	-2.294283	1.894226	-0.260107
6	-1.780633	-2.071195	0.418577	6	-3.652815	1.470132	-0.488242
6	-2.917433	-2.327116	1.200210	7	-1.739258	1.642644	1.031218
6	-4.166700	-2.413449	0.609251	6	-4.361924	0.914794	0.518576
6	-4.308417	-2.215875	-0.772554	1	-4.075750	1.618648	-1.481675
1	-3.252825	-1.800778	-2.632347	6	-2.483723	1.056730	2.053539
1	-1.043841	-1.702466	-1.582831	6	-3.764473	0.718156	1.824988
1	-2.812328	-2.459727	2.279165	1	-5.389562	0.587836	0.352849
1	-5.060727	-2.623789	1.198668	1	-1.961479	0.881932	2.991757
15	-0.144828	-2.089557	1.171256	1	-4.342191	0.261164	2.627459
15	1.254703	0.432191	-1.029978	6	0.370674	1.988944	2.285861

1	0.307685	1.026660	2.811278	6	3.350742	-0.323648	0.810403
1	1.415518	2.188210	2.019181	6	5.173489	-1.066550	-1.179885
1	-0.017	2.804666	2.926504	1	3.573198	-0.683145	-2.573256
8	6.727914	-1.324176	0.502505	6	4.630239	-0.706512	1.158575
8	-5.565208	-2.270731	-1.251005	1	2.631646	-0.074719	1.594997
6	-5.779465	-2.125593	-2.630897	6	5.554202	-1.081295	0.167133
1	-5.252420	-2.903604	-3.208532	1	5.865125	-1.363723	-1.967386
1	-6.858657	-2.231166	-2.793125	1	4.942252	-0.751373	2.202665
1	-5.457570	-1.133795	-2.992948	6	-1.259323	2.317572	-1.164140
6	7.710217	-1.655491	-0.441341	1	-1.249632	2.391875	-2.247601
1	7.396408	-2.500346	-1.078466	6	-0.177029	2.813205	-0.252263
1	7.964569	-0.796779	-1.086835	6	-0.635421	2.368511	1.099140
1	8.602663	-1.949790	0.124095	6	-0.272731	4.389621	-0.296240
16	1.181886	-3.059719	0.192042	6	0.280509	5.058179	-1.524446
16	-0.119421	-1.612237	3.046705	1	1.355874	5.235971	-1.367935
16	0.652561	-0.068708	-2.812270	1	0.183132	4.439202	-2.425103
16	1.490240	2.601542	-0.849478	1	-0.219588	6.026323	-1.650874
O,O-H9				8	0.299291	-0.094611	0.198509
6	-3.295755	-2.115964	-1.439484	8	-0.775008	4.986953	0.615387
6	-2.028189	-1.834386	-0.932063	6	-2.244800	1.803612	-0.400201
6	-1.792156	-1.803927	0.444251	6	-3.543915	1.257379	-0.693518
6	-2.849895	-2.092699	1.313774	7	-1.835276	1.850189	0.975670
6	-4.114710	-2.383476	0.820724	6	-4.339739	0.839880	0.313830
6	-4.349950	-2.387395	-0.560299	1	-3.845543	1.193736	-1.738406
1	-3.441757	-2.124485	-2.519822	6	-2.659791	1.365906	2.002303
1	-1.210302	-1.639719	-1.630538	6	-3.878623	0.895957	1.686871
1	-2.667777	-2.079867	2.391304	1	-5.322460	0.416415	0.105150
1	-4.944977	-2.616249	1.490348	1	-2.228768	1.359277	3.210
15	-0.095241	-1.583604	1.089829	1	-4.513113	0.512890	2.485581
15	1.312252	0.221423	-0.998943	6	0.079524	2.528547	2.367760
6	2.967424	-0.301254	-0.542754	1	0.246753	1.510799	2.782805
6	3.880250	-0.678390	-1.524859	1	1.043953	3.020078	2.202632

1	-0.523205	3.108006	3.083356	1	3.477782	-0.816162	-2.519901
8	6.771766	-1.441957	0.604767	6	4.119	-1.807945	1.174393
8	-5.619225	-2.643369	-0.947984	1	2.200439	-0.951910	1.611721
6	-5.906248	-2.732495	-2.316682	6	5.065591	-2.119553	0.193612
1	-5.316508	-3.524891	-2.808632	1	5.553600	-1.995548	-1.924380
1	-6.971848	-2.978454	-2.400826	1	4.303140	-2.106674	2.205115
1	-5.721212	-1.777088	-2.839295	6	-0.531882	2.940971	-1.147905
6	7.734124	-1.877395	-0.318789	1	-0.440010	3.094507	-2.216579
1	7.395625	-2.773346	-0.866639	6	0.469246	3.259018	-0.149304
1	7.990321	-1.087483	-1.045685	6	-0.103754	2.840646	1.149754
1	8.630707	-2.131619	0.259067	6	1.422439	4.431227	-0.328039
16	1.072057	-3.004872	0.457188	6	2.006093	4.559460	-1.707096
16	-0.132958	-0.972616	2.975586	1	2.221733	3.570821	-2.139438
16	0.735513	-0.127839	-2.814070	1	1.268090	5.054822	-2.358154
16	1.555507	2.349012	-0.600540	1	2.909589	5.179140	-1.666059
O,O-H10				8	-0.108643	-0.500258	-0.416965
6	-4.385	-1.906621	-1.371683	8	1.667285	5.176471	0.585108
6	-2.666784	-1.793436	-0.982256	6	-1.593287	2.364868	-0.505596
6	-2.315950	-1.697509	0.364884	6	-2.847568	1.856484	-0.968650
6	-3.327311	-1.740633	1.330372	7	-1.330556	2.315535	0.875014
6	-4.658902	-1.861941	0.957433	6	-3.762943	1.422992	-0.065172
6	-5.006773	-1.941467	-0.398065	1	-3.030085	1.830705	-2.042246
1	-4.237934	-1.974185	-2.433467	6	-2.259977	1.835373	1.785827
1	-1.886410	-1.771567	-1.745613	6	-3.470184	1.433254	1.341329
1	-3.058226	-1.663421	2.386796	1	-4.723355	1.028692	-0.400551
1	-5.456038	-1.901933	1.701922	1	-1.951340	1.803440	2.826763
15	-0.564178	-1.663255	0.865755	1	-4.202505	1.064090	2.056891
15	1.223308	0.103468	-0.996706	6	0.273691	3.237910	2.535178
6	2.702779	-0.792998	-0.508023	1	0.275195	2.352648	3.187952
6	3.658401	-1.098373	-1.480700	1	1.260250	3.710422	2.543739
6	2.939663	-1.159211	0.832054	1	-0.461353	3.969135	2.907618
6	4.832434	-1.762685	-1.141741	8	6.166110	-2.754677	0.622386

8	-6.325566	-2.040325	-0.670617	1	-2.610558	-1.624612	3.539619
6	-6.737655	-2.189871	-2.001537	1	0.623666	1.240933	3.377360
1	-6.305595	-3.093467	-2.465013	1	-0.441878	-0.778172	4.457513
1	-7.829915	-2.287998	-1.983565	6	-0.399732	3.854772	2.197893
1	-6.469237	-1.312703	-2.616964	1	0.301469	3.716694	3.033377
6	7.157188	-3.121781	-0.301695	1	-0.092668	4.723131	1.603593
1	6.765526	-3.816457	-1.063985	1	-1.410150	4.026328	2.597755
1	7.591216	-2.240848	-0.804741	6	5.553033	-0.550364	-0.568093
1	7.944298	-3.628297	0.269252	6	5.088057	0.298728	-1.584525
16	0.321473	-3.347172	0.470470	6	3.753471	0.663122	-1.630494
16	-0.311985	-0.705640	2.582858	6	2.861862	0.196237	-0.654629
16	1.135834	0.652916	-2.848655	6	3.324599	-0.647493	0.359522
16	1.629023	1.769400	0.415235	6	4.661839	-1.024147	0.404717
O,O-H11				8	6.860178	-0.859378	-0.607131
6	-2.392954	1.820656	0.326324	6	7.386949	-1.736233	0.354029
1	-3.260225	1.655559	-0.308905	15	1.140048	0.703	-0.687099
6	-1.418252	2.735552	0.170225	8	0.263456	-0.325963	0.163949
6	-0.404106	2.619814	1.288131	16	0.441761	1.326493	-2.388106
6	-1.349321	3.807317	-0.875439	1	5.797945	0.646458	-2.336121
6	-2.282606	3.673047	-2.049228	1	3.387395	1.305239	-2.434782
1	-2.168599	2.682869	-2.512281	1	2.634939	-1.050144	1.106761
1	-3.325439	3.789583	-1.713398	1	4.989726	-1.704441	1.189923
1	-2.050679	4.456756	-2.779286	1	8.452740	-1.850950	0.123388
16	1.321725	2.305382	0.777323	1	7.284223	-1.330242	1.375117
8	-0.606080	4.747772	-0.725917	1	6.902370	-2.726245	0.310311
6	-2.098433	1.007623	1.491293	6	-4.531121	-1.924435	-0.856265
6	-2.749727	-0.086987	2.044101	6	-4.020793	-2.817065	0.097849
7	-0.944975	1.451039	2.037714	6	-2.657502	-2.855935	0.360262
6	-2.152740	-0.728137	3.120194	6	-1.770740	-2.011276	-0.318310
1	-3.666570	-0.458530	1.586577	6	-2.279944	-1.146809	-1.287760
6	-0.346022	0.845688	3.074389	6	-3.649492	-1.084913	-1.550913
6	-0.941463	-0.258987	3.641755	8	-5.867617	-1.946023	-1.041800

6	-6.431490	-1.133050	-2.033787	1	-2.684373	3.090837	-2.617118
15	0.033022	-2.096648	-0.003575	6	-4.290675	-1.735541	-1.805890
16	0.999930	-2.676102	-1.588892	1	-3.969965	-1.488250	-2.827895
16	0.383226	-2.788406	1.810709	1	-4.297390	-2.824167	-1.676667
1	-4.718218	-3.478997	0.614443	1	-5.306230	-1.346446	-1.640516
1	-2.261060	-3.541962	1.113302	6	3.658777	-1.902538	-1.596187
1	-1.599803	-0.503765	-1.854024	6	3.379003	-2.257381	-0.267661
1	-4.009714	-0.398481	-2.318263	6	2.160493	-1.929537	0.298949
1	-7.509143	-1.336499	-2.033795	6	1.197893	-1.235803	-0.448155
1	-6.273421	-0.059572	-1.825785	6	1.477231	-0.883868	-1.772476
1	-6.023563	-1.362964	-3.033083	6	2.697484	-1.217033	-2.350431
O,O-H12				8	4.872251	-2.249203	-2.056969
6	-4.056313	-0.193041	1.254421	6	5.234568	-1.902131	-3.367550
1	-4.379468	-0.040788	2.281861	15	-0.370965	-0.765958	0.300932
6	-3.778369	-1.361608	0.650456	8	-0.688732	0.764980	0.002840
6	-3.334503	-1.125007	-0.776717	16	-0.633627	-1.344924	2.136244
6	-3.903317	-2.734320	1.234910	1	4.148698	-2.778425	0.302997
6	-4.046040	-2.831785	2.729489	1	1.944047	-2.193789	1.336300
1	-3.166138	-2.375676	3.207663	1	0.762499	-0.292575	-2.349649
1	-4.943359	-2.293980	3.072122	1	2.893966	-0.913255	-3.378116
1	-4.124233	-3.887821	3.011908	1	6.251037	-2.282972	-3.522160
16	-1.652072	-1.747652	-1.156640	1	4.562903	-2.362555	-4.112243
8	-3.895555	-3.702130	0.510611	1	5.235296	-0.808423	-3.514021
6	-3.807803	0.895526	0.326654	6	4.134752	0.770308	1.667084
6	-3.883533	2.266612	0.471106	6	4.099931	1.125558	0.311090
7	-3.386452	0.359525	-0.849206	6	2.934514	1.620799	-0.249428
6	-3.482812	3.067950	-0.597401	6	1.782012	1.780447	0.529839
1	-4.186422	2.697573	1.424018	6	1.834903	1.469115	1.889008
6	-2.993588	1.108871	-1.887344	6	2.997770	0.957821	2.461511
6	-3.054822	2.484795	-1.792961	8	5.297204	0.252751	2.114740
1	-3.488027	4.152620	-0.494877	6	5.387781	-0.163239	3.449204
1	-2.584347	0.583846	-2.750747	15	0.199005	2.297512	-0.207627

16	-0.736078	3.582620	0.944442	1	3.793483	0.331853	3.004211
16	0.317515	2.545948	-2.161557	1	2.633620	-0.984655	3.326196
1	5.001232	0.977275	-0.285866	1	4.320834	-1.378807	2.885633
1	2.892686	1.868999	-1.312459	6	-2.423419	-2.485013	-0.649800
1	0.947116	1.612976	2.509134	6	-1.710369	-2.226549	-1.831761
1	2.997662	0.705221	3.521614	6	-0.670350	-1.310650	-1.832668
1	6.396268	-0.573132	3.584022	6	-0.316510	-0.634623	-0.654657
1	5.247232	0.675448	4.153123	6	-1.018487	-0.911378	0.519916
1	4.648719	-0.949399	3.683703	6	-2.055589	-1.837614	0.533878
O,O-H13				8	-3.441314	-3.359825	-0.745054
6	3.187361	-2.326578	-0.433764	6	-4.171433	-3.683568	0.415057
1	2.986086	-3.165668	-1.095030	15	0.897499	0.708813	-0.731654
6	2.526890	-1.984242	0.710306	8	0.044938	2.059556	-0.910328
6	3.065438	-0.726739	1.248175	16	2.195864	0.541942	-2.163134
6	1.429315	-2.766838	1.361374	1	-2.003657	-2.750975	-2.742589
6	0.828443	-3.894828	0.563228	1	-0.121605	-1.104694	-2.754747
1	0.381991	-3.499988	-0.362695	1	-0.758510	-0.397673	1.446849
1	1.597580	-4.630643	0.283804	1	-2.583324	-2.018080	1.468911
1	0.053722	-4.384212	1.164129	1	-4.932400	-4.410926	0.108295
16	1.673772	0.843133	1.289650	1	-3.524535	-4.144389	1.180833
8	1.057312	-2.497767	2.480571	1	-4.667582	-2.795582	0.840310
6	4.202754	-1.346788	-0.670274	6	-4.646628	0.250534	0.161206
6	5.156853	-1.195906	-1.684162	6	-4.155599	0.759706	1.369664
7	4.130508	-0.420329	0.327902	6	-3.040569	1.586529	1.376668
6	5.982164	-0.091360	-1.660167	6	-2.407298	1.937260	0.179714
1	5.209633	-1.938827	-2.479412	6	-2.931780	1.463791	-1.024556
6	4.909627	0.685505	0.347383	6	-4.036622	0.617698	-1.043564
6	5.849362	0.867613	-0.635570	8	-5.692435	-0.604027	0.248964
1	6.726879	0.053474	-2.444405	6	-6.219162	-1.153058	-0.931533
1	4.723163	1.399770	1.148771	15	-0.919517	2.991401	0.139177
1	6.471118	1.762183	-0.618210	16	-1.236380	4.726158	-0.638614
6	3.486388	-0.681929	2.708347	16	0.097989	2.812673	1.889301

1	-4.652994	0.472869	2.297826
1	-2.631960	1.945894	2.324287
1	-2.455563	1.738624	-1.968598
1	-4.398429	0.239791	-1.999356
1	-7.052374	-1.800100	-0.630413
1	-6.603199	-0.371866	-1.609354
1	-5.467854	-1.760132	-1.466538

O,O-H14

Indolizine

6	-3.314580	0.544323	-0.058
6	-3.369348	-0.887307	-0.111
6	-2.211924	-1.609901	-0.039
6	-0.953112	-0.945392	0.077
7	-0.944977	0.460093	0.035
6	-2.118347	1.186485	0.064
6	0.365875	-1.361996	0.179
6	1.178830	-0.196662	0.142
6	0.342390	0.923968	-0.033
6	0.643869	2.382512	-0.063
6	2.661096	-0.167381	-0.032
6	3.367767	-1.507089	-0.152
8	3.296388	0.867672	0.005
1	-4.231497	1.134345	-0.047
1	-4.337378	-1.390285	-0.226
1	-2.220273	-2.700963	-0.013
1	-2.014550	2.270881	0.222
1	0.695744	-2.397669	0.318
1	1.729765	2.520303	-0.890
1	0.223807	2.879683	-0.890290
1	0.225345	2.879394	0.891066
1	3.083900	-2.092583	0.887620
1	3.082298	-2.093631	-0.886705

1	4.451489	-1.340867	-0.001188
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LR 5 Members Ring Cis

6	-1.584941	2.466711	-0.970421
6	-0.329368	1.908147	-1.188544
6	0.635886	1.898048	-0.177956
6	0.336520	2.478113	1.060920
6	-0.912740	3.033092	1.288940
6	-1.886979	3.025912	0.278824
1	-2.318772	2.452286	-1.775599
1	-0.111675	1.459991	-2.160847
1	1.081776	2.477223	1.859035
1	-1.164375	3.482164	2.250642
8	-3.074165	3.569504	0.595848
6	-4.091365	3.610994	-0.370623
1	-4.953854	4.094307	0.103027
1	-3.791494	4.243	-1.253948
1	-4.383854	2.598049	-0.698221
15	2.208602	1.084556	-0.540951
15	1.443065	-1.740140	0.053103
16	1.699443	-0.734298	1.965053
8	1.691677	-0.437613	-0.932571
16	2.555198	-3.246505	-0.339415
6	-0.343668	-1.984597	0.002584
6	-1.235262	-0.992789	0.425240
6	-0.853466	-3.184263	-0.518772
6	-2.609905	-1.181346	0.326092
1	-0.864437	-0.057243	0.846820
6	-2.219542	-3.378773	-0.622739
1	-0.160971	-3.964672	-0.842463
6	-3.111572	-2.378315	-0.204005
1	-3.274313	-0.388320	0.668080
1	-2.630621	-4.304596	-1.027432

8	-4.417388	-2.652672	-0.344296
6	-5.369973	-1.711359	0.077218
1	-5.279211	-0.762524	-0.479039
1	-6.353689	-2.150557	-0.125352
1	-5.285375	-1.504148	1.157474
16	3.365254	1.907306	-1.819716
16	3.165926	0.617907	1.306774

Figure 24

O,O-I1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603

6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104

1	-1.995603	-2.616824	0.099871	6	2.490809	-0.781376	0.315290
6	-2.769395	1.109466	-0.122320	6	3.153407	0.389017	0.699605
6	-3.846604	0.226048	-0.023242	6	3.216076	-1.815551	-0.301885
1	-4.384517	-1.864961	0.130790	6	4.518843	0.533126	0.484738
1	-2.942230	2.188329	-0.193797	1	2.590010	1.198244	1.169247
1	-4.870163	0.603990	-0.011555	6	4.574104	-1.679850	-0.516320
6	1.239675	2.194562	-0.935888	1	2.700275	-2.728593	-0.606940
1	1.074718	3.239890	-0.646013	6	5.239282	-0.503636	-0.127213
1	2.245811	2.082825	-1.369636	1	5.008365	1.456113	0.793375
1	0.497232	1.881452	-1.682557	1	5.155828	-2.472745	-0.988319
O,O-I2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	O,O-I3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410

1	-4.625439	1.226573	0.899941	6	2.712662	-1.064653	-0.522233
1	-4.622697	1.228758	-0.898633	6	4.044366	-1.211129	-0.135774
O,O-I4				8	6.065983	-0.118937	0.651254
6	-3.334661	0.397287	-0.108530	6	6.750251	-1.342013	0.655008
1	-4.118597	0.841972	-0.722543	15	0.365113	0.365313	-1.020351
6	-2.413161	1.137904	0.523965	16	-0.395518	-1.250449	-1.791788
6	-1.331402	0.469811	1.339344	16	-0.068646	2.175	-1.599652
6	-2.423406	2.642127	0.573366	1	4.751288	2.038421	0.583111
6	-3.226687	3.371879	-0.471469	1	2.366028	2.293570	-0.127409
1	-2.942736	3.028651	-1.475901	1	2.137963	-1.937187	-0.842338
1	-4.301678	3.184930	-0.320741	1	4.497353	-2.202090	-0.158553
1	-3.035202	4.446410	-0.371560	1	7.772680	-1.129256	0.989940
8	-0.181966	0.303263	0.873581	1	6.291452	-2.066358	1.350436
8	-1.840026	3.212329	1.466614	1	6.791949	-1.791956	-0.352023
6 -3.262443 -1.057243 0.047002				O,O-I5			
6 -4.026569 -1.984634 -0.659766				6	-3.140294	1.584731	-0.280793
7 -2.344662 -1.437919 0.937046				1	-3.709346	2.314968	-0.851029
6 -3.781158 -3.337644 -0.441352				6	-1.835213	1.665546	0.090194
1 -4.772442 -1.650062 -1.381820				6	-1.480183	0.491734	1.008572
6 -2.094447 -2.720682 1.142669				6	-0.930	2.850856	-0.038497
6 -2.797807 -3.718820 0.469015				6	-1.271552	3.857357	-1.106844
1 -4.347532 -4.093322 -0.989262				1	-1.458073	3.363216	-2.069440
1 -1.306134 -2.962164 1.861521				1	-2.182418	4.403799	-0.811958
1 -2.572631 -4.769972 0.652262				1	-0.445870	4.572077	-1.201154
6 -1.475502 0.477469 2.828198				8	-0.317280	-0.179641	0.828175
1 -0.772198 -0.234987 3.276436				8	-0.016499	3.007072	0.741074
1 -1.221252 1.499873 3.148804				6	-3.641042	0.282075	0.068685
1 -2.506781 0.258154 3.129696				6	-4.848867	-0.366933	-0.195334
6 4.776332 -0.086964 0.264722				7	-2.680203	-0.390818	0.748746
6 4.160975 1.175118 0.271815				6	-4.992672	-1.686546	0.211374
6 2.839920 1.309386 -0.118334				1	-5.639784	0.157630	-0.730794
6 2.099257 0.186979 -0.519755				6	-2.779272	-1.671388	1.127676

6	-3.951747	-2.354049	0.871303	6	-1.068109	3.811276	-1.203859
1	-5.923496	-2.216349	-0.626	1	-1.280202	3.343998	-2.174774
1	-1.897723	-2.106604	1.599296	1	-1.953273	4.393761	-0.900663
1	-4.039900	-3.400726	1.158560	1	-0.211021	4.489582	-1.287191
6	-1.536444	0.938450	2.474250	8	-0.349369	-0.266441	0.897599
1	-1.392286	0.061315	3.119785	8	0.112	2.919999	0.669410
1	-0.715143	1.646720	2.632687	6	-3.623798	0.390288	-0.023018
1	-2.495026	1.423241	2.705257	6	-4.890438	-0.189011	-0.242197
6	4.722340	-0.478309	0.214403	7	-2.714320	-0.334889	0.690066
6	4.147210	-1.725998	-0.061687	6	-5.131906	-1.461224	0.232518
6	2.789598	-1.825263	-0.329545	1	-5.643177	0.367222	-0.800347
6	1.981623	-0.683022	-0.334273	6	-2.922611	-1.581489	1.149019
6	2.557916	0.559332	-0.060484	6	-4.138567	-2.181494	0.931193
6	3.917767	0.669611	0.217513	1	-6.103297	-1.926686	0.052873
8	6.048008	-0.475075	0.464652	1	-2.076555	-2.056875	1.647020
6	6.684189	0.737929	0.757572	1	-4.311228	-3.199385	1.276797
15	0.206411	-0.789886	-0.700188	6	-1.595970	1.044416	2.378809
16	-0.436380	-2.634319	-0.905621	1	-1.571487	0.208965	3.091747
16	-0.346921	0.608717	-2.010456	1	-0.736349	1.700298	2.554668
1	4.791428	-2.606844	-0.058579	1	-2.528019	1.612350	2.502307
1	2.335118	-2.797119	-0.537347	6	4.731689	-0.444499	0.178297
1	1.938599	1.459807	-0.058644	6	4.208352	-1.680602	-0.226165
1	4.336146	1.653318	0.429602	6	2.846407	-1.824713	-0.442131
1	7.743047	0.506438	0.926120	6	1.981595	-0.738272	-0.264937
1	6.605952	1.456258	-0.077134	6	2.504811	0.493408	0.136641
1	6.272880	1.206956	1.668523	6	3.870046	0.646163	0.361495
O,O-I6				8	6.064662	-0.396778	0.368521
6	-3.043024	1.615854	-0.424540	6	6.657464	0.810499	0.762681
1	-3.550137	2.357962	-1.035124	15	0.206803	-0.911107	-0.574946
6	-1.693679	1.592308	-0.090715	16	-0.387124	-2.749520	-0.831471
6	-1.486268	0.486157	0.957232	16	-0.440168	0.512659	-1.871444
6	-0.777777	2.779544	-0.142998	1	4.896774	-2.516276	-0.361195

1	2.433887	-2.789243	-0.747939	6	-5.161418	-1.601271	0.164088
1	1.842490	1.349510	0.287800	1	-5.638720	0.117596	-1.030777
1	4.247329	1.618022	0.679087	6	-2.982541	-1.668508	1.165883
1	7.732382	0.615912	0.860160	6	-4.185434	-2.274728	0.968358
1	6.505316	1.605167	0.011691	1	-6.132445	-2.074842	0.002160
1	6.269772	1.160440	1.735250	1	-2.164351	-2.101798	1.743542
O,O-I7				1	-4.383785	-3.253846	1.400537
15	0.296444	-0.904243	-0.428162	6	-1.793268	1.043678	2.264052
6	2.030900	-0.520070	-0.137545	1	-1.900362	0.251902	3.018046
6	3.017294	-1.441893	-0.483827	1	-0.942153	1.681752	2.520454
6	2.403187	0.711716	0.429052	1	-2.712623	1.645142	2.238533
6	4.365612	-1.156383	-0.275039	8	6.119	0.438366	0.542909
1	2.725651	-2.401860	-0.916517	6	7.047297	-0.437097	0.217718
6	3.738244	0.999194	0.644011	1	6.966977	-1.391228	0.766202
1	1.642077	1.444383	0.707914	1	7.081005	-0.647887	-0.865011
6	4.732325	0.068742	0.294007	1	7.977252	0.064347	0.510775
1	5.114101	-1.896849	-0.555611	16	-0.089138	-2.737366	-0.889894
1	4.047584	1.946106	1.088737	16	-0.557179	0.561452	-1.689995
6	-3.060115	1.387318	-0.672971	O,O-I8			
1	-3.523747	2.058146	-1.390502	6	-3.176366	-1.962081	-1.557479
6	-1.627126	1.389576	-0.299267	6	-1.920802	-1.902966	-0.961774
6	-1.565539	0.395579	0.903921	6	-1.780633	-2.071195	0.418577
6	-0.930807	2.734875	-0.116813	6	-2.917433	-2.327116	1.200210
6	-1.346157	3.831190	-1.065139	6	-4.166700	-2.413449	0.609251
1	-2.325832	4.220322	-0.746455	6	-4.308417	-2.215875	-0.772554
1	-0.606726	4.639587	-1.031161	1	-3.252825	-1.800778	-2.632347
1	-1.456389	3.455297	-2.092335	1	-1.043841	-1.702466	-1.582831
8	-0.385900	-0.333136	0.973482	1	-2.812328	-2.459727	2.279165
8	-0.085370	2.911640	0.729031	1	-5.060727	-2.623789	1.198668
6	-3.619909	0.225401	-0.214364	15	-0.144828	-2.089557	1.171256
6	-4.901874	-0.392671	-0.410305	15	1.254703	0.432191	-1.029978
7	-2.723987	-0.468691	0.587688	6	2.925583	-0.109628	-0.607024

6	3.856924	-0.404005	-1.647	1	1.415518	2.188210	2.019181
6	3.293506	-0.243282	0.741448	1	-0.017	2.804666	2.926504
6	5.149287	-0.810617	-1.268932	8	6.727914	-1.324176	0.502505
1	3.562374	-0.328568	-2.649612	8	-5.565208	-2.270731	-1.251005
6	4.570509	-0.650217	1.080398	6	-5.779465	-2.125593	-2.630897
1	2.557251	-0.059077	1.526776	1	-5.252420	-2.903604	-3.208532
6	5.511952	-0.934153	0.077294	1	-6.858657	-2.231166	-2.793125
1	5.855023	-1.037460	-2.067619	1	-5.457570	-1.133795	-2.992948
1	4.867338	-0.778058	2.122275	6	7.710217	-1.655491	-0.441341
6	-1.376270	2.514739	-1.029560	1	7.396408	-2.500346	-1.078466
1	-1.491252	2.814405	-2.066853	1	7.964569	-0.796779	-1.086835
6	-0.176895	2.812244	-0.166392	1	8.602663	-1.949790	0.124095
6	-0.442264	1.960804	1.054029	16	1.181886	-3.059719	0.192042
6	-0.354109	4.321080	0.236581	16	-0.119421	-1.612237	3.046705
6	-0.012731	5.336112	-0.823064	16	0.652561	-0.068708	-2.812270
1	1.065980	5.549154	-0.758636	16	1.490240	2.601542	-0.849478
1	-0.213514	4.971407	-1.838175	O,O-I9			
1	-0.564913	6.261485	-0.617730	6	-3.295755	-2.115964	-1.439484
8	0.332211	0.208114	0.215068	6	-2.028189	-1.834386	-0.932063
8	-0.756347	4.631041	1.326641	6	-1.792156	-1.803927	0.444251
6	-2.294283	1.894226	-0.260107	6	-2.849895	-2.092699	1.313774
6	-3.652815	1.470132	-0.488242	6	-4.114710	-2.383476	0.820724
7	-1.739258	1.642644	1.031218	6	-4.349950	-2.387395	-0.560299
6	-4.361924	0.914794	0.518576	1	-3.441757	-2.124485	-2.519822
1	-4.075750	1.618648	-1.481675	1	-1.210302	-1.639719	-1.630538
6	-2.483723	1.056730	2.053539	1	-2.667777	-2.079867	2.391304
6	-3.764473	0.718156	1.824988	1	-4.944977	-2.616249	1.490348
1	-5.389562	0.587836	0.352849	15	-0.095241	-1.583604	1.089829
1	-1.961479	0.881932	2.991757	15	1.312252	0.221423	-0.998943
1	-4.342191	0.261164	2.627459	6	2.967424	-0.301254	-0.542754
6	0.370674	1.988944	2.285861	6	3.880250	-0.678390	-1.524859
1	0.307685	1.026660	2.811278	6	3.350742	-0.323648	0.810403

6	5.173489	-1.066550	-1.179885	8	6.771766	-1.441957	0.604767
1	3.573198	-0.683145	-2.573256	8	-5.619225	-2.643369	-0.947984
6	4.630239	-0.706512	1.158575	6	-5.906248	-2.732495	-2.316682
1	2.631646	-0.074719	1.594997	1	-5.316508	-3.524891	-2.808632
6	5.554202	-1.081295	0.167133	1	-6.971848	-2.978454	-2.400826
1	5.865125	-1.363723	-1.967386	1	-5.721212	-1.777088	-2.839295
1	4.942252	-0.751373	2.202665	6	7.734124	-1.877395	-0.318789
6	-1.259323	2.317572	-1.164140	1	7.395625	-2.773346	-0.866639
1	-1.249632	2.391875	-2.247601	1	7.990321	-1.087483	-1.045685
6	-0.177029	2.813205	-0.252263	1	8.630707	-2.131619	0.259067
6	-0.635421	2.368511	1.099140	16	1.072057	-3.004872	0.457188
6	-0.272731	4.389621	-0.296240	16	-0.132958	-0.972616	2.975586
6	0.280509	5.058179	-1.524446	16	0.735513	-0.127839	-2.814070
1	1.355874	5.235971	-1.367935	16	1.555507	2.349012	-0.600540
1	0.183132	4.439202	-2.425103	O,O-I10			
1	-0.219588	6.026323	-1.650874	6	-4.385	-1.906621	-1.371683
8	0.299291	-0.094611	0.198509	6	-2.666784	-1.793436	-0.982256
8	-0.775008	4.986953	0.615387	6	-2.315950	-1.697509	0.364884
6	-2.244800	1.803612	-0.400201	6	-3.327311	-1.740633	1.330372
6	-3.543915	1.257379	-0.693518	6	-4.658902	-1.861941	0.957433
7	-1.835276	1.850189	0.975670	6	-5.006773	-1.941467	-0.398065
6	-4.339739	0.839880	0.313830	1	-4.237934	-1.974185	-2.433467
1	-3.845543	1.193736	-1.738406	1	-1.886410	-1.771567	-1.745613
6	-2.659791	1.365906	2.002303	1	-3.058226	-1.663421	2.386796
6	-3.878623	0.895957	1.686871	1	-5.456038	-1.901933	1.701922
1	-5.322460	0.416415	0.105150	15	-0.564178	-1.663255	0.865755
1	-2.228768	1.359277	3.210	15	1.223308	0.103468	-0.996706
1	-4.513113	0.512890	2.485581	6	2.702779	-0.792998	-0.508023
6	0.079524	2.528547	2.367760	6	3.658401	-1.098373	-1.480700
1	0.246753	1.510799	2.782805	6	2.939663	-1.159211	0.832054
1	1.043953	3.020078	2.202632	6	4.832434	-1.762685	-1.141741
1	-0.523205	3.108006	3.083356	1	3.477782	-0.816162	-2.519901

6	4.119	-1.807945	1.174393	6	-6.737655	-2.189871	-2.001537
1	2.200439	-0.951910	1.611721	1	-6.305595	-3.093467	-2.465013
6	5.065591	-2.119553	0.193612	1	-7.829915	-2.287998	-1.983565
1	5.553600	-1.995548	-1.924380	1	-6.469237	-1.312703	-2.616964
1	4.303140	-2.106674	2.205115	6	7.157188	-3.121781	-0.301695
6	-0.531882	2.940971	-1.147905	1	6.765526	-3.816457	-1.063985
1	-0.440010	3.094507	-2.216579	1	7.591216	-2.240848	-0.804741
6	0.469246	3.259018	-0.149304	1	7.944298	-3.628297	0.269252
6	-0.103754	2.840646	1.149754	16	0.321473	-3.347172	0.470470
6	1.422439	4.431227	-0.328039	16	-0.311985	-0.705640	2.582858
6	2.006093	4.559460	-1.707096	16	1.135834	0.652916	-2.848655
1	2.221733	3.570821	-2.139438	16	1.629023	1.769400	0.415235
1	1.268090	5.054822	-2.358154	O,O-I11			
1	2.909589	5.179140	-1.666059	6	-4.056313	-0.193041	1.254421
8	-0.108643	-0.500258	-0.416965	1	-4.379468	-0.040788	2.281861
8	1.667285	5.176471	0.585108	6	-3.778369	-1.361608	0.650456
6	-1.593287	2.364868	-0.505596	6	-3.334503	-1.125007	-0.776717
6	-2.847568	1.856484	-0.968650	6	-3.903317	-2.734320	1.234910
7	-1.330556	2.315535	0.875014	6	-4.046040	-2.831785	2.729489
6	-3.762943	1.422992	-0.065172	1	-3.166138	-2.375676	3.207663
1	-3.030085	1.830705	-2.042246	1	-4.943359	-2.293980	3.072122
6	-2.259977	1.835373	1.785827	1	-4.124233	-3.887821	3.011908
6	-3.470184	1.433254	1.341329	16	-1.652072	-1.747652	-1.156640
1	-4.723355	1.028692	-0.400551	8	-3.895555	-3.702130	0.510611
1	-1.951340	1.803440	2.826763	6	-3.807803	0.895526	0.326654
1	-4.202505	1.064090	2.056891	6	-3.883533	2.266612	0.471106
6	0.273691	3.237910	2.535178	7	-3.386452	0.359525	-0.849206
1	0.275195	2.352648	3.187952	6	-3.482812	3.067950	-0.597401
1	1.260250	3.710422	2.543739	1	-4.186422	2.697573	1.424018
1	-0.461353	3.969135	2.907618	6	-2.993588	1.108871	-1.887344
8	6.166110	-2.754677	0.622386	6	-3.054822	2.484795	-1.792961
8	-6.325566	-2.040325	-0.670617	1	-3.488027	4.152620	-0.494877

1	-2.584347	0.583846	-2.750747	15	0.199005	2.297512	-0.207627
1	-2.684373	3.090837	-2.617118	16	-0.736078	3.582620	0.944442
6	-4.290675	-1.735541	-1.805890	16	0.317515	2.545948	-2.161557
1	-3.969965	-1.488250	-2.827895	1	5.001232	0.977275	-0.285866
1	-4.297390	-2.824167	-1.676667	1	2.892686	1.868999	-1.312459
1	-5.306230	-1.346446	-1.640516	1	0.947116	1.612976	2.509134
6	3.658777	-1.902538	-1.596187	1	2.997662	0.705221	3.521614
6	3.379003	-2.257381	-0.267661	1	6.396268	-0.573132	3.584022
6	2.160493	-1.929537	0.298949	1	5.247232	0.675448	4.153123
6	1.197893	-1.235803	-0.448155	1	4.648719	-0.949399	3.683703
6	1.477231	-0.883868	-1.772476	O,O-I12			
6	2.697484	-1.217033	-2.350431	6	-4.026713	-1.833140	-1.386613
8	4.872251	-2.249203	-2.056969	6	-2.689651	-1.752704	-0.995860
6	5.234568	-1.902131	-3.367550	6	-2.333831	-1.763442	0.352700
15	-0.370965	-0.765958	0.300932	6	-3.342870	-1.882221	1.314861
8	-0.688732	0.764980	0.002840	6	-4.677101	-1.963290	0.941443
16	-0.633627	-1.344924	2.136244	6	-5.030210	-1.940531	-0.414691
1	4.148698	-2.778425	0.302997	1	-4.269680	-1.822471	-2.449573
1	1.944047	-2.193789	1.336300	1	-1.911721	-1.669122	-1.757810
1	0.762499	-0.292575	-2.349649	1	-3.066521	-1.891580	2.372658
1	2.893966	-0.913255	-3.378116	1	-5.470960	-2.060483	1.684344
1	6.251037	-2.282972	-3.522160	15	-0.580236	-1.735343	0.862075
1	4.562903	-2.362555	-4.112243	15	1.205460	0.182411	-0.810743
1	5.235296	-0.808423	-3.514021	6	2.683847	-0.778516	-0.438925
6	4.134752	0.770308	1.667084	6	3.618970	-1.039152	-1.442254
6	4.099931	1.125558	0.311090	6	2.940475	-1.219901	0.873835
6	2.934514	1.620799	-0.249428	6	4.800155	-1.720830	-1.155649
6	1.782012	1.780447	0.529839	1	3.422785	-0.698887	-2.461602
6	1.834903	1.469115	1.889008	6	4.116076	-1.882269	1.165809
6	2.997770	0.957821	2.461511	1	2.213493	-1.054606	1.673385
8	5.297204	0.252751	2.114740	6	5.058868	-2.136113	0.157888
6	5.387781	-0.163239	3.449204	1	5.510031	-1.912272	-1.959891

1	4.325451	-2.233560	2.176593	6	7.155174	-3.097424	-0.400866
6	-0.705042	3.353353	-1.255803	1	6.762133	-3.768763	-1.183422
1	-0.809392	3.705034	-2.278580	1	7.572949	-2.194309	-0.878193
6	0.267762	3.649087	-0.375343	1	7.956266	-3.614605	0.140725
6	0.123177	2.814802	0.866802	16	0.313077	-3.409989	0.455164
6	1.438942	4.567337	-0.563570	16	-0.390972	-0.862491	2.638536
6	2.038937	4.616251	-1.936498	16	1.055995	0.844584	-2.635490
1	2.323533	3.593580	-2.234186	16	1.553116	1.620773	0.783470
1	1.297703	4.967207	-2.670990	O,O-I13			
1	2.906895	5.285647	-1.938068	Indolizine			
8	-0.134110	-0.542821	-0.345097	6	-3.314580	0.544323	-0.058
8	1.856386	5.203756	0.375565	6	-3.369348	-0.887307	-0.111
6	-1.664493	2.478433	-0.605042	6	-2.211924	-1.609901	-0.039
6	-2.909519	2.021185	-1.286	6	-0.953112	-0.945392	0.077
7	-1.214229	2.216262	0.653795	7	-0.944977	0.460093	0.035
6	-3.712329	1.385444	-0.053754	6	-2.118347	1.186485	0.064
1	-3.252025	2.202697	-2.017858	6	0.365875	-1.361996	0.179
6	-1.971624	1.615476	1.584819	6	1.178830	-0.196662	0.142
6	-3.255680	1.216656	1.250595	6	0.342390	0.923968	-0.033
1	-4.707446	1.030180	-0.326505	6	0.643869	2.382512	-0.063
1	-1.541116	1.471037	2.570886	6	2.661096	-0.167381	-0.032
1	-3.875617	0.745322	2.009780	6	3.367767	-1.507089	-0.152
6	0.220258	3.494921	2.224603	8	3.296388	0.867672	0.005
1	0.177410	2.742565	3.024099	1	-4.231497	1.134345	-0.047
1	1.171006	4.034225	2.291234	1	-4.337378	-1.390285	-0.226
1	-0.597227	4.221342	2.341588	1	-2.220273	-2.700963	-0.013
8	6.173118	-2.776611	0.547427	1	-2.014550	2.270881	0.222
8	-6.350046	-2.020449	-0.689171	1	0.695744	-2.397669	0.318
6	-6.761317	-2.157156	-2.021898	1	1.729765	2.520303	-0.890
1	-6.308935	-3.043253	-2.499318	1	0.223807	2.879683	-0.890290
1	-7.851089	-2.279435	-2.004123	1	0.225345	2.879394	0.891066
1	-6.514428	-1.264793	-2.624503	1	3.083900	-2.092583	0.887620

1	3.082298	-2.093631	-0.886705
1	4.451489	-1.340867	-0.001188
LR 5 Members Ring Trans			
6	-4.873230	0.922247	0.943235
6	-3.644647	1.358178	0.452580
6	-2.658407	0.439795	0.093137
6	-2.903794	-0.938528	0.232279
6	-4.119009	-1.376322	0.721976
6	-5.115654	-0.450607	1.081361
1	-5.626347	1.659923	1.218013
1	-3.447016	2.428104	0.352361
1	-2.132813	-1.666170	-0.036277
1	-4.328538	-2.439448	0.846374
8	-6.259435	-0.971697	1.547917
6	-7.303213	-0.115108	1.935281
1	-8.120520	-0.757725	2.282648
1	-6.996732	0.552303	2.758466
1	-7.662176	0.496250	1.089986
15	-1.086296	1.017265	-0.544484
15	1.086300	-1.016866	-0.545057
16	1.038550	-0.121873	-2.511642
8	0.405	0.329	0.172602
16	0.659623	-2.881768	-0.374579
6	2.658719	-0.439912	0.092317
6	3.644845	-1.358439	0.451617
6	2.904128	0.938378	0.232012
6	4.873365	-0.922745	0.942674
1	3.447162	-2.428317	0.350945
6	4.119262	1.375935	0.722091
1	2.133243	1.666151	-0.036454
6	5.115778	0.450039	1.081398
1	5.626450	-1.660519	1.217281

1	4.328813	2.439007	0.846931
8	6.259488	0.970918	1.548355
6	7.303030	0.114141	1.935903
1	7.662361	-0.496934	1.090560
1	8.120201	0.756591	2.283896
1	6.996124	-0.553570	2.758689
16	-0.659933	2.882211	-0.373649
16	-1.038924	0.122658	-2.511284

Figure 25

O,O-J1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603

6	-2.652613	-0.746168	-0.150	1	-1.995603	-2.616824	0.099871
6	-3.051857	0.594301	0.287	6	-2.769395	1.109466	-0.122320
6	-3.625394	-1.755670	-0.493	6	-3.846604	0.226048	-0.023242
6	-4.400241	0.930604	0.362	1	-4.384517	-1.864961	0.130790
1	-2.307453	1.395396	0.536	1	-2.942230	2.188329	-0.193797
6	-4.970864	-1.427866	-0.432	1	-4.870163	0.603990	-0.011555
1	-3.315267	-2.803163	-0.809	6	1.239675	2.194562	-0.935888
6	-5.371350	-0.082808	0.013	1	1.074718	3.239890	-0.646013
1	-4.679935	1.983600	0.725	1	2.245811	2.082825	-1.369636
1	-5.741489	-2.199662	-0.707	1	0.497232	1.881452	-1.682557
8	-6.693755	0.139912	0.103	O,O-J2			
6	-7.175115	1.459861	0.447	6	5.400901	0.930783	-0.445015
1	-6.850662	2.011249	-0.898237	6	4.170740	0.289473	-0.348337
1	-8.269204	1.391129	0.340	6	4.075699	-0.988954	0.209562
1	-6.850803	2.010720	0.899507	6	5.234665	-1.623743	0.673728
Preindolizine				6	6.464553	-0.991663	0.580373
6	0.178997	-1.007094	-0.061471	6	6.558715	0.290524	0.020328
1	0.344103	-2.083841	-0.158607	1	5.444108	1.926190	-0.886203
6	1.241723	-0.189608	0.035834	1	3.277414	0.800138	-0.719737
6	1.157013	1.312645	0.278992	1	5.158382	-2.622565	1.110036
6	2.649285	-0.701640	-0.049454	1	7.377073	-1.471636	0.936858
6	2.902049	-2.193470	-0.049733	8	7.790575	0.827890	-0.031130
1	2.462099	-2.668778	0.839244	6	7.958765	2.110480	-0.574263
1	2.458138	-2.665040	-0.939439	1	9.028499	2.341043	-0.503791
1	3.985338	-2.360717	-0.058901	1	7.654085	2.149482	-1.634360
8	1.125	1.721883	1.410299	1	7.391231	2.870606	-0.010402
8	3.564577	0.088276	-0.125556	15	2.468145	-1.818563	0.336135
6	-1.233616	-0.593404	-0.052625	15	0.198846	-0.091680	-0.593392
6	-2.248065	-1.556404	0.038139	16	1.143715	-0.428518	1.289048
7	-1.504383	0.713443	-0.139051	16	1.524720	-1.553892	-1.550099
6	-3.574545	-1.136383	0.056104	16	2.515777	-3.597406	1.102665
				16	0.356210	1.561320	-1.622572

6	-1.372734	-0.995702	-0.701262	6	-5.157745	-0.400158	1.297520
6	-1.578158	-2.178103	0.006753	1	-6.937237	-0.030281	0.134765
6	-2.373994	-0.519672	-1.552920	1	-3.180089	-0.445564	2.261065
6	-2.787953	-2.862988	-0.095396	1	-5.532584	-1.310677	1.764063
1	-0.788267	-2.579419	0.647337	6	-2.067645	2.484372	2.660219
6	-3.576057	-1.200609	-1.668690	1	-2.114290	1.681481	3.409497
1	-2.201255	0.398613	-2.119582	1	-1.166127	3.084189	2.836377
6	-3.799794	-2.367753	-0.927297	1	-2.954767	3.130521	2.743035
1	-2.921528	-3.783120	0.473243	O,O-J3			
1	-4.368365	-0.843402	-2.328483	6	3.686977	-0.808271	1.612083
8	-5.019805	-2.931034	-1.059844	6	2.409009	-1.361495	1.520336
6	-5.290400	-4.133112	-0.389993	6	2.058657	-2.176344	0.448052
1	-5.219724	-4.016670	0.706196	6	3.024865	-2.472274	-0.528796
1	-6.317648	-4.415053	-0.650909	6	4.290377	-1.922656	-0.451218
1	-4.606505	-4.939606	-0.704280	6	4.626306	-1.068175	0.611914
6	-3.290482	2.936849	-0.414187	1	3.922193	-0.163005	2.457925
1	-3.641970	3.642149	-1.166710	1	1.672480	-1.135585	2.292493
6	-2.080601	2.929262	0.174555	1	2.772866	-3.136992	-1.358928
6	-1.908720	1.851642	1.266910	1	5.046070	-2.130603	-1.210189
6	-1.022982	3.972004	-0.031407	15	0.366584	-2.791382	0.195903
6	-1.031525	4.722482	-1.342055	15	-1.119988	-0.104547	-0.014699
1	-1.844339	5.467126	-1.325505	6	-2.926758	-0.134712	-0.009791
1	-0.077466	5.250906	-1.454120	6	-3.630255	-1.333253	-0.123385
1	-1.192510	4.046363	-2.192023	6	-3.628156	1.076602	0.086229
8	-0.999533	0.966831	1.179026	6	-5.022121	-1.339044	-0.135859
8	-0.260321	4.246149	0.864464	1	-3.091929	-2.279963	-0.200104
6	-4.123966	1.850867	0.091616	6	-5.012651	1.073809	0.095302
6	-5.419283	1.453489	-0.237203	1	-3.091636	2.025196	0.155132
7	-3.432720	1.160631	1.006175	6	-5.722856	-0.131675	-0.015443
6	-5.932504	0.317074	0.382303	1	-5.542986	-2.290906	-0.233487
1	-5.997481	2.014590	-0.971788	1	-5.574991	2.004438	0.182359
6	-3.879252	0.056667	1.586863	6	1.695256	2.854300	0.520219

1	2.221844	3.272	1.374704	1	-7.635636	-1.899558	0.725312
6	0.232990	2.580377	0.464362	1	-8.887878	-0.880552	-0.047371
6	-0.016529	2.148153	-1.021318	16	0.225718	-4.674528	-0.203590
6	-0.719994	3.629303	1.036283	16	-0.908680	-1.893714	1.577910
6	-0.215886	4.410958	2.222636	16	-0.285869	-1.471575	-1.403009
1	0.562656	5.112659	1.886125	16	-0.138446	1.013521	1.463604
1	-1.046468	4.968416	2.670648	O,O-J4			
1	0.242460	3.745281	2.969096	6	-3.875052	0.901114	1.414838
8	-0.987585	1.175268	-1.147922	6	-2.559214	1.356687	1.467151
8	-1.826745	3.805762	0.584303	6	-2.045550	2.170107	0.456732
6	2.290576	2.191036	-0.513963	6	-2.870748	2.528096	-0.622287
6	3.667113	1.939386	-0.843881	6	-4.168966	2.061202	-0.693792
7	1.341453	1.651974	-1.375319	6	-4.680958	1.239206	0.323946
6	3.975934	1.228549	-1.962376	1	-4.247364	0.267385	2.219251
1	4.440463	2.314308	-0.173373	1	-1.922751	1.074879	2.307658
6	1.654608	0.994532	-2.521876	1	-2.479834	3.177751	-1.408825
6	2.953659	0.745703	-2.843072	1	-4.820120	2.319772	-1.529976
1	5.022963	1.015819	-2.188801	15	-0.338323	2.753655	0.510051
1	0.808530	0.665260	-3.126328	15	1.193159	-0.173719	-0.582264
1	3.198061	0.183510	-3.742603	6	2.967187	-0.032914	-0.451392
6	-0.370309	3.301879	-1.952221	6	3.583426	1.208209	-0.616700
1	-0.360164	2.936290	-2.988096	6	3.738021	-1.159924	-0.112460
1	-1.367460	3.684067	-1.713495	6	4.960275	1.339044	-0.458204
1	0.371790	4.106	-1.847346	1	2.983034	2.085391	-0.869028
8	-7.062831	-0.033512	0.001697	6	5.105784	-1.034355	0.037911
8	5.866789	-0.543079	0.577287	1	3.260106	-2.131353	0.037829
6	6.282676	0.289966	1.625232	6	5.729629	0.214865	-0.132387
1	6.264081	-0.233775	2.596301	1	5.416	2.319542	-0.590217
1	7.314666	0.585959	1.401569	1	5.726873	-1.893413	0.295409
1	5.657586	1.197151	1.699372	6	-1.635972	-2.598693	0.935503
6	-7.839700	-1.197869	-0.101445	1	-2.099353	-2.778259	1.901613
1	-7.671972	-1.715771	-1.061284	6	-0.180285	-2.446875	0.687895

6	-0.065786	-2.449337	-0.852119	16	-0.030912	4.521454	-0.179015
6	0.811380	-3.294342	1.448109	16	0.746578	1.824492	1.861938
6	0.443871	-3.635610	2.870358	16	0.353051	1.303298	-1.609871
1	-0.362165	-4.385707	2.862979	16	0.294215	-0.592997	1.272581
1	1.320147	-4.045329	3.385918	O,O-J5			
1	0.067095	-2.749961	3.403080	15	0.296444	-0.904243	-0.428162
8	0.968779	-1.616230	-1.315875	6	2.030900	-0.520070	-0.137545
8	1.860676	-3.654226	0.958897	6	3.017294	-1.441893	-0.483827
6	-2.295736	-2.179495	-0.183284	6	2.403187	0.711716	0.429052
6	-3.681313	-1.933923	-0.477328	6	4.365612	-1.156383	-0.275039
7	-1.395233	-1.924896	-1.218215	1	2.725651	-2.401860	-0.916517
6	-4.041046	-1.446573	-1.695405	6	3.738244	0.999194	0.644011
1	-4.418009	-2.125809	0.302564	1	1.642077	1.444383	0.707914
6	-1.759300	-1.469836	-2.446206	6	4.732325	0.068742	0.294007
6	-3.064117	-1.197508	-2.717030	1	5.114101	-1.896849	-0.555611
1	-5.091856	-1.226760	-1.895702	1	4.047584	1.946106	1.088737
1	-0.945499	-1.308335	-3.155049	6	-3.060115	1.387318	-0.672971
1	-3.349154	-0.790451	-3.685452	1	-3.523747	2.058146	-1.390502
6	0.139301	-3.814596	-1.492001	6	-1.627126	1.389576	-0.299267
1	0.064104	-3.715064	-2.583701	6	-1.565539	0.395579	0.903921
1	1.125324	-4.207766	-1.225034	6	-0.930807	2.734875	-0.116813
1	-0.641609	-4.502077	-1.138115	6	-1.346157	3.831190	-1.065139
8	7.060291	0.235018	0.037769	1	-2.325832	4.220322	-0.746455
8	-5.950103	0.819613	0.160264	1	-0.606726	4.639587	-1.031161
6	-6.570664	0.096392	1.189318	1	-1.456389	3.455297	-2.092335
1	-6.581762	0.663485	2.135649	8	-0.385900	-0.333136	0.973482
1	-7.603745	-0.083692	0.868950	8	-0.085370	2.911640	0.729031
1	-6.078134	-0.875628	1.364095	6	-3.619909	0.225401	-0.214364
6	7.753916	1.449141	-0.094005	6	-4.901874	-0.392671	-0.410305
1	7.647319	1.871575	-1.107656	7	-2.723987	-0.468691	0.587688
1	7.411266	2.194462	0.643611	6	-5.161418	-1.601271	0.164088
1	8.811621	1.226733	0.089313	1	-5.638720	0.117596	-1.030777

6	-2.982541	-1.668508	1.165883	6	5.149287	-0.810617	-1.268932
6	-4.185434	-2.274728	0.968358	1	3.562374	-0.328568	-2.649612
1	-6.132445	-2.074842	0.002160	6	4.570509	-0.650217	1.080398
1	-2.164351	-2.101798	1.743542	1	2.557251	-0.059077	1.526776
1	-4.383785	-3.253846	1.400537	6	5.511952	-0.934153	0.077294
6	-1.793268	1.043678	2.264052	1	5.855023	-1.037460	-2.067619
1	-1.900362	0.251902	3.018046	1	4.867338	-0.778058	2.122275
1	-0.942153	1.681752	2.520454	6	-1.376270	2.514739	-1.029560
1	-2.712623	1.645142	2.238533	1	-1.491252	2.814405	-2.066853
8	6.119	0.438366	0.542909	6	-0.176895	2.812244	-0.166392
6	7.047297	-0.437097	0.217718	6	-0.442264	1.960804	1.054029
1	6.966977	-1.391228	0.766202	6	-0.354109	4.321080	0.236581
1	7.081005	-0.647887	-0.865011	6	-0.012731	5.336112	-0.823064
1	7.977252	0.064347	0.510775	1	1.065980	5.549154	-0.758636
16	-0.089138	-2.737366	-0.889894	1	-0.213514	4.971407	-1.838175
16	-0.557179	0.561452	-1.689995	1	-0.564913	6.261485	-0.617730
O,O-J6				8	0.332211	0.208114	0.215068
6	-3.176366	-1.962081	-1.557479	8	-0.756347	4.631041	1.326641
6	-1.920802	-1.902966	-0.961774	6	-2.294283	1.894226	-0.260107
6	-1.780633	-2.071195	0.418577	6	-3.652815	1.470132	-0.488242
6	-2.917433	-2.327116	1.200210	7	-1.739258	1.642644	1.031218
6	-4.166700	-2.413449	0.609251	6	-4.361924	0.914794	0.518576
6	-4.308417	-2.215875	-0.772554	1	-4.075750	1.618648	-1.481675
1	-3.252825	-1.800778	-2.632347	6	-2.483723	1.056730	2.053539
1	-1.043841	-1.702466	-1.582831	6	-3.764473	0.718156	1.824988
1	-2.812328	-2.459727	2.279165	1	-5.389562	0.587836	0.352849
1	-5.060727	-2.623789	1.198668	1	-1.961479	0.881932	2.991757
15	-0.144828	-2.089557	1.171256	1	-4.342191	0.261164	2.627459
15	1.254703	0.432191	-1.029978	6	0.370674	1.988944	2.285861
6	2.925583	-0.109628	-0.607024	1	0.307685	1.026660	2.811278
6	3.856924	-0.404005	-1.647	1	1.415518	2.188210	2.019181
6	3.293506	-0.243282	0.741448	1	-0.017	2.804666	2.926504

8	6.727914	-1.324176	0.502505	6	4.630239	-0.706512	1.158575
8	-5.565208	-2.270731	-1.251005	1	2.631646	-0.074719	1.594997
6	-5.779465	-2.125593	-2.630897	6	5.554202	-1.081295	0.167133
1	-5.252420	-2.903604	-3.208532	1	5.865125	-1.363723	-1.967386
1	-6.858657	-2.231166	-2.793125	1	4.942252	-0.751373	2.202665
1	-5.457570	-1.133795	-2.992948	6	-1.259323	2.317572	-1.164140
6	7.710217	-1.655491	-0.441341	1	-1.249632	2.391875	-2.247601
1	7.396408	-2.500346	-1.078466	6	-0.177029	2.813205	-0.252263
1	7.964569	-0.796779	-1.086835	6	-0.635421	2.368511	1.099140
1	8.602663	-1.949790	0.124095	6	-0.272731	4.389621	-0.296240
16	1.181886	-3.059719	0.192042	6	0.280509	5.058179	-1.524446
16	-0.119421	-1.612237	3.046705	1	1.355874	5.235971	-1.367935
16	0.652561	-0.068708	-2.812270	1	0.183132	4.439202	-2.425103
16	1.490240	2.601542	-0.849478	1	-0.219588	6.026323	-1.650874
O,O-J7				8	0.299291	-0.094611	0.198509
6	-3.295755	-2.115964	-1.439484	8	-0.775008	4.986953	0.615387
6	-2.028189	-1.834386	-0.932063	6	-2.244800	1.803612	-0.400201
6	-1.792156	-1.803927	0.444251	6	-3.543915	1.257379	-0.693518
6	-2.849895	-2.092699	1.313774	7	-1.835276	1.850189	0.975670
6	-4.114710	-2.383476	0.820724	6	-4.339739	0.839880	0.313830
6	-4.349950	-2.387395	-0.560299	1	-3.845543	1.193736	-1.738406
1	-3.441757	-2.124485	-2.519822	6	-2.659791	1.365906	2.002303
1	-1.210302	-1.639719	-1.630538	6	-3.878623	0.895957	1.686871
1	-2.667777	-2.079867	2.391304	1	-5.322460	0.416415	0.105150
1	-4.944977	-2.616249	1.490348	1	-2.228768	1.359277	3.210
15	-0.095241	-1.583604	1.089829	1	-4.513113	0.512890	2.485581
15	1.312252	0.221423	-0.998943	6	0.079524	2.528547	2.367760
6	2.967424	-0.301254	-0.542754	1	0.246753	1.510799	2.782805
6	3.880250	-0.678390	-1.524859	1	1.043953	3.020078	2.202632
6	3.350742	-0.323648	0.810403	1	-0.523205	3.108006	3.083356
6	5.173489	-1.066550	-1.179885	8	6.771766	-1.441957	0.604767
1	3.573198	-0.683145	-2.573256	8	-5.619225	-2.643369	-0.947984

6	-5.906248	-2.732495	-2.316682	6	5.065591	-2.119553	0.193612
1	-5.316508	-3.524891	-2.808632	1	5.553600	-1.995548	-1.924380
1	-6.971848	-2.978454	-2.400826	1	4.303140	-2.106674	2.205115
1	-5.721212	-1.777088	-2.839295	6	-0.531882	2.940971	-1.147905
6	7.734124	-1.877395	-0.318789	1	-0.440010	3.094507	-2.216579
1	7.395625	-2.773346	-0.866639	6	0.469246	3.259018	-0.149304
1	7.990321	-1.087483	-1.045685	6	-0.103754	2.840646	1.149754
1	8.630707	-2.131619	0.259067	6	1.422439	4.431227	-0.328039
16	1.072057	-3.004872	0.457188	6	2.006093	4.559460	-1.707096
16	-0.132958	-0.972616	2.975586	1	2.221733	3.570821	-2.139438
16	0.735513	-0.127839	-2.814070	1	1.268090	5.054822	-2.358154
16	1.555507	2.349012	-0.600540	1	2.909589	5.179140	-1.666059
O,O-J8				8	-0.108643	-0.500258	-0.416965
6	-4.385	-1.906621	-1.371683	8	1.667285	5.176471	0.585108
6	-2.666784	-1.793436	-0.982256	6	-1.593287	2.364868	-0.505596
6	-2.315950	-1.697509	0.364884	6	-2.847568	1.856484	-0.968650
6	-3.327311	-1.740633	1.330372	7	-1.330556	2.315535	0.875014
6	-4.658902	-1.861941	0.957433	6	-3.762943	1.422992	-0.065172
6	-5.006773	-1.941467	-0.398065	1	-3.030085	1.830705	-2.042246
1	-4.237934	-1.974185	-2.433467	6	-2.259977	1.835373	1.785827
1	-1.886410	-1.771567	-1.745613	6	-3.470184	1.433254	1.341329
1	-3.058226	-1.663421	2.386796	1	-4.723355	1.028692	-0.400551
1	-5.456038	-1.901933	1.701922	1	-1.951340	1.803440	2.826763
15	-0.564178	-1.663255	0.865755	1	-4.202505	1.064090	2.056891
15	1.223308	0.103468	-0.996706	6	0.273691	3.237910	2.535178
6	2.702779	-0.792998	-0.508023	1	0.275195	2.352648	3.187952
6	3.658401	-1.098373	-1.480700	1	1.260250	3.710422	2.543739
6	2.939663	-1.159211	0.832054	1	-0.461353	3.969135	2.907618
6	4.832434	-1.762685	-1.141741	8	6.166110	-2.754677	0.622386
1	3.477782	-0.816162	-2.519901	8	-6.325566	-2.040325	-0.670617
6	4.119	-1.807945	1.174393	6	-6.737655	-2.189871	-2.001537
1	2.200439	-0.951910	1.611721	1	-6.305595	-3.093467	-2.465013

1	-7.829915	-2.287998	-1.983565	6	-0.399732	3.854772	2.197893
1	-6.469237	-1.312703	-2.616964	1	0.301469	3.716694	3.033377
6	7.157188	-3.121781	-0.301695	1	-0.092668	4.723131	1.603593
1	6.765526	-3.816457	-1.063985	1	-1.410150	4.026328	2.597755
1	7.591216	-2.240848	-0.804741	6	5.553033	-0.550364	-0.568093
1	7.944298	-3.628297	0.269252	6	5.088057	0.298728	-1.584525
16	0.321473	-3.347172	0.470470	6	3.753471	0.663122	-1.630494
16	-0.311985	-0.705640	2.582858	6	2.861862	0.196237	-0.654629
16	1.135834	0.652916	-2.848655	6	3.324599	-0.647493	0.359522
16	1.629023	1.769400	0.415235	6	4.661839	-1.024147	0.404717
O,O-J9				8	6.860178	-0.859378	-0.607131
6	-2.392954	1.820656	0.326324	6	7.386949	-1.736233	0.354029
1	-3.260225	1.655559	-0.308905	15	1.140048	0.703	-0.687099
6	-1.418252	2.735552	0.170225	8	0.263456	-0.325963	0.163949
6	-0.404106	2.619814	1.288131	16	0.441761	1.326493	-2.388106
6	-1.349321	3.807317	-0.875439	1	5.797945	0.646458	-2.336121
6	-2.282606	3.673047	-2.049228	1	3.387395	1.305239	-2.434782
1	-2.168599	2.682869	-2.512281	1	2.634939	-1.050144	1.106761
1	-3.325439	3.789583	-1.713398	1	4.989726	-1.704441	1.189923
1	-2.050679	4.456756	-2.779286	1	8.452740	-1.850950	0.123388
16	1.321725	2.305382	0.777323	1	7.284223	-1.330242	1.375117
8	-0.606080	4.747772	-0.725917	1	6.902370	-2.726245	0.310311
6	-2.098433	1.007623	1.491293	6	-4.531121	-1.924435	-0.856265
6	-2.749727	-0.086987	2.044101	6	-4.020793	-2.817065	0.097849
7	-0.944975	1.451039	2.037714	6	-2.657502	-2.855935	0.360262
6	-2.152740	-0.728137	3.120194	6	-1.770740	-2.011276	-0.318310
1	-3.666570	-0.458530	1.586577	6	-2.279944	-1.146809	-1.287760
6	-0.346022	0.845688	3.074389	6	-3.649492	-1.084913	-1.550913
6	-0.941463	-0.258987	3.641755	8	-5.867617	-1.946023	-1.041800
1	-2.610558	-1.624612	3.539619	6	-6.431490	-1.133050	-2.033787
1	0.623666	1.240933	3.377360	15	0.033022	-2.096648	-0.003575
1	-0.441878	-0.778172	4.457513	16	0.999930	-2.676102	-1.588892

16	0.383226	-2.788406	1.810709	1	-4.297390	-2.824167	-1.676667
1	-4.718218	-3.478997	0.614443	1	-5.306230	-1.346446	-1.640516
1	-2.261060	-3.541962	1.113302	6	3.658777	-1.902538	-1.596187
1	-1.599803	-0.503765	-1.854024	6	3.379003	-2.257381	-0.267661
1	-4.009714	-0.398481	-2.318263	6	2.160493	-1.929537	0.298949
1	-7.509143	-1.336499	-2.033795	6	1.197893	-1.235803	-0.448155
1	-6.273421	-0.059572	-1.825785	6	1.477231	-0.883868	-1.772476
1	-6.023563	-1.362964	-3.033083	6	2.697484	-1.217033	-2.350431
O,O-J10				8	4.872251	-2.249203	-2.056969
6	-4.056313	-0.193041	1.254421	6	5.234568	-1.902131	-3.367550
1	-4.379468	-0.040788	2.281861	15	-0.370965	-0.765958	0.300932
6	-3.778369	-1.361608	0.650456	8	-0.688732	0.764980	0.002840
6	-3.334503	-1.125007	-0.776717	16	-0.633627	-1.344924	2.136244
6	-3.903317	-2.734320	1.234910	1	4.148698	-2.778425	0.302997
6	-4.046040	-2.831785	2.729489	1	1.944047	-2.193789	1.336300
1	-3.166138	-2.375676	3.207663	1	0.762499	-0.292575	-2.349649
1	-4.943359	-2.293980	3.072122	1	2.893966	-0.913255	-3.378116
1	-4.124233	-3.887821	3.011908	1	6.251037	-2.282972	-3.522160
16	-1.652072	-1.747652	-1.156640	1	4.562903	-2.362555	-4.112243
8	-3.895555	-3.702130	0.510611	1	5.235296	-0.808423	-3.514021
6	-3.807803	0.895526	0.326654	6	4.134752	0.770308	1.667084
6	-3.883533	2.266612	0.471106	6	4.099931	1.125558	0.311090
7	-3.386452	0.359525	-0.849206	6	2.934514	1.620799	-0.249428
6	-3.482812	3.067950	-0.597401	6	1.782012	1.780447	0.529839
1	-4.186422	2.697573	1.424018	6	1.834903	1.469115	1.889008
6	-2.993588	1.108871	-1.887344	6	2.997770	0.957821	2.461511
6	-3.054822	2.484795	-1.792961	8	5.297204	0.252751	2.114740
1	-3.488027	4.152620	-0.494877	6	5.387781	-0.163239	3.449204
1	-2.584347	0.583846	-2.750747	15	0.199005	2.297512	-0.207627
1	-2.684373	3.090837	-2.617118	16	-0.736078	3.582620	0.944442
6	-4.290675	-1.735541	-1.805890	16	0.317515	2.545948	-2.161557
1	-3.969965	-1.488250	-2.827895	1	5.001232	0.977275	-0.285866

1	2.892686	1.868999	-1.312459	6	-2.423419	-2.485013	-0.649800
1	0.947116	1.612976	2.509134	6	-1.710369	-2.226549	-1.831761
1	2.997662	0.705221	3.521614	6	-0.670350	-1.310650	-1.832668
1	6.396268	-0.573132	3.584022	6	-0.316510	-0.634623	-0.654657
1	5.247232	0.675448	4.153123	6	-1.018487	-0.911378	0.519916
1	4.648719	-0.949399	3.683703	6	-2.055589	-1.837614	0.533878
O,O-J11				8	-3.441314	-3.359825	-0.745054
6	3.187361	-2.326578	-0.433764	6	-4.171433	-3.683568	0.415057
1	2.986086	-3.165668	-1.095030	15	0.897499	0.708813	-0.731654
6	2.526890	-1.984242	0.710306	8	0.044938	2.059556	-0.910328
6	3.065438	-0.726739	1.248175	16	2.195864	0.541942	-2.163134
6	1.429315	-2.766838	1.361374	1	-2.003657	-2.750975	-2.742589
6	0.828443	-3.894828	0.563228	1	-0.121605	-1.104694	-2.754747
1	0.381991	-3.499988	-0.362695	1	-0.758510	-0.397673	1.446849
1	1.597580	-4.630643	0.283804	1	-2.583324	-2.018080	1.468911
1	0.053722	-4.384212	1.164129	1	-4.932400	-4.410926	0.108295
16	1.673772	0.843133	1.289650	1	-3.524535	-4.144389	1.180833
8	1.057312	-2.497767	2.480571	1	-4.667582	-2.795582	0.840310
6	4.202754	-1.346788	-0.670274	6	-4.646628	0.250534	0.161206
6	5.156853	-1.195906	-1.684162	6	-4.155599	0.759706	1.369664
7	4.130508	-0.420329	0.327902	6	-3.040569	1.586529	1.376668
6	5.982164	-0.091360	-1.660167	6	-2.407298	1.937260	0.179714
1	5.209633	-1.938827	-2.479412	6	-2.931780	1.463791	-1.024556
6	4.909627	0.685505	0.347383	6	-4.036622	0.617698	-1.043564
6	5.849362	0.867613	-0.635570	8	-5.692435	-0.604027	0.248964
1	6.726879	0.053474	-2.444405	6	-6.219162	-1.153058	-0.931533
1	4.723163	1.399770	1.148771	15	-0.919517	2.991401	0.139177
1	6.471118	1.762183	-0.618210	16	-1.236380	4.726158	-0.638614
6	3.486388	-0.681929	2.708347	16	0.097989	2.812673	1.889301
1	3.793483	0.331853	3.004211	1	-4.652994	0.472869	2.297826
1	2.633620	-0.984655	3.326196	1	-2.631960	1.945894	2.324287
1	4.320834	-1.378807	2.885633	1	-2.455563	1.738624	-1.968598

1	-4.398429	0.239791	-1.999356	6	-0.329368	1.908147	-1.188544
1	-7.052374	-1.800100	-0.630413	6	0.635886	1.898048	-0.177956
1	-6.603199	-0.371866	-1.609354	6	0.336520	2.478113	1.060920
1	-5.467854	-1.760132	-1.466538	6	-0.912740	3.033092	1.288940
O,O-J12				6	-1.886979	3.025912	0.278824
Indolizine				1	-2.318772	2.452286	-1.775599
6	-3.314580	0.544323	-0.058	1	-0.111675	1.459991	-2.160847
6	-3.369348	-0.887307	-0.111	1	1.081776	2.477223	1.859035
6	-2.211924	-1.609901	-0.039	1	-1.164375	3.482164	2.250642
6	-0.953112	-0.945392	0.077	8	-3.074165	3.569504	0.595848
7	-0.944977	0.460093	0.035	6	-4.091365	3.610994	-0.370623
6	-2.118347	1.186485	0.064	1	-4.953854	4.094307	0.103027
6	0.365875	-1.361996	0.179	1	-3.791494	4.243	-1.253948
6	1.178830	-0.196662	0.142	1	-4.383854	2.598049	-0.698221
6	0.342390	0.923968	-0.033	15	2.208602	1.084556	-0.540951
6	0.643869	2.382512	-0.063	15	1.443065	-1.740140	0.053103
6	2.661096	-0.167381	-0.032	16	1.699443	-0.734298	1.965053
6	3.367767	-1.507089	-0.152	8	1.691677	-0.437613	-0.932571
8	3.296388	0.867672	0.005	16	2.555198	-3.246505	-0.339415
1	-4.231497	1.134345	-0.047	6	-0.343668	-1.984597	0.002584
1	-4.337378	-1.390285	-0.226	6	-1.235262	-0.992789	0.425240
1	-2.220273	-2.700963	-0.013	6	-0.853466	-3.184263	-0.518772
1	-2.014550	2.270881	0.222	6	-2.609905	-1.181346	0.326092
1	0.695744	-2.397669	0.318	1	-0.864437	-0.057243	0.846820
1	1.729765	2.520303	-0.890	6	-2.219542	-3.378773	-0.622739
1	0.223807	2.879683	-0.890290	1	-0.160971	-3.964672	-0.842463
1	0.225345	2.879394	0.891066	6	-3.111572	-2.378315	-0.204005
1	3.083900	-2.092583	0.887620	1	-3.274313	-0.388320	0.668080
1	3.082298	-2.093631	-0.886705	1	-2.630621	-4.304596	-1.027432
1	4.451489	-1.340867	-0.001188	8	-4.417388	-2.652672	-0.344296
LR 5 Members Ring Cis				6	-5.369973	-1.711359	0.077218
6	-1.584941	2.466711	-0.970421	1	-5.279211	-0.762524	-0.479039

1	-6.353689	-2.150557	-0.125352
1	-5.285375	-1.504148	1.157474
16	3.365254	1.907306	-1.819716
16	3.165926	0.617907	1.306774

Figure 26

O,O-H1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287

6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320

6	-3.846604	0.226048	-0.023242	6	3.216076	-1.815551	-0.301885
1	-4.384517	-1.864961	0.130790	6	4.518843	0.533126	0.484738
1	-2.942230	2.188329	-0.193797	1	2.590010	1.198244	1.169247
1	-4.870163	0.603990	-0.011555	6	4.574104	-1.679850	-0.516320
6	1.239675	2.194562	-0.935888	1	2.700275	-2.728593	-0.606940
1	1.074718	3.239890	-0.646013	6	5.239282	-0.503636	-0.127213
1	2.245811	2.082825	-1.369636	1	5.008365	1.456113	0.793375
1	0.497232	1.881452	-1.682557	1	5.155828	-2.472745	-0.988319
O,O-H2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	O,O-H3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633

O,O-H4				8	6.065983	-0.118937	0.651254
6	-3.334661	0.397287	-0.108530	6	6.750251	-1.342013	0.655008
1	-4.118597	0.841972	-0.722543	15	0.365113	0.365313	-1.020351
6	-2.413161	1.137904	0.523965	16	-0.395518	-1.250449	-1.791788
6	-1.331402	0.469811	1.339344	16	-0.068646	2.175	-1.599652
6	-2.423406	2.642127	0.573366	1	4.751288	2.038421	0.583111
6	-3.226687	3.371879	-0.471469	1	2.366028	2.293570	-0.127409
1	-2.942736	3.028651	-1.475901	1	2.137963	-1.937187	-0.842338
1	-4.301678	3.184930	-0.320741	1	4.497353	-2.202090	-0.158553
1	-3.035202	4.446410	-0.371560	1	7.772680	-1.129256	0.989940
8	-0.181966	0.303263	0.873581	1	6.291452	-2.066358	1.350436
8	-1.840026	3.212329	1.466614	1	6.791949	-1.791956	-0.352023
6	-3.262443	-1.057243	0.047002	O,O-H5			
6	-4.026569	-1.984634	-0.659766	6	-3.140294	1.584731	-0.280793
7	-2.344662	-1.437919	0.937046	1	-3.709346	2.314968	-0.851029
6	-3.781158	-3.337644	-0.441352	6	-1.835213	1.665546	0.090194
1	-4.772442	-1.650062	-1.381820	6	-1.480183	0.491734	1.008572
6	-2.094447	-2.720682	1.142669	6	-0.930	2.850856	-0.038497
6	-2.797807	-3.718820	0.469015	6	-1.271552	3.857357	-1.106844
1	-4.347532	-4.093322	-0.989262	1	-1.458073	3.363216	-2.069440
1	-1.306134	-2.962164	1.861521	1	-2.182418	4.403799	-0.811958
1	-2.572631	-4.769972	0.652262	1	-0.445870	4.572077	-1.201154
6	-1.475502	0.477469	2.828198	8	-0.317280	-0.179641	0.828175
1	-0.772198	-0.234987	3.276436	8	-0.016499	3.007072	0.741074
1	-1.221252	1.499873	3.148804	6	-3.641042	0.282075	0.068685
1	-2.506781	0.258154	3.129696	6	-4.848867	-0.366933	-0.195334
6	4.776332	-0.086964	0.264722	7	-2.680203	-0.390818	0.748746
6	4.160975	1.175118	0.271815	6	-4.992672	-1.686546	0.211374
6	2.839920	1.309386	-0.118334	1	-5.639784	0.157630	-0.730794
6	2.099257	0.186979	-0.519755	6	-2.779272	-1.671388	1.127676
6	2.712662	-1.064653	-0.522233	6	-3.951747	-2.354049	0.871303
6	4.044366	-1.211129	-0.135774	1	-5.923496	-2.216349	-0.626

1	-1.897723	-2.106604	1.599296	1	-1.953273	4.393761	-0.900663
1	-4.039900	-3.400726	1.158560	1	-0.211021	4.489582	-1.287191
6	-1.536444	0.938450	2.474250	8	-0.349369	-0.266441	0.897599
1	-1.392286	0.061315	3.119785	8	0.112	2.919999	0.669410
1	-0.715143	1.646720	2.632687	6	-3.623798	0.390288	-0.023018
1	-2.495026	1.423241	2.705257	6	-4.890438	-0.189011	-0.242197
6	4.722340	-0.478309	0.214403	7	-2.714320	-0.334889	0.690066
6	4.147210	-1.725998	-0.061687	6	-5.131906	-1.461224	0.232518
6	2.789598	-1.825263	-0.329545	1	-5.643177	0.367222	-0.800347
6	1.981623	-0.683022	-0.334273	6	-2.922611	-1.581489	1.149019
6	2.557916	0.559332	-0.060484	6	-4.138567	-2.181494	0.931193
6	3.917767	0.669611	0.217513	1	-6.103297	-1.926686	0.052873
8	6.048008	-0.475075	0.464652	1	-2.076555	-2.056875	1.647020
6	6.684189	0.737929	0.757572	1	-4.311228	-3.199385	1.276797
15	0.206411	-0.789886	-0.700188	6	-1.595970	1.044416	2.378809
16	-0.436380	-2.634319	-0.905621	1	-1.571487	0.208965	3.091747
16	-0.346921	0.608717	-2.010456	1	-0.736349	1.700298	2.554668
1	4.791428	-2.606844	-0.058579	1	-2.528019	1.612350	2.502307
1	2.335118	-2.797119	-0.537347	6	4.731689	-0.444499	0.178297
1	1.938599	1.459807	-0.058644	6	4.208352	-1.680602	-0.226165
1	4.336146	1.653318	0.429602	6	2.846407	-1.824713	-0.442131
1	7.743047	0.506438	0.926120	6	1.981595	-0.738272	-0.264937
1	6.605952	1.456258	-0.077134	6	2.504811	0.493408	0.136641
1	6.272880	1.206956	1.668523	6	3.870046	0.646163	0.361495
O,O-H6				8	6.064662	-0.396778	0.368521
6	-3.043024	1.615854	-0.424540	6	6.657464	0.810499	0.762681
1	-3.550137	2.357962	-1.035124	15	0.206803	-0.911107	-0.574946
6	-1.693679	1.592308	-0.090715	16	-0.387124	-2.749520	-0.831471
6	-1.486268	0.486157	0.957232	16	-0.440168	0.512659	-1.871444
6	-0.777777	2.779544	-0.142998	1	4.896774	-2.516276	-0.361195
6	-1.068109	3.811276	-1.203859	1	2.433887	-2.789243	-0.747939
1	-1.280202	3.343998	-2.174774	1	1.842490	1.349510	0.287800

1	4.247329	1.618022	0.679087	6	-2.982541	-1.668508	1.165883
1	7.732382	0.615912	0.860160	6	-4.185434	-2.274728	0.968358
1	6.505316	1.605167	0.011691	1	-6.132445	-2.074842	0.002160
1	6.269772	1.160440	1.735250	1	-2.164351	-2.101798	1.743542
O,O-H7				1	-4.383785	-3.253846	1.400537
15	0.296444	-0.904243	-0.428162	6	-1.793268	1.043678	2.264052
6	2.030900	-0.520070	-0.137545	1	-1.900362	0.251902	3.018046
6	3.017294	-1.441893	-0.483827	1	-0.942153	1.681752	2.520454
6	2.403187	0.711716	0.429052	1	-2.712623	1.645142	2.238533
6	4.365612	-1.156383	-0.275039	8	6.119	0.438366	0.542909
1	2.725651	-2.401860	-0.916517	6	7.047297	-0.437097	0.217718
6	3.738244	0.999194	0.644011	1	6.966977	-1.391228	0.766202
1	1.642077	1.444383	0.707914	1	7.081005	-0.647887	-0.865011
6	4.732325	0.068742	0.294007	1	7.977252	0.064347	0.510775
1	5.114101	-1.896849	-0.555611	16	-0.089138	-2.737366	-0.889894
1	4.047584	1.946106	1.088737	16	-0.557179	0.561452	-1.689995
6	-3.060115	1.387318	-0.672971	O,O-H8			
1	-3.523747	2.058146	-1.390502	6	-3.176366	-1.962081	-1.557479
6	-1.627126	1.389576	-0.299267	6	-1.920802	-1.902966	-0.961774
6	-1.565539	0.395579	0.903921	6	-1.780633	-2.071195	0.418577
6	-0.930807	2.734875	-0.116813	6	-2.917433	-2.327116	1.200210
6	-1.346157	3.831190	-1.065139	6	-4.166700	-2.413449	0.609251
1	-2.325832	4.220322	-0.746455	6	-4.308417	-2.215875	-0.772554
1	-0.606726	4.639587	-1.031161	1	-3.252825	-1.800778	-2.632347
1	-1.456389	3.455297	-2.092335	1	-1.043841	-1.702466	-1.582831
8	-0.385900	-0.333136	0.973482	1	-2.812328	-2.459727	2.279165
8	-0.085370	2.911640	0.729031	1	-5.060727	-2.623789	1.198668
6	-3.619909	0.225401	-0.214364	15	-0.144828	-2.089557	1.171256
6	-4.901874	-0.392671	-0.410305	15	1.254703	0.432191	-1.029978
7	-2.723987	-0.468691	0.587688	6	2.925583	-0.109628	-0.607024
6	-5.161418	-1.601271	0.164088	6	3.856924	-0.404005	-1.647
1	-5.638720	0.117596	-1.030777	6	3.293506	-0.243282	0.741448

6	5.149287	-0.810617	-1.268932	8	6.727914	-1.324176	0.502505
1	3.562374	-0.328568	-2.649612	8	-5.565208	-2.270731	-1.251005
6	4.570509	-0.650217	1.080398	6	-5.779465	-2.125593	-2.630897
1	2.557251	-0.059077	1.526776	1	-5.252420	-2.903604	-3.208532
6	5.511952	-0.934153	0.077294	1	-6.858657	-2.231166	-2.793125
1	5.855023	-1.037460	-2.067619	1	-5.457570	-1.133795	-2.992948
1	4.867338	-0.778058	2.122275	6	7.710217	-1.655491	-0.441341
6	-1.376270	2.514739	-1.029560	1	7.396408	-2.500346	-1.078466
1	-1.491252	2.814405	-2.066853	1	7.964569	-0.796779	-1.086835
6	-0.176895	2.812244	-0.166392	1	8.602663	-1.949790	0.124095
6	-0.442264	1.960804	1.054029	16	1.181886	-3.059719	0.192042
6	-0.354109	4.321080	0.236581	16	-0.119421	-1.612237	3.046705
6	-0.012731	5.336112	-0.823064	16	0.652561	-0.068708	-2.812270
1	1.065980	5.549154	-0.758636	16	1.490240	2.601542	-0.849478
1	-0.213514	4.971407	-1.838175	O,O-H9			
1	-0.564913	6.261485	-0.617730	6	-3.295755	-2.115964	-1.439484
8	0.332211	0.208114	0.215068	6	-2.028189	-1.834386	-0.932063
8	-0.756347	4.631041	1.326641	6	-1.792156	-1.803927	0.444251
6	-2.294283	1.894226	-0.260107	6	-2.849895	-2.092699	1.313774
6	-3.652815	1.470132	-0.488242	6	-4.114710	-2.383476	0.820724
7	-1.739258	1.642644	1.031218	6	-4.349950	-2.387395	-0.560299
6	-4.361924	0.914794	0.518576	1	-3.441757	-2.124485	-2.519822
1	-4.075750	1.618648	-1.481675	1	-1.210302	-1.639719	-1.630538
6	-2.483723	1.056730	2.053539	1	-2.667777	-2.079867	2.391304
6	-3.764473	0.718156	1.824988	1	-4.944977	-2.616249	1.490348
1	-5.389562	0.587836	0.352849	15	-0.095241	-1.583604	1.089829
1	-1.961479	0.881932	2.991757	15	1.312252	0.221423	-0.998943
1	-4.342191	0.261164	2.627459	6	2.967424	-0.301254	-0.542754
6	0.370674	1.988944	2.285861	6	3.880250	-0.678390	-1.524859
1	0.307685	1.026660	2.811278	6	3.350742	-0.323648	0.810403
1	1.415518	2.188210	2.019181	6	5.173489	-1.066550	-1.179885
1	-0.017	2.804666	2.926504	1	3.573198	-0.683145	-2.573256

6	4.630239	-0.706512	1.158575	6	-5.906248	-2.732495	-2.316682
1	2.631646	-0.074719	1.594997	1	-5.316508	-3.524891	-2.808632
6	5.554202	-1.081295	0.167133	1	-6.971848	-2.978454	-2.400826
1	5.865125	-1.363723	-1.967386	1	-5.721212	-1.777088	-2.839295
1	4.942252	-0.751373	2.202665	6	7.734124	-1.877395	-0.318789
6	-1.259323	2.317572	-1.164140	1	7.395625	-2.773346	-0.866639
1	-1.249632	2.391875	-2.247601	1	7.990321	-1.087483	-1.045685
6	-0.177029	2.813205	-0.252263	1	8.630707	-2.131619	0.259067
6	-0.635421	2.368511	1.099140	16	1.072057	-3.004872	0.457188
6	-0.272731	4.389621	-0.296240	16	-0.132958	-0.972616	2.975586
6	0.280509	5.058179	-1.524446	16	0.735513	-0.127839	-2.814070
1	1.355874	5.235971	-1.367935	16	1.555507	2.349012	-0.600540
1	0.183132	4.439202	-2.425103	O,O-H10			
1	-0.219588	6.026323	-1.650874	6	-4.385	-1.906621	-1.371683
8	0.299291	-0.094611	0.198509	6	-2.666784	-1.793436	-0.982256
8	-0.775008	4.986953	0.615387	6	-2.315950	-1.697509	0.364884
6	-2.244800	1.803612	-0.400201	6	-3.327311	-1.740633	1.330372
6	-3.543915	1.257379	-0.693518	6	-4.658902	-1.861941	0.957433
7	-1.835276	1.850189	0.975670	6	-5.006773	-1.941467	-0.398065
6	-4.339739	0.839880	0.313830	1	-4.237934	-1.974185	-2.433467
1	-3.845543	1.193736	-1.738406	1	-1.886410	-1.771567	-1.745613
6	-2.659791	1.365906	2.002303	1	-3.058226	-1.663421	2.386796
6	-3.878623	0.895957	1.686871	1	-5.456038	-1.901933	1.701922
1	-5.322460	0.416415	0.105150	15	-0.564178	-1.663255	0.865755
1	-2.228768	1.359277	3.210	15	1.223308	0.103468	-0.996706
1	-4.513113	0.512890	2.485581	6	2.702779	-0.792998	-0.508023
6	0.079524	2.528547	2.367760	6	3.658401	-1.098373	-1.480700
1	0.246753	1.510799	2.782805	6	2.939663	-1.159211	0.832054
1	1.043953	3.020078	2.202632	6	4.832434	-1.762685	-1.141741
1	-0.523205	3.108006	3.083356	1	3.477782	-0.816162	-2.519901
8	6.771766	-1.441957	0.604767	6	4.119	-1.807945	1.174393
8	-5.619225	-2.643369	-0.947984	1	2.200439	-0.951910	1.611721

6	5.065591	-2.119553	0.193612	1	-7.829915	-2.287998	-1.983565
1	5.553600	-1.995548	-1.924380	1	-6.469237	-1.312703	-2.616964
1	4.303140	-2.106674	2.205115	6	7.157188	-3.121781	-0.301695
6	-0.531882	2.940971	-1.147905	1	6.765526	-3.816457	-1.063985
1	-0.440010	3.094507	-2.216579	1	7.591216	-2.240848	-0.804741
6	0.469246	3.259018	-0.149304	1	7.944298	-3.628297	0.269252
6	-0.103754	2.840646	1.149754	16	0.321473	-3.347172	0.470470
6	1.422439	4.431227	-0.328039	16	-0.311985	-0.705640	2.582858
6	2.006093	4.559460	-1.707096	16	1.135834	0.652916	-2.848655
1	2.221733	3.570821	-2.139438	16	1.629023	1.769400	0.415235
1	1.268090	5.054822	-2.358154	O,O-H11			
1	2.909589	5.179140	-1.666059	6	-2.392954	1.820656	0.326324
8	-0.108643	-0.500258	-0.416965	1	-3.260225	1.655559	-0.308905
8	1.667285	5.176471	0.585108	6	-1.418252	2.735552	0.170225
6	-1.593287	2.364868	-0.505596	6	-0.404106	2.619814	1.288131
6	-2.847568	1.856484	-0.968650	6	-1.349321	3.807317	-0.875439
7	-1.330556	2.315535	0.875014	6	-2.282606	3.673047	-2.049228
6	-3.762943	1.422992	-0.065172	1	-2.168599	2.682869	-2.512281
1	-3.030085	1.830705	-2.042246	1	-3.325439	3.789583	-1.713398
6	-2.259977	1.835373	1.785827	1	-2.050679	4.456756	-2.779286
6	-3.470184	1.433254	1.341329	16	1.321725	2.305382	0.777323
1	-4.723355	1.028692	-0.400551	8	-0.606080	4.747772	-0.725917
1	-1.951340	1.803440	2.826763	6	-2.098433	1.007623	1.491293
1	-4.202505	1.064090	2.056891	6	-2.749727	-0.086987	2.044101
6	0.273691	3.237910	2.535178	7	-0.944975	1.451039	2.037714
1	0.275195	2.352648	3.187952	6	-2.152740	-0.728137	3.120194
1	1.260250	3.710422	2.543739	1	-3.666570	-0.458530	1.586577
1	-0.461353	3.969135	2.907618	6	-0.346022	0.845688	3.074389
8	6.166110	-2.754677	0.622386	6	-0.941463	-0.258987	3.641755
8	-6.325566	-2.040325	-0.670617	1	-2.610558	-1.624612	3.539619
6	-6.737655	-2.189871	-2.001537	1	0.623666	1.240933	3.377360
1	-6.305595	-3.093467	-2.465013	1	-0.441878	-0.778172	4.457513

6	-0.399732	3.854772	2.197893	16	0.383226	-2.788406	1.810709
1	0.301469	3.716694	3.033377	1	-4.718218	-3.478997	0.614443
1	-0.092668	4.723131	1.603593	1	-2.261060	-3.541962	1.113302
1	-1.410150	4.026328	2.597755	1	-1.599803	-0.503765	-1.854024
6	5.553033	-0.550364	-0.568093	1	-4.009714	-0.398481	-2.318263
6	5.088057	0.298728	-1.584525	1	-7.509143	-1.336499	-2.033795
6	3.753471	0.663122	-1.630494	1	-6.273421	-0.059572	-1.825785
6	2.861862	0.196237	-0.654629	1	-6.023563	-1.362964	-3.033083
6	3.324599	-0.647493	0.359522	O,O-H12			
6	4.661839	-1.024147	0.404717	6	-4.056313	-0.193041	1.254421
8	6.860178	-0.859378	-0.607131	1	-4.379468	-0.040788	2.281861
6	7.386949	-1.736233	0.354029	6	-3.778369	-1.361608	0.650456
15	1.140048	0.703	-0.687099	6	-3.334503	-1.125007	-0.776717
8	0.263456	-0.325963	0.163949	6	-3.903317	-2.734320	1.234910
16	0.441761	1.326493	-2.388106	6	-4.046040	-2.831785	2.729489
1	5.797945	0.646458	-2.336121	1	-3.166138	-2.375676	3.207663
1	3.387395	1.305239	-2.434782	1	-4.943359	-2.293980	3.072122
1	2.634939	-1.050144	1.106761	1	-4.124233	-3.887821	3.011908
1	4.989726	-1.704441	1.189923	16	-1.652072	-1.747652	-1.156640
1	8.452740	-1.850950	0.123388	8	-3.895555	-3.702130	0.510611
1	7.284223	-1.330242	1.375117	6	-3.807803	0.895526	0.326654
1	6.902370	-2.726245	0.310311	6	-3.883533	2.266612	0.471106
6	-4.531121	-1.924435	-0.856265	7	-3.386452	0.359525	-0.849206
6	-4.020793	-2.817065	0.097849	6	-3.482812	3.067950	-0.597401
6	-2.657502	-2.855935	0.360262	1	-4.186422	2.697573	1.424018
6	-1.770740	-2.011276	-0.318310	6	-2.993588	1.108871	-1.887344
6	-2.279944	-1.146809	-1.287760	6	-3.054822	2.484795	-1.792961
6	-3.649492	-1.084913	-1.550913	1	-3.488027	4.152620	-0.494877
8	-5.867617	-1.946023	-1.041800	1	-2.584347	0.583846	-2.750747
6	-6.431490	-1.133050	-2.033787	1	-2.684373	3.090837	-2.617118
15	0.033022	-2.096648	-0.003575	6	-4.290675	-1.735541	-1.805890
16	0.999930	-2.676102	-1.588892	1	-3.969965	-1.488250	-2.827895

1	-4.297390	-2.824167	-1.676667	1	2.892686	1.868999	-1.312459
1	-5.306230	-1.346446	-1.640516	1	0.947116	1.612976	2.509134
6	3.658777	-1.902538	-1.596187	1	2.997662	0.705221	3.521614
6	3.379003	-2.257381	-0.267661	1	6.396268	-0.573132	3.584022
6	2.160493	-1.929537	0.298949	1	5.247232	0.675448	4.153123
6	1.197893	-1.235803	-0.448155	1	4.648719	-0.949399	3.683703
6	1.477231	-0.883868	-1.772476	O,O-H13			
6	2.697484	-1.217033	-2.350431	6	3.187361	-2.326578	-0.433764
8	4.872251	-2.249203	-2.056969	1	2.986086	-3.165668	-1.095030
6	5.234568	-1.902131	-3.367550	6	2.526890	-1.984242	0.710306
15	-0.370965	-0.765958	0.300932	6	3.065438	-0.726739	1.248175
8	-0.688732	0.764980	0.002840	6	1.429315	-2.766838	1.361374
16	-0.633627	-1.344924	2.136244	6	0.828443	-3.894828	0.563228
1	4.148698	-2.778425	0.302997	1	0.381991	-3.499988	-0.362695
1	1.944047	-2.193789	1.336300	1	1.597580	-4.630643	0.283804
1	0.762499	-0.292575	-2.349649	1	0.053722	-4.384212	1.164129
1	2.893966	-0.913255	-3.378116	16	1.673772	0.843133	1.289650
1	6.251037	-2.282972	-3.522160	8	1.057312	-2.497767	2.480571
1	4.562903	-2.362555	-4.112243	6	4.202754	-1.346788	-0.670274
1	5.235296	-0.808423	-3.514021	6	5.156853	-1.195906	-1.684162
6	4.134752	0.770308	1.667084	7	4.130508	-0.420329	0.327902
6	4.099931	1.125558	0.311090	6	5.982164	-0.091360	-1.660167
6	2.934514	1.620799	-0.249428	1	5.209633	-1.938827	-2.479412
6	1.782012	1.780447	0.529839	6	4.909627	0.685505	0.347383
6	1.834903	1.469115	1.889008	6	5.849362	0.867613	-0.635570
6	2.997770	0.957821	2.461511	1	6.726879	0.053474	-2.444405
8	5.297204	0.252751	2.114740	1	4.723163	1.399770	1.148771
6	5.387781	-0.163239	3.449204	1	6.471118	1.762183	-0.618210
15	0.199005	2.297512	-0.207627	6	3.486388	-0.681929	2.708347
16	-0.736078	3.582620	0.944442	1	3.793483	0.331853	3.004211
16	0.317515	2.545948	-2.161557	1	2.633620	-0.984655	3.326196
1	5.001232	0.977275	-0.285866	1	4.320834	-1.378807	2.885633

6	-2.423419	-2.485013	-0.649800	1	-4.398429	0.239791	-1.999356
6	-1.710369	-2.226549	-1.831761	1	-7.052374	-1.800100	-0.630413
6	-0.670350	-1.310650	-1.832668	1	-6.603199	-0.371866	-1.609354
6	-0.316510	-0.634623	-0.654657	1	-5.467854	-1.760132	-1.466538
6	-1.018487	-0.911378	0.519916	O,O-H14			
6	-2.055589	-1.837614	0.533878	Indolizine			
8	-3.441314	-3.359825	-0.745054	6	-3.314580	0.544323	-0.058
6	-4.171433	-3.683568	0.415057	6	-3.369348	-0.887307	-0.111
15	0.897499	0.708813	-0.731654	6	-2.211924	-1.609901	-0.039
8	0.044938	2.059556	-0.910328	6	-0.953112	-0.945392	0.077
16	2.195864	0.541942	-2.163134	7	-0.944977	0.460093	0.035
1	-2.003657	-2.750975	-2.742589	6	-2.118347	1.186485	0.064
1	-0.121605	-1.104694	-2.754747	6	0.365875	-1.361996	0.179
1	-0.758510	-0.397673	1.446849	6	1.178830	-0.196662	0.142
1	-2.583324	-2.018080	1.468911	6	0.342390	0.923968	-0.033
1	-4.932400	-4.410926	0.108295	6	0.643869	2.382512	-0.063
1	-3.524535	-4.144389	1.180833	6	2.661096	-0.167381	-0.032
1	-4.667582	-2.795582	0.840310	6	3.367767	-1.507089	-0.152
6	-4.646628	0.250534	0.161206	8	3.296388	0.867672	0.005
6	-4.155599	0.759706	1.369664	1	-4.231497	1.134345	-0.047
6	-3.040569	1.586529	1.376668	1	-4.337378	-1.390285	-0.226
6	-2.407298	1.937260	0.179714	1	-2.220273	-2.700963	-0.013
6	-2.931780	1.463791	-1.024556	1	-2.014550	2.270881	0.222
6	-4.036622	0.617698	-1.043564	1	0.695744	-2.397669	0.318
8	-5.692435	-0.604027	0.248964	1	1.729765	2.520303	-0.890
6	-6.219162	-1.153058	-0.931533	1	0.223807	2.879683	-0.890290
15	-0.919517	2.991401	0.139177	1	0.225345	2.879394	0.891066
16	-1.236380	4.726158	-0.638614	1	3.083900	-2.092583	0.887620
16	0.097989	2.812673	1.889301	1	3.082298	-2.093631	-0.886705
1	-4.652994	0.472869	2.297826	1	4.451489	-1.340867	-0.001188
1	-2.631960	1.945894	2.324287	LR 5 Members Ring Cis			
1	-2.455563	1.738624	-1.968598	6	-1.584941	2.466711	-0.970421

6	-0.329368	1.908147	-1.188544	1	-6.353689	-2.150557	-0.125352
6	0.635886	1.898048	-0.177956	1	-5.285375	-1.504148	1.157474
6	0.336520	2.478113	1.060920	16	3.365254	1.907306	-1.819716
6	-0.912740	3.033092	1.288940	16	3.165926	0.617907	1.306774
6	-1.886979	3.025912	0.278824				
1	-2.318772	2.452286	-1.775599		O,O-J1		
1	-0.111675	1.459991	-2.160847		LR		
1	1.081776	2.477223	1.859035	6	4.399900	-0.931020	0.078
1	-1.164375	3.482164	2.250642	6	3.051574	-0.594451	0.074
8	-3.074165	3.569504	0.595848	6	2.652608	0.746089	0.098
6	-4.091365	3.610994	-0.370623	6	3.625607	1.755391	0.006
1	-4.953854	4.094307	0.103027	6	4.971010	1.427326	0.027
1	-3.791494	4.243	-1.253948	6	5.371218	0.082184	0.079
1	-4.383854	2.598049	-0.698221	1	4.679398	-1.984067	0.068
15	2.208602	1.084556	-0.540951	1	2.307030	-1.395415	0.071
15	1.443065	-1.740140	0.053103	1	3.315697	2.802948	-0.108
16	1.699443	-0.734298	1.965053	1	5.741782	2.198979	-0.020
8	1.691677	-0.437613	-0.932571	8	6.693580	-0.140809	0.086
16	2.555198	-3.246505	-0.339415	6	7.174688	-1.460847	0.183
6	-0.343668	-1.984597	0.002584	1	8.268794	-1.392340	0.326
6	-1.235262	-0.992789	0.425240	1	6.850105	-2.011894	0.899028
6	-0.853466	-3.184263	-0.518772	1	6.850302	-2.011911	-0.898728
6	-2.609905	-1.181346	0.326092	15	0.901258	1.184195	-0.247
1	-0.864437	-0.057243	0.846820	15	-0.901144	-1.183693	-0.071
6	-2.219542	-3.378773	-0.622739	16	-0.184	0.609	-1.552090
1	-0.160971	-3.964672	-0.842463	16	-0.116	0.185	1.553327
6	-3.111572	-2.378315	-0.204005	16	0.492940	3.068803	-0.771
1	-3.274313	-0.388320	0.668080	16	-0.492242	-3.068189	-0.603
1	-2.630621	-4.304596	-1.027432	6	-2.652613	-0.746168	-0.150
8	-4.417388	-2.652672	-0.344296	6	-3.051857	0.594301	0.287
6	-5.369973	-1.711359	0.077218	6	-3.625394	-1.755670	-0.493
1	-5.279211	-0.762524	-0.479039	6	-4.400241	0.930604	0.362

1	-2.307453	1.395396	0.536	1	-2.942230	2.188329	-0.193797
6	-4.970864	-1.427866	-0.432	1	-4.870163	0.603990	-0.011555
1	-3.315267	-2.803163	-0.809	6	1.239675	2.194562	-0.935888
6	-5.371350	-0.082808	0.013	1	1.074718	3.239890	-0.646013
1	-4.679935	1.983600	0.725	1	2.245811	2.082825	-1.369636
1	-5.741489	-2.199662	-0.707	1	0.497232	1.881452	-1.682557
8	-6.693755	0.139912	0.103	O,O-J2			
6	-7.175115	1.459861	0.447	6	5.400901	0.930783	-0.445015
1	-6.850662	2.011249	-0.898237	6	4.170740	0.289473	-0.348337
1	-8.269204	1.391129	0.340	6	4.075699	-0.988954	0.209562
1	-6.850803	2.010720	0.899507	6	5.234665	-1.623743	0.673728
Preindolizine				6	6.464553	-0.991663	0.580373
6	0.178997	-1.007094	-0.061471	6	6.558715	0.290524	0.020328
1	0.344103	-2.083841	-0.158607	1	5.444108	1.926190	-0.886203
6	1.241723	-0.189608	0.035834	1	3.277414	0.800138	-0.719737
6	1.157013	1.312645	0.278992	1	5.158382	-2.622565	1.110036
6	2.649285	-0.701640	-0.049454	1	7.377073	-1.471636	0.936858
6	2.902049	-2.193470	-0.049733	8	7.790575	0.827890	-0.031130
1	2.462099	-2.668778	0.839244	6	7.958765	2.110480	-0.574263
1	2.458138	-2.665040	-0.939439	1	9.028499	2.341043	-0.503791
1	3.985338	-2.360717	-0.058901	1	7.654085	2.149482	-1.634360
8	1.125	1.721883	1.410299	1	7.391231	2.870606	-0.010402
8	3.564577	0.088276	-0.125556	15	2.468145	-1.818563	0.336135
6	-1.233616	-0.593404	-0.052625	15	0.198846	-0.091680	-0.593392
6	-2.248065	-1.556404	0.038139	16	1.143715	-0.428518	1.289048
7	-1.504383	0.713443	-0.139051	16	1.524720	-1.553892	-1.550099
6	-3.574545	-1.136383	0.056104	16	2.515777	-3.597406	1.102665
1	-1.995603	-2.616824	0.099871	16	0.356210	1.561320	-1.622572
6	-2.769395	1.109466	-0.122320	6	-1.372734	-0.995702	-0.701262
6	-3.846604	0.226048	-0.023242	6	-1.578158	-2.178103	0.006753
1	-4.384517	-1.864961	0.130790	6	-2.373994	-0.519672	-1.552920
				6	-2.787953	-2.862988	-0.095396

1	-0.788267	-2.579419	0.647337	6	-2.067645	2.484372	2.660219
6	-3.576057	-1.200609	-1.668690	1	-2.114290	1.681481	3.409497
1	-2.201255	0.398613	-2.119582	1	-1.166127	3.084189	2.836377
6	-3.799794	-2.367753	-0.927297	1	-2.954767	3.130521	2.743035
1	-2.921528	-3.783120	0.473243	O,O-J3			
1	-4.368365	-0.843402	-2.328483	6	3.686977	-0.808271	1.612083
8	-5.019805	-2.931034	-1.059844	6	2.409009	-1.361495	1.520336
6	-5.290400	-4.133112	-0.389993	6	2.058657	-2.176344	0.448052
1	-5.219724	-4.016670	0.706196	6	3.024865	-2.472274	-0.528796
1	-6.317648	-4.415053	-0.650909	6	4.290377	-1.922656	-0.451218
1	-4.606505	-4.939606	-0.704280	6	4.626306	-1.068175	0.611914
6	-3.290482	2.936849	-0.414187	1	3.922193	-0.163005	2.457925
1	-3.641970	3.642149	-1.166710	1	1.672480	-1.135585	2.292493
6	-2.080601	2.929262	0.174555	1	2.772866	-3.136992	-1.358928
6	-1.908720	1.851642	1.266910	1	5.046070	-2.130603	-1.210189
6	-1.022982	3.972004	-0.031407	15	0.366584	-2.791382	0.195903
6	-1.031525	4.722482	-1.342055	15	-1.119988	-0.104547	-0.014699
1	-1.844339	5.467126	-1.325505	6	-2.926758	-0.134712	-0.009791
1	-0.077466	5.250906	-1.454120	6	-3.630255	-1.333253	-0.123385
1	-1.192510	4.046363	-2.192023	6	-3.628156	1.076602	0.086229
8	-0.999533	0.966831	1.179026	6	-5.022121	-1.339044	-0.135859
8	-0.260321	4.246149	0.864464	1	-3.091929	-2.279963	-0.200104
6	-4.123966	1.850867	0.091616	6	-5.012651	1.073809	0.095302
6	-5.419283	1.453489	-0.237203	1	-3.091636	2.025196	0.155132
7	-3.432720	1.160631	1.006175	6	-5.722856	-0.131675	-0.015443
6	-5.932504	0.317074	0.382303	1	-5.542986	-2.290906	-0.233487
1	-5.997481	2.014590	-0.971788	1	-5.574991	2.004438	0.182359
6	-3.879252	0.056667	1.586863	6	1.695256	2.854300	0.520219
6	-5.157745	-0.400158	1.297520	1	2.221844	3.272	1.374704
1	-6.937237	-0.030281	0.134765	6	0.232990	2.580377	0.464362
1	-3.180089	-0.445564	2.261065	6	-0.016529	2.148153	-1.021318
1	-5.532584	-1.310677	1.764063	6	-0.719994	3.629303	1.036283

6	-0.215886	4.410958	2.222636	16	-0.285869	-1.471575	-1.403009
1	0.562656	5.112659	1.886125	16	-0.138446	1.013521	1.463604
1	-1.046468	4.968416	2.670648	O,O-J4			
1	0.242460	3.745281	2.969096	6	-3.875052	0.901114	1.414838
8	-0.987585	1.175268	-1.147922	6	-2.559214	1.356687	1.467151
8	-1.826745	3.805762	0.584303	6	-2.045550	2.170107	0.456732
6	2.290576	2.191036	-0.513963	6	-2.870748	2.528096	-0.622287
6	3.667113	1.939386	-0.843881	6	-4.168966	2.061202	-0.693792
7	1.341453	1.651974	-1.375319	6	-4.680958	1.239206	0.323946
6	3.975934	1.228549	-1.962376	1	-4.247364	0.267385	2.219251
1	4.440463	2.314308	-0.173373	1	-1.922751	1.074879	2.307658
6	1.654608	0.994532	-2.521876	1	-2.479834	3.177751	-1.408825
6	2.953659	0.745703	-2.843072	1	-4.820120	2.319772	-1.529976
1	5.022963	1.015819	-2.188801	15	-0.338323	2.753655	0.510051
1	0.808530	0.665260	-3.126328	15	1.193159	-0.173719	-0.582264
1	3.198061	0.183510	-3.742603	6	2.967187	-0.032914	-0.451392
6	-0.370309	3.301879	-1.952221	6	3.583426	1.208209	-0.616700
1	-0.360164	2.936290	-2.988096	6	3.738021	-1.159924	-0.112460
1	-1.367460	3.684067	-1.713495	6	4.960275	1.339044	-0.458204
1	0.371790	4.106	-1.847346	1	2.983034	2.085391	-0.869028
8	-7.062831	-0.033512	0.001697	6	5.105784	-1.034355	0.037911
8	5.866789	-0.543079	0.577287	1	3.260106	-2.131353	0.037829
6	6.282676	0.289966	1.625232	6	5.729629	0.214865	-0.132387
1	6.264081	-0.233775	2.596301	1	5.416	2.319542	-0.590217
1	7.314666	0.585959	1.401569	1	5.726873	-1.893413	0.295409
1	5.657586	1.197151	1.699372	6	-1.635972	-2.598693	0.935503
6	-7.839700	-1.197869	-0.101445	1	-2.099353	-2.778259	1.901613
1	-7.671972	-1.715771	-1.061284	6	-0.180285	-2.446875	0.687895
1	-7.635636	-1.899558	0.725312	6	-0.065786	-2.449337	-0.852119
1	-8.887878	-0.880552	-0.047371	6	0.811380	-3.294342	1.448109
16	0.225718	-4.674528	-0.203590	6	0.443871	-3.635610	2.870358
16	-0.908680	-1.893714	1.577910	1	-0.362165	-4.385707	2.862979

1	1.320147	-4.045329	3.385918	O,O-J5			
1	0.067095	-2.749961	3.403080	15	0.296444	-0.904243	-0.428162
8	0.968779	-1.616230	-1.315875	6	2.030900	-0.520070	-0.137545
8	1.860676	-3.654226	0.958897	6	3.017294	-1.441893	-0.483827
6	-2.295736	-2.179495	-0.183284	6	2.403187	0.711716	0.429052
6	-3.681313	-1.933923	-0.477328	6	4.365612	-1.156383	-0.275039
7	-1.395233	-1.924896	-1.218215	1	2.725651	-2.401860	-0.916517
6	-4.041046	-1.446573	-1.695405	6	3.738244	0.999194	0.644011
1	-4.418009	-2.125809	0.302564	1	1.642077	1.444383	0.707914
6	-1.759300	-1.469836	-2.446206	6	4.732325	0.068742	0.294007
6	-3.064117	-1.197508	-2.717030	1	5.114101	-1.896849	-0.555611
1	-5.091856	-1.226760	-1.895702	1	4.047584	1.946106	1.088737
1	-0.945499	-1.308335	-3.155049	6	-3.060115	1.387318	-0.672971
1	-3.349154	-0.790451	-3.685452	1	-3.523747	2.058146	-1.390502
6	0.139301	-3.814596	-1.492001	6	-1.627126	1.389576	-0.299267
1	0.064104	-3.715064	-2.583701	6	-1.565539	0.395579	0.903921
1	1.125324	-4.207766	-1.225034	6	-0.930807	2.734875	-0.116813
1	-0.641609	-4.502077	-1.138115	6	-1.346157	3.831190	-1.065139
8	7.060291	0.235018	0.037769	1	-2.325832	4.220322	-0.746455
8	-5.950103	0.819613	0.160264	1	-0.606726	4.639587	-1.031161
6	-6.570664	0.096392	1.189318	1	-1.456389	3.455297	-2.092335
1	-6.581762	0.663485	2.135649	8	-0.385900	-0.333136	0.973482
1	-7.603745	-0.083692	0.868950	8	-0.085370	2.911640	0.729031
1	-6.078134	-0.875628	1.364095	6	-3.619909	0.225401	-0.214364
6	7.753916	1.449141	-0.094005	6	-4.901874	-0.392671	-0.410305
1	7.647319	1.871575	-1.107656	7	-2.723987	-0.468691	0.587688
1	7.411266	2.194462	0.643611	6	-5.161418	-1.601271	0.164088
1	8.811621	1.226733	0.089313	1	-5.638720	0.117596	-1.030777
16	-0.030912	4.521454	-0.179015	6	-2.982541	-1.668508	1.165883
16	0.746578	1.824492	1.861938	6	-4.185434	-2.274728	0.968358
16	0.353051	1.303298	-1.609871	1	-6.132445	-2.074842	0.002160
16	0.294215	-0.592997	1.272581	1	-2.164351	-2.101798	1.743542

1	-4.383785	-3.253846	1.400537	6	5.511952	-0.934153	0.077294
6	-1.793268	1.043678	2.264052	1	5.855023	-1.037460	-2.067619
1	-1.900362	0.251902	3.018046	1	4.867338	-0.778058	2.122275
1	-0.942153	1.681752	2.520454	6	-1.376270	2.514739	-1.029560
1	-2.712623	1.645142	2.238533	1	-1.491252	2.814405	-2.066853
8	6.119	0.438366	0.542909	6	-0.176895	2.812244	-0.166392
6	7.047297	-0.437097	0.217718	6	-0.442264	1.960804	1.054029
1	6.966977	-1.391228	0.766202	6	-0.354109	4.321080	0.236581
1	7.081005	-0.647887	-0.865011	6	-0.012731	5.336112	-0.823064
1	7.977252	0.064347	0.510775	1	1.065980	5.549154	-0.758636
16	-0.089138	-2.737366	-0.889894	1	-0.213514	4.971407	-1.838175
16	-0.557179	0.561452	-1.689995	1	-0.564913	6.261485	-0.617730
O,O-J6				8	0.332211	0.208114	0.215068
6	-3.176366	-1.962081	-1.557479	8	-0.756347	4.631041	1.326641
6	-1.920802	-1.902966	-0.961774	6	-2.294283	1.894226	-0.260107
6	-1.780633	-2.071195	0.418577	6	-3.652815	1.470132	-0.488242
6	-2.917433	-2.327116	1.200210	7	-1.739258	1.642644	1.031218
6	-4.166700	-2.413449	0.609251	6	-4.361924	0.914794	0.518576
6	-4.308417	-2.215875	-0.772554	1	-4.075750	1.618648	-1.481675
1	-3.252825	-1.800778	-2.632347	6	-2.483723	1.056730	2.053539
1	-1.043841	-1.702466	-1.582831	6	-3.764473	0.718156	1.824988
1	-2.812328	-2.459727	2.279165	1	-5.389562	0.587836	0.352849
1	-5.060727	-2.623789	1.198668	1	-1.961479	0.881932	2.991757
15	-0.144828	-2.089557	1.171256	1	-4.342191	0.261164	2.627459
15	1.254703	0.432191	-1.029978	6	0.370674	1.988944	2.285861
6	2.925583	-0.109628	-0.607024	1	0.307685	1.026660	2.811278
6	3.856924	-0.404005	-1.647	1	1.415518	2.188210	2.019181
6	3.293506	-0.243282	0.741448	1	-0.017	2.804666	2.926504
6	5.149287	-0.810617	-1.268932	8	6.727914	-1.324176	0.502505
1	3.562374	-0.328568	-2.649612	8	-5.565208	-2.270731	-1.251005
6	4.570509	-0.650217	1.080398	6	-5.779465	-2.125593	-2.630897
1	2.557251	-0.059077	1.526776	1	-5.252420	-2.903604	-3.208532

1	-6.858657	-2.231166	-2.793125	1	4.942252	-0.751373	2.202665
1	-5.457570	-1.133795	-2.992948	6	-1.259323	2.317572	-1.164140
6	7.710217	-1.655491	-0.441341	1	-1.249632	2.391875	-2.247601
1	7.396408	-2.500346	-1.078466	6	-0.177029	2.813205	-0.252263
1	7.964569	-0.796779	-1.086835	6	-0.635421	2.368511	1.099140
1	8.602663	-1.949790	0.124095	6	-0.272731	4.389621	-0.296240
16	1.181886	-3.059719	0.192042	6	0.280509	5.058179	-1.524446
16	-0.119421	-1.612237	3.046705	1	1.355874	5.235971	-1.367935
16	0.652561	-0.068708	-2.812270	1	0.183132	4.439202	-2.425103
16	1.490240	2.601542	-0.849478	1	-0.219588	6.026323	-1.650874
O,O-J7				8	0.299291	-0.094611	0.198509
6	-3.295755	-2.115964	-1.439484	8	-0.775008	4.986953	0.615387
6	-2.028189	-1.834386	-0.932063	6	-2.244800	1.803612	-0.400201
6	-1.792156	-1.803927	0.444251	6	-3.543915	1.257379	-0.693518
6	-2.849895	-2.092699	1.313774	7	-1.835276	1.850189	0.975670
6	-4.114710	-2.383476	0.820724	6	-4.339739	0.839880	0.313830
6	-4.349950	-2.387395	-0.560299	1	-3.845543	1.193736	-1.738406
1	-3.441757	-2.124485	-2.519822	6	-2.659791	1.365906	2.002303
1	-1.210302	-1.639719	-1.630538	6	-3.878623	0.895957	1.686871
1	-2.667777	-2.079867	2.391304	1	-5.322460	0.416415	0.105150
1	-4.944977	-2.616249	1.490348	1	-2.228768	1.359277	3.210
15	-0.095241	-1.583604	1.089829	1	-4.513113	0.512890	2.485581
15	1.312252	0.221423	-0.998943	6	0.079524	2.528547	2.367760
6	2.967424	-0.301254	-0.542754	1	0.246753	1.510799	2.782805
6	3.880250	-0.678390	-1.524859	1	1.043953	3.020078	2.202632
6	3.350742	-0.323648	0.810403	1	-0.523205	3.108006	3.083356
6	5.173489	-1.066550	-1.179885	8	6.771766	-1.441957	0.604767
1	3.573198	-0.683145	-2.573256	8	-5.619225	-2.643369	-0.947984
6	4.630239	-0.706512	1.158575	6	-5.906248	-2.732495	-2.316682
1	2.631646	-0.074719	1.594997	1	-5.316508	-3.524891	-2.808632
6	5.554202	-1.081295	0.167133	1	-6.971848	-2.978454	-2.400826
1	5.865125	-1.363723	-1.967386	1	-5.721212	-1.777088	-2.839295

6	7.734124	-1.877395	-0.318789	1	-0.440010	3.094507	-2.216579
1	7.395625	-2.773346	-0.866639	6	0.469246	3.259018	-0.149304
1	7.990321	-1.087483	-1.045685	6	-0.103754	2.840646	1.149754
1	8.630707	-2.131619	0.259067	6	1.422439	4.431227	-0.328039
16	1.072057	-3.004872	0.457188	6	2.006093	4.559460	-1.707096
16	-0.132958	-0.972616	2.975586	1	2.221733	3.570821	-2.139438
16	0.735513	-0.127839	-2.814070	1	1.268090	5.054822	-2.358154
16	1.555507	2.349012	-0.600540	1	2.909589	5.179140	-1.666059
O,O-J8				8	-0.108643	-0.500258	-0.416965
6	-4.385	-1.906621	-1.371683	8	1.667285	5.176471	0.585108
6	-2.666784	-1.793436	-0.982256	6	-1.593287	2.364868	-0.505596
6	-2.315950	-1.697509	0.364884	6	-2.847568	1.856484	-0.968650
6	-3.327311	-1.740633	1.330372	7	-1.330556	2.315535	0.875014
6	-4.658902	-1.861941	0.957433	6	-3.762943	1.422992	-0.065172
6	-5.006773	-1.941467	-0.398065	1	-3.030085	1.830705	-2.042246
1	-4.237934	-1.974185	-2.433467	6	-2.259977	1.835373	1.785827
1	-1.886410	-1.771567	-1.745613	6	-3.470184	1.433254	1.341329
1	-3.058226	-1.663421	2.386796	1	-4.723355	1.028692	-0.400551
1	-5.456038	-1.901933	1.701922	1	-1.951340	1.803440	2.826763
15	-0.564178	-1.663255	0.865755	1	-4.202505	1.064090	2.056891
15	1.223308	0.103468	-0.996706	6	0.273691	3.237910	2.535178
6	2.702779	-0.792998	-0.508023	1	0.275195	2.352648	3.187952
6	3.658401	-1.098373	-1.480700	1	1.260250	3.710422	2.543739
6	2.939663	-1.159211	0.832054	1	-0.461353	3.969135	2.907618
6	4.832434	-1.762685	-1.141741	8	6.166110	-2.754677	0.622386
1	3.477782	-0.816162	-2.519901	8	-6.325566	-2.040325	-0.670617
6	4.119	-1.807945	1.174393	6	-6.737655	-2.189871	-2.001537
1	2.200439	-0.951910	1.611721	1	-6.305595	-3.093467	-2.465013
6	5.065591	-2.119553	0.193612	1	-7.829915	-2.287998	-1.983565
1	5.553600	-1.995548	-1.924380	1	-6.469237	-1.312703	-2.616964
1	4.303140	-2.106674	2.205115	6	7.157188	-3.121781	-0.301695
6	-0.531882	2.940971	-1.147905	1	6.765526	-3.816457	-1.063985

1	7.591216	-2.240848	-0.804741	6	5.553033	-0.550364	-0.568093
1	7.944298	-3.628297	0.269252	6	5.088057	0.298728	-1.584525
16	0.321473	-3.347172	0.470470	6	3.753471	0.663122	-1.630494
16	-0.311985	-0.705640	2.582858	6	2.861862	0.196237	-0.654629
16	1.135834	0.652916	-2.848655	6	3.324599	-0.647493	0.359522
16	1.629023	1.769400	0.415235	6	4.661839	-1.024147	0.404717
O,O-J9				8	6.860178	-0.859378	-0.607131
6	-2.392954	1.820656	0.326324	6	7.386949	-1.736233	0.354029
1	-3.260225	1.655559	-0.308905	15	1.140048	0.703	-0.687099
6	-1.418252	2.735552	0.170225	8	0.263456	-0.325963	0.163949
6	-0.404106	2.619814	1.288131	16	0.441761	1.326493	-2.388106
6	-1.349321	3.807317	-0.875439	1	5.797945	0.646458	-2.336121
6	-2.282606	3.673047	-2.049228	1	3.387395	1.305239	-2.434782
1	-2.168599	2.682869	-2.512281	1	2.634939	-1.050144	1.106761
1	-3.325439	3.789583	-1.713398	1	4.989726	-1.704441	1.189923
1	-2.050679	4.456756	-2.779286	1	8.452740	-1.850950	0.123388
16	1.321725	2.305382	0.777323	1	7.284223	-1.330242	1.375117
8	-0.606080	4.747772	-0.725917	1	6.902370	-2.726245	0.310311
6	-2.098433	1.007623	1.491293	6	-4.531121	-1.924435	-0.856265
6	-2.749727	-0.086987	2.044101	6	-4.020793	-2.817065	0.097849
7	-0.944975	1.451039	2.037714	6	-2.657502	-2.855935	0.360262
6	-2.152740	-0.728137	3.120194	6	-1.770740	-2.011276	-0.318310
1	-3.666570	-0.458530	1.586577	6	-2.279944	-1.146809	-1.287760
6	-0.346022	0.845688	3.074389	6	-3.649492	-1.084913	-1.550913
6	-0.941463	-0.258987	3.641755	8	-5.867617	-1.946023	-1.041800
1	-2.610558	-1.624612	3.539619	6	-6.431490	-1.133050	-2.033787
1	0.623666	1.240933	3.377360	15	0.033022	-2.096648	-0.003575
1	-0.441878	-0.778172	4.457513	16	0.999930	-2.676102	-1.588892
6	-0.399732	3.854772	2.197893	16	0.383226	-2.788406	1.810709
1	0.301469	3.716694	3.033377	1	-4.718218	-3.478997	0.614443
1	-0.092668	4.723131	1.603593	1	-2.261060	-3.541962	1.113302
1	-1.410150	4.026328	2.597755	1	-1.599803	-0.503765	-1.854024

1	-4.009714	-0.398481	-2.318263	6	2.160493	-1.929537	0.298949
1	-7.509143	-1.336499	-2.033795	6	1.197893	-1.235803	-0.448155
1	-6.273421	-0.059572	-1.825785	6	1.477231	-0.883868	-1.772476
1	-6.023563	-1.362964	-3.033083	6	2.697484	-1.217033	-2.350431
O,O-J10				8	4.872251	-2.249203	-2.056969
6	-4.056313	-0.193041	1.254421	6	5.234568	-1.902131	-3.367550
1	-4.379468	-0.040788	2.281861	15	-0.370965	-0.765958	0.300932
6	-3.778369	-1.361608	0.650456	8	-0.688732	0.764980	0.002840
6	-3.334503	-1.125007	-0.776717	16	-0.633627	-1.344924	2.136244
6	-3.903317	-2.734320	1.234910	1	4.148698	-2.778425	0.302997
6	-4.046040	-2.831785	2.729489	1	1.944047	-2.193789	1.336300
1	-3.166138	-2.375676	3.207663	1	0.762499	-0.292575	-2.349649
1	-4.943359	-2.293980	3.072122	1	2.893966	-0.913255	-3.378116
1	-4.124233	-3.887821	3.011908	1	6.251037	-2.282972	-3.522160
16	-1.652072	-1.747652	-1.156640	1	4.562903	-2.362555	-4.112243
8	-3.895555	-3.702130	0.510611	1	5.235296	-0.808423	-3.514021
6	-3.807803	0.895526	0.326654	6	4.134752	0.770308	1.667084
6	-3.883533	2.266612	0.471106	6	4.099931	1.125558	0.311090
7	-3.386452	0.359525	-0.849206	6	2.934514	1.620799	-0.249428
6	-3.482812	3.067950	-0.597401	6	1.782012	1.780447	0.529839
1	-4.186422	2.697573	1.424018	6	1.834903	1.469115	1.889008
6	-2.993588	1.108871	-1.887344	6	2.997770	0.957821	2.461511
6	-3.054822	2.484795	-1.792961	8	5.297204	0.252751	2.114740
1	-3.488027	4.152620	-0.494877	6	5.387781	-0.163239	3.449204
1	-2.584347	0.583846	-2.750747	15	0.199005	2.297512	-0.207627
1	-2.684373	3.090837	-2.617118	16	-0.736078	3.582620	0.944442
6	-4.290675	-1.735541	-1.805890	16	0.317515	2.545948	-2.161557
1	-3.969965	-1.488250	-2.827895	1	5.001232	0.977275	-0.285866
1	-4.297390	-2.824167	-1.676667	1	2.892686	1.868999	-1.312459
1	-5.306230	-1.346446	-1.640516	1	0.947116	1.612976	2.509134
6	3.658777	-1.902538	-1.596187	1	2.997662	0.705221	3.521614
6	3.379003	-2.257381	-0.267661	1	6.396268	-0.573132	3.584022

1	5.247232	0.675448	4.153123	6	-1.018487	-0.911378	0.519916
1	4.648719	-0.949399	3.683703	6	-2.055589	-1.837614	0.533878
O,O-J11				8	-3.441314	-3.359825	-0.745054
6	3.187361	-2.326578	-0.433764	6	-4.171433	-3.683568	0.415057
1	2.986086	-3.165668	-1.095030	15	0.897499	0.708813	-0.731654
6	2.526890	-1.984242	0.710306	8	0.044938	2.059556	-0.910328
6	3.065438	-0.726739	1.248175	16	2.195864	0.541942	-2.163134
6	1.429315	-2.766838	1.361374	1	-2.003657	-2.750975	-2.742589
6	0.828443	-3.894828	0.563228	1	-0.121605	-1.104694	-2.754747
1	0.381991	-3.499988	-0.362695	1	-0.758510	-0.397673	1.446849
1	1.597580	-4.630643	0.283804	1	-2.583324	-2.018080	1.468911
1	0.053722	-4.384212	1.164129	1	-4.932400	-4.410926	0.108295
16	1.673772	0.843133	1.289650	1	-3.524535	-4.144389	1.180833
8	1.057312	-2.497767	2.480571	1	-4.667582	-2.795582	0.840310
6	4.202754	-1.346788	-0.670274	6	-4.646628	0.250534	0.161206
6	5.156853	-1.195906	-1.684162	6	-4.155599	0.759706	1.369664
7	4.130508	-0.420329	0.327902	6	-3.040569	1.586529	1.376668
6	5.982164	-0.091360	-1.660167	6	-2.407298	1.937260	0.179714
1	5.209633	-1.938827	-2.479412	6	-2.931780	1.463791	-1.024556
6	4.909627	0.685505	0.347383	6	-4.036622	0.617698	-1.043564
6	5.849362	0.867613	-0.635570	8	-5.692435	-0.604027	0.248964
1	6.726879	0.053474	-2.444405	6	-6.219162	-1.153058	-0.931533
1	4.723163	1.399770	1.148771	15	-0.919517	2.991401	0.139177
1	6.471118	1.762183	-0.618210	16	-1.236380	4.726158	-0.638614
6	3.486388	-0.681929	2.708347	16	0.097989	2.812673	1.889301
1	3.793483	0.331853	3.004211	1	-4.652994	0.472869	2.297826
1	2.633620	-0.984655	3.326196	1	-2.631960	1.945894	2.324287
1	4.320834	-1.378807	2.885633	1	-2.455563	1.738624	-1.968598
6	-2.423419	-2.485013	-0.649800	1	-4.398429	0.239791	-1.999356
6	-1.710369	-2.226549	-1.831761	1	-7.052374	-1.800100	-0.630413
6	-0.670350	-1.310650	-1.832668	1	-6.603199	-0.371866	-1.609354
6	-0.316510	-0.634623	-0.654657	1	-5.467854	-1.760132	-1.466538

O,O-J12				6	-1.886979	3.025912	0.278824
Indolizine				1	-2.318772	2.452286	-1.775599
6	-3.314580	0.544323	-0.058	1	-0.111675	1.459991	-2.160847
6	-3.369348	-0.887307	-0.111	1	1.081776	2.477223	1.859035
6	-2.211924	-1.609901	-0.039	1	-1.164375	3.482164	2.250642
6	-0.953112	-0.945392	0.077	8	-3.074165	3.569504	0.595848
7	-0.944977	0.460093	0.035	6	-4.091365	3.610994	-0.370623
6	-2.118347	1.186485	0.064	1	-4.953854	4.094307	0.103027
6	0.365875	-1.361996	0.179	1	-3.791494	4.243	-1.253948
6	1.178830	-0.196662	0.142	1	-4.383854	2.598049	-0.698221
6	0.342390	0.923968	-0.033	15	2.208602	1.084556	-0.540951
6	0.643869	2.382512	-0.063	15	1.443065	-1.740140	0.053103
6	2.661096	-0.167381	-0.032	16	1.699443	-0.734298	1.965053
6	3.367767	-1.507089	-0.152	8	1.691677	-0.437613	-0.932571
8	3.296388	0.867672	0.005	16	2.555198	-3.246505	-0.339415
1	-4.231497	1.134345	-0.047	6	-0.343668	-1.984597	0.002584
1	-4.337378	-1.390285	-0.226	6	-1.235262	-0.992789	0.425240
1	-2.220273	-2.700963	-0.013	6	-0.853466	-3.184263	-0.518772
1	-2.014550	2.270881	0.222	6	-2.609905	-1.181346	0.326092
1	0.695744	-2.397669	0.318	1	-0.864437	-0.057243	0.846820
1	1.729765	2.520303	-0.890	6	-2.219542	-3.378773	-0.622739
1	0.223807	2.879683	-0.890290	1	-0.160971	-3.964672	-0.842463
1	0.225345	2.879394	0.891066	6	-3.111572	-2.378315	-0.204005
1	3.083900	-2.092583	0.887620	1	-3.274313	-0.388320	0.668080
1	3.082298	-2.093631	-0.886705	1	-2.630621	-4.304596	-1.027432
1	4.451489	-1.340867	-0.001188	8	-4.417388	-2.652672	-0.344296
LR 5 Members Ring Cis				6	-5.369973	-1.711359	0.077218
6	-1.584941	2.466711	-0.970421	1	-5.279211	-0.762524	-0.479039
6	-0.329368	1.908147	-1.188544	1	-6.353689	-2.150557	-0.125352
6	0.635886	1.898048	-0.177956	1	-5.285375	-1.504148	1.157474
6	0.336520	2.478113	1.060920	16	3.365254	1.907306	-1.819716
6	-0.912740	3.033092	1.288940	16	3.165926	0.617907	1.306774

Figure 28

O,O-WC1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172
1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061
1	-4.199996	1.376948	0.207
6	-5.069288	-1.919326	-0.038
1	-3.674079	-3.572737	-0.154
1	-6.213733	-0.087007	0.087
34	0.079	-0.183	1.668777
34	-0.077	0.194	-1.668768
34	1.718838	-2.850294	-0.372
34	-1.718852	2.850296	0.392
1	5.952123	2.562719	0.021
1	-5.952103	-2.562746	-0.087

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-WC2

6	-2.249958	-2.496176	1.050638
1	-1.878248	-3.497771	1.289137
6	-2.341971	-2.144448	-0.245719
6	-2.722954	-0.740491	-0.657819
6	-2.135928	-3.200818	-1.298660

6	-1.084157	-4.259564	-1.046715	15	-0.437197	0.835641	-0.842079
1	-0.159225	-3.814391	-0.652688	34	1.735485	1.352791	-1.571643
1	-1.445299	-4.997546	-0.313894	15	2.466889	0.453479	0.377113
1	-0.888103	-4.781103	-1.991208	34	3.690649	1.599995	1.613454
8	-2.241860	0.232941	0.029778	34	0.324491	0.078349	1.125059
8	-2.789592	-3.198052	-2.316548	1	1.461522	-1.701081	-1.368948
6	-2.649680	-1.685791	2.221072	6	2.381458	-2.052596	-0.892616
6	-1.880730	-1.728728	3.391026	6	3.095280	-1.221989	-0.017879
7	-3.762318	-0.951719	2.123528	6	4.275875	-1.677211	0.572094
6	-2.257373	-0.936354	4.470689	1	4.829063	-1.019920	1.247471
1	-0.991894	-2.361352	3.440356	1	5.663249	-3.316309	0.756069
6	-4.120032	-0.204729	3.160171	6	4.739408	-2.963576	0.293243
6	-3.399094	-0.149589	4.354207	6	4.028200	-3.791232	-0.571557
1	-1.667924	-0.934305	5.390024	1	4.394225	-4.796998	-0.789198
1	-5.036080	0.383221	3.041109	6	2.849888	-3.333018	-1.165409
1	-3.735282	0.489229	5.172451	1	2.293253	-3.974706	-
6	-4.066349	-0.562733	-1.300449	1.851646O,O-WC3			
1	-4.163218	0.450163	-1.709775	6	-2.624171	-2.195308	1.254230
1	-4.251911	-1.327374	-2.063068	1	-2.466623	-3.158384	1.749128
1	-4.789868	-0.684889	-0.476252	6	-2.478419	-2.141552	-0.082968
34	-1.074134	-0.469441	-2.470663	6	-2.546726	-0.859274	-0.894159
1	-2.513957	2.189419	-2.353411	6	-2.314565	-3.407097	-0.870732
6	-2.126312	2.904943	-1.624897	6	-2.100189	-4.723392	-0.159959
6	-2.632339	4.201630	-1.567889	1	-1.219167	-4.675086	0.497215
1	-3.423008	4.502784	-2.257960	1	-2.970926	-4.988518	0.457379
6	-2.132216	5.108191	-0.634531	1	-1.949728	-5.500111	-0.918582
1	-2.534794	6.122344	-0.588843	8	-2.116970	0.261929	-0.164303
6	-1.115503	4.721729	0.238663	8	-2.365203	-3.366567	-2.084036
1	-0.717461	5.430971	0.967001	6	-2.993475	-1.089598	2.167144
6	-0.596613	3.431039	0.182921	6	-2.297931	-0.922624	3.370704
6	-1.111228	2.523401	-0.745943	7	-4.016366	-0.305045	1.816584
1	0.210677	3.136816	0.858335	6	-2.641922	0.139523	4.200986

1	-1.487501	-1.604540	3.636067	1	5.716470	-3.296282	1.213188
6	-4.347985	0.697371	2.620399	6	4.768811	-3.026686	0.742583
6	-3.685759	0.975071	3.816977	6	4.018667	-3.990257	0.073415
1	-2.102927	0.310181	5.135111	1	4.378466	-5.020027	0.015466
1	-5.189096	1.320373	2.298610	6	2.808827	-3.638828	-0.529838
1	-3.991921	1.821457	4.433889	1	2.220583	-4.389437	-1.062086
6	-3.917212	-0.636565	-1.506333	O,O-WC4			
1	-3.916595	0.250390	-2.154553	6	-1.548875	-2.779960	0.218955
1	-4.214533	-1.508762	-2.103543	1	-1.068766	-3.704865	-0.125256
1	-4.628078	-0.490169	-0.680399	6	-2.129048	-2.037628	-0.741093
34	-1.050825	-0.854561	-2.248344	6	-2.838119	-0.718291	-0.654870
1	-2.826790	2.110182	-1.863991	6	-2.255013	-2.689588	-2.115471
6	-2.137225	2.867624	-1.491155	6	-0.985460	-2.958067	-2.879681
6	-2.453404	4.219150	-1.615039	1	-0.499195	-1.993175	-3.089491
1	-3.384659	4.513233	-2.103258	1	-0.277771	-3.552136	-2.282800
6	-1.588549	5.187346	-1.109246	1	-1.218802	-3.477184	-3.817101
1	-1.838812	6.246340	-1.202837	8	-1.858127	0.100681	0.807598
6	-0.401945	4.804334	-0.483278	8	-3.350616	-2.978578	-2.525617
1	0.276817	5.558054	-0.079731	6	-1.433680	-2.578149	1.681894
6	-0.067382	3.457694	-0.379679	6	-0.232829	-2.920459	2.318342
6	-0.936957	2.486699	-0.886353	7	-2.489190	-2.127449	2.366567
1	0.874	3.169150	0.094416	6	-0.113018	-2.723957	3.689786
15	-0.546062	0.707860	-0.743675	1	0.604918	-3.314204	1.740485
34	1.737027	0.954643	-1.715934	6	-2.372030	-1.948090	3.675798
15	2.508973	0.373855	0.302877	6	-1.202888	-2.216044	4.388912
34	3.785048	1.687059	1.309866	1	0.821185	-2.962252	4.202515
34	0.409256	0.160685	1.223808	1	-3.260626	-1.572779	4.194520
1	1.406456	-2.056651	-0.943026	1	-1.158821	-2.042388	5.465317
6	2.351203	-2.327389	-0.464385	6	-4.179004	-0.761852	0.003513
6	3.106084	-1.358284	0.209463	1	-4.635154	0.234598	0.053964
6	4.315020	-1.709059	0.812533	1	-4.801189	-1.410356	-0.636896
1	4.896887	-0.944181	1.332758	1	-4.088963	-1.229170	0.993634

34	-2.594894	0.478844	-2.066956	6	-2.297163	-1.936427	0.158
1	-3.158431	2.265534	0.931164	6	-2.564136	-0.559891	-0.010
6	-2.410656	3.054555	0.838457	6	-3.882724	-0.098023	-0.139
6	-2.771200	4.397772	0.930332	6	-4.935650	-1.012306	-0.100
1	-3.815484	4.666583	1.100164	6	-4.672986	-2.379727	0.071
6	-1.802288	5.390353	0.800627	1	-3.145092	-3.910749	0.336
1	-2.087976	6.442127	0.872087	1	-1.271438	-2.315908	0.258
6	-0.466052	5.048731	0.578648	1	-4.077533	0.976933	-0.273
1	0.291149	5.827986	0.474538	1	-5.965124	-0.648648	-0.203
6	-0.094340	3.712181	0.487702	15	-1.199802	0.654798	-0.073
6	-1.071969	2.718376	0.618531	15	1.351406	-1.081416	0.121
1	0.952697	3.448128	0.309954	6	3.047170	-0.458360	0.102
15	-0.647816	0.974067	0.479910	6	3.340566	0.910495	-0.016
34	0.321032	0.588020	-1.533914	6	4.072707	-1.408916	0.207
15	2.310199	0.528701	-0.254716	6	4.668157	1.324397	-0.031
34	3.761337	2.010342	-0.473616	1	2.531895	1.646252	-0.097
34	1.127704	0.529986	1.755748	6	5.400347	-0.983441	0.192
1	0.950198	-2.059502	-0.385321	1	3.820269	-2.471415	0.300
6	2.024240	-2.254173	-0.433467	6	5.696001	0.378306	0.073
6	2.932507	-1.188340	-0.386772	1	4.903010	2.390515	-0.126
6	4.304672	-1.438806	-0.458481	1	6.205311	-1.720856	0.271
1	5.006975	-0.601874	-0.432523	34	0.229558	-0.008556	1.668190
1	5.839221	-2.941721	-0.627930	34	0.229634	-0.008824	-1.668166
6	4.765882	-2.750564	-0.570058	34	-1.746619	2.657493	-0.246
6	3.862436	-3.812	-0.614016	8	1.268867	-2.568118	0.243
1	4.226804	-4.835387	-0.706453	1	-5.498268	-3.095024	0.103
6	2.490303	-3.559709	-0.546304	1	6.737008	0.708957	0.059
1	1.778978	-4.388452	-0.584893	Selenone			
O,O-WC5				6	-0.333324	1.424558	-0.066121
WR Subs				1	-0.345046	2.474424	-0.368625
6	-3.354373	-2.839392	0.199	6	0.856921	0.843079	0.179511
				6	1.056228	-0.594387	0.526165

6	2.130367	1.654854	0.149592
6	2.106200	3.042644	-0.454031
1	1.689058	3.028820	-1.471245
1	1.492253	3.722032	0.156358
1	3.134291	3.422171	-0.479560
8	3.147381	1.194873	0.614710
6	-1.657576	0.789505	0.010450
6	-2.765949	1.420956	-0.573416
7	-1.766728	-0.381801	0.646685
6	-4.007829	0.798383	-0.507961
1	-2.647307	2.382914	-1.075995
6	-2.953370	-0.970851	0.707346
6	-4.109016	-0.427877	0.142932
1	-4.885664	1.264749	-0.960087
1	-2.993795	-1.929383	1.235493
1	-5.061858	-0.953802	0.220351
6	1.143527	-0.917404	1.980875
1	1.261761	-1.994777	2.147695
1	2.012494	-0.383174	2.416
1	0.237273	-0.553248	2.488249
34	1.308750	-1.757290	-0.773799

Figure 29

O,O-WA1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172

1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061
1	-4.199996	1.376948	0.207
6	-5.069288	-1.919326	-0.038
1	-3.674079	-3.572737	-0.154
1	-6.213733	-0.087007	0.087
34	0.079	-0.183	1.668777
34	-0.077	0.194	-1.668768
34	1.718838	-2.850294	-0.372
34	-1.718852	2.850296	0.392
1	5.952123	2.562719	0.021
1	-5.952103	-2.562746	-0.087

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556

6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-WA2

6	-4.298518	-1.963420	-0.528116
6	-3.071957	-1.342369	-0.742646
6	-2.849875	-0.055080	-0.237604
6	-3.852878	0.602052	0.486252
6	-5.075471	-0.028108	0.696660
6	-5.299179	-1.308838	0.189851
1	-4.471791	-2.965818	-0.924006
1	-2.281363	-1.850636	-1.298863
1	-3.671442	1.605768	0.877116
1	-5.859036	0.485695	1.257006
15	-1.249960	0.753638	-0.511858
15	1.447068	-1.018601	0.481954
6	2.450864	0.477482	0.344280
6	2.171597	1.588598	1.149129
6	3.511477	0.516787	-0.572830
6	2.952875	2.736757	1.030735

1	1.353496	1.549383	1.870424
6	4.282064	1.666040	-0.683251
1	3.723975	-0.354289	-1.196789
6	4.001653	2.777575	0.116699
1	2.733472	3.603363	1.656848
1	5.103962	1.698888	-1.400837
34	-0.237548	-0.828342	1.742395
34	-0.026076	-0.175282	-1.963588
34	-1.127504	2.747712	0.001490
34	2.347861	-2.793628	-0.023433
1	-6.260687	-1.799511	0.355688
1	4.607957	3.681126	0.023607

O,O-WA3

15	-0.591699	-0.001	0.018
6	1.224915	-0.033	0.037
6	1.925949	-1.213933	0.362
6	1.925953	1.213872	-0.263
6	3.317418	-1.209159	0.309
1	1.375344	-2.157190	0.621
6	3.317417	1.209103	-0.330
1	1.375330	2.157122	-0.465
6	4.013078	-0.031	-0.054
1	3.860472	-2.156115	0.558
1	3.860482	2.156052	-0.594
34	-1.486067	-1.854380	-0.121
34	-1.485986	1.854417	0.102
1	5.105294	-0.023	-0.108

O,O-WA4

6	-2.630869	0.252267	0.100611
1	-3.418819	0.085793	0.840787
6	-2.058780	-0.825472	-0.475028
6	-0.878415	-0.694164	-1.347667

6	-2.647320	-2.202578	-0.252135	34	0.586618	-2.508163	0.122213
6	-3.040250	-2.543457	1.163158	34	0.194662	0.506553	2.236234
1	-2.257327	-2.223402	1.865632	1	6.004341	1.480389	-1.251542
1	-3.977949	-2.029759	1.428008	O,O-WA5			
1	-3.206211	-3.624879	1.232802	6	2.786055	0.661909	0.309
8	0.074074	0.124472	-1.218	1	3.739640	0.748395	-0.529514
8	-2.795520	-2.965397	-1.175616	6	2.342505	-0.567258	0.314156
6	-2.375039	1.659272	-0.261218	6	0.994493	-0.833536	0.954986
6	-2.520874	2.670768	0.694396	6	3.220789	-1.767958	0.118631
7	-2.030419	1.911981	-1.528710	6	4.514073	-1.635184	-0.651911
6	-2.260449	3.984159	0.320386	1	4.338263	-1.209522	-1.650506
1	-2.803194	2.420514	1.718250	1	5.220039	-0.979173	-0.121480
6	-1.786727	3.168906	-1.879505	1	4.958124	-2.632432	-0.749928
6	-1.882525	4.243136	-0.994158	8	0.066160	0.217014	0.674932
1	-2.347422	4.793803	1.047678	8	2.894096	-2.833956	0.598277
1	-1.504701	3.336973	-2.923945	6	2.128948	1.952798	0.324662
1	-1.671111	5.257981	-1.334751	6	1.808997	2.855659	-0.693731
6	-0.901449	-1.171054	-2.743629	7	1.891877	2.203244	1.614768
1	0.114355	-1.256760	-3.144848	6	1.171950	4.043394	-0.352242
1	-1.468637	-2.107653	-2.812770	1	2.020735	2.607364	-1.734973
1	-1.455497	-0.391298	-3.297081	6	1.297914	3.348852	1.932493
15	0.909079	-0.392595	0.495542	6	0.907443	4.299451	0.990292
6	2.548420	0.199001	-0.035038	1	0.881651	4.757591	-1.125438
6	3.222324	-0.472066	-1.062501	1	1.117487	3.522535	2.998636
6	3.123842	1.326568	0.557796	1	0.410167	5.217960	1.306256
6	4.460377	-0.008940	-1.498304	6	1.085407	-1.052480	2.449317
1	2.777189	-1.365452	-1.506887	1	0.100188	-1.291547	2.871517
6	4.364313	1.784518	0.118224	1	1.776784	-1.875929	2.667553
1	2.595372	1.836531	1.366784	1	1.464979	-0.120084	2.894234
6	5.031334	1.120020	-0.909823	15	-0.919575	-0.332802	-0.536513
1	4.984584	-0.535227	-2.298747	6	-2.580775	-0.202341	0.183365
1	4.812352	2.664341	0.584551	6	-2.755304	-0.396338	1.559228

6	-3.684114	0.082260	-0.626204	1	-2.503794	5.052877	-0.748534
6	-4.025601	-0.303756	2.118265	6	-1.335003	-0.637976	-2.694006
1	-1.893532	-0.612194	2.191976	1	-0.454169	-0.478707	-3.324712
6	-4.955528	0.167920	-0.061831	1	-1.929878	-1.487877	-3.085883
1	-3.536834	0.246700	-1.696131	1	-2.007798	0.234744	-2.648609
6	-5.127006	-0.023718	1.307816	15	0.872426	0.202326	0.323963
1	-4.157749	-0.450358	3.192034	6	2.616827	0.514663	-0.042048
1	-5.815126	0.391190	-0.696984	6	2.919277	1.132419	-1.261638
34	0.057581	-2.314713	-0.053135	6	3.640931	0.156160	0.840652
34	-0.716827	0.501718	-2.423729	6	4.246646	1.394385	-1.591425
1	-6.123498	0.048169	1.749174	1	2.106549	1.407954	-1.936575
O,O-WA6				6	4.966225	0.411380	0.499115
6	-2.729497	-0.139572	0.265726	1	3.391787	-0.312645	1.795643
1	-3.365805	-0.412875	1.113858	6	5.268618	1.031043	-0.714337
6	-2.030411	-1.145947	-0.295102	1	4.484584	1.882877	-2.538643
6	-0.988185	-1.048493	-1.330183	1	5.766954	0.130795	1.186374
6	-2.311741	-2.581209	0.131041	34	0.633766	-1.926406	-0.954794
6	-2.390078	-2.884914	1.601820	34	0.433989	0.019583	2.353734
1	-1.473999	-2.521842	2.093979	1	6.309626	1.233438	-0.976191
1	-3.239045	-2.366435	2.072017	O,O-WA7			
1	-2.508216	-3.966068	1.739523	WR Sub HexaCycle			
8	-0.037356	0.936050	-0.653330	15	0.442837	1.493299	-0.811896
8	-2.455188	-3.415983	-0.728924	15	0.444308	-1.491102	-0.815858
6	-2.689093	1.309795	-0.014152	15	-1.193904	-0.002061	1.282005
6	-2.543609	2.185704	1.068450	8	1.144299	0.001385	-0.811865
7	-2.808760	1.735999	-1.273968	8	-0.632608	1.271766	0.415812
6	-2.460868	3.549	0.815215	8	-0.633740	-1.272322	0.410294
1	-2.448993	1.790334	2.081069	6	1.745096	2.469616	-0.046261
6	-2.744282	3.042534	-1.504612	6	2.428839	3.430960	-0.795838
6	-2.561154	3.991808	-0.500540	6	2.092017	2.234102	1.290264
1	-2.318330	4.257096	1.634068	6	3.469036	4.149306	-0.209873
1	-2.845463	3.356215	-2.548824	1	2.142614	3.613661	-1.834246

6	4.093206	-0.289717	-0.218	1	2.462099	-2.668778	0.839244
6	5.218069	0.534573	-0.176	1	2.458138	-2.665040	-0.939439
6	5.069304	1.919305	-0.011	1	3.985338	-2.360717	-0.058901
1	3.674106	3.572726	0.245	8	1.125	1.721883	1.410299
1	1.671888	2.128423	0.172	8	3.564577	0.088276	-0.125556
1	4.199989	-1.376962	-0.346	6	-1.233616	-0.593404	-0.052625
1	6.213736	0.086979	-0.273	6	-2.248065	-1.556404	0.038139
15	1.349546	-0.804254	-0.147	7	-1.504383	0.713443	-0.139051
15	-1.349549	0.804259	0.157	6	-3.574545	-1.136383	0.056104
6	-2.817832	-0.280777	0.091	1	-1.995603	-2.616824	0.099871
6	-2.666465	-1.674016	-0.013	6	-2.769395	1.109466	-0.122320
6	-4.093205	0.289704	0.128	6	-3.846604	0.226048	-0.023242
6	-3.793899	-2.487737	-0.074	1	-4.384517	-1.864961	0.130790
1	-1.671870	-2.128420	-0.047	1	-2.942230	2.188329	-0.193797
6	-5.218063	-0.534594	0.061	1	-4.870163	0.603990	-0.011555
1	-4.199996	1.376948	0.207	6	1.239675	2.194562	-0.935888
6	-5.069288	-1.919326	-0.038	1	1.074718	3.239890	-0.646013
1	-3.674079	-3.572737	-0.154	1	2.245811	2.082825	-1.369636
1	-6.213733	-0.087007	0.087	1	0.497232	1.881452	-1.682557
34	0.079	-0.183	1.668777	O,O-WD2			
34	-0.077	0.194	-1.668768	6	2.601478	-3.057628	-2.239605
34	1.718838	-2.850294	-0.372	6	2.258194	-1.874751	-1.594014
34	-1.718852	2.850296	0.392	6	3.164291	-1.277956	-0.707411
1	5.952123	2.562719	0.021	6	4.407960	-1.868929	-0.475598
1	-5.952103	-2.562746	-0.087	6	4.745231	-3.055683	-1.127368
Preindolizine				6	3.844698	-3.649924	-2.008128
6	0.178997	-1.007094	-0.061471	1	1.894075	-3.515087	-2.934522
1	0.344103	-2.083841	-0.158607	1	1.283926	-1.416737	-1.789237
6	1.241723	-0.189608	0.035834	1	5.108331	-1.391707	0.214455
6	1.157013	1.312645	0.278992	1	5.720108	-3.513306	-0.946378
6	2.649285	-0.701640	-0.049454	15	2.712053	0.275578	0.159302
6	2.902049	-2.193470	-0.049733				

15	-0.356237	0.957117	-0.470202	1	-2.677643	-5.117718	0.347636
6	-0.939051	2.583166	0.120884	6	-1.608521	-2.188115	2.619792
6	-0.137187	3.359011	0.961033	6	-1.192654	-3.466833	2.950023
6	-2.194438	3.039341	-0.282368	1	-1.265	-5.547037	2.367554
6	-0.598375	4.598066	1.398592	1	-1.348414	-1.288938	3.183425
1	0.847861	3.002464	1.272781	1	-0.566906	-3.626241	3.827545
6	-2.644138	4.283450	0.153485	6	-3.998551	-0.272	2.053509
1	-2.826097	2.418254	-0.919198	1	-3.526970	0.010767	3.023602
6	-1.849337	5.062812	0.992965	1	-4.469724	0.717421	1.681839
1	0.028487	5.204747	2.055258	1	-4.761699	-0.985185	2.167456
1	-3.626646	4.639805	-0.162831	O,O-WD3			
34	1.728270	1.610527	-1.375582	6	2.129327	-3.641190	-1.389810
34	0.713576	-0.163058	1.186670	6	1.898855	-2.322010	-1.017411
34	4.210625	1.064508	1.386049	6	2.964185	-1.525652	-0.577328
34	-1.318558	0.059561	-2.135411	6	4.255161	-2.053918	-0.519851
1	4.111944	-4.577009	-2.520530	6	4.479987	-3.377832	-0.898137
1	-2.206663	6.037054	1.334563	6	3.420085	-4.171207	-1.330069
6	-3.526903	-2.426557	-0.366005	1	1.294901	-4.259613	-1.726706
1	-3.979808	-3.032677	-1.148636	1	0.886401	-1.913819	-1.066652
6	-3.559250	-1.082002	-0.256358	1	5.078212	-1.423235	-0.174792
6	-2.894246	-0.572669	1.042333	1	5.490334	-3.789146	-0.850215
6	-4.359890	-0.173277	-1.137011	15	2.664361	0.206170	-0.056369
6	-4.795729	-0.710624	-2.479760	15	-0.533070	0.910340	0.055275
1	-3.992082	-1.262915	-2.984113	6	-0.761199	2.704303	0.295426
1	-5.646768	-1.395199	-2.329095	6	0.320563	3.518183	0.644790
1	-5.128783	0.125729	-3.105431	6	-2.041785	3.245632	0.154143
8	-1.929403	0.297386	1.020811	6	0.116445	4.879167	0.849530
8	-4.721245	0.909743	-0.734785	1	1.322397	3.096749	0.757392
6	-2.752021	-2.992806	0.720441	6	-2.229129	4.614757	0.336859
6	-2.369972	-4.305124	1.005797	1	-2.893367	2.607699	-0.091228
7	-2.367922	-2.001858	1.542609	6	-1.154894	5.430300	0.687038
6	-1.582620	-4.531763	2.128472	1	0.959963	5.512052	1.131794

1	-3.226590	5.040793	0.211556	O,O-WD4			
34	1.364968	1.208014	-1.575991	6	-2.392583	-3.646771	1.673185
34	0.958874	-0.010281	1.477730	6	-2.131513	-2.306700	1.404407
34	4.350799	1.223803	0.638514	6	-3.007775	-1.574458	0.594774
34	-1.515781	-0.162934	-1.631944	6	-4.144504	-2.188562	0.062986
1	3.597841	-5.208883	-1.621095	6	-4.401057	-3.531316	0.337197
1	-1.308243	6.501121	0.837805	6	-3.526588	-4.261274	1.139486
6	-3.347149	-2.190116	-0.664389	1	-1.707731	-4.215052	2.306075
1	-3.733548	-2.718322	-1.531526	1	-1.246861	-1.822664	1.824583
6	-3.163293	-0.718325	-0.565949	1	-4.827007	-1.605656	-0.560386
6	-2.750819	-0.486443	0.934075	1	-5.292425	-4.006134	-0.078141
6	-4.271475	0.172483	-1.117504	15	-2.646217	0.180959	0.193693
6	-5.038666	-0.367589	-2.299180	15	0.661549	0.862614	-0.294468
1	-4.361661	-0.774394	-3.065150	6	0.626951	2.658536	-0.470884
1	-5.684109	-1.192957	-1.961734	6	-0.536433	3.333169	-0.851582
1	-5.655497	0.431391	-2.726200	6	1.824591	3.348924	-0.253809
8	-1.816363	0.506876	1.143006	6	-0.495535	4.714215	-1.015485
8	-4.517055	1.261530	-0.652966	1	-1.474620	2.795553	-1.009203
6	-2.699732	-2.783191	0.379719	6	1.847191	4.732223	-0.413773
6	-2.428011	-4.159254	0.702571	1	2.736049	2.815475	0.027184
7	-2.216332	-1.832867	1.271839	6	0.691339	5.412937	-0.793889
6	-1.768511	-4.465207	1.853366	1	-1.402461	5.244381	-1.311195
1	-2.762604	-4.931747	0.009867	1	2.778119	5.276319	-0.243591
6	-1.607040	-2.145923	2.445152	34	-1.514183	1.154481	1.766510
6	-1.347144	-3.442336	2.766522	34	-0.914990	-0.213039	-1.408632
1	-1.559462	-5.510495	2.091919	34	-4.232309	1.183516	-0.734114
1	-1.332295	-1.300371	3.078482	34	1.456956	-0.028322	1.554916
1	-0.826334	-3.685149	3.691013	1	-3.729386	-5.313171	1.353182
6	-3.942362	-0.202601	1.846590	1	0.715283	6.497629	-0.920073
1	-3.603016	-0.230457	2.890953	6	3.468105	-2.006257	0.801609
1	-4.354396	0.787038	1.627976	1	3.828306	-2.466910	1.717199
1	-4.718243	-0.967751	1.700348	6	3.227873	-0.555725	0.603884

6	2.923903	-0.437351	-0.923945	8	0.110815	0.019859	1.114181
6	4.227193	0.439075	1.172888	8	0.237307	3.226981	0.971490
6	4.945601	0.025877	2.432460	6	-3.172785	0.296433	0.099160
1	4.247323	-0.387991	3.175351	6	-4.331999	-0.419710	-0.217886
1	5.670544	-0.765797	2.188335	7	-2.226730	-0.312543	0.860623
1	5.471325	0.891418	2.851431	6	-4.445780	-1.727094	0.228897
8	1.973483	0.532593	-1.258853	1	-5.107943	0.049967	-0.821725
8	4.424019	1.514897	0.654937	6	-2.302995	-1.580518	1.290920
6	2.901819	-2.683393	-0.239817	6	-3.424388	-2.322936	0.985674
6	2.699039	-4.083485	-0.501666	1	-5.336524	-2.306154	-0.023186
7	2.433055	-1.800200	-1.208786	1	-1.443502	-1.957622	1.846218
6	2.110069	-4.474356	-1.664266	1	-3.489853	-3.359390	1.313204
1	3.025009	-4.805512	0.247104	6	-1.288694	1.122216	2.618067
6	1.889475	-2.197423	-2.392453	1	-1.165119	0.270528	3.300865
6	1.693770	-3.517248	-2.650294	1	-0.512551	1.868319	2.821796
1	1.950024	-5.537547	-1.856099	1	-2.281289	1.572797	2.755621
1	1.606262	-1.397495	-3.079145	6	5.187969	0.178270	0.966040
1	1.221424	-3.830481	-3.579619	6	4.824248	-1.075118	0.479327
6	4.157133	-0.163166	-1.777828	6	3.502771	-1.324602	0.107864
1	3.889211	-0.265649	-2.838109	6	2.547558	-0.313594	0.217069
1	4.524623	0.850397	-1.591121	6	2.912192	0.948596	0.704333
1	4.941130	-0.893673	-1.533536	6	4.229745	1.187710	1.081246
O,O-WD5				15	0.825490	-0.597562	-0.314943
6	-2.718507	1.608747	-0.251372	1	5.570945	-1.867084	0.389794
1	-3.287197	2.296858	-0.871837	1	3.202831	-2.307696	-0.263806
6	-1.436561	1.764757	0.192949	1	2.164765	1.741061	0.791601
6	-1.100394	0.636590	1.175872	1	4.511340	2.170310	1.466054
6	-0.616391	3.015223	0.137798	34	0.330766	-2.635619	-0.559393
6	-0.984550	4.028754	-0.916782	34	0.267226	0.800886	-1.847959
1	-1.183954	3.554950	-1.886728	1	6.223041	0.372028	1.257106
1	-1.895315	4.559806	-0.594164	O,O-WD6			
1	-0.170248	4.756403	-1.011479	6	-1.802925	-3.837599	0.496542

6	-1.607180	-2.505061	0.139981	6	4.149101	-0.298897	2.956097
6	-2.634944	-1.576144	0.341145	1	4.729668	-1.231709	3.022602
6	-3.850780	-1.990449	0.900962	1	4.701591	0.518620	3.434202
6	-4.034011	-3.322602	1.258906	1	3.202182	-0.464038	3.494720
6	-3.010936	-4.248005	1.056526	8	2.133648	0.387518	-1.337904
1	-0.999759	-4.555168	0.322688	8	4.316957	1.108910	1.041901
1	-0.656142	-2.207238	-0.304897	6	2.294124	-2.903565	0.027729
1	-4.656179	-1.266407	1.043347	6	1.734663	-4.207137	-0.209455
1	-4.985123	-3.638776	1.691862	7	2.447666	-2.062737	-1.104614
15	-2.457350	0.206101	-0.025531	6	1.404102	-4.592287	-1.468459
15	0.876584	0.945174	-0.600510	1	1.594078	-4.868283	0.647134
6	1.002072	2.737079	-0.590344	6	2.131588	-2.473636	-2.377582
6	-0.079875	3.564362	-0.904895	6	1.605918	-3.702044	-2.591202
6	2.242822	3.273977	-0.217411	1	0.979299	-5.582609	-1.644379
6	0.085167	4.946274	-0.854510	1	2.292069	-1.741268	-3.169515
1	-1.045652	3.136270	-1.183287	1	1.334502	-4.006036	-3.601326
6	2.390250	4.656685	-0.173634	6	4.331282	-0.507319	-1.508121
1	3.075650	2.616022	0.053664	1	4.146855	-0.447168	-2.588911
6	1.316695	5.490111	-0.492697	1	4.735202	0.445231	-1.152019
1	-0.755431	5.598314	-1.098576	1	5.060349	-1.307481	-1.310984
1	3.351759	5.084908	0.115666	O,O-WD7			
34	-1.408095	1.189859	1.687870	6	-3.888107	-3.461076	0.245897
34	-0.903308	0.269462	-1.764716	6	-3.878915	-2.071169	0.284706
34	-4.211425	1.202717	-0.560057	6	-2.843034	-1.362264	-0.340150
34	0.801575	0.067208	1.466092	6	-1.824551	-2.050429	-1.006926
1	-3.159130	-5.295272	1.328658	6	-1.845900	-3.444054	-1.042662
1	1.441139	6.574538	-0.453628	6	-2.870906	-4.148835	-0.417947
6	2.716135	-2.238918	1.133742	1	-4.698426	-4.008971	0.730877
1	2.667938	-2.620399	2.150551	1	-4.682977	-1.530692	0.789801
6	3.075791	-0.877088	0.736655	1	-1.003995	-1.527958	-1.501680
6	3.061009	-0.835632	-0.750554	1	-1.044379	-3.971291	-1.562413
6	3.886721	0.058254	1.507405	15	-2.900153	0.454536	-0.191827

15	0.589950	0.621592	-0.689140
6	1.603602	2.111861	-0.557351
6	1.207234	3.211251	0.215614
6	2.829768	2.114509	-1.225490
6	2.052692	4.309642	0.321164
1	0.243684	3.205873	0.732094
6	3.672147	3.219697	-1.111419
1	3.130240	1.241574	-1.807177
6	3.284573	4.311708	-0.339747
1	1.752180	5.168856	0.924020
1	4.644362	3.207363	-1.605628
34	-1.945017	0.994195	1.801260
34	-1.369701	1.361784	-1.613982
34	-4.766743	1.359427	-0.369011
34	0.076062	-0.122546	1.427205
1	-2.883306	-5.240607	-0.451754
1	3.948851	5.173532	-0.246383
6	3.171706	-1.263179	1.518158
1	3.030613	-0.919220	2.539527
6	4.026690	-0.701991	0.529032
6	3.940577	-1.489066	-0.620657
6	4.831064	0.531782	0.670140
6	4.528817	1.401182	1.870795
1	3.479213	1.735149	1.829297
1	4.662432	0.843305	2.809728
1	5.193426	2.273275	1.861669
8	1.240777	-0.474778	-1.466314
8	5.667429	0.866222	-0.147120
6	2.584908	-2.389043	0.962818
6	1.660685	-3.365894	1.430639
7	3.066412	-2.503999	-0.347698
6	1.235446	-4.357002	0.596355

1	1.296841	-3.287568	2.456102
6	2.610329	-3.487263	-1.196887
6	1.721686	-4.411052	-0.749760
1	0.518600	-5.102579	0.943210
1	3.002646	-3.468625	-2.212262
1	1.382439	-5.190189	-1.433233
6	4.534556	-1.321777	-1.973696
1	3.741452	-1.131351	-2.716566
1	5.231473	-0.477641	-1.956728
1	5.090281	-2.220204	-2.288431

Figure 31

O,O-WG1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172
1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061

1	-4.199996	1.376948	0.207	6	1.239675	2.194562	-0.935888
6	-5.069288	-1.919326	-0.038	1	1.074718	3.239890	-0.646013
1	-3.674079	-3.572737	-0.154	1	2.245811	2.082825	-1.369636
1	-6.213733	-0.087007	0.087	1	0.497232	1.881452	-1.682557
34	0.079	-0.183	1.668777				
34	-0.077	0.194	-1.668768		O,O-WG2		
34	1.718838	-2.850294	-0.372	6	-4.298518	-1.963420	-0.528116
34	-1.718852	2.850296	0.392	6	-3.071957	-1.342369	-0.742646
1	5.952123	2.562719	0.021	6	-2.849875	-0.055080	-0.237604
1	-5.952103	-2.562746	-0.087	6	-3.852878	0.602052	0.486252
Preindolizine				6	-5.075471	-0.028108	0.696660
6	0.178997	-1.007094	-0.061471	6	-5.299179	-1.308838	0.189851
1	0.344103	-2.083841	-0.158607	1	-4.471791	-2.965818	-0.924006
6	1.241723	-0.189608	0.035834	1	-2.281363	-1.850636	-1.298863
6	1.157013	1.312645	0.278992	1	-3.671442	1.605768	0.877116
6	2.649285	-0.701640	-0.049454	1	-5.859036	0.485695	1.257006
6	2.902049	-2.193470	-0.049733	15	-1.249960	0.753638	-0.511858
1	2.462099	-2.668778	0.839244	15	1.447068	-1.018601	0.481954
1	2.458138	-2.665040	-0.939439	6	2.450864	0.477482	0.344280
1	3.985338	-2.360717	-0.058901	6	2.171597	1.588598	1.149129
8	1.125	1.721883	1.410299	6	3.511477	0.516787	-0.572830
8	3.564577	0.088276	-0.125556	6	2.952875	2.736757	1.030735
6	-1.233616	-0.593404	-0.052625	1	1.353496	1.549383	1.870424
6	-2.248065	-1.556404	0.038139	6	4.282064	1.666040	-0.683251
7	-1.504383	0.713443	-0.139051	1	3.723975	-0.354289	-1.196789
6	-3.574545	-1.136383	0.056104	6	4.001653	2.777575	0.116699
1	-1.995603	-2.616824	0.099871	1	2.733472	3.603363	1.656848
6	-2.769395	1.109466	-0.122320	1	5.103962	1.698888	-1.400837
6	-3.846604	0.226048	-0.023242	34	-0.237548	-0.828342	1.742395
1	-4.384517	-1.864961	0.130790	34	-0.026076	-0.175282	-1.963588
1	-2.942230	2.188329	-0.193797	34	-1.127504	2.747712	0.001490
1	-4.870163	0.603990	-0.011555	34	2.347861	-2.793628	-0.023433

1	-6.260687	-1.799511	0.355688	6	-4.331966	-0.419689	-0.217895
1	4.607957	3.681126	0.023607	7	-2.226714	-0.312511	0.860645
O,O-WG3				6	-4.445743	-1.727077	0.228882
15	-0.591699	-0.001	0.018	1	-5.107905	0.049981	-0.821747
6	1.224915	-0.033	0.037	6	-2.302974	-1.580490	1.290933
6	1.925949	-1.213933	0.362	6	-3.424359	-2.322914	0.985672
6	1.925953	1.213872	-0.263	1	-5.336478	-2.306143	-0.023219
6	3.317418	-1.209159	0.309	1	-1.443486	-1.957590	1.846241
1	1.375344	-2.157190	0.621	1	-3.489822	-3.359370	1.313196
6	3.317417	1.209103	-0.330	6	-1.288655	1.122237	2.618083
1	1.375330	2.157122	-0.465	1	-1.165072	0.270549	3.300881
6	4.013078	-0.031	-0.054	1	-0.512511	1.868341	2.821803
1	3.860472	-2.156115	0.558	1	-2.281249	1.572817	2.755652
1	3.860482	2.156052	-0.594	6	5.187946	0.178270	0.966018
34	-1.486067	-1.854380	-0.121	6	4.824226	-1.075120	0.479319
34	-1.485986	1.854417	0.102	6	3.502750	-1.324612	0.107859
1	5.105294	-0.023	-0.108	6	2.547539	-0.313601	0.217048
O,O-WG4				6	2.912177	0.948595	0.704297
O,O-WG5				6	4.229730	1.187711	1.081212
6	-2.718484	1.608775	-0.251363	15	0.825470	-0.597573	-0.314947
1	-3.287168	2.296882	-0.871839	34	0.330732	-2.635631	-0.559352
6	-1.436542	1.764784	0.192963	34	0.267206	0.800843	-1.847984
6	-1.100375	0.636617	1.175886	1	5.570926	-1.867085	0.389795
6	-0.616354	3.015239	0.137800	1	3.202811	-2.307712	-0.263799
6	-0.984521	4.028774	-0.916774	1	2.164747	1.741061	0.791552
1	-1.183896	3.554969	-1.886726	1	4.511331	2.170313	1.466011
1	-1.895308	4.559798	-0.594173	1	6.223021	0.372033	1.257086
1	-0.170233	4.756440	-1.011452	O,O-WG6			
8	0.110834	0.019882	1.114177	6	0.263257	2.741729	0.477855
8	0.237363	3.226982	0.971474	1	0.803875	3.524236	-0.046774
6	-3.172764	0.296461	0.099170	6	0.885566	1.552602	1.083792
				6	-0.326407	0.674705	1.562406

6	2.018331	1.791195	2.090871	34	0.891981	-0.150289	-2.262109
6	2.566564	3.189064	2.185851	8	-0.467596	-0.311374	0.536720
1	1.770245	3.900795	2.446820	34	3.264713	1.975786	-1.424375
1	3.365752	3.209085	2.935863	6	2.952891	-0.881384	0.290048
1	2.965800	3.486870	1.202807	6	2.267036	-1.909328	0.950498
8	2.464115	0.882606	2.752140	6	4.348730	-0.916888	0.205054
6	-1.064937	2.757993	0.768171	6	2.976800	-2.965144	1.512396
6	-2.102173	3.725377	0.512079	1	1.182304	-1.892501	1.030864
7	-1.439128	1.619419	1.487514	6	5.051720	-1.975914	0.774655
6	-3.360902	3.505623	0.972736	1	4.878395	-0.111791	-0.309431
1	-1.843315	4.623809	-0.048655	6	4.368379	-3.257	1.426605
6	-2.712343	1.398351	1.928651	1	2.434160	-3.764152	2.021263
6	-3.690688	2.312205	1.702873	1	6.141161	-1.998186	0.705475
1	-4.143162	4.243001	0.779646	34	-2.266457	-2.817242	1.367668
1	-2.892086	0.451329	2.439982	34	-0.368930	-2.227857	-1.616530
1	-4.702743	2.124984	2.056535	1	4.921560	-3.830103	1.871813
6	-0.224813	0.012480	2.923529	1	-5.763270	1.864077	-2.202240
1	-1.119303	-0.593438	3.117384	O,O-WG7			
1	0.655889	-0.635327	2.959218	6	0.254485	2.599701	0.124366
1	-0.121673	0.776180	3.705194	1	0.731946	3.301471	-0.553008
6	-3.634151	1.612700	-1.952506	6	0.976481	1.481671	0.822409
6	-2.617483	0.834232	-1.409690	6	-0.206527	0.667342	1.477890
6	-2.940271	-0.319904	-0.684062	6	2.017569	1.973575	1.881507
6	-4.277736	-0.692712	-0.517102	6	2.210559	3.454945	2.031415
6	-5.288804	0.093100	-1.063869	1	1.253033	3.951588	2.242995
6	-4.968432	1.246662	-1.777913	1	2.935993	3.641500	2.831930
1	-3.379648	2.517958	-2.506834	1	2.585132	3.861145	1.079399
1	-1.575867	1.131790	-1.542026	8	2.630476	1.170092	2.538832
1	-4.518914	-1.592982	0.052778	6	-1.007948	2.686339	0.600950
1	-6.332612	-0.196446	-0.927205	6	-2.064699	3.649292	0.391268
15	-1.625850	-1.349246	0.033983	7	-1.288050	1.638558	1.491271
15	2.073181	0.522751	-0.463438	6	-3.257045	3.492586	1.017278

1	-1.871703	4.487322	-0.278932	6	4.246619	-3.043518	1.547906
6	-2.509567	1.469449	2.084870	1	2.292069	-3.891982	1.919650
6	-3.504751	2.368016	1.884230	1	6.040775	-1.955454	1.033882
1	-4.052596	4.223492	0.856941	34	-2.209887	-2.852777	1.350201
1	-2.629129	0.578656	2.703292	34	-0.390374	-2.140306	-1.698371
1	-4.470755	2.227281	2.365489	1	4.784668	-3.874053	2.010221
6	0.023234	0.017449	2.829383	1	-5.873642	1.903096	-1.964676
1	-0.814661	-0.651581	3.067888	O,O-WG8			
1	0.946342	-0.570904	2.811279	6	0.096778	2.652029	-0.211885
1	0.119292	0.782919	3.609643	1	0.350581	3.074525	-1.180679
6	-3.739592	1.590394	-1.895046	6	1.024573	1.859445	0.630044
6	-2.701063	0.803421	-1.408788	6	0.190659	1.460836	1.784792
6	-2.991986	-0.306257	-0.604079	6	2.325825	2.564828	1.126367
6	-4.319175	-0.625182	-0.299145	6	2.551168	3.970830	0.648078
6	-5.351387	0.171177	-0.787642	1	1.699348	4.597712	0.955756
6	-5.062440	1.278817	-1.583419	1	3.482921	4.354167	1.080255
1	-3.510047	2.459972	-2.513715	1	2.604643	3.985445	-0.449097
1	-1.666398	1.061483	-1.642402	8	3.047305	2.013044	1.913745
1	-4.533947	-1.494080	0.327273	6	-1.104439	2.714205	0.405260
1	-6.387047	-0.075807	-0.545747	6	-2.373979	3.296561	0.058879
15	-1.647024	-1.349046	0.025639	7	-1.013473	2.011213	1.640449
15	2.041157	0.503310	-0.427878	6	-3.440192	3.120713	0.871231
34	0.835532	-0.196171	-2.234953	1	-2.444751	3.851028	-0.876543
8	-0.464501	-0.334708	0.495092	6	-2.135966	1.796237	2.442602
34	3.333790	1.878448	-1.380719	6	-3.316046	2.335516	2.080588
6	2.866555	-0.916914	0.368911	1	-4.411084	3.541956	0.609118
6	2.161942	-1.998443	0.915187	1	-1.996123	1.154416	3.309977
6	4.265411	-0.913571	0.409748	1	-4.191042	2.147879	2.702616
6	2.853598	-3.054845	1.500554	6	0.576776	0.699520	2.992263
1	1.076171	-2.030632	0.890912	1	0.011301	-0.248513	3.008456
6	4.949540	-1.972125	1.001143	1	1.648572	0.482054	2.973559
1	4.814127	-0.074859	-0.023763	1	0.335792	1.270434	3.902324

6	-3.569257	1.222415	-2.357568	6	-3.369348	-0.887307	-0.111
6	-2.543555	0.509341	-1.743257	6	-2.211924	-1.609901	-0.039
6	-2.817142	-0.295816	-0.628797	6	-0.953112	-0.945392	0.077
6	-4.119446	-0.358540	-0.127076	7	-0.944977	0.460093	0.035
6	-5.140425	0.372056	-0.735098	6	-2.118347	1.186485	0.064
6	-4.868652	1.157260	-1.853807	6	0.365875	-1.361996	0.179
1	-3.350376	1.833355	-3.236262	6	1.178830	-0.196662	0.142
1	-1.527553	0.570660	-2.139015	6	0.342390	0.923968	-0.033
1	-4.324223	-0.986497	0.743661	6	0.643869	2.382512	-0.063
1	-6.156150	0.313743	-0.337534	6	2.661096	-0.167381	-0.032
15	-1.462648	-1.239595	0.162231	6	3.367767	-1.507089	-0.152
15	1.650228	0.291255	-0.523841	8	3.296388	0.867672	0.005
34	0.852909	-0.935010	-2.282305	1	-4.231497	1.134345	-0.047
8	-0.279805	-0.242219	0.365101	1	-4.337378	-1.390285	-0.226
34	2.901860	1.401540	-1.875897	1	-2.220273	-2.700963	-0.013
6	2.586780	-0.797132	0.609255	1	-2.014550	2.270881	0.222
6	1.986082	-1.822953	1.350694	1	0.695744	-2.397669	0.318
6	3.974511	-0.616430	0.679324	1	1.729765	2.520303	-0.890
6	2.768950	-2.650959	2.150621	1	0.223807	2.879683	-0.890290
1	0.911377	-1.982958	1.322871	1	0.225345	2.879394	0.891066
6	4.747088	-1.442197	1.490346	1	3.083900	-2.092583	0.887620
1	4.446927	0.173614	0.093309	1	3.082298	-2.093631	-0.886705
6	4.147257	-2.461990	2.226664	1	4.451489	-1.340867	-0.001188
1	2.286202	-3.450571	2.715912	WR Pentacycle			
1	5.826173	-1.285191	1.542869	6	1.916598	3.720572	-0.991460
34	-2.059353	-2.299322	1.884041	6	1.758485	2.352668	-1.187786
34	-0.561	-2.630040	-1.399042	6	1.846398	1.476358	-0.096750
1	4.756328	-3.112352	2.858546	6	2.108245	1.974959	1.180764
1	-5.672483	1.716765	-2.338074	6	2.268805	3.347196	1.369287
O,O-WG9				6	2.168591	4.219603	0.287827
Indolizine				1	1.846535	4.401238	-1.842233
6	-3.314580	0.544323	-0.058	1	1.566925	1.961845	-2.189955

1	2.181736	1.293977	2.031050
1	2.471173	3.734232	2.369805
15	1.579852	-0.289762	-0.443689
15	-1.401995	-0.660078	-0.169895
34	-0.684800	-0.387931	2.012596
8	-0.003364	-0.247176	-0.943129
34	-2.209502	-2.475985	-0.709538
6	-2.403970	0.834309	-0.400833
6	-1.819762	2.100129	-0.254347
6	-3.760983	0.715243	-0.711753
6	-2.598310	3.240162	-0.422024
1	-0.759535	2.197706	-0.012903
6	-4.534511	1.863601	-0.873937
1	-4.203219	-0.276807	-0.831414
6	-3.954993	3.122547	-0.739
1	-2.141096	4.225308	-0.311283
1	-5.594946	1.770298	-1.115625
34	2.900790	-1.185035	-1.746051
34	1.355058	-1.427550	1.503481
1	-4.562930	4.020596	-0.859219
1	2.294289	5.293611	0.440076

Figure 32

O,O-WH1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172

1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061
1	-4.199996	1.376948	0.207
6	-5.069288	-1.919326	-0.038
1	-3.674079	-3.572737	-0.154
1	-6.213733	-0.087007	0.087
34	0.079	-0.183	1.668777
34	-0.077	0.194	-1.668768
34	1.718838	-2.850294	-0.372
34	-1.718852	2.850296	0.392
1	5.952123	2.562719	0.021
1	-5.952103	-2.562746	-0.087

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556

6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-WH2

6	-4.298518	-1.963420	-0.528116
6	-3.071957	-1.342369	-0.742646
6	-2.849875	-0.055080	-0.237604
6	-3.852878	0.602052	0.486252
6	-5.075471	-0.028108	0.696660
6	-5.299179	-1.308838	0.189851
1	-4.471791	-2.965818	-0.924006
1	-2.281363	-1.850636	-1.298863
1	-3.671442	1.605768	0.877116
1	-5.859036	0.485695	1.257006
15	-1.249960	0.753638	-0.511858
15	1.447068	-1.018601	0.481954
6	2.450864	0.477482	0.344280
6	2.171597	1.588598	1.149129
6	3.511477	0.516787	-0.572830
6	2.952875	2.736757	1.030735

1	1.353496	1.549383	1.870424
6	4.282064	1.666040	-0.683251
1	3.723975	-0.354289	-1.196789
6	4.001653	2.777575	0.116699
1	2.733472	3.603363	1.656848
1	5.103962	1.698888	-1.400837
34	-0.237548	-0.828342	1.742395
34	-0.026076	-0.175282	-1.963588
34	-1.127504	2.747712	0.001490
34	2.347861	-2.793628	-0.023433
1	-6.260687	-1.799511	0.355688
1	4.607957	3.681126	0.023607

O,O-WH3

15	-0.591699	-0.001	0.018
6	1.224915	-0.033	0.037
6	1.925949	-1.213933	0.362
6	1.925953	1.213872	-0.263
6	3.317418	-1.209159	0.309
1	1.375344	-2.157190	0.621
6	3.317417	1.209103	-0.330
1	1.375330	2.157122	-0.465
6	4.013078	-0.031	-0.054
1	3.860472	-2.156115	0.558
1	3.860482	2.156052	-0.594
34	-1.486067	-1.854380	-0.121
34	-1.485986	1.854417	0.102
1	5.105294	-0.023	-0.108

O,O-WH4

O,O-WH5

6	-2.718484	1.608775	-0.251363
1	-3.287168	2.296882	-0.871839
6	-1.436542	1.764784	0.192963

6	-1.100375	0.636617	1.175886	1	3.202811	-2.307712	-0.263799
6	-0.616354	3.015239	0.137800	1	2.164747	1.741061	0.791552
6	-0.984521	4.028774	-0.916774	1	4.511331	2.170313	1.466011
1	-1.183896	3.554969	-1.886726	1	6.223021	0.372033	1.257086
1	-1.895308	4.559798	-0.594173	O,O-WH6			
1	-0.170233	4.756440	-1.011452	6	-2.659557	1.580226	-0.391480
8	0.110834	0.019882	1.114177	1	-3.190126	2.265824	-1.046212
8	0.237363	3.226982	0.971474	6	-1.301469	1.667662	-0.003146
6	-3.172764	0.296461	0.099170	6	-1.098154	0.609037	1.103672
6	-4.331966	-0.419689	-0.217895	6	-0.553485	2.971361	0.058520
7	-2.226714	-0.312511	0.860645	6	-0.947569	4.020108	-0.953071
6	-4.445743	-1.727077	0.228882	1	-1.118269	3.590093	-1.949397
1	-5.107905	0.049981	-0.821747	1	-1.887206	4.489955	-0.620741
6	-2.302974	-1.580490	1.290933	1	-0.165727	4.786940	-0.998919
6	-3.424359	-2.322914	0.985672	8	0.106930	-0.050452	1.155709
1	-5.336478	-2.306143	-0.023219	8	0.283163	3.185035	0.907864
1	-1.443486	-1.957590	1.846241	6	-3.156689	0.337620	0.011379
1	-3.489822	-3.359370	1.313196	6	-4.378556	-0.340163	-0.234920
6	-1.288655	1.122237	2.618083	7	-2.226283	-0.312437	0.782595
1	-1.165072	0.270549	3.300881	6	-4.559633	-1.599890	0.280778
1	-0.512511	1.868341	2.821803	1	-5.141962	0.146501	-0.841578
1	-2.281249	1.572817	2.755652	6	-2.390541	-1.549076	1.298329
6	5.187946	0.178270	0.966018	6	-3.552980	-2.230263	1.057507
6	4.824226	-1.075120	0.479319	1	-5.492589	-2.132029	0.082911
6	3.502750	-1.324612	0.107859	1	-1.547054	-1.947952	1.863541
6	2.547539	-0.313601	0.217048	1	-3.683036	-3.238948	1.445911
6	2.912177	0.948595	0.704297	6	-1.347447	1.193042	2.496223
6	4.229730	1.187711	1.081212	1	-1.333440	0.376480	3.230828
15	0.825470	-0.597573	-0.314947	1	-0.549757	1.906672	2.727039
34	0.330732	-2.635631	-0.559352	1	-2.320280	1.702186	2.527872
34	0.267206	0.800843	-1.847984	6	5.208852	0.382762	0.847404
1	5.570926	-1.867085	0.389795	6	4.908446	-0.878215	0.337062

6	3.589970	-1.209534	0.026650	1	-1.619395	-1.907209	1.944878
6	2.574154	-0.272371	0.223400	1	-3.797427	-3.133383	1.602235
6	2.873716	0.997315	0.734895	6	-1.370709	1.258954	2.407446
6	4.191193	1.317531	1.047587	1	-1.450619	0.477615	3.175374
15	0.856220	-0.681279	-0.213021	1	-0.553737	1.940871	2.662037
34	0.482840	-2.715247	-0.521903	1	-2.316393	1.816158	2.357138
34	0.101265	0.730999	-1.716686	6	5.215688	0.494739	0.783433
1	5.701554	-1.612725	0.182384	6	4.950341	-0.758543	0.235346
1	3.339977	-2.199513	-0.362788	6	3.636710	-1.135820	-0.038679
1	2.080774	1.732503	0.892205	6	2.590213	-0.251671	0.233765
1	4.423728	2.305065	1.451479	6	2.853900	1.010775	0.781966
1	6.242236	0.640054	1.091353	6	4.168137	1.376064	1.056871
O,O-WH7				15	0.880123	-0.727794	-0.143087
6	-2.607652	1.516424	-0.531641	34	0.563848	-2.747832	-0.516227
1	-3.096724	2.166846	-1.251249	34	0.003764	0.698636	-1.636174
6	-1.186303	1.576699	-0.148160	1	5.767261	-1.450971	0.022506
6	-1.093199	0.594605	1.061838	1	3.415549	-2.120684	-0.456923
6	-0.527824	2.937698	0.012974	1	2.037906	1.705649	0.994113
6	-0.984055	4.016193	-0.938939	1	4.373881	2.357283	1.489346
1	-1.113169	3.634007	-1.961506	1	6.245588	0.787561	0.999955
1	-1.962482	4.390797	-0.599050	O,O-WH8			
1	-0.259737	4.838780	-0.928368	6	3.180682	-1.225909	2.450297
8	0.109232	-0.089058	1.183723	6	2.018640	-1.359079	1.696085
8	0.311614	3.151677	0.857247	6	2.082358	-1.963674	0.435517
6	-3.130414	0.337235	-0.065875	6	3.303708	-2.432339	-0.062045
6	-4.387739	-0.324118	-0.265528	6	4.457152	-2.312196	0.710269
7	-2.215060	-0.316600	0.746129	6	4.396717	-1.708083	1.965552
6	-4.613655	-1.532191	0.325785	1	3.128497	-0.744722	3.429096
1	-5.134928	0.152372	-0.900258	1	1.066107	-0.990995	2.086977
6	-2.443144	-1.511321	1.348573	1	3.346600	-2.898211	-1.049031
6	-3.625368	-2.157603	1.151546	1	5.405407	-2.697446	0.328588
1	-5.567151	-2.039584	0.162724	15	0.560022	-2.305592	-0.494050

15	-1.382232	0.457635	0.718507	6	0.306033	1.435647	-2.597636
6	-2.848983	-0.422757	0.094759	1	0.552371	0.383749	-2.796189
6	-3.929781	-0.714307	0.929058	1	-0.776558	1.575732	-2.700806
6	-2.868269	-0.820243	-1.247616	1	0.822252	2.094643	-3.314187
6	-5.031266	-1.399748	0.418680	34	-0.867070	-3.297724	0.602141
1	-3.891022	-0.421148	1.981053	34	0.791806	-2.295382	-2.562872
6	-3.967692	-1.507717	-1.749519	34	-1.174160	0.484303	2.804870
1	-2.006015	-0.619201	-1.887214	34	-1.860552	2.582304	-0.121290
6	-5.050499	-1.796063	-0.917418	1	-5.911500	-2.339789	-1.312704
1	-5.873779	-1.634152	1.072778	1	5.301953	-1.616676	2.570679
1	-3.973182	-1.833313	-2.791688	O,O-WH9			
6	0.958903	2.998172	0.782466	6	3.017089	-1.884792	2.699
1	0.757068	3.580933	1.676378	6	1.889482	-1.688491	1.807393
6	0.053687	2.889726	-0.408717	6	1.943637	-1.944726	0.431895
6	0.718770	1.827378	-1.238446	6	3.134163	-2.403133	-0.136630
6	0.213556	4.266873	-1.152078	6	4.260062	-2.606066	0.662497
6	-0.444613	5.459116	-0.504608	6	4.203719	-2.348857	2.031603
1	-1.435678	5.593998	-0.966531	1	2.960875	-1.687790	3.673142
1	-0.592878	5.337372	0.575055	1	0.956754	-1.351031	2.265548
1	0.154985	6.351850	-0.723479	1	3.169772	-2.603724	-1.210539
8	-0.165676	0.100875	-0.187074	1	5.182268	-2.981234	0.212101
8	0.845143	4.356362	-2.170598	15	0.405223	-1.879115	-0.568196
6	2.090862	2.317078	0.505451	15	-1.392269	0.270146	0.771718
6	3.346326	2.165896	1.194270	6	-2.913674	-0.444315	0.097069
7	1.944557	1.659261	-0.754252	6	-3.996753	-0.708540	0.937939
6	4.336350	1.438693	0.632374	6	-2.994210	-0.713949	-1.276493
1	3.461611	2.656182	2.160738	6	-5.166445	-1.243360	0.402665
6	2.964643	0.875200	-1.295057	1	-3.910783	-0.511818	2.008859
6	4.135611	0.777484	-0.641105	6	-4.165395	-1.247467	-1.799813
1	5.293643	1.321429	1.141519	1	-2.134885	-0.543011	-1.930626
1	2.731913	0.353565	-2.222212	6	-5.250207	-1.511826	-0.962164
1	4.925512	0.158898	-1.064644	1	-6.011726	-1.459904	1.058780

1	-4.224537	-1.475111	-2.865541	O,O-WH10			
6	1.052471	2.613595	0.999187	6	-4.112717	-1.598506	-1.627312
1	0.789185	2.926832	2.005319	6	-2.793372	-1.552486	-1.180852
6	0.266457	2.902521	-0.237009	6	-2.494493	-1.584521	0.182024
6	1.027802	2.204732	-1.309492	6	-3.543119	-1.682275	1.102721
6	0.282640	4.449226	-0.489661	6	-4.861246	-1.734561	0.670768
6	-0.470142	5.306966	0.492934	6	-5.157142	-1.691277	-0.698505
1	-1.456818	5.535989	0.060700	1	-4.310856	-1.566528	-2.698820
1	-0.637127	4.817594	1.459907	1	-1.984317	-1.485957	-1.911321
1	0.071159	6.253740	0.616399	1	-3.315302	-1.709592	2.171430
8	-0.127387	-0.267121	-0.052567	1	-5.687253	-1.816883	1.379466
8	0.881150	4.899631	-1.428114	15	-0.760339	-1.650525	0.744074
6	2.153801	1.919533	0.642453	15	1.121380	0.180876	-0.990068
6	3.296991	1.435156	1.369247	6	2.582239	-0.778278	-0.547857
7	2.106305	1.679050	-0.770919	6	3.549936	-1.044977	-1.520956
6	4.292762	0.806450	0.708253	6	2.788730	-1.231416	0.771488
1	3.324309	1.598666	2.446043	6	4.704196	-1.751130	-1.201968
6	3.122041	0.966835	-1.425163	1	3.394474	-0.698635	-2.544868
6	4.190781	0.563649	-0.715346	6	3.940591	-1.922454	1.094803
1	5.167294	0.438860	1.244304	1	2.039463	-1.062679	1.551421
1	2.953593	0.745341	-2.475997	6	4.906980	-2.193615	0.113347
1	4.975624	0.007590	-1.227160	1	5.434439	-1.950754	-1.985383
6	0.687714	2.108936	-2.733499	1	4.105368	-2.291583	2.107428
1	0.512271	1.035016	-2.960695	6	-0.580124	3.157370	-0.985923
1	-0.216948	2.683245	-2.956909	1	-0.446076	3.343303	-2.045010
1	1.520079	2.465170	-3.358636	6	0.367797	3.455606	0.062421
34	-0.934426	-3.331550	0.126737	6	-0.252334	2.996851	1.319037
34	0.822061	-1.611045	-2.645581	6	1.331511	4.625731	-0.039434
34	-1.226463	0.398602	2.844003	6	1.878066	4.877116	-1.417758
34	-1.633664	2.329093	-0.258804	1	2.103324	3.931741	-1.933991
1	-6.165509	-1.939043	-1.377707	1	1.117034	5.409737	-2.009983
1	5.082616	-2.520126	2.657906	1	2.772523	5.506685	-1.345149

8	-0.223900	-0.419077	-0.423478	1	-3.784988	0.948	2.243826
8	1.614134	5.285272	0.928341	6	-3.765970	-0.095252	0.322761
6	-1.664670	2.552222	-0.409210	6	-3.105122	0.181884	-1.002680
6	-2.892449	2.050465	-0.940746	6	-4.604653	-1.310173	0.566960
7	-1.457728	2.466267	0.978879	6	-4.917687	-1.647602	1.998892
6	-3.841036	1.579967	-0.090901	1	-3.974308	-1.838517	2.534352
1	-3.029731	2.059883	-2.021363	1	-5.429796	-0.812291	2.499845
6	-2.419093	1.945752	1.833408	1	-5.553858	-2.539588	2.027399
6	-3.604120	1.542731	1.324432	34	-1.781917	-1.216214	-1.492733
1	-4.783464	1.191171	-0.478783	8	-4.990968	-1.977417	-0.364916
1	-2.156625	1.886073	2.885702	6	-2.647820	1.877017	0.551367
1	-4.359107	1.139532	1.997175	6	-2.089840	3.055232	1.006977
6	0.070734	3.333586	2.733899	7	-2.428023	1.468729	-0.728440
1	0.051924	2.423003	3.351367	6	-1.290800	3.793164	0.133292
1	1.052159	3.812598	2.801635	1	-2.242450	3.363562	2.040169
1	-0.682414	4.044167	3.111530	6	-1.650547	2.155123	-1.581178
8	5.986096	-2.876651	0.520138	6	-1.087028	3.346812	-1.177232
8	-6.465483	-1.733051	-1.028833	1	-0.827272	4.720271	0.467062
6	-6.824617	-1.770625	-2.382988	1	-1.460757	1.704151	-2.555597
1	-6.387515	-2.643635	-2.897435	1	-0.422218	3.876194	-1.857328
1	-7.918055	-1.849258	-2.417390	6	-4.084816	0.318832	-2.168731
1	-6.517410	-0.853493	-2.916267	1	-3.559005	0.578183	-3.098553
6	6.982612	-3.216595	-0.409044	1	-4.615133	-0.631745	-2.300476
1	6.584918	-3.855702	-1.215341	1	-4.819801	1.105048	-1.938873
1	7.447341	-2.320387	-0.854195	6	2.780684	-3.866339	-1.810550
1	7.746556	-3.775582	0.143952	6	2.289517	-4.166753	-0.541316
34	0.126634	-3.477288	0.229668	6	1.387558	-3.306554	0.080259
34	-0.515720	-0.789666	2.683211	6	0.984602	-2.139874	-0.573283
34	1.004307	0.832348	-2.966262	6	1.488335	-1.827716	-1.844421
34	1.645165	1.836770	0.586125	6	2.382999	-2.697340	-2.459456
O,O-WH11				15	-0.220396	-1.019874	0.198217
6	-3.483139	0.884377	1.200891	8	0.271455	0.485818	0.016930

34	-0.875474	-1.538866	2.114172	6	-3.681997	0.779695	0.479324
1	2.610265	-5.075835	-0.029051	6	-3.668112	2.117979	0.820067
1	0.994603	-3.528580	1.075	7	-3.305424	0.391130	-0.769629
1	1.218990	-0.886532	-2.332070	6	-3.247920	3.042457	-0.136646
1	2.783961	-2.450072	-3.444233	1	-3.939523	2.423703	1.829433
6	4.541231	-1.927612	1.584447	6	-2.880835	1.261816	-1.699747
6	4.711981	-1.420443	0.297507	6	-2.871248	2.609875	-1.413293
6	3.894514	-0.390079	-0.161963	1	-3.219206	4.104244	0.103164
6	2.904535	0.138911	0.667952	1	-2.513625	0.847562	-2.639087
6	2.750457	-0.353689	1.969547	1	-2.487802	3.307883	-2.155264
6	3.561747	-1.391141	2.420312	6	-4.308371	-1.459236	-2.075727
15	1.761997	1.439839	0.065866	1	-3.913509	-1.090125	-3.032959
34	1.484777	2.908751	1.562089	1	-4.402078	-2.551002	-2.113992
34	2.097178	1.975014	-1.961769	1	-5.305326	-1.024676	-1.906222
1	5.481496	-1.832776	-0.358607	6	3.703638	-2.316293	-1.481416
1	4.009302	0.005770	-1.173822	6	3.361777	-2.646441	-0.160922
1	1.988697	0.074734	2.624895	6	2.169494	-2.202337	0.382726
1	3.426465	-1.782144	3.430926	6	1.295263	-1.415907	-0.380433
1	5.178186	-2.740813	1.940277	6	1.639591	-1.083178	-1.695608
1	3.486228	-4.544829	-2.295370	6	2.832153	-1.534170	-2.250551
O,O-WH12				8	4.884564	-2.781917	-1.919438
6	-4.035606	-0.410672	1.230479	6	5.308369	-2.468101	-3.220317
1	-4.340191	-0.389745	2.274333	15	-0.269603	-0.826799	0.305137
6	-3.886458	-1.489621	0.439870	8	-0.462279	0.718566	-0.045051
6	-3.384479	-1.077366	-0.919495	34	-0.672893	-1.359528	2.288275
6	-4.147427	-2.917600	0.802141	1	4.062699	-3.244774	0.422260
6	-4.274064	-3.238388	2.266197	1	1.906648	-2.450961	1.413519
1	-3.330597	-2.977078	2.771328	1	0.998774	-0.422712	-2.286615
1	-5.081777	-2.654410	2.732497	1	3.078857	-1.243986	-3.271251
1	-4.479465	-4.308434	2.384010	1	6.285220	-2.947288	-3.355150
34	-1.588313	-1.838250	-1.301771	1	4.610570	-2.857093	-3.981436
8	-4.233961	-3.757937	-0.063514	1	5.421470	-1.379504	-3.360449

6	4.372976	0.312973	1.560976	7	-4.202218	0.614831	0.490023
6	4.330931	0.727684	0.222317	6	-6.019857	0.124629	-1.522055
6	3.194519	1.334544	-0.284058	1	-5.191435	1.859748	-2.497969
6	2.078154	1.550325	0.533711	6	-5.032588	-0.464446	0.599351
6	2.145284	1.185694	1.879551	6	-5.941053	-0.722990	-0.385666
6	3.278488	0.561953	2.396676	1	-6.744905	-0.090877	-2.308089
8	5.498175	-0.319370	1.949646	1	-4.909058	-1.086173	1.484655
6	5.585743	-0.810702	3.258759	1	-6.594192	-1.589987	-0.289344
15	0.511541	2.197589	-0.140118	6	-3.449046	0.827243	2.859247
34	-0.362737	3.567783	1.216838	1	-3.563795	-0.230864	3.140399
34	0.606205	2.607632	-2.223351	1	-2.604810	1.247706	3.417139
1	5.200909	0.534020	-0.407226	1	-4.367984	1.363837	3.147880
1	3.147629	1.628476	-1.335378	6	2.158783	3.206505	-0.759534
1	1.292476	1.376983	2.535049	6	1.524686	2.812661	-1.949050
1	3.286175	0.268787	3.446228	6	0.622487	1.760538	-1.945061
1	6.561235	-1.304638	3.345371	6	0.333575	1.074538	-0.754493
1	5.529818	-0.001761	4.007549	6	0.954452	1.486610	0.425712
1	4.791438	-1.547489	3.472105	6	1.849633	2.550047	0.434933
O,O-WH13				8	3.046095	4.213804	-0.856341
6	-3.261606	2.445201	-0.419238	6	3.657940	4.693560	0.318003
1	-3.026709	3.221729	-1.141896	15	-0.702592	-0.418111	-0.816732
6	-2.642304	2.201672	0.796902	8	0.353170	-1.648764	-1.012294
6	-3.188557	1.007730	1.383641	34	-2.125200	-0.468293	-2.330661
6	-1.594094	3.058062	1.420070	1	1.764943	3.346625	-2.869773
6	-1.136811	4.256097	0.623523	1	0.132589	1.457876	-2.873708
1	-0.718696	3.931436	-0.342048	1	0.737177	0.982017	1.367609
1	-1.981640	4.930324	0.416618	1	2.309746	2.835159	1.379467
1	-0.368304	4.791610	1.192617	1	4.328495	5.504373	0.009448
34	-1.479260	-0.676320	1.335864	1	2.911744	5.094242	1.024982
8	-1.137055	2.807851	2.514707	1	4.245754	3.905998	0.818301
6	-4.244557	1.454437	-0.602350	6	4.682804	0.819655	0.307066
6	-5.175105	1.198389	-1.631600	6	4.201585	0.221925	1.478816

6	3.224003	-0.761650	1.412082	6	-2.403970	0.834309	-0.400833
6	2.718059	-1.172118	0.174775	6	-1.819762	2.100129	-0.254347
6	3.226484	-0.595567	-0.992487	6	-3.760983	0.715243	-0.711753
6	4.197922	0.396512	-0.936282	6	-2.598310	3.240162	-0.422024
8	5.591722	1.806407	0.463797	1	-0.759535	2.197706	-0.012903
6	6.139676	2.411951	-0.680583	6	-4.534511	1.863601	-0.873937
15	1.437536	-2.448286	-0.019412	1	-4.203219	-0.276807	-0.831414
34	2.128328	-4.205930	-0.870388	6	-3.954993	3.122547	-0.739
34	0.259526	-2.678989	1.841768	1	-2.141096	4.225308	-0.311283
1	4.664	0.558702	2.437208	1	-5.594946	1.770298	-1.115625
1	2.831484	-1.202257	2.331788	34	2.900790	-1.185035	-1.746051
1	2.847754	-0.913789	-1.966575	34	1.355058	-1.427550	1.503481
1	4.552437	0.841983	-1.864950	1	-4.562930	4.020596	-0.859219
1	6.862922	3.155390	-0.323851	1	2.294289	5.293611	0.440076
1	6.666414	1.678846	-1.314458	Indolizine			
1	5.365464	2.921025	-1.280574	6	-3.314580	0.544323	-0.058
O,O-WH14				6	-3.369348	-0.887307	-0.111
6	1.916598	3.720572	-0.991460	6	-2.211924	-1.609901	-0.039
6	1.758485	2.352668	-1.187786	6	-0.953112	-0.945392	0.077
6	1.846398	1.476358	-0.096750	7	-0.944977	0.460093	0.035
6	2.108245	1.974959	1.180764	6	-2.118347	1.186485	0.064
6	2.268805	3.347196	1.369287	6	0.365875	-1.361996	0.179
6	2.168591	4.219603	0.287827	6	1.178830	-0.196662	0.142
1	1.846535	4.401238	-1.842233	6	0.342390	0.923968	-0.033
1	1.566925	1.961845	-2.189955	6	0.643869	2.382512	-0.063
1	2.181736	1.293977	2.031050	6	2.661096	-0.167381	-0.032
1	2.471173	3.734232	2.369805	6	3.367767	-1.507089	-0.152
15	1.579852	-0.289762	-0.443689	8	3.296388	0.867672	0.005
15	-1.401995	-0.660078	-0.169895	1	-4.231497	1.134345	-0.047
34	-0.684800	-0.387931	2.012596	1	-4.337378	-1.390285	-0.226
8	-0.003364	-0.247176	-0.943129	1	-2.220273	-2.700963	-0.013
34	-2.209502	-2.475985	-0.709538	1	-2.014550	2.270881	0.222

1	0.695744	-2.397669	0.318
1	1.729765	2.520303	-0.890
1	0.223807	2.879683	-0.890290
1	0.225345	2.879394	0.891066
1	3.083900	-2.092583	0.887620
1	3.082298	-2.093631	-0.886705
1	4.451489	-1.340867	-0.001188

Figure 33

O,O-WJ1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172
1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061
1	-4.199996	1.376948	0.207
6	-5.069288	-1.919326	-0.038
1	-3.674079	-3.572737	-0.154

1	-6.213733	-0.087007	0.087
34	0.079	-0.183	1.668777
34	-0.077	0.194	-1.668768
34	1.718838	-2.850294	-0.372
34	-1.718852	2.850296	0.392
1	5.952123	2.562719	0.021
1	-5.952103	-2.562746	-0.087

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636

1	0.497232	1.881452	-1.682557	1	-3.979808	-3.032677	-1.148636
				6	-3.559250	-1.082002	-0.256358
O,O-WJ2				6	-2.894246	-0.572669	1.042333
6	2.601478	-3.057628	-2.239605	6	-4.359890	-0.173277	-1.137011
6	2.258194	-1.874751	-1.594014	6	-4.795729	-0.710624	-2.479760
6	3.164291	-1.277956	-0.707411	1	-3.992082	-1.262915	-2.984113
6	4.407960	-1.868929	-0.475598	1	-5.646768	-1.395199	-2.329095
6	4.745231	-3.055683	-1.127368	1	-5.128783	0.125729	-3.105431
6	3.844698	-3.649924	-2.008128	8	-1.929403	0.297386	1.020811
1	1.894075	-3.515087	-2.934522	8	-4.721245	0.909743	-0.734785
1	1.283926	-1.416737	-1.789237	6	-2.752021	-2.992806	0.720441
1	5.108331	-1.391707	0.214455	6	-2.369972	-4.305124	1.005797
1	5.720108	-3.513306	-0.946378	7	-2.367922	-2.001858	1.542609
15	2.712053	0.275578	0.159302	6	-1.582620	-4.531763	2.128472
15	-0.356237	0.957117	-0.470202	1	-2.677643	-5.117718	0.347636
6	-0.939051	2.583166	0.120884	6	-1.608521	-2.188115	2.619792
6	-0.137187	3.359011	0.961033	6	-1.192654	-3.466833	2.950023
6	-2.194438	3.039341	-0.282368	1	-1.265	-5.547037	2.367554
6	-0.598375	4.598066	1.398592	1	-1.348414	-1.288938	3.183425
1	0.847861	3.002464	1.272781	1	-0.566906	-3.626241	3.827545
6	-2.644138	4.283450	0.153485	6	-3.998551	-0.272	2.053509
1	-2.826097	2.418254	-0.919198	1	-3.526970	0.010767	3.023602
6	-1.849337	5.062812	0.992965	1	-4.469724	0.717421	1.681839
1	0.028487	5.204747	2.055258	1	-4.761699	-0.985185	2.167456
1	-3.626646	4.639805	-0.162831	O,O-WJ3			
34	1.728270	1.610527	-1.375582	6	2.129327	-3.641190	-1.389810
34	0.713576	-0.163058	1.186670	6	1.898855	-2.322010	-1.017411
34	4.210625	1.064508	1.386049	6	2.964185	-1.525652	-0.577328
34	-1.318558	0.059561	-2.135411	6	4.255161	-2.053918	-0.519851
1	4.111944	-4.577009	-2.520530	6	4.479987	-3.377832	-0.898137
1	-2.206663	6.037054	1.334563	6	3.420085	-4.171207	-1.330069
6	-3.526903	-2.426557	-0.366005	1	1.294901	-4.259613	-1.726706

1	0.886401	-1.913819	-1.066652	6	-2.699732	-2.783191	0.379719
1	5.078212	-1.423235	-0.174792	6	-2.428011	-4.159254	0.702571
1	5.490334	-3.789146	-0.850215	7	-2.216332	-1.832867	1.271839
15	2.664361	0.206170	-0.056369	6	-1.768511	-4.465207	1.853366
15	-0.533070	0.910340	0.055275	1	-2.762604	-4.931747	0.009867
6	-0.761199	2.704303	0.295426	6	-1.607040	-2.145923	2.445152
6	0.320563	3.518183	0.644790	6	-1.347144	-3.442336	2.766522
6	-2.041785	3.245632	0.154143	1	-1.559462	-5.510495	2.091919
6	0.116445	4.879167	0.849530	1	-1.332295	-1.300371	3.078482
1	1.322397	3.096749	0.757392	1	-0.826334	-3.685149	3.691013
6	-2.229129	4.614757	0.336859	6	-3.942362	-0.202601	1.846590
1	-2.893367	2.607699	-0.091228	1	-3.603016	-0.230457	2.890953
6	-1.154894	5.430300	0.687038	1	-4.354396	0.787038	1.627976
1	0.959963	5.512052	1.131794	1	-4.718243	-0.967751	1.700348
1	-3.226590	5.040793	0.211556	O,O-WJ4			
34	1.364968	1.208014	-1.575991	6	-2.392583	-3.646771	1.673185
34	0.958874	-0.010281	1.477730	6	-2.131513	-2.306700	1.404407
34	4.350799	1.223803	0.638514	6	-3.007775	-1.574458	0.594774
34	-1.515781	-0.162934	-1.631944	6	-4.144504	-2.188562	0.062986
1	3.597841	-5.208883	-1.621095	6	-4.401057	-3.531316	0.337197
1	-1.308243	6.501121	0.837805	6	-3.526588	-4.261274	1.139486
6	-3.347149	-2.190116	-0.664389	1	-1.707731	-4.215052	2.306075
1	-3.733548	-2.718322	-1.531526	1	-1.246861	-1.822664	1.824583
6	-3.163293	-0.718325	-0.565949	1	-4.827007	-1.605656	-0.560386
6	-2.750819	-0.486443	0.934075	1	-5.292425	-4.006134	-0.078141
6	-4.271475	0.172483	-1.117504	15	-2.646217	0.180959	0.193693
6	-5.038666	-0.367589	-2.299180	15	0.661549	0.862614	-0.294468
1	-4.361661	-0.774394	-3.065150	6	0.626951	2.658536	-0.470884
1	-5.684109	-1.192957	-1.961734	6	-0.536433	3.333169	-0.851582
1	-5.655497	0.431391	-2.726200	6	1.824591	3.348924	-0.253809
8	-1.816363	0.506876	1.143006	6	-0.495535	4.714215	-1.015485
8	-4.517055	1.261530	-0.652966	1	-1.474620	2.795553	-1.009203

6	1.847191	4.732223	-0.413773	6	4.157133	-0.163166	-1.777828
1	2.736049	2.815475	0.027184	1	3.889211	-0.265649	-2.838109
6	0.691339	5.412937	-0.793889	1	4.524623	0.850397	-1.591121
1	-1.402461	5.244381	-1.311195	1	4.941130	-0.893673	-1.533536
1	2.778119	5.276319	-0.243591	O,O-WJ5			
34	-1.514183	1.154481	1.766510	6	-2.718507	1.608747	-0.251372
34	-0.914990	-0.213039	-1.408632	1	-3.287197	2.296858	-0.871837
34	-4.232309	1.183516	-0.734114	6	-1.436561	1.764757	0.192949
34	1.456956	-0.028322	1.554916	6	-1.100394	0.636590	1.175872
1	-3.729386	-5.313171	1.353182	6	-0.616391	3.015223	0.137798
1	0.715283	6.497629	-0.920073	6	-0.984550	4.028754	-0.916782
6	3.468105	-2.006257	0.801609	1	-1.183954	3.554950	-1.886728
1	3.828306	-2.466910	1.717199	1	-1.895315	4.559806	-0.594164
6	3.227873	-0.555725	0.603884	1	-0.170248	4.756403	-1.011479
6	2.923903	-0.437351	-0.923945	8	0.110815	0.019859	1.114181
6	4.227193	0.439075	1.172888	8	0.237307	3.226981	0.971490
6	4.945601	0.025877	2.432460	6	-3.172785	0.296433	0.099160
1	4.247323	-0.387991	3.175351	6	-4.331999	-0.419710	-0.217886
1	5.670544	-0.765797	2.188335	7	-2.226730	-0.312543	0.860623
1	5.471325	0.891418	2.851431	6	-4.445780	-1.727094	0.228897
8	1.973483	0.532593	-1.258853	1	-5.107943	0.049967	-0.821725
8	4.424019	1.514897	0.654937	6	-2.302995	-1.580518	1.290920
6	2.901819	-2.683393	-0.239817	6	-3.424388	-2.322936	0.985674
6	2.699039	-4.083485	-0.501666	1	-5.336524	-2.306154	-0.023186
7	2.433055	-1.800200	-1.208786	1	-1.443502	-1.957622	1.846218
6	2.110069	-4.474356	-1.664266	1	-3.489853	-3.359390	1.313204
1	3.025009	-4.805512	0.247104	6	-1.288694	1.122216	2.618067
6	1.889475	-2.197423	-2.392453	1	-1.165119	0.270528	3.300865
6	1.693770	-3.517248	-2.650294	1	-0.512551	1.868319	2.821796
1	1.950024	-5.537547	-1.856099	1	-2.281289	1.572797	2.755621
1	1.606262	-1.397495	-3.079145	6	5.187969	0.178270	0.966040
1	1.221424	-3.830481	-3.579619	6	4.824248	-1.075118	0.479327

6	3.502771	-1.324602	0.107864	1	-3.797427	-3.133383	1.602235
6	2.547558	-0.313594	0.217069	6	-1.370709	1.258954	2.407446
6	2.912192	0.948596	0.704333	1	-1.450619	0.477615	3.175374
6	4.229745	1.187710	1.081246	1	-0.553737	1.940871	2.662037
15	0.825490	-0.597562	-0.314943	1	-2.316393	1.816158	2.357138
1	5.570945	-1.867084	0.389794	6	5.215688	0.494739	0.783433
1	3.202831	-2.307696	-0.263806	6	4.950341	-0.758543	0.235346
1	2.164765	1.741061	0.791601	6	3.636710	-1.135820	-0.038679
1	4.511340	2.170310	1.466054	6	2.590213	-0.251671	0.233765
34	0.330766	-2.635619	-0.559393	6	2.853900	1.010775	0.781966
34	0.267226	0.800886	-1.847959	6	4.168137	1.376064	1.056871
1	6.223041	0.372028	1.257106	15	0.880123	-0.727794	-0.143087
6	-2.607652	1.516424	-0.531641	34	0.563848	-2.747832	-0.516227
1	-3.096724	2.166846	-1.251249	34	0.003764	0.698636	-1.636174
6	-1.186303	1.576699	-0.148160	1	5.767261	-1.450971	0.022506
6	-1.093199	0.594605	1.061838	1	3.415549	-2.120684	-0.456923
6	-0.527824	2.937698	0.012974	1	2.037906	1.705649	0.994113
6	-0.984055	4.016193	-0.938939	1	4.373881	2.357283	1.489346
1	-1.113169	3.634007	-1.961506	1	6.245588	0.787561	0.999955
1	-1.962482	4.390797	-0.599050	O,O-WJ6			
1	-0.259737	4.838780	-0.928368	6	3.180682	-1.225909	2.450297
8	0.109232	-0.089058	1.183723	6	2.018640	-1.359079	1.696085
8	0.311614	3.151677	0.857247	6	2.082358	-1.963674	0.435517
6	-3.130414	0.337235	-0.065875	6	3.303708	-2.432339	-0.062045
6	-4.387739	-0.324118	-0.265528	6	4.457152	-2.312196	0.710269
7	-2.215060	-0.316600	0.746129	6	4.396717	-1.708083	1.965552
6	-4.613655	-1.532191	0.325785	1	3.128497	-0.744722	3.429096
1	-5.134928	0.152372	-0.900258	1	1.066107	-0.990995	2.086977
6	-2.443144	-1.511321	1.348573	1	3.346600	-2.898211	-1.049031
6	-3.625368	-2.157603	1.151546	1	5.405407	-2.697446	0.328588
1	-5.567151	-2.039584	0.162724	15	0.560022	-2.305592	-0.494050
1	-1.619395	-1.907209	1.944878	15	-1.382232	0.457635	0.718507

6	-2.848983	-0.422757	0.094759	1	0.552371	0.383749	-2.796189
6	-3.929781	-0.714307	0.929058	1	-0.776558	1.575732	-2.700806
6	-2.868269	-0.820243	-1.247616	1	0.822252	2.094643	-3.314187
6	-5.031266	-1.399748	0.418680	34	-0.867070	-3.297724	0.602141
1	-3.891022	-0.421148	1.981053	34	0.791806	-2.295382	-2.562872
6	-3.967692	-1.507717	-1.749519	34	-1.174160	0.484303	2.804870
1	-2.006015	-0.619201	-1.887214	34	-1.860552	2.582304	-0.121290
6	-5.050499	-1.796063	-0.917418	1	-5.911500	-2.339789	-1.312704
1	-5.873779	-1.634152	1.072778	1	5.301953	-1.616676	2.570679
1	-3.973182	-1.833313	-2.791688	O,O-WJ7			
6	0.958903	2.998172	0.782466	6	3.017089	-1.884792	2.699
1	0.757068	3.580933	1.676378	6	1.889482	-1.688491	1.807393
6	0.053687	2.889726	-0.408717	6	1.943637	-1.944726	0.431895
6	0.718770	1.827378	-1.238446	6	3.134163	-2.403133	-0.136630
6	0.213556	4.266873	-1.152078	6	4.260062	-2.606066	0.662497
6	-0.444613	5.459116	-0.504608	6	4.203719	-2.348857	2.031603
1	-1.435678	5.593998	-0.966531	1	2.960875	-1.687790	3.673142
1	-0.592878	5.337372	0.575055	1	0.956754	-1.351031	2.265548
1	0.154985	6.351850	-0.723479	1	3.169772	-2.603724	-1.210539
8	-0.165676	0.100875	-0.187074	1	5.182268	-2.981234	0.212101
8	0.845143	4.356362	-2.170598	15	0.405223	-1.879115	-0.568196
6	2.090862	2.317078	0.505451	15	-1.392269	0.270146	0.771718
6	3.346326	2.165896	1.194270	6	-2.913674	-0.444315	0.097069
7	1.944557	1.659261	-0.754252	6	-3.996753	-0.708540	0.937939
6	4.336350	1.438693	0.632374	6	-2.994210	-0.713949	-1.276493
1	3.461611	2.656182	2.160738	6	-5.166445	-1.243360	0.402665
6	2.964643	0.875200	-1.295057	1	-3.910783	-0.511818	2.008859
6	4.135611	0.777484	-0.641105	6	-4.165395	-1.247467	-1.799813
1	5.293643	1.321429	1.141519	1	-2.134885	-0.543011	-1.930626
1	2.731913	0.353565	-2.222212	6	-5.250207	-1.511826	-0.962164
1	4.925512	0.158898	-1.064644	1	-6.011726	-1.459904	1.058780
6	0.306033	1.435647	-2.597636	1	-4.224537	-1.475111	-2.865541

6	1.052471	2.613595	0.999187	6	-4.112717	-1.598506	-1.627312
1	0.789185	2.926832	2.005319	6	-2.793372	-1.552486	-1.180852
6	0.266457	2.902521	-0.237009	6	-2.494493	-1.584521	0.182024
6	1.027802	2.204732	-1.309492	6	-3.543119	-1.682275	1.102721
6	0.282640	4.449226	-0.489661	6	-4.861246	-1.734561	0.670768
6	-0.470142	5.306966	0.492934	6	-5.157142	-1.691277	-0.698505
1	-1.456818	5.535989	0.060700	1	-4.310856	-1.566528	-2.698820
1	-0.637127	4.817594	1.459907	1	-1.984317	-1.485957	-1.911321
1	0.071159	6.253740	0.616399	1	-3.315302	-1.709592	2.171430
8	-0.127387	-0.267121	-0.052567	1	-5.687253	-1.816883	1.379466
8	0.881150	4.899631	-1.428114	15	-0.760339	-1.650525	0.744074
6	2.153801	1.919533	0.642453	15	1.121380	0.180876	-0.990068
6	3.296991	1.435156	1.369247	6	2.582239	-0.778278	-0.547857
7	2.106305	1.679050	-0.770919	6	3.549936	-1.044977	-1.520956
6	4.292762	0.806450	0.708253	6	2.788730	-1.231416	0.771488
1	3.324309	1.598666	2.446043	6	4.704196	-1.751130	-1.201968
6	3.122041	0.966835	-1.425163	1	3.394474	-0.698635	-2.544868
6	4.190781	0.563649	-0.715346	6	3.940591	-1.922454	1.094803
1	5.167294	0.438860	1.244304	1	2.039463	-1.062679	1.551421
1	2.953593	0.745341	-2.475997	6	4.906980	-2.193615	0.113347
1	4.975624	0.007590	-1.227160	1	5.434439	-1.950754	-1.985383
6	0.687714	2.108936	-2.733499	1	4.105368	-2.291583	2.107428
1	0.512271	1.035016	-2.960695	6	-0.580124	3.157370	-0.985923
1	-0.216948	2.683245	-2.956909	1	-0.446076	3.343303	-2.045010
1	1.520079	2.465170	-3.358636	6	0.367797	3.455606	0.062421
34	-0.934426	-3.331550	0.126737	6	-0.252334	2.996851	1.319037
34	0.822061	-1.611045	-2.645581	6	1.331511	4.625731	-0.039434
34	-1.226463	0.398602	2.844003	6	1.878066	4.877116	-1.417758
34	-1.633664	2.329093	-0.258804	1	2.103324	3.931741	-1.933991
1	-6.165509	-1.939043	-1.377707	1	1.117034	5.409737	-2.009983
1	5.082616	-2.520126	2.657906	1	2.772523	5.506685	-1.345149
O,O-WJ8				8	-0.223900	-0.419077	-0.423478

8	1.614134	5.285272	0.928341	6	-3.765970	-0.095252	0.322761
6	-1.664670	2.552222	-0.409210	6	-3.105122	0.181884	-1.002680
6	-2.892449	2.050465	-0.940746	6	-4.604653	-1.310173	0.566960
7	-1.457728	2.466267	0.978879	6	-4.917687	-1.647602	1.998892
6	-3.841036	1.579967	-0.090901	1	-3.974308	-1.838517	2.534352
1	-3.029731	2.059883	-2.021363	1	-5.429796	-0.812291	2.499845
6	-2.419093	1.945752	1.833408	1	-5.553858	-2.539588	2.027399
6	-3.604120	1.542731	1.324432	34	-1.781917	-1.216214	-1.492733
1	-4.783464	1.191171	-0.478783	8	-4.990968	-1.977417	-0.364916
1	-2.156625	1.886073	2.885702	6	-2.647820	1.877017	0.551367
1	-4.359107	1.139532	1.997175	6	-2.089840	3.055232	1.006977
6	0.070734	3.333586	2.733899	7	-2.428023	1.468729	-0.728440
1	0.051924	2.423003	3.351367	6	-1.290800	3.793164	0.133292
1	1.052159	3.812598	2.801635	1	-2.242450	3.363562	2.040169
1	-0.682414	4.044167	3.111530	6	-1.650547	2.155123	-1.581178
8	5.986096	-2.876651	0.520138	6	-1.087028	3.346812	-1.177232
8	-6.465483	-1.733051	-1.028833	1	-0.827272	4.720271	0.467062
6	-6.824617	-1.770625	-2.382988	1	-1.460757	1.704151	-2.555597
1	-6.387515	-2.643635	-2.897435	1	-0.422218	3.876194	-1.857328
1	-7.918055	-1.849258	-2.417390	6	-4.084816	0.318832	-2.168731
1	-6.517410	-0.853493	-2.916267	1	-3.559005	0.578183	-3.098553
6	6.982612	-3.216595	-0.409044	1	-4.615133	-0.631745	-2.300476
1	6.584918	-3.855702	-1.215341	1	-4.819801	1.105048	-1.938873
1	7.447341	-2.320387	-0.854195	6	2.780684	-3.866339	-1.810550
1	7.746556	-3.775582	0.143952	6	2.289517	-4.166753	-0.541316
34	0.126634	-3.477288	0.229668	6	1.387558	-3.306554	0.080259
34	-0.515720	-0.789666	2.683211	6	0.984602	-2.139874	-0.573283
34	1.004307	0.832348	-2.966262	6	1.488335	-1.827716	-1.844421
34	1.645165	1.836770	0.586125	6	2.382999	-2.697340	-2.459456
O,O-WJ9				15	-0.220396	-1.019874	0.198217
6	-3.483139	0.884377	1.200891	8	0.271455	0.485818	0.016930
1	-3.784988	0.948	2.243826	34	-0.875474	-1.538866	2.114172

1	2.610265	-5.075835	-0.029051	6	-3.668112	2.117979	0.820067
1	0.994603	-3.528580	1.075	7	-3.305424	0.391130	-0.769629
1	1.218990	-0.886532	-2.332070	6	-3.247920	3.042457	-0.136646
1	2.783961	-2.450072	-3.444233	1	-3.939523	2.423703	1.829433
6	4.541231	-1.927612	1.584447	6	-2.880835	1.261816	-1.699747
6	4.711981	-1.420443	0.297507	6	-2.871248	2.609875	-1.413293
6	3.894514	-0.390079	-0.161963	1	-3.219206	4.104244	0.103164
6	2.904535	0.138911	0.667952	1	-2.513625	0.847562	-2.639087
6	2.750457	-0.353689	1.969547	1	-2.487802	3.307883	-2.155264
6	3.561747	-1.391141	2.420312	6	-4.308371	-1.459236	-2.075727
15	1.761997	1.439839	0.065866	1	-3.913509	-1.090125	-3.032959
34	1.484777	2.908751	1.562089	1	-4.402078	-2.551002	-2.113992
34	2.097178	1.975014	-1.961769	1	-5.305326	-1.024676	-1.906222
1	5.481496	-1.832776	-0.358607	6	3.703638	-2.316293	-1.481416
1	4.009302	0.005770	-1.173822	6	3.361777	-2.646441	-0.160922
1	1.988697	0.074734	2.624895	6	2.169494	-2.202337	0.382726
1	3.426465	-1.782144	3.430926	6	1.295263	-1.415907	-0.380433
1	5.178186	-2.740813	1.940277	6	1.639591	-1.083178	-1.695608
1	3.486228	-4.544829	-2.295370	6	2.832153	-1.534170	-2.250551
O,O-WJ10				8	4.884564	-2.781917	-1.919438
6	-4.035606	-0.410672	1.230479	6	5.308369	-2.468101	-3.220317
1	-4.340191	-0.389745	2.274333	15	-0.269603	-0.826799	0.305137
6	-3.886458	-1.489621	0.439870	8	-0.462279	0.718566	-0.045051
6	-3.384479	-1.077366	-0.919495	34	-0.672893	-1.359528	2.288275
6	-4.147427	-2.917600	0.802141	1	4.062699	-3.244774	0.422260
6	-4.274064	-3.238388	2.266197	1	1.906648	-2.450961	1.413519
1	-3.330597	-2.977078	2.771328	1	0.998774	-0.422712	-2.286615
1	-5.081777	-2.654410	2.732497	1	3.078857	-1.243986	-3.271251
1	-4.479465	-4.308434	2.384010	1	6.285220	-2.947288	-3.355150
34	-1.588313	-1.838250	-1.301771	1	4.610570	-2.857093	-3.981436
8	-4.233961	-3.757937	-0.063514	1	5.421470	-1.379504	-3.360449
6	-3.681997	0.779695	0.479324	6	4.372976	0.312973	1.560976

6	4.330931	0.727684	0.222317	6	-6.019857	0.124629	-1.522055
6	3.194519	1.334544	-0.284058	1	-5.191435	1.859748	-2.497969
6	2.078154	1.550325	0.533711	6	-5.032588	-0.464446	0.599351
6	2.145284	1.185694	1.879551	6	-5.941053	-0.722990	-0.385666
6	3.278488	0.561953	2.396676	1	-6.744905	-0.090877	-2.308089
8	5.498175	-0.319370	1.949646	1	-4.909058	-1.086173	1.484655
6	5.585743	-0.810702	3.258759	1	-6.594192	-1.589987	-0.289344
15	0.511541	2.197589	-0.140118	6	-3.449046	0.827243	2.859247
34	-0.362737	3.567783	1.216838	1	-3.563795	-0.230864	3.140399
34	0.606205	2.607632	-2.223351	1	-2.604810	1.247706	3.417139
1	5.200909	0.534020	-0.407226	1	-4.367984	1.363837	3.147880
1	3.147629	1.628476	-1.335378	6	2.158783	3.206505	-0.759534
1	1.292476	1.376983	2.535049	6	1.524686	2.812661	-1.949050
1	3.286175	0.268787	3.446228	6	0.622487	1.760538	-1.945061
1	6.561235	-1.304638	3.345371	6	0.333575	1.074538	-0.754493
1	5.529818	-0.001761	4.007549	6	0.954452	1.486610	0.425712
1	4.791438	-1.547489	3.472105	6	1.849633	2.550047	0.434933
O,O-WJ11				8	3.046095	4.213804	-0.856341
6	-3.261606	2.445201	-0.419238	6	3.657940	4.693560	0.318003
1	-3.026709	3.221729	-1.141896	15	-0.702592	-0.418111	-0.816732
6	-2.642304	2.201672	0.796902	8	0.353170	-1.648764	-1.012294
6	-3.188557	1.007730	1.383641	34	-2.125200	-0.468293	-2.330661
6	-1.594094	3.058062	1.420070	1	1.764943	3.346625	-2.869773
6	-1.136811	4.256097	0.623523	1	0.132589	1.457876	-2.873708
1	-0.718696	3.931436	-0.342048	1	0.737177	0.982017	1.367609
1	-1.981640	4.930324	0.416618	1	2.309746	2.835159	1.379467
1	-0.368304	4.791610	1.192617	1	4.328495	5.504373	0.009448
34	-1.479260	-0.676320	1.335864	1	2.911744	5.094242	1.024982
8	-1.137055	2.807851	2.514707	1	4.245754	3.905998	0.818301
6	-4.244557	1.454437	-0.602350	6	4.682804	0.819655	0.307066
6	-5.175105	1.198389	-1.631600	6	4.201585	0.221925	1.478816
7	-4.202218	0.614831	0.490023	6	3.224003	-0.761650	1.412082

6	2.718059	-1.172118	0.174775	6	-1.819762	2.100129	-0.254347
6	3.226484	-0.595567	-0.992487	6	-3.760983	0.715243	-0.711753
6	4.197922	0.396512	-0.936282	6	-2.598310	3.240162	-0.422024
8	5.591722	1.806407	0.463797	1	-0.759535	2.197706	-0.012903
6	6.139676	2.411951	-0.680583	6	-4.534511	1.863601	-0.873937
15	1.437536	-2.448286	-0.019412	1	-4.203219	-0.276807	-0.831414
34	2.128328	-4.205930	-0.870388	6	-3.954993	3.122547	-0.739
34	0.259526	-2.678989	1.841768	1	-2.141096	4.225308	-0.311283
1	4.664	0.558702	2.437208	1	-5.594946	1.770298	-1.115625
1	2.831484	-1.202257	2.331788	34	2.900790	-1.185035	-1.746051
1	2.847754	-0.913789	-1.966575	34	1.355058	-1.427550	1.503481
1	4.552437	0.841983	-1.864950	1	-4.562930	4.020596	-0.859219
1	6.862922	3.155390	-0.323851	1	2.294289	5.293611	0.440076
1	6.666414	1.678846	-1.314458	Indolizine			
1	5.365464	2.921025	-1.280574	6	-3.314580	0.544323	-0.058
O,O-WJ12				6	-3.369348	-0.887307	-0.111
6	1.916598	3.720572	-0.991460	6	-2.211924	-1.609901	-0.039
6	1.758485	2.352668	-1.187786	6	-0.953112	-0.945392	0.077
6	1.846398	1.476358	-0.096750	7	-0.944977	0.460093	0.035
6	2.108245	1.974959	1.180764	6	-2.118347	1.186485	0.064
6	2.268805	3.347196	1.369287	6	0.365875	-1.361996	0.179
6	2.168591	4.219603	0.287827	6	1.178830	-0.196662	0.142
1	1.846535	4.401238	-1.842233	6	0.342390	0.923968	-0.033
1	1.566925	1.961845	-2.189955	6	0.643869	2.382512	-0.063
1	2.181736	1.293977	2.031050	6	2.661096	-0.167381	-0.032
1	2.471173	3.734232	2.369805	6	3.367767	-1.507089	-0.152
15	1.579852	-0.289762	-0.443689	8	3.296388	0.867672	0.005
15	-1.401995	-0.660078	-0.169895	1	-4.231497	1.134345	-0.047
34	-0.684800	-0.387931	2.012596	1	-4.337378	-1.390285	-0.226
8	-0.003364	-0.247176	-0.943129	1	-2.220273	-2.700963	-0.013
34	-2.209502	-2.475985	-0.709538	1	-2.014550	2.270881	0.222
6	-2.403970	0.834309	-0.400833	1	0.695744	-2.397669	0.318

1	1.729765	2.520303	-0.890
1	0.223807	2.879683	-0.890290
1	0.225345	2.879394	0.891066
1	3.083900	-2.092583	0.887620
1	3.082298	-2.093631	-0.886705
1	4.451489	-1.340867	-0.001188

Figure 40

N,O-A1

6	-1.930290	0.408578	-1.367349
1	-1.689527	-0.219937	-2.237521
6	-0.670027	0.957777	-0.728202
6	-0.661971	2.309311	-0.178057
6	0.448768	0.142603	-0.608671
6	0.412915	-1.291340	-1.070791
1	1.197865	-1.888977	-0.592444
1	-0.554921	-1.746003	-0.826527
1	0.548861	-1.363429	-2.161532
8	0.320394	2.796580	0.394728
6	-2.829272	-0.375414	-0.429555
6	-3.333834	-1.633406	-0.781114
7	-3.122863	0.193842	0.742669
6	-4.155681	-2.311521	0.115318
1	-3.081530	-2.073296	-1.748706
6	-3.909095	-0.454993	1.594845
6	-4.451567	-1.713437	1.336515
1	-4.557872	-3.295573	-0.136339
1	-4.121709	0.052896	2.542020
1	-5.087973	-2.205476	2.073792
6	-1.909145	3.160048	-0.292752
1	-2.758714	2.642232	0.175015
1	-1.723006	4.114851	0.212788
1	-2.160851	3.355870	-1.346914

7	1.589	0.608752	-0.028432
1	1.442024	1.561599	0.355050
6	2.837381	0.001943	0.106181
6	3.464265	-0.685960	-0.941875
6	3.517384	0.149321	1.323508
6	4.726894	-1.245524	-0.758146
1	2.971318	-0.761556	-1.911971
6	4.786073	-0.395952	1.493279
1	3.031530	0.691116	2.137866
6	5.394161	-1.105380	0.457483
1	5.200807	-1.780062	-1.584507
1	5.300129	-0.272304	2.448964
1	6.386079	-1.540296	0.594635
1	-2.527440	1.237618	-1.774861

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6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247

15	-0.901144	-1.183693	-0.071	6	-6.575757	-2.137635	-0.229085
16	-0.184	0.609	-1.552090	1	-7.598145	-2.349814	0.104217
16	-0.116	0.185	1.553327	1	-6.550899	-2.137520	-1.331831
16	0.492940	3.068803	-0.771	1	-5.902560	-2.925468	0.148168
16	-0.492242	-3.068189	-0.603	15	-0.937468	1.631443	-0.512316
6	-2.652613	-0.746168	-0.150	15	0.725823	-0.944103	0.573580
6	-3.051857	0.594301	0.287	16	-0.037424	0.374100	1.823646
6	-3.625394	-1.755670	-0.493	16	0.299548	0.620838	-1.668058
6	-4.400241	0.930604	0.362	16	-0.803876	3.498794	-0.124871
1	-2.307453	1.395396	0.536	16	-0.045896	-2.658290	0.185837
6	-4.970864	-1.427866	-0.432	6	2.490809	-0.781376	0.315290
1	-3.315267	-2.803163	-0.809	6	3.153407	0.389017	0.699605
6	-5.371350	-0.082808	0.013	6	3.216076	-1.815551	-0.301885
1	-4.679935	1.983600	0.725	6	4.518843	0.533126	0.484738
1	-5.741489	-2.199662	-0.707	1	2.590010	1.198244	1.169247
8	-6.693755	0.139912	0.103	6	4.574104	-1.679850	-0.516320
6	-7.175115	1.459861	0.447	1	2.700275	-2.728593	-0.606940
1	-6.850662	2.011249	-0.898237	6	5.239282	-0.503636	-0.127213
1	-8.269204	1.391129	0.340	1	5.008365	1.456113	0.793375
1	-6.850803	2.010720	0.899507	1	5.155828	-2.472745	-0.988319
N,O-A2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	N,O-A3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948

8	-3.885436	-0.498129	-0.230	1	3.267094	3.237489	-0.099520
6	-4.759250	0.603778	-0.315	8	0.022801	-0.252040	1.194807
15	2.021612	0.066269	-0.039	6	-0.679651	3.137631	-0.021047
16	2.707743	1.856016	-0.605	6	-1.281146	4.069735	-0.867564
16	2.982996	-1.591296	0.363	7	-1.360960	2.096844	0.440637
1	-2.254777	-2.424604	-0.001081	6	-2.613077	3.877870	-1.224613
1	0.236002	-2.243390	-0.730	1	-0.711497	4.919826	-1.246911
1	-0.098402	2.054262	0.001405	6	-2.636977	1.905013	0.123732
1	-2.554405	1.881627	0.001668	6	-3.310819	2.779919	-0.721033
1	-5.775254	0.192793	-0.002410	1	-3.106513	4.581597	-1.898511
1	-4.625439	1.226573	0.899941	1	-3.125265	1.023316	0.548801
1	-4.622697	1.228758	-0.898633	1	-4.353706	2.595968	-0.981681
N,O-A4				6	-0.310217	1.368038	2.839957
15	-0.031410	-1.175269	-0.460215	1	-0.349027	2.455499	2.975508
6	-1.839669	-1.370891	-0.352772	1	-1.297298	0.924995	3.023739
6	-2.413751	-1.939466	0.785931	1	0.402128	0.951809	3.570770
6	-2.673950	-0.960591	-1.399535	8	-5.970426	-1.722537	-0.126185
6	-3.796091	-2.066929	0.905314	6	-6.610010	-2.282509	0.988639
1	-1.766431	-2.286246	1.594500	1	-6.316272	-3.334872	1.144234
6	-4.050904	-1.098678	-1.300855	1	-6.400181	-1.714044	1.911596
1	-2.226581	-0.512056	-2.289429	1	-7.687045	-2.241607	0.786117
6	-4.625294	-1.642873	-0.143371	16	0.470521	0.018979	-1.922244
1	-4.212558	-2.508772	1.810499	16	0.941610	-2.788691	0.043941
1	-4.712367	-0.787629	-2.111225	7	2.858582	0.042937	0.787496
6	0.748570	3.206621	0.472065	1	2.154353	-0.650873	1.032698
1	1.372913	3.661579	-0.305523	6	4.076164	-0.533059	0.313130
6	1.208495	1.809727	0.817421	6	5.222123	-0.496750	1.110019
6	0.192527	0.984556	1.474134	6	4.108041	-1.163777	-0.932847
6	2.453676	1.311534	0.503333	6	6.406809	-1.072624	0.654768
6	3.498285	2.170523	-0.155808	1	5.171911	-0.014079	2.088522
1	4.483735	2.010269	0.298899	6	5.293117	-1.744735	-1.379839
1	3.577856	1.878160	-1.214674	1	3.194046	-1.195515	-1.530131

6	6.442852	-1.697585	-0.591433	6	1.653853	2.194787	-1.353224
1	7.302263	-1.040606	1.279430	6	2.503903	3.272159	-1.220751
1	5.315501	-2.241849	-2.351822	1	2.708676	5.270118	-0.421831
1	7.368871	-2.154596	-0.947228	1	1.930048	1.244649	-1.813599
1	0.774150	3.900601	1.335136	1	3.514789	3.214561	-1.622782
N,O-A5				6	-0.985656	0.834950	-2.316166
15	0.726542	-0.389811	1.131278	1	-0.143415	0.478042	-2.926108
6	2.296530	-1.119739	0.536765	1	-1.757714	0.055891	-2.300413
6	3.503120	-0.433995	0.652092	1	-1.406944	1.750518	-2.754143
6	2.292642	-2.379644	-0.081688	8	5.766843	-2.842429	-0.969055
6	4.693260	-0.976107	0.159951	6	7.019530	-2.234630	-0.822228
1	3.509361	0.538701	1.151321	1	7.071481	-1.264378	-1.347555
6	3.463300	-2.924886	-0.581564	1	7.275348	-2.075807	0.239943
1	1.353720	-2.934410	-0.149536	1	7.755213	-2.916615	-1.266013
6	4.676401	-2.227966	-0.463048	16	-0.487238	-1.774318	1.833767
1	5.622545	-0.419354	0.283376	16	1.068152	1.289601	2.125055
1	3.474304	-3.905158	-1.061047	7	-2.873306	-0.424308	-0.015126
6	-1.385475	3.026706	0.428002	1	-2.064809	-0.984450	0.283048
1	-1.314063	3.125795	1.525243	6	-4.044151	-1.127479	-0.273595
6	-1.663905	1.612561	-0.003592	6	-5.145514	-0.524357	-0.900568
6	-0.540804	1.075322	-0.875029	6	-4.113555	-2.492071	0.054084
6	-2.785367	0.924624	0.296398	6	-6.296801	-1.263527	-1.163473
6	-3.896934	1.585987	1.075265	1	-5.090223	0.524115	-1.200998
1	-4.391453	2.384249	0.499837	6	-5.260724	-3.223327	-0.231485
1	-4.659127	0.860431	1.382417	1	-3.254704	-2.963260	0.538157
1	-3.479036	2.042449	1.985803	6	-6.364704	-2.615498	-0.832907
8	0.159913	-0.030331	-0.475733	1	-7.146321	-0.775894	-1.647710
6	-0.039158	3.312964	-0.147918	1	-5.296250	-4.283700	0.029178
6	0.771392	4.433634	-0.015	1	-7.266477	-3.192251	-1.046992
7	0.412468	2.270405	-0.855593	1	-2.129613	3.758445	0.067288
6	2.047979	4.409836	-0.544592	N,O-A6			
1	0.408780	5.287538	0.571820	15	0.752995	-0.599143	1.028289

6	2.394225	-1.156947	0.485632	1	-1.949466	-0.065340	-2.034576
6	3.380709	-0.231036	0.139314	1	-1.787044	1.662836	-2.463588
6	2.673881	-2.523745	0.363902	8	6.064020	-2.524796	-0.885105
6	4.624999	-0.649030	-0.326437	6	7.103365	-1.651249	-1.233552
1	3.185038	0.837810	0.256663	1	6.817841	-0.986725	-2.067611
6	3.909001	-2.951757	-0.097397	1	7.422677	-1.032399	-0.377032
1	1.906491	-3.250419	0.640970	1	7.945767	-2.277029	-1.551994
6	4.895188	-2.018947	-0.448557	16	-0.381915	-2.038024	1.710391
1	5.375534	0.099608	-0.579556	16	1.097604	1.019444	2.260389
1	4.139907	-4.013563	-0.195158	7	-2.885386	-0.590090	0.130902
6	-1.136895	2.654603	0.971350	1	-2.145285	-1.258909	0.364102
1	-0.104094	1.940577	1.786103	6	-4.085030	-1.104546	-0.331127
6	-1.632244	1.423370	0.335035	6	-5.095888	-0.266832	-0.832272
6	-0.629377	1.033602	-0.750162	6	-4.287251	-2.495644	-0.357130
6	-2.713430	0.688853	0.675848	6	-6.282495	-0.810011	-1.319225
6	-3.657356	1.122124	1.766847	1	-4.937037	0.813846	-0.854937
1	-3.763058	2.213880	1.822863	6	-5.469123	-3.025035	-0.862175
1	-4.654338	0.683869	1.627906	1	-3.504241	-3.153711	0.027844
1	-3.271859	0.760571	2.734868	6	-6.480632	-2.189292	-1.340143
8	0.217269	-0.049421	-0.463593	1	-7.057327	-0.140460	-1.700662
6	-0.151398	3.194373	0.127155	1	-5.605615	-4.109042	-0.874395
6	0.591614	4.402780	0.178861	1	-7.409059	-2.610627	-1.729980
7	0.218952	2.266502	-0.807868	1	-1.729983	3.276415	1.641139
6	1.663699	4.568021	-0.659225	N,O-A7			
1	0.305084	5.166279	0.901759	15	0.863804	-0.251673	1.096794
6	1.299589	2.400370	-1.610272	6	2.404668	-1.010574	0.541364
6	2.045329	3.544826	-1.569615	6	3.294538	-0.301722	-0.270765
1	2.241987	5.493612	-0.619834	6	2.711732	-2.328716	0.903124
1	1.527665	1.550777	-2.255218	6	4.474046	-0.888537	-0.719185
1	2.910573	3.657307	-2.221096	1	3.078154	0.731831	-0.552440
6	-1.247705	0.771270	-2.117157	6	3.880656	-2.923496	0.457723
1	-0.468028	0.503392	-2.844049	1	2.019328	-2.884943	1.539402

6	4.772042	-2.210406	-0.357919	16	-0.229957	-1.328804	2.287654
1	5.150751	-0.308226	-1.345898	16	1.572281	1.564589	1.917565
1	4.131805	-3.950290	0.727315	7	-2.779819	-0.730682	0.267064
6	-1.620903	2.846098	0.659890	1	-1.992012	-1.250919	0.652430
1	0.326980	2.055524	2.135032	6	-3.833416	-1.461773	-0.248815
6	-1.835359	1.464543	0.257536	6	-4.882383	-0.842201	-0.950868
6	-0.739626	1.103708	-0.753466	6	-3.845021	-2.862744	-0.121848
6	-2.835471	0.627961	0.623141	6	-5.919513	-1.604400	-1.482968
6	-3.933401	1.059259	1.558404	1	-4.868071	0.241060	-1.091263
1	-4.158642	2.130125	1.465384	6	-4.877898	-3.612229	-0.672484
1	-4.858410	0.496129	1.373238	1	-3.031683	-3.353723	0.418829
1	-3.633109	0.856698	2.600807	6	-5.929102	-2.991965	-1.350678
8	0.196059	0.089922	-0.358333	1	-6.727434	-1.102006	-2.020811
6	-0.560386	3.350247	-0.037389	1	-4.865428	-4.699185	-0.560999
6	0.101482	4.628899	-0.038086	1	-6.742182	-3.584129	-1.774473
7	-0.018779	2.376107	-0.878780	1	-2.217907	3.405927	1.374108
6	1.211051	4.819175	-0.800472	N,O-A8			
1	-0.299259	5.420821	0.595484	15	0.728350	-0.953167	-0.009945
6	1.097788	2.567261	-1.627951	6	2.503019	-1.305901	-0.006939
6	1.741730	3.764653	-1.622545	6	3.430419	-0.267738	-0.088619
1	1.714578	5.788307	-0.788242	6	2.961499	-2.627622	0.100598
1	1.432604	1.708007	-2.211646	6	4.800378	-0.530776	-0.068
1	2.633689	3.913204	-2.228854	1	3.077028	0.760919	-0.184593
6	-1.280505	0.645740	-2.101799	6	4.317881	-2.897896	0.134669
1	-0.453729	0.443980	-2.797762	1	2.240272	-3.447152	0.147134
1	-1.862792	-0.272541	-1.969838	6	5.250726	-1.850721	0.056221
1	-1.925961	1.429887	-2.518843	1	5.502196	0.300127	-0.130792
8	5.878743	-2.867391	-0.741185	1	4.692220	-3.919426	0.217219
6	6.815326	-2.223142	-1.564376	6	-1.144305	2.729319	1.276295
1	6.371900	-1.925134	-2.529883	1	0.775980	0.132343	2.364289
1	7.245042	-1.332344	-1.075130	6	-1.572030	1.635484	0.417774
1	7.616870	-2.947580	-1.750608	6	-0.668421	1.624725	-0.751537

6	-2.658611	0.823069	0.657560	6	-6.543773	-1.028133	-0.396310
6	-3.534343	1.126638	1.845383	1	-5.363319	0.779893	-0.335395
1	-3.992198	2.122925	1.766212	6	-5.314062	-3.096616	-0.289088
1	-4.324202	0.380423	1.981552	1	-3.166562	-2.910537	-0.062532
1	-2.905276	1.118087	2.748539	6	-6.530679	-2.422389	-0.396339
8	0.672707	0.545402	-0.468853	1	-7.488836	-0.489732	-0.496228
6	-0.190929	3.432471	0.614556	1	-5.291044	-4.188578	-0.292474
6	0.584975	4.602185	0.932839	1	-7.464658	-2.980316	-0.487021
7	0.020161	2.840286	-0.655458	1	-1.530349	2.971084	2.262085
6	1.503111	5.071071	0.052998	N,O-A9			
1	0.414370	5.086137	1.895468	15	1.042001	-0.221214	-0.238197
6	0.998226	3.296039	-1.512380	6	2.751486	-0.825441	-0.098950
6	1.727662	4.392177	-1.204855	6	3.782339	0.109130	-0.157607
1	2.090209	5.959745	0.292834	6	3.069549	-2.181459	0.063643
1	1.145817	2.726554	-2.428565	6	5.118156	-0.285744	-0.050383
1	2.484850	4.747020	-1.903200	1	3.528096	1.162394	-0.296477
6	-1.110539	1.188005	-2.125187	6	4.388877	-2.585383	0.174666
1	-0.326110	1.379609	-2.866592	1	2.267768	-2.923159	0.092660
1	-1.319457	0.114665	-2.162415	6	5.425356	-1.638846	0.120120
1	-2.013614	1.748672	-2.406936	1	5.901739	0.470178	-0.103757
8	6.547512	-2.209786	0.096927	1	4.653408	-3.636466	0.301801
6	7.535649	-1.219575	0.005401	6	-1.993549	2.549467	1.363105
1	7.478211	-0.673065	-0.951942	1	0.746729	0.570040	2.262444
1	7.468542	-0.494661	0.835086	6	-2.266229	1.595711	0.336030
1	8.502318	-1.734120	0.062639	6	-1.678885	2.048764	-0.858063
16	-0.339618	-2.291202	-0.976953	6	-2.990087	0.374176	0.552285
16	0.128471	-1.008532	2.037263	6	-3.907839	0.299540	1.731351
7	-2.917437	-0.295622	-0.072440	1	-4.562813	1.178829	1.773619
1	-2.120197	-0.792349	-0.482685	1	-4.501852	-0.618760	1.756993
6	-4.135675	-0.989200	-0.160036	1	-3.263811	0.314557	2.625663
6	-5.354137	-0.311394	-0.294244	8	1.056476	1.256145	-0.525898
6	-4.121693	-2.390318	-0.163215	6	-1.213723	3.531732	0.798298

6	-0.595224	4.716500	1.297645	1	-5.361405	-5.296127	-0.037530
7	-1.048708	3.214840	-0.558390	1	-2.279283	2.495936	2.409513
6	0.156093	5.489738	0.467241	N,O-A10			
1	-0.737164	4.970186	2.348921	15	1.114303	-0.007919	-0.150396
6	-0.244359	3.976472	-1.382116	6	2.813902	-0.624507	-0.068678
6	0.341069	5.099440	-0.901382	6	3.837010	0.308736	-0.227568
1	0.636609	6.396181	0.838555	6	3.141638	-1.968382	0.163785
1	-0.094912	3.601896	-2.392382	6	5.175580	-0.077369	-0.153613
1	0.978851	5.686809	-1.561856	1	3.575757	1.352390	-0.416643
6	-1.711597	1.528788	-2.250392	6	4.466667	-2.361817	0.241284
1	-0.743872	1.066917	-2.502395	1	2.349088	-2.712848	0.272834
1	-2.484538	0.759472	-2.366096	6	5.495608	-1.418478	0.084694
1	-1.929965	2.337856	-2.964690	1	5.952923	0.675228	-0.284852
8	6.678902	-2.127153	0.238244	1	4.740467	-3.402902	0.418972
6	7.761313	-1.241330	0.182365	6	-2.306753	2.383860	1.321049
1	7.811295	-0.713909	-0.786497	1	0.009037	1.131220	1.869372
1	7.721978	-0.491624	0.992078	6	-2.435968	1.413351	0.286119
1	8.669875	-1.844112	0.303183	6	-1.859263	1.927847	-0.878426
16	-0.011435	-1.479654	-1.403223	6	-3.047065	0.136	0.462876
16	0.229779	-0.567413	1.751018	6	-4.086093	-0.025450	1.542173
7	-2.783911	-0.672999	-0.205885	1	-4.595308	-0.994911	1.526668
1	-1.878656	-0.734455	-0.761513	1	-3.577416	0.080127	2.513667
6	-3.492143	-1.908207	-0.145171	1	-4.821836	0.786353	1.466542
6	-4.853633	-1.956304	-0.452957	8	1.062986	1.420532	-0.602990
6	-2.790466	-3.070250	0.179212	6	-1.618066	3.456091	0.786577
6	-5.524781	-3.175182	-0.404528	6	-1.152622	4.698860	1.304850
1	-5.378184	-1.040440	-0.734417	7	-1.365430	3.161360	-0.559402
6	-3.470692	-4.285378	0.214257	6	-0.460862	5.553984	0.499614
1	-1.719642	-3.006167	0.380322	1	-1.357635	4.934070	2.350159
6	-4.834696	-4.340325	-0.069614	6	-0.632310	4.011657	-1.357468
1	-6.590174	-3.215936	-0.639732	6	-0.190	5.193862	-0.860072
1	-2.926284	-5.197308	0.466668	1	-0.095796	6.505963	0.888544

1	-0.419978	3.664180	-2.366414	6	5.283438	-0.182370	-0.351303
1	0.395066	5.851990	-1.502389	1	3.713444	1.205184	-0.879998
6	-1.772110	1.405887	-2.268691	6	4.531945	-2.288786	0.588721
1	-0.727379	1.164441	-2.519558	1	2.411430	-2.551424	0.777254
1	-2.360958	0.487758	-2.373029	6	5.577872	-1.442569	0.182089
1	-2.151071	2.146772	-2.991384	1	6.073817	0.492563	-0.678786
8	6.752389	-1.894981	0.176175	1	4.786882	-3.267402	0.997888
6	7.830444	-1.010801	0.032616	6	-2.404873	2.402378	1.324533
1	7.838228	-0.531744	-0.961799	1	-0.439642	0.934141	1.519112
1	7.820505	-0.224464	0.807134	6	-2.550801	1.432211	0.292158
1	8.744017	-1.606964	0.145271	6	-1.911550	1.908166	-0.855021
16	0.081794	-1.426493	-1.234677	6	-3.214808	0.130577	0.457552
16	0.387023	-0.165498	1.870140	6	-4.266828	0.042478	1.533883
7	-2.644325	-0.902937	-0.243560	1	-4.786725	-0.922252	1.526989
1	-1.336558	-1.009227	-0.768952	1	-3.784382	0.166795	2.516048
6	-3.226526	-2.189611	-0.159148	1	-4.996711	0.857087	1.425073
6	-4.439484	-2.463604	-0.799434	8	1.153227	1.353595	-0.892478
6	-2.542398	-3.208566	0.510481	6	-1.652738	3.442528	0.804336
6	-4.976800	-3.747225	-0.746049	6	-1.152396	4.667776	1.327382
1	-4.953722	-1.662955	-1.335733	7	-1.366060	3.121802	-0.527989
6	-3.086975	-4.490236	0.556054	6	-0.403317	5.488637	0.536024
1	-1.589086	-2.980355	0.990250	1	-1.378658	4.919984	2.364271
6	-4.303746	-4.763449	-0.067817	6	-0.581884	3.937416	-1.312618
1	-5.927111	-3.954883	-1.242532	6	-0.109322	5.107432	-0.811644
1	-2.552826	-5.282774	1.084494	1	-0.012302	6.428682	0.928766
1	-4.727053	-5.769091	-0.028777	1	-0.355193	3.571633	-2.311842
1	-2.644535	2.301852	2.350696	1	0.515349	5.738808	-1.443520
N,O-A11				6	-1.808408	1.369965	-2.239280
15	1.236202	0.021168	-0.220767	1	-0.762022	1.123598	-2.478315
6	2.915955	-0.614668	-0.062336	1	-2.405878	0.456902	-2.333145
6	3.954256	0.223077	-0.466712	1	-2.170825	2.106580	-2.975379
6	3.215816	-1.880138	0.465864	8	6.821990	-1.927194	0.341169

6	7.919247	-1.144105	-0.047681	6	-2.107143	2.204152	1.351387
1	7.898033	-0.920900	-1.128302	1	0.343716	-0.238	-2.184001
1	7.963607	-0.195028	0.513745	6	-2.406371	1.337221	0.270206
1	8.818277	-1.730593	0.176286	6	-2.051984	1.976628	-0.922109
16	0.238645	-1.557250	-1.190925	6	-2.942161	-0.016623	0.421819
16	0.561437	0.063717	1.794662	6	-3.733036	-0.307100	1.666397
7	-2.834923	-0.861121	-0.260887	1	-4.318441	-1.229892	1.576750
1	-1.029208	-1.114897	-0.875896	1	-3.014599	-0.435469	2.492658
6	-3.418513	-2.135789	-0.165337	1	-4.390797	0.534885	1.917735
6	-4.617236	-2.430648	-0.827185	8	0.931568	1.531757	0.128047
6	-2.751676	-3.147934	0.537073	6	-1.542954	3.345053	0.814873
6	-5.150575	-3.716004	-0.766077	6	-0.999153	4.537255	1.366356
1	-5.123670	-1.641432	-1.387321	7	-1.535372	3.193965	-0.578599
6	-3.293983	-4.429582	0.593612	6	-0.496301	5.504145	0.545681
1	-1.807954	-2.913007	1.034015	1	-0.993611	4.648758	2.451445
6	-4.494140	-4.720238	-0.055077	6	-1.024666	4.171008	-1.403886
1	-6.088954	-3.933711	-1.281244	6	-0.514455	5.311758	-0.872419
1	-2.769557	-5.210348	1.149192	1	-0.073902	6.420152	0.961450
1	-4.915313	-5.726462	-0.009373	1	-1.050651	3.966727	-2.473358
1	-2.785942	2.349669	2.341066	1	-0.111839	6.072173	-1.542138
N,O-A12				6	-2.233909	1.596974	-2.350829
15	1.106312	0.153713	0.663547	1	-1.270068	1.519420	-2.882309
6	2.790217	-0.432590	0.412118	1	-2.734449	0.624759	-2.421283
6	3.658565	0.367324	-0.333329	1	-2.842417	2.342801	-2.889649
6	3.252969	-1.649552	0.934675	8	6.675612	-1.723593	-0.206253
6	4.973843	-0.030367	-0.563538	6	7.610776	-0.967125	-0.928388
1	3.295004	1.317830	-0.729887	1	7.293668	-0.815037	-1.974426
6	4.556553	-2.054410	0.709030	1	7.787324	0.016597	-0.460425
1	2.578612	-2.270625	1.528670	1	8.547621	-1.536853	-0.920926
6	5.428700	-1.248699	-0.042754	16	0.163679	-0.694444	2.123813
1	5.630486	0.616264	-1.145178	16	0.212994	-1.119877	-1.445801
1	4.937695	-2.995046	1.109474	7	-2.663466	-0.907543	-0.465462

1	-1.172191	-0.896279	-1.118224
6	-3.102383	-2.244802	-0.362806
6	-4.235973	-2.673915	-1.061568
6	-2.348110	-3.167670	0.371834
6	-4.621310	-4.011596	-1.007526
1	-4.810300	-1.949527	-1.642894
6	-2.738164	-4.504584	0.414270
1	-1.463042	-2.819506	0.911326
6	-3.874525	-4.931731	-0.271646
1	-5.512183	-4.338007	-1.548880
1	-2.146445	-5.217223	0.993020
1	-4.176854	-5.980290	-0.234621
1	-2.213521	1.992271	2.411253

N,O-A13

15	2.252970	-0.311363	0.059
6	0.470387	-0.246430	0.187
6	-0.225123	0.967400	-0.116
6	-0.247728	-1.457799	0.327
6	-1.614959	0.987136	-0.333
1	0.331623	1.907244	-0.257
6	-1.628908	-1.445210	0.085
1	0.297965	-2.403358	0.721
6	-2.326275	-0.223223	-0.304
1	-2.132009	1.946032	-0.551
1	-2.205794	-2.371032	0.144
8	2.769476	-1.699347	-0.143
8	-3.661125	-0.310474	-0.781
6	-4.436775	0.862771	0.655
1	-4.246574	1.471815	0.900148
1	-4.248424	1.472794	-0.898566
1	-5.484946	0.542378	0.001493
16	3.192693	1.344705	0.023

N,O-A14

6	4.318757	0.672768	0.549301
6	3.007812	0.295985	0.821227
6	2.455768	-0.843743	0.229606
6	3.237891	-1.610693	-0.650214
6	4.542178	-1.244502	-0.923317
6	5.095125	-0.097197	-0.328250
1	4.721154	1.566358	1.025136
1	2.401279	0.898206	1.501049
1	2.807766	-2.499704	-1.116126
1	5.165970	-1.829512	-1.600446
8	6.365235	0.182217	-0.655797
6	6.989430	1.313836	-0.105382
1	8.984	1.347450	-0.526655
1	6.459284	2.242991	-0.374569
1	7.060798	1.243954	0.993366
15	0.755097	-1.302601	0.562906
15	-0.717118	1.269408	-0.482370
16	-0.118	-0.309251	2.010575
16	0.186949	-3.003177	-0.121978
16	-0.126303	3.047084	-0.177730
6	-2.437239	0.884799	-0.349828
6	-2.854727	-0.423412	-0.633898
6	-3.381814	1.849427	0.047111
6	-4.194349	-0.770818	-0.526144
1	-2.121749	-1.178159	-0.927144
6	-4.714999	1.509052	0.150939
1	-3.054727	2.866745	0.272828
6	-5.134352	0.195034	-0.133722
1	-4.492206	-1.795754	-0.743625
1	-5.466546	2.238095	0.455771
8	-6.443230	-0.040432	-0.003760

6	-6.951007	-1.327213	-0.263285	1	-0.772545	-2.585576	0.886934
1	-6.520333	-2.077140	0.420667	1	-2.258292	-2.137879	0.001850
1	-8.032886	-1.271210	-0.097689	7	-1.485013	0.380974	0.036
1	-6.761710	-1.632839	-1.305683	6	-2.877677	0.254942	-0.065
8	0.080789	0.133712	-1.073399	6	-3.589396	0.228687	1.208005
N,O-A15				6	-3.588945	0.225536	-1.208323
Acid				6	-4.980270	0.155930	1.202951
1	0.	-0.973735	-0.828280	1	-3.036023	0.266837	2.148729
1	0.	0.973735	-0.828280	6	-4.979825	0.152821	-1.203612
16	0.	0.	0.103535	1	-3.035221	0.261232	-2.148940
Indolizine				6	-5.684186	0.116365	-0.415
6	5.128981	0.895505	-0.570	1	-5.519220	0.130534	2.153075
6	5.368585	-0.515622	-0.066	1	-5.518405	0.124954	-2.153875
6	4.312860	-1.381334	0.357	1	-6.774578	0.060126	-0.544
6	2.980491	-0.883551	0.311	LR-Substituted			
7	2.789383	0.507256	-0.156	6	4.305405	0.899139	-0.213571
6	3.858699	1.377955	-0.611	6	2.954360	0.605738	-0.070665
6	1.726257	-1.467199	0.647	6	2.517319	-0.721821	-0.004248
6	0.765165	-0.420686	0.360	6	3.457540	-1.760747	-0.078879
6	1.450481	0.799784	-0.114	6	4.804457	-1.475674	-0.217267
6	0.976893	2.212235	-0.549	6	5.241729	-0.143139	-0.287336
6	-0.698142	-0.626356	0.496	1	4.613880	1.942601	-0.268695
6	-1.164617	-2.063820	0.001252	1	2.239764	1.431187	-0.015062
1	5.960448	1.600801	-0.932	1	3.118688	-2.798112	-0.033058
1	6.393171	-0.890623	-0.030	1	5.549083	-2.270318	-0.278238
1	4.461109	-2.462317	0.747	8	6.562862	0.037852	-0.425215
1	3.618796	2.440411	-0.001015	6	7.079190	1.342052	-0.510688
1	1.540749	-2.537787	0.001040	1	8.164420	1.239123	-0.625662
1	-0.117813	2.218836	-0.056	1	6.675697	1.881645	-1.383961
1	1.334750	2.756360	0.889823	1	6.868076	1.922787	0.403120
1	1.333862	2.755521	-0.891795	15	0.772537	-1.096982	0.173845
1	-0.773504	-2.586202	-0.884491	15	-0.772523	1.096903	0.175282

16	-0.056	-0.652	1.856818	6	-3.333834	-1.633406	-0.781114
16	0.265562	-2.938220	-0.020532	7	-3.122863	0.193842	0.742669
16	-0.265734	2.938333	-0.018391	6	-4.155681	-2.311521	0.115318
6	-2.517295	0.721728	-0.003248	1	-3.081530	-2.073296	-1.748706
6	-2.954693	-0.605799	-0.067517	6	-3.909095	-0.454993	1.594845
6	-3.457173	1.760787	-0.080646	6	-4.451567	-1.713437	1.336515
6	-4.305688	-0.899093	-0.211098	1	-4.557872	-3.295573	-0.136339
1	-2.240362	-1.431335	-0.009700	1	-4.121709	0.052896	2.542020
6	-4.804047	1.475841	-0.219691	1	-5.087973	-2.205476	2.073792
1	-3.118035	2.798127	-0.036427	6	-1.909145	3.160048	-0.292752
6	-5.241652	0.143308	-0.287685	1	-2.758714	2.642232	0.175015
1	-4.614423	-1.942573	-0.264459	1	-1.723006	4.114851	0.212788
1	-5.548387	2.270594	-0.282760	1	-2.160851	3.355870	-1.346914
8	-6.562706	-0.037575	-0.426382	7	1.589	0.608752	-0.028432
6	-7.079239	-1.341792	-0.510494	1	1.442024	1.561599	0.355050
1	-6.869497	-1.921122	0.404516	6	2.837381	0.001943	0.106181
1	-8.164289	-1.238770	-0.627059	6	3.464265	-0.685960	-0.941875
1	-6.674708	-1.882853	-1.382376	6	3.517384	0.149321	1.323508
8	0.126	0.431	-0.816553	6	4.726894	-1.245524	-0.758146
Figure 41				1	2.971318	-0.761556	-1.911971
N,O-D1				6	4.786073	-0.395952	1.493279
6	-1.930290	0.408578	-1.367349	1	3.031530	0.691116	2.137866
1	-1.689527	-0.219937	-2.237521	6	5.394161	-1.105380	0.457483
6	-0.670027	0.957777	-0.728202	1	5.200807	-1.780062	-1.584507
6	-0.661971	2.309311	-0.178057	1	5.300129	-0.272304	2.448964
6	0.448768	0.142603	-0.608671	1	6.386079	-1.540296	0.594635
6	0.412915	-1.291340	-1.070791	1	-2.527440	1.237618	-1.774861
1	1.197865	-1.888977	-0.592444	LR			
1	-0.554921	-1.746003	-0.826527	6	4.399900	-0.931020	0.078
1	0.548861	-1.363429	-2.161532	6	3.051574	-0.594451	0.074
8	0.320394	2.796580	0.394728	6	2.652608	0.746089	0.098
6	-2.829272	-0.375414	-0.429555				

6	3.625607	1.755391	0.006	1	-6.850803	2.010720	0.899507
6	4.971010	1.427326	0.027				
6	5.371218	0.082184	0.079		N,O-D2		
1	4.679398	-1.984067	0.068	6	-4.040100	-0.995309	-0.715057
1	2.307030	-1.395415	0.071	6	-2.806060	-0.380074	-0.894362
1	3.315697	2.802948	-0.108	6	-2.537931	0.861547	-0.308140
1	5.741782	2.198979	-0.020	6	-3.531311	1.490869	0.464960
8	6.693580	-0.140809	0.086	6	-4.758656	0.886153	0.643939
6	7.174688	-1.460847	0.183	6	-5.024024	-0.367057	0.059747
1	8.268794	-1.392340	0.326	1	-4.217340	-1.963686	-1.181138
1	6.850105	-2.011894	0.899028	1	-2.040794	-0.873401	-1.495921
1	6.850302	-2.011911	-0.898728	1	-3.326587	2.460132	0.924601
15	0.901258	1.184195	-0.247	1	-5.542149	1.356584	1.239391
15	-0.901144	-1.183693	-0.071	8	-6.239018	-0.877646	0.295638
16	-0.184	0.609	-1.552090	6	-6.575757	-2.137635	-0.229085
16	-0.116	0.185	1.553327	1	-7.598145	-2.349814	0.104217
16	0.492940	3.068803	-0.771	1	-6.550899	-2.137520	-1.331831
16	-0.492242	-3.068189	-0.603	1	-5.902560	-2.925468	0.148168
6	-2.652613	-0.746168	-0.150	15	-0.937468	1.631443	-0.512316
6	-3.051857	0.594301	0.287	15	0.725823	-0.944103	0.573580
6	-3.625394	-1.755670	-0.493	16	-0.037424	0.374100	1.823646
6	-4.400241	0.930604	0.362	16	0.299548	0.620838	-1.668058
1	-2.307453	1.395396	0.536	16	-0.803876	3.498794	-0.124871
6	-4.970864	-1.427866	-0.432	16	-0.045896	-2.658290	0.185837
1	-3.315267	-2.803163	-0.809	6	2.490809	-0.781376	0.315290
6	-5.371350	-0.082808	0.013	6	3.153407	0.389017	0.699605
1	-4.679935	1.983600	0.725	6	3.216076	-1.815551	-0.301885
1	-5.741489	-2.199662	-0.707	6	4.518843	0.533126	0.484738
8	-6.693755	0.139912	0.103	1	2.590010	1.198244	1.169247
6	-7.175115	1.459861	0.447	6	4.574104	-1.679850	-0.516320
1	-6.850662	2.011249	-0.898237	1	2.700275	-2.728593	-0.606940
1	-8.269204	1.391129	0.340	6	5.239282	-0.503636	-0.127213

1	5.008365	1.456113	0.793375	1	-1.766431	-2.286246	1.594500
1	5.155828	-2.472745	-0.988319	6	-4.050904	-1.098678	-1.300855
8	6.554046	-0.461539	-0.378351	1	-2.226581	-0.512056	-2.289429
6	7.292017	0.681090	-0.023996	6	-4.625294	-1.642873	-0.143371
1	7.259570	0.862974	1.063412	1	-4.212558	-2.508772	1.810499
1	8.328884	0.487145	-0.321802	1	-4.712367	-0.787629	-2.111225
1	6.928185	1.578435	-0.551917	6	0.748570	3.206621	0.472065
N,O-D3				1	1.372913	3.661579	-0.305523
6	-2.563014	-0.295727	0.078	6	1.208495	1.809727	0.817421
6	-1.761443	-1.451863	-0.463	6	0.192527	0.984556	1.474134
6	-0.384385	-1.344393	-0.361	6	2.453676	1.311534	0.503333
6	0.230510	-0.078248	0.234	6	3.498285	2.170523	-0.155808
6	-0.571133	1.069674	0.902	1	4.483735	2.010269	0.298899
6	-1.957541	0.970024	0.948	1	3.577856	1.878160	-1.214674
8	-3.885436	-0.498129	-0.230	1	3.267094	3.237489	-0.099520
6	-4.759250	0.603778	-0.315	8	0.022801	-0.252040	1.194807
15	2.021612	0.066269	-0.039	6	-0.679651	3.137631	-0.021047
16	2.707743	1.856016	-0.605	6	-1.281146	4.069735	-0.867564
16	2.982996	-1.591296	0.363	7	-1.360960	2.096844	0.440637
1	-2.254777	-2.424604	-0.001081	6	-2.613077	3.877870	-1.224613
1	0.236002	-2.243390	-0.730	1	-0.711497	4.919826	-1.246911
1	-0.098402	2.054262	0.001405	6	-2.636977	1.905013	0.123732
1	-2.554405	1.881627	0.001668	6	-3.310819	2.779919	-0.721033
1	-5.775254	0.192793	-0.002410	1	-3.106513	4.581597	-1.898511
1	-4.625439	1.226573	0.899941	1	-3.125265	1.023316	0.548801
1	-4.622697	1.228758	-0.898633	1	-4.353706	2.595968	-0.981681
N,O-D4				6	-0.310217	1.368038	2.839957
15	-0.031410	-1.175269	-0.460215	1	-0.349027	2.455499	2.975508
6	-1.839669	-1.370891	-0.352772	1	-1.297298	0.924995	3.023739
6	-2.413751	-1.939466	0.785931	1	0.402128	0.951809	3.570770
6	-2.673950	-0.960591	-1.399535	8	-5.970426	-1.722537	-0.126185
6	-3.796091	-2.066929	0.905314	6	-6.610010	-2.282509	0.988639

1	-6.316272	-3.334872	1.144234	1	-1.314063	3.125795	1.525243
1	-6.400181	-1.714044	1.911596	6	-1.663905	1.612561	-0.003592
1	-7.687045	-2.241607	0.786117	6	-0.540804	1.075322	-0.875029
16	0.470521	0.018979	-1.922244	6	-2.785367	0.924624	0.296398
16	0.941610	-2.788691	0.043941	6	-3.896934	1.585987	1.075265
7	2.858582	0.042937	0.787496	1	-4.391453	2.384249	0.499837
1	2.154353	-0.650873	1.032698	1	-4.659127	0.860431	1.382417
6	4.076164	-0.533059	0.313130	1	-3.479036	2.042449	1.985803
6	5.222123	-0.496750	1.110019	8	0.159913	-0.030331	-0.475733
6	4.108041	-1.163777	-0.932847	6	-0.039158	3.312964	-0.147918
6	6.406809	-1.072624	0.654768	6	0.771392	4.433634	-0.015
1	5.171911	-0.014079	2.088522	7	0.412468	2.270405	-0.855593
6	5.293117	-1.744735	-1.379839	6	2.047979	4.409836	-0.544592
1	3.194046	-1.195515	-1.530131	1	0.408780	5.287538	0.571820
6	6.442852	-1.697585	-0.591433	6	1.653853	2.194787	-1.353224
1	7.302263	-1.040606	1.279430	6	2.503903	3.272159	-1.220751
1	5.315501	-2.241849	-2.351822	1	2.708676	5.270118	-0.421831
1	7.368871	-2.154596	-0.947228	1	1.930048	1.244649	-1.813599
1	0.774150	3.900601	1.335136	1	3.514789	3.214561	-1.622782
N,O-D5				6	-0.985656	0.834950	-2.316166
15	0.726542	-0.389811	1.131278	1	-0.143415	0.478042	-2.926108
6	2.296530	-1.119739	0.536765	1	-1.757714	0.055891	-2.300413
6	3.503120	-0.433995	0.652092	1	-1.406944	1.750518	-2.754143
6	2.292642	-2.379644	-0.081688	8	5.766843	-2.842429	-0.969055
6	4.693260	-0.976107	0.159951	6	7.019530	-2.234630	-0.822228
1	3.509361	0.538701	1.151321	1	7.071481	-1.264378	-1.347555
6	3.463300	-2.924886	-0.581564	1	7.275348	-2.075807	0.239943
1	1.353720	-2.934410	-0.149536	1	7.755213	-2.916615	-1.266013
6	4.676401	-2.227966	-0.463048	16	-0.487238	-1.774318	1.833767
1	5.622545	-0.419354	0.283376	16	1.068152	1.289601	2.125055
1	3.474304	-3.905158	-1.061047	7	-2.873306	-0.424308	-0.015126
6	-1.385475	3.026706	0.428002	1	-2.064809	-0.984450	0.283048

6	-4.044151	-1.127479	-0.273595	1	-3.271859	0.760571	2.734868
6	-5.145514	-0.524357	-0.900568	8	0.217269	-0.049421	-0.463593
6	-4.113555	-2.492071	0.054084	6	-0.151398	3.194373	0.127155
6	-6.296801	-1.263527	-1.163473	6	0.591614	4.402780	0.178861
1	-5.090223	0.524115	-1.200998	7	0.218952	2.266502	-0.807868
6	-5.260724	-3.223327	-0.231485	6	1.663699	4.568021	-0.659225
1	-3.254704	-2.963260	0.538157	1	0.305084	5.166279	0.901759
6	-6.364704	-2.615498	-0.832907	6	1.299589	2.400370	-1.610272
1	-7.146321	-0.775894	-1.647710	6	2.045329	3.544826	-1.569615
1	-5.296250	-4.283700	0.029178	1	2.241987	5.493612	-0.619834
1	-7.266477	-3.192251	-1.046992	1	1.527665	1.550777	-2.255218
1	-2.129613	3.758445	0.067288	1	2.910573	3.657307	-2.221096
N,O-D6				6	-1.247705	0.771270	-2.117157
15	0.752995	-0.599143	1.028289	1	-0.468028	0.503392	-2.844049
6	2.394225	-1.156947	0.485632	1	-1.949466	-0.065340	-2.034576
6	3.380709	-0.231036	0.139314	1	-1.787044	1.662836	-2.463588
6	2.673881	-2.523745	0.363902	8	6.064020	-2.524796	-0.885105
6	4.624999	-0.649030	-0.326437	6	7.103365	-1.651249	-1.233552
1	3.185038	0.837810	0.256663	1	6.817841	-0.986725	-2.067611
6	3.909001	-2.951757	-0.097397	1	7.422677	-1.032399	-0.377032
1	1.906491	-3.250419	0.640970	1	7.945767	-2.277029	-1.551994
6	4.895188	-2.018947	-0.448557	16	-0.381915	-2.038024	1.710391
1	5.375534	0.099608	-0.579556	16	1.097604	1.019444	2.260389
1	4.139907	-4.013563	-0.195158	7	-2.885386	-0.590090	0.130902
6	-1.136895	2.654603	0.971350	1	-2.145285	-1.258909	0.364102
1	-0.104094	1.940577	1.786103	6	-4.085030	-1.104546	-0.331127
6	-1.632244	1.423370	0.335035	6	-5.095888	-0.266832	-0.832272
6	-0.629377	1.033602	-0.750162	6	-4.287251	-2.495644	-0.357130
6	-2.713430	0.688853	0.675848	6	-6.282495	-0.810011	-1.319225
6	-3.657356	1.122124	1.766847	1	-4.937037	0.813846	-0.854937
1	-3.763058	2.213880	1.822863	6	-5.469123	-3.025035	-0.862175
1	-4.654338	0.683869	1.627906	1	-3.504241	-3.153711	0.027844

6	-6.480632	-2.189292	-1.340143	6	1.097788	2.567261	-1.627951
1	-7.057327	-0.140460	-1.700662	6	1.741730	3.764653	-1.622545
1	-5.605615	-4.109042	-0.874395	1	1.714578	5.788307	-0.788242
1	-7.409059	-2.610627	-1.729980	1	1.432604	1.708007	-2.211646
1	-1.729983	3.276415	1.641139	1	2.633689	3.913204	-2.228854
N,O-D7				6	-1.280505	0.645740	-2.101799
15	0.863804	-0.251673	1.096794	1	-0.453729	0.443980	-2.797762
6	2.404668	-1.010574	0.541364	1	-1.862792	-0.272541	-1.969838
6	3.294538	-0.301722	-0.270765	1	-1.925961	1.429887	-2.518843
6	2.711732	-2.328716	0.903124	8	5.878743	-2.867391	-0.741185
6	4.474046	-0.888537	-0.719185	6	6.815326	-2.223142	-1.564376
1	3.078154	0.731831	-0.552440	1	6.371900	-1.925134	-2.529883
6	3.880656	-2.923496	0.457723	1	7.245042	-1.332344	-1.075130
1	2.019328	-2.884943	1.539402	1	7.616870	-2.947580	-1.750608
6	4.772042	-2.210406	-0.357919	16	-0.229957	-1.328804	2.287654
1	5.150751	-0.308226	-1.345898	16	1.572281	1.564589	1.917565
1	4.131805	-3.950290	0.727315	7	-2.779819	-0.730682	0.267064
6	-1.620903	2.846098	0.659890	1	-1.992012	-1.250919	0.652430
1	0.326980	2.055524	2.135032	6	-3.833416	-1.461773	-0.248815
6	-1.835359	1.464543	0.257536	6	-4.882383	-0.842201	-0.950868
6	-0.739626	1.103708	-0.753466	6	-3.845021	-2.862744	-0.121848
6	-2.835471	0.627961	0.623141	6	-5.919513	-1.604400	-1.482968
6	-3.933401	1.059259	1.558404	1	-4.868071	0.241060	-1.091263
1	-4.158642	2.130125	1.465384	6	-4.877898	-3.612229	-0.672484
1	-4.858410	0.496129	1.373238	1	-3.031683	-3.353723	0.418829
1	-3.633109	0.856698	2.600807	6	-5.929102	-2.991965	-1.350678
8	0.196059	0.089922	-0.358333	1	-6.727434	-1.102006	-2.020811
6	-0.560386	3.350247	-0.037389	1	-4.865428	-4.699185	-0.560999
6	0.101482	4.628899	-0.038086	1	-6.742182	-3.584129	-1.774473
7	-0.018779	2.376107	-0.878780	1	-2.217907	3.405927	1.374108
6	1.211051	4.819175	-0.800472	N,O-D8			
1	-0.299259	5.420821	0.595484	15	0.728350	-0.953167	-0.009945

6	2.503019	-1.305901	-0.006939	1	-1.319457	0.114665	-2.162415
6	3.430419	-0.267738	-0.088619	1	-2.013614	1.748672	-2.406936
6	2.961499	-2.627622	0.100598	8	6.547512	-2.209786	0.096927
6	4.800378	-0.530776	-0.068	6	7.535649	-1.219575	0.005401
1	3.077028	0.760919	-0.184593	1	7.478211	-0.673065	-0.951942
6	4.317881	-2.897896	0.134669	1	7.468542	-0.494661	0.835086
1	2.240272	-3.447152	0.147134	1	8.502318	-1.734120	0.062639
6	5.250726	-1.850721	0.056221	16	-0.339618	-2.291202	-0.976953
1	5.502196	0.300127	-0.130792	16	0.128471	-1.008532	2.037263
1	4.692220	-3.919426	0.217219	7	-2.917437	-0.295622	-0.072440
6	-1.144305	2.729319	1.276295	1	-2.120197	-0.792349	-0.482685
1	0.775980	0.132343	2.364289	6	-4.135675	-0.989200	-0.160036
6	-1.572030	1.635484	0.417774	6	-5.354137	-0.311394	-0.294244
6	-0.668421	1.624725	-0.751537	6	-4.121693	-2.390318	-0.163215
6	-2.658611	0.823069	0.657560	6	-6.543773	-1.028133	-0.396310
6	-3.534343	1.126638	1.845383	1	-5.363319	0.779893	-0.335395
1	-3.992198	2.122925	1.766212	6	-5.314062	-3.096616	-0.289088
1	-4.324202	0.380423	1.981552	1	-3.166562	-2.910537	-0.062532
1	-2.905276	1.118087	2.748539	6	-6.530679	-2.422389	-0.396339
8	0.672707	0.545402	-0.468853	1	-7.488836	-0.489732	-0.496228
6	-0.190929	3.432471	0.614556	1	-5.291044	-4.188578	-0.292474
6	0.584975	4.602185	0.932839	1	-7.464658	-2.980316	-0.487021
7	0.020161	2.840286	-0.655458	1	-1.530349	2.971084	2.262085
6	1.503111	5.071071	0.052998	N,O-D9			
1	0.414370	5.086137	1.895468	15	-0.937013	-0.264341	-0.100101
6	0.998226	3.296039	-1.512380	6	-2.677645	-0.794289	-0.152558
6	1.727662	4.392177	-1.204855	6	-3.632769	0.013675	0.460211
1	2.090209	5.959745	0.292834	6	-3.090308	-1.973625	-0.788444
1	1.145817	2.726554	-2.428565	6	-4.984231	-0.339507	0.455945
1	2.484850	4.747020	-1.903200	1	-3.305317	0.939727	0.938221
6	-1.110539	1.188005	-2.125187	6	-4.425953	-2.338288	-0.795001
1	-0.326110	1.379609	-2.866592	1	-2.347150	-2.596790	-1.291782

6	-5.384614	-1.523528	-0.170909	16	0.006885	-0.768153	-1.770263
1	-5.708118	0.317895	0.938028	16	-0.104593	-1.646941	1.427628
1	-4.765116	-3.252216	-1.285644	7	2.787505	-0.589572	0.379855
6	1.990105	2.541710	-1.378867	1	1.962324	-0.573660	1.002964
1	-0.696175	-1.030605	2.473100	6	3.407817	-1.878356	0.275110
6	2.269989	1.646398	-0.304154	6	4.653436	-2.091019	0.864456
6	1.685282	2.162171	0.865984	6	2.735604	-2.903657	-0.388834
6	2.947103	0.396715	-0.472349	6	5.244496	-3.349391	0.773762
6	3.782459	0.181020	-1.689136	1	5.152302	-1.271593	1.386414
1	4.257623	1.111591	-2.016920	6	3.334363	-4.159505	-0.467261
1	4.534814	-0.602869	-1.549361	1	1.761735	-2.694163	-0.841970
1	3.079510	-0.156825	-2.470756	6	4.584599	-4.382933	0.109168
8	-0.866324	1.112083	0.511194	1	6.221122	-3.523169	1.229769
6	1.217465	3.554158	-0.863327	1	2.816680	-4.969185	-0.985211
6	0.594077	4.707879	-1.424908	1	5.048336	-5.369173	0.041296
7	1.059517	3.311563	0.512012	1	2.246315	2.414608	-2.426190
6	-0.152418	5.527631	-0.636555	N,O-D10			
1	0.727019	4.898167	-2.490462	15	1.106312	0.153713	0.663547
6	0.263724	4.124663	1.296276	6	2.790217	-0.432590	0.412118
6	-0.325337	5.217241	0.754392	6	3.658565	0.367324	-0.333329
1	-0.638081	6.409740	-1.056104	6	3.252969	-1.649552	0.934675
1	0.126759	3.819091	2.331302	6	4.973843	-0.030367	-0.563538
1	-0.955241	5.843913	1.385968	1	3.295004	1.317830	-0.729887
6	1.676783	1.677926	2.271610	6	4.556553	-2.054410	0.709030
1	0.707492	1.197032	2.476717	1	2.578612	-2.270625	1.528670
1	2.478126	0.949581	2.447987	6	5.428700	-1.248699	-0.042754
1	1.823968	2.505331	2.981933	1	5.630486	0.616264	-1.145178
8	-6.661753	-1.959622	-0.230973	1	4.937695	-2.995046	1.109474
6	-7.670675	-1.191261	0.360868	6	-2.107143	2.204152	1.351387
1	-7.512313	-1.069511	1.446949	1	0.343716	-0.238	-2.184001
1	-7.749226	-0.190553	-0.099616	6	-2.406371	1.337221	0.270206
1	-8.613515	-1.728327	0.199311	6	-2.051984	1.976628	-0.922109

6	-2.942161	-0.016623	0.421819	6	-4.621310	-4.011596	-1.007526
6	-3.733036	-0.307100	1.666397	1	-4.810300	-1.949527	-1.642894
1	-4.318441	-1.229892	1.576750	6	-2.738164	-4.504584	0.414270
1	-3.014599	-0.435469	2.492658	1	-1.463042	-2.819506	0.911326
1	-4.390797	0.534885	1.917735	6	-3.874525	-4.931731	-0.271646
8	0.931568	1.531757	0.128047	1	-5.512183	-4.338007	-1.548880
6	-1.542954	3.345053	0.814873	1	-2.146445	-5.217223	0.993020
6	-0.999153	4.537255	1.366356	1	-4.176854	-5.980290	-0.234621
7	-1.535372	3.193965	-0.578599	1	-2.213521	1.992271	2.411253
6	-0.496301	5.504145	0.545681	N,O-D11			
1	-0.993611	4.648758	2.451445	15	2.252970	-0.311363	0.059
6	-1.024666	4.171008	-1.403886	6	0.470387	-0.246430	0.187
6	-0.514455	5.311758	-0.872419	6	-0.225123	0.967400	-0.116
1	-0.073902	6.420152	0.961450	6	-0.247728	-1.457799	0.327
1	-1.050651	3.966727	-2.473358	6	-1.614959	0.987136	-0.333
1	-0.111839	6.072173	-1.542138	1	0.331623	1.907244	-0.257
6	-2.233909	1.596974	-2.350829	6	-1.628908	-1.445210	0.085
1	-1.270068	1.519420	-2.882309	1	0.297965	-2.403358	0.721
1	-2.734449	0.624759	-2.421283	6	-2.326275	-0.223223	-0.304
1	-2.842417	2.342801	-2.889649	1	-2.132009	1.946032	-0.551
8	6.675612	-1.723593	-0.206253	1	-2.205794	-2.371032	0.144
6	7.610776	-0.967125	-0.928388	8	2.769476	-1.699347	-0.143
1	7.293668	-0.815037	-1.974426	8	-3.661125	-0.310474	-0.781
1	7.787324	0.016597	-0.460425	6	-4.436775	0.862771	0.655
1	8.547621	-1.536853	-0.920926	1	-4.246574	1.471815	0.900148
16	0.163679	-0.694444	2.123813	1	-4.248424	1.472794	-0.898566
16	0.212994	-1.119877	-1.445801	1	-5.484946	0.542378	0.001493
7	-2.663466	-0.907543	-0.465462	16	3.192693	1.344705	0.023
1	-1.172191	-0.896279	-1.118224	N,O-D12			
6	-3.102383	-2.244802	-0.362806	6	4.318757	0.672768	0.549301
6	-4.235973	-2.673915	-1.061568	6	3.007812	0.295985	0.821227
6	-2.348110	-3.167670	0.371834	6	2.455768	-0.843743	0.229606

6	3.237891	-1.610693	-0.650214
6	4.542178	-1.244502	-0.923317
6	5.095125	-0.097197	-0.328250
1	4.721154	1.566358	1.025136
1	2.401279	0.898206	1.501049
1	2.807766	-2.499704	-1.116126
1	5.165970	-1.829512	-1.600446
8	6.365235	0.182217	-0.655797
6	6.989430	1.313836	-0.105382
1	8.984	1.347450	-0.526655
1	6.459284	2.242991	-0.374569
1	7.060798	1.243954	0.993366
15	0.755097	-1.302601	0.562906
15	-0.717118	1.269408	-0.482370
16	-0.118	-0.309251	2.010575
16	0.186949	-3.003177	-0.121978
16	-0.126303	3.047084	-0.177730
6	-2.437239	0.884799	-0.349828
6	-2.854727	-0.423412	-0.633898
6	-3.381814	1.849427	0.047111
6	-4.194349	-0.770818	-0.526144
1	-2.121749	-1.178159	-0.927144
6	-4.714999	1.509052	0.150939
1	-3.054727	2.866745	0.272828
6	-5.134352	0.195034	-0.133722
1	-4.492206	-1.795754	-0.743625
1	-5.466546	2.238095	0.455771
8	-6.443230	-0.040432	-0.003760
6	-6.951007	-1.327213	-0.263285
1	-6.520333	-2.077140	0.420667
1	-8.032886	-1.271210	-0.097689
1	-6.761710	-1.632839	-1.305683

8	0.080789	0.133712	-1.073399
N,O-D13			
Acid			
1	0.	-0.973735	-0.828280
1	0.	0.973735	-0.828280
16	0.	0.	0.103535
Indolizine			
6	5.128981	0.895505	-0.570
6	5.368585	-0.515622	-0.066
6	4.312860	-1.381334	0.357
6	2.980491	-0.883551	0.311
7	2.789383	0.507256	-0.156
6	3.858699	1.377955	-0.611
6	1.726257	-1.467199	0.647
6	0.765165	-0.420686	0.360
6	1.450481	0.799784	-0.114
6	0.976893	2.212235	-0.549
6	-0.698142	-0.626356	0.496
6	-1.164617	-2.063820	0.001252
1	5.960448	1.600801	-0.932
1	6.393171	-0.890623	-0.030
1	4.461109	-2.462317	0.747
1	3.618796	2.440411	-0.001015
1	1.540749	-2.537787	0.001040
1	-0.117813	2.218836	-0.056
1	1.334750	2.756360	0.889823
1	1.333862	2.755521	-0.891795
1	-0.773504	-2.586202	-0.884491
1	-0.772545	-2.585576	0.886934
1	-2.258292	-2.137879	0.001850
7	-1.485013	0.380974	0.036
6	-2.877677	0.254942	-0.065

6	-3.589396	0.228687	1.208005
6	-3.588945	0.225536	-1.208323
6	-4.980270	0.155930	1.202951
1	-3.036023	0.266837	2.148729
6	-4.979825	0.152821	-1.203612
1	-3.035221	0.261232	-2.148940
6	-5.684186	0.116365	-0.415
1	-5.519220	0.130534	2.153075
1	-5.518405	0.124954	-2.153875
1	-6.774578	0.060126	-0.544
LR-Substituted			
6	4.305405	0.899139	-0.213571
6	2.954360	0.605738	-0.070665
6	2.517319	-0.721821	-0.004248
6	3.457540	-1.760747	-0.078879
6	4.804457	-1.475674	-0.217267
6	5.241729	-0.143139	-0.287336
1	4.613880	1.942601	-0.268695
1	2.239764	1.431187	-0.015062
1	3.118688	-2.798112	-0.033058
1	5.549083	-2.270318	-0.278238
8	6.562862	0.037852	-0.425215
6	7.079190	1.342052	-0.510688
1	8.164420	1.239123	-0.625662
1	6.675697	1.881645	-1.383961
1	6.868076	1.922787	0.403120
15	0.772537	-1.096982	0.173845
15	-0.772523	1.096903	0.175282
16	-0.056	-0.652	1.856818
16	0.265562	-2.938220	-0.020532
16	-0.265734	2.938333	-0.018391
6	-2.517295	0.721728	-0.003248

6	-2.954693	-0.605799	-0.067517
6	-3.457173	1.760787	-0.080646
6	-4.305688	-0.899093	-0.211098
1	-2.240362	-1.431335	-0.009700
6	-4.804047	1.475841	-0.219691
1	-3.118035	2.798127	-0.036427
6	-5.241652	0.143308	-0.287685
1	-4.614423	-1.942573	-0.264459
1	-5.548387	2.270594	-0.282760
8	-6.562706	-0.037575	-0.426382
6	-7.079239	-1.341792	-0.510494
1	-6.869497	-1.921122	0.404516
1	-8.164289	-1.238770	-0.627059
1	-6.674708	-1.882853	-1.382376
8	0.126	0.431	-0.816553

Figure 42

N,O-W1

6	-2.814181	0.191697	-0.525126
6	-3.286756	2.364780	0.048782
6	-4.250497	1.981258	0.978116
6	-4.486881	0.618955	1.149530
6	-3.760679	-0.290428	0.388794
6	-1.975296	-0.757248	-1.353379
6	-0.661538	-1.101446	-0.675583
6	0.482803	-0.423738	-0.987400
6	-0.785220	-2.164411	0.355735
6	0.289943	-2.393303	1.408475
6	0.468239	0.769278	-1.911142
7	1.735417	-0.873292	-0.598767
8	-1.804840	-2.829240	0.425358

6	2.803394	-0.086716	-0.146126	1	3.674106	3.572726	0.245
6	4.108032	-0.592004	-0.236768	1	1.671888	2.128423	0.172
6	5.184487	0.151686	0.235710	1	4.199989	-1.376962	-0.346
6	4.982175	1.416697	0.787999	1	6.213736	0.086979	-0.273
6	3.685825	1.920420	0.880884	15	1.349546	-0.804254	-0.147
6	2.598509	1.172919	0.433865	15	-1.349549	0.804259	0.157
1	-3.071029	3.426289	-0.115876	6	-2.817832	-0.280777	0.091
1	-4.798611	2.732147	1.549837	6	-2.666465	-1.674016	-0.013
1	-5.230615	0.268331	1.868907	6	-4.093205	0.289704	0.128
1	-3.898733	-1.366988	0.498519	6	-3.793899	-2.487737	-0.074
1	-2.527875	-1.693841	-1.503915	1	-1.671870	-2.128420	-0.047
1	-1.806831	-0.297645	-2.334729	6	-5.218063	-0.534594	0.061
1	0.823339	-1.475995	1.690322	1	-4.199996	1.376948	0.207
1	-0.205320	-2.827663	2.286030	6	-5.069288	-1.919326	-0.038
1	1.029048	-3.133537	1.058984	1	-3.674079	-3.572737	-0.154
1	0.278399	0.416014	-2.938270	1	-6.213733	-0.087007	0.087
1	-0.336885	1.467294	-1.645530	34	0.079	-0.183	1.668777
1	1.432941	1.289467	-1.921616	34	-0.077	0.194	-1.668768
1	1.825660	-1.861885	-0.414344	34	1.718838	-2.850294	-0.372
1	4.271672	-1.571920	-0.692018	34	-1.718852	2.850296	0.392
1	6.193834	-0.258547	0.158835	1	5.952123	2.562719	0.021
1	5.829131	2.002796	1.149272	1	-5.952103	-2.562746	-0.087
1	3.511670	2.902159	1.326823				
1	1.583503	1.558881	0.549480	N,O-W2			
7	-2.586666	1.500176	-0.682343	6	-4.298518	-1.963420	-0.528116
WR				6	-3.071957	-1.342369	-0.742646
6	3.793919	2.487725	0.113	6	-2.849875	-0.055080	-0.237604
6	2.666479	1.674012	0.072	6	-3.852878	0.602052	0.486252
6	2.817837	0.280772	-0.094	6	-5.075471	-0.028108	0.696660
6	4.093206	-0.289717	-0.218	6	-5.299179	-1.308838	0.189851
6	5.218069	0.534573	-0.176	1	-4.471791	-2.965818	-0.924006
6	5.069304	1.919305	-0.011	1	-2.281363	-1.850636	-1.298863

1	-3.671442	1.605768	0.877116	34	-1.486067	-1.854380	-0.121
1	-5.859036	0.485695	1.257006	34	-1.485986	1.854417	0.102
15	-1.249960	0.753638	-0.511858	1	5.105294	-0.023	-0.108
15	1.447068	-1.018601	0.481954	N,O-W4			
6	2.450864	0.477482	0.344280	15	-0.293852	-1.211100	-0.250633
6	2.171597	1.588598	1.149129	6	-2.025609	-1.773153	-0.023688
6	3.511477	0.516787	-0.572830	6	-2.425988	-2.295766	1.212811
6	2.952875	2.736757	1.030735	6	-2.944896	-1.691859	-1.071256
1	1.353496	1.549383	1.870424	6	-3.745385	-2.694471	1.406393
6	4.282064	1.666040	-0.683251	1	-1.696374	-2.382988	2.020335
1	3.723975	-0.354289	-1.196789	6	-4.262126	-2.109962	-0.879113
6	4.001653	2.777575	0.116699	1	-2.624402	-1.277314	-2.029778
1	2.733472	3.603363	1.656848	6	-4.667494	-2.599726	0.360916
1	5.103962	1.698888	-1.400837	1	-4.055468	-3.091724	2.375507
34	-0.237548	-0.828342	1.742395	1	-4.975952	-2.046928	-1.703500
34	-0.026076	-0.175282	-1.963588	6	-0.433221	3.275802	0.573548
34	-1.127504	2.747712	0.001490	1	0.051341	3.850725	-0.223598
34	2.347861	-2.793628	-0.023433	6	0.330998	2.017307	0.908423
1	-6.260687	-1.799511	0.355688	6	-0.461958	1.007735	1.605234
1	4.607957	3.681126	0.023607	6	1.644821	1.793416	0.550612
N,O-W3				6	2.455067	2.837681	-0.167373
15	-0.591699	-0.001	0.018	1	3.442057	2.956216	0.297588
6	1.224915	-0.033	0.037	1	2.622941	2.499142	-1.201637
6	1.925949	-1.213933	0.362	1	1.967526	3.815040	-0.190459
6	1.925953	1.213872	-0.263	8	-0.350217	-0.247829	1.353521
6	3.317418	-1.209159	0.309	6	-1.823961	2.887800	0.124224
1	1.375344	-2.157190	0.621	6	-2.635944	3.654138	-0.711963
6	3.317417	1.209103	-0.330	7	-2.246138	1.727286	0.610071
1	1.375330	2.157122	-0.465	6	-3.899769	3.168717	-1.034910
6	4.013078	-0.031	-0.054	1	-2.275342	4.603265	-1.112267
1	3.860472	-2.156115	0.558	6	-3.457462	1.256406	0.329709
1	3.860482	2.156052	-0.594	6	-4.326040	1.951126	-0.504588

1	-4.551354	3.738186	-1.701148	1	0.550857	-3.379114	-0.724048
1	-3.733004	0.297960	0.778334	6	3.777299	-3.691418	-1.786592
1	-5.308413	1.538368	-0.736451	1	5.383004	-2.340476	-1.277724
6	-1.004769	1.288566	2.979780	1	1.994621	-4.871563	-2.100622
1	-1.251783	2.348127	3.116500	6	-0.186114	3.030870	0.537785
1	-1.882794	0.662578	3.183865	1	0.030335	2.949226	1.618039
1	-0.211543	1.021018	3.696499	6	-0.871288	1.806791	-0.005552
34	-0.112926	0.062760	-1.916354	6	-0.005489	1.106451	-1.037593
34	1.102244	-2.695857	0.258643	6	-2.122167	1.420280	0.322437
7	2.327106	0.655209	0.843181	6	-2.952124	2.250492	1.270842
1	1.808750	-0.165274	1.152301	1	-3.158254	3.255225	0.870393
6	3.640247	0.360602	0.365027	1	-3.908496	1.766784	1.500496
6	4.753604	0.687073	1.141763	1	-2.401971	2.373852	2.216797
6	3.805663	-0.280904	-0.864630	8	0.425699	-0.177277	-0.807631
6	6.035338	0.391671	0.681169	6	1.115331	3.056922	-0.190366
1	4.602835	1.173173	2.108205	6	2.186107	3.935391	-0.063694
6	5.089205	-0.580029	-1.317293	7	1.212965	2.024910	-1.038299
1	2.919870	-0.543112	-1.447944	6	3.347699	3.678139	-0.778343
6	6.203555	-0.241456	-0.549969	1	2.110066	4.779088	0.621912
1	6.904910	0.651250	1.288977	6	2.337060	1.716958	-1.700239
1	5.217300	-1.084541	-2.277159	6	3.433337	2.546211	-1.597185
1	7.207558	-0.476445	-0.910185	1	4.206955	4.343983	-0.678860
1	-0.535063	3.965200	1.434300	1	2.321775	0.785792	-2.269177
1	-5.700970	-2.919221	0.513486	1	4.349711	2.299688	-2.132215
N,O-W5				6	-0.621559	1.126814	-2.435419
15	1.033554	-0.866473	0.662535	1	0.044076	0.631432	-3.156521
6	2.146832	-2.008958	-0.258394	1	-1.566717	0.571758	-2.396447
6	3.506395	-1.723545	-0.409440	1	-0.822776	2.158591	-2.755295
6	1.609327	-3.148169	-0.867088	34	-0.567368	-1.910186	1.585005
6	4.318558	-2.563317	-1.172066	34	2.151140	0.563862	1.783015
1	3.922134	-0.844268	0.090282	7	-2.603196	0.197553	-0.121320
6	2.421740	-3.982885	-1.630517	1	-1.972078	-0.594186	0.053042

6	-3.935704	-0.119521	-0.360872	1	-2.300397	-1.323922	-2.723224
6	-4.847573	0.835553	-0.836102	1	-2.998824	-2.678447	-1.803493
6	-4.372963	-1.441438	-0.175109	8	0.517032	0.075948	0.894282
6	-6.170828	0.479709	-1.088231	6	0.859219	-3.059667	-0.171292
1	-4.511897	1.857315	-1.026440	6	1.845461	-4.073020	-0.323027
6	-5.690992	-1.788211	-0.448953	7	0.978098	-2.221775	0.910218
1	-3.662523	-2.187014	0.190303	6	2.878762	-4.145354	0.571739
6	-6.603087	-0.831296	-0.898283	1	1.766826	-4.761780	-1.164121
1	-6.868197	1.237706	-1.452827	6	2.013567	-2.266804	1.782895
1	-6.012435	-2.821373	-0.298454	6	2.982424	-3.219062	1.649064
1	-7.639329	-1.106623	-1.103022	1	3.642419	-4.917212	0.454844
1	-0.747547	3.966776	0.373032	1	2.019983	-1.501612	2.559949
1	4.414399	-4.350464	-2.381129	1	3.811191	-3.257974	2.354259
N,O-W6				6	-0.841778	-1.258695	2.276655
15	1.002115	0.986934	-0.417497	1	-0.173975	-0.979	3.100300
6	2.461419	1.745272	0.381861	1	-1.685088	-0.560780	2.250689
6	3.530089	0.934067	0.786200	1	-1.220274	-2.275688	2.444340
6	2.505958	3.119609	0.618837	34	-0.456990	2.376652	-1.021319
6	4.628062	1.497459	1.427727	34	1.831085	-0.338083	-1.994907
1	3.509881	-0.138362	0.576956	7	-2.643108	0.022534	0.086148
6	3.611157	3.681042	1.259021	1	-2.041858	0.851541	0.083275
1	1.668943	3.745012	0.298435	6	-3.979425	0.225853	0.395150
6	4.670039	2.872901	1.665396	6	-4.860831	-0.850823	0.586882
1	5.460598	0.861560	1.736812	6	-4.462823	1.533937	0.571067
1	3.642171	4.757669	1.438715	6	-6.193816	-0.617699	0.916473
6	-0.175338	-2.620950	-1.002828	1	-4.490814	-1.874030	0.491056
1	0.779246	-1.592152	-1.689688	6	-5.790914	1.751918	0.918260
6	-0.933774	-1.602637	-0.264749	1	-3.780558	2.375407	0.426579
6	-0.101352	-1.193606	0.946679	6	-6.670955	0.680845	1.085367
6	-2.135238	-1.080774	-0.601879	1	-6.865460	-1.468298	1.055711
6	-2.873072	-1.585451	-1.818376	1	-6.146584	2.776412	1.050894
1	-3.863883	-1.124007	-1.907688	1	-7.715592	0.857636	1.347678

1	-0.587009	-3.234311	-1.803084	1	-1.840338	1.470850	2.609425
1	5.535897	3.314929	2.163385	1	-3.657215	3.193775	2.482350
N,O-W7				6	1.005331	1.193121	2.211295
15	-1.059136	-0.863093	-0.466670	1	0.352772	0.880730	3.038891
6	-2.133295	-1.992576	0.471788	1	1.833941	0.482044	2.127559
6	-3.012972	-1.477367	1.433608	1	1.404258	2.194903	2.417668
6	-2.083645	-3.367139	0.234306	34	0.251606	-1.769677	-1.822010
6	-3.838373	-2.338558	2.149303	34	-2.605303	0.491187	-1.405073
1	-3.059238	-0.401248	1.616109	7	2.658294	-0.060488	-0.106272
6	-2.909376	-4.225583	0.959048	1	2.048016	-0.857239	-0.284146
1	-1.392004	-3.756546	-0.516872	6	3.950029	-0.339003	0.303650
6	-3.785068	-3.713631	1.913846	6	4.818159	0.679660	0.733239
1	-4.526667	-1.936417	2.895452	6	4.401973	-1.670091	0.345438
1	-2.865225	-5.300768	0.774662	6	6.105912	0.371025	1.164247
6	0.363759	2.840838	-0.878029	1	4.467704	1.714367	0.742105
1	-1.556317	1.318360	-2.028403	6	5.683769	-1.965583	0.794509
6	1.049768	1.695847	-0.300122	1	3.732658	-2.468667	0.014994
6	0.225537	1.224519	0.903392	6	6.551161	-0.949533	1.293
6	2.233490	1.153642	-0.672544	1	6.766588	1.178221	1.489955
6	3.034993	1.704528	-1.821212	1	6.013398	-3.007128	0.819341
1	2.907843	2.789466	-1.933327	1	7.559782	-1.185329	1.544305
1	4.105965	1.494304	-1.696932	1	0.672131	3.394996	-1.759764
1	2.713694	1.219047	-2.758840	1	-4.431386	-4.387879	2.479901
8	-0.376516	-0.081026	0.797972	N,O-W8			
6	-0.726139	3.134429	-0.111954	15	1.020590	-1.058759	-0.101303
6	-1.754397	4.138631	-0.203069	6	2.741178	-1.654840	-0.111267
7	-0.841393	2.227538	0.945985	6	3.788758	-0.730028	-0.170577
6	-2.771844	4.153762	0.698150	6	3.015658	-3.023546	-0.032256
1	-1.695284	4.870236	-1.009574	6	5.108253	-1.178720	-0.145504
6	-1.863743	2.246042	1.841929	1	3.564069	0.335583	-0.244159
6	-2.844595	3.182802	1.757984	6	4.336138	-3.463983	-0.005338
1	-3.551132	4.915098	0.620842	1	2.191994	-3.741189	-0.001165

6	5.382736	-2.542709	-0.060525	6	-4.857972	0.848014	-0.299659
1	5.925750	-0.456153	-0.194286	6	-4.147713	-1.463196	-0.198543
1	4.548789	-4.533254	0.056592	6	-6.182558	0.432288	-0.408042
6	-0.110090	2.908451	1.201308	1	-4.611135	1.911590	-0.325575
1	1.346978	0.078446	2.408037	6	-5.472689	-1.868133	-0.331872
6	-0.774140	1.924909	0.359514	1	-3.343137	-2.196171	-0.106439
6	0.072855	1.739210	-0.837297	6	-6.496982	-0.925874	-0.427379
6	-1.990511	1.341810	0.632911	1	-6.973805	1.179941	-0.497211
6	-2.751374	1.800829	1.849410	1	-5.706218	-2.934897	-0.350613
1	-2.950255	2.881265	1.818671	1	-7.535346	-1.248769	-0.524338
1	-3.698278	1.265912	1.976368	1	-0.405138	3.212881	2.201133
1	-2.130239	1.599406	2.736421	1	6.417698	-2.891666	-0.040298
8	1.181907	0.423908	-0.586367	N,O-W9			
6	0.941478	3.411842	0.506481	15	-1.154644	-0.854960	-0.070659
6	1.946754	4.401083	0.795316	6	-2.479397	-2.117137	-0.084420
7	0.989081	2.795501	-0.768663	6	-3.673062	-1.806570	0.572284
6	2.908717	4.681993	-0.117178	6	-2.333107	-3.354414	-0.718652
1	1.909747	4.903786	1.762649	6	-4.714466	-2.734271	0.600239
6	2.005589	3.054238	-1.662231	1	-3.770532	-0.828748	1.048946
6	2.949070	3.980871	-1.382117	6	-3.372691	-4.279360	-0.684735
1	3.670304	5.432894	0.101461	1	-1.402342	-3.579221	-1.245585
1	2.003107	2.473297	-2.583115	6	-4.564132	-3.970944	-0.024623
1	3.735831	4.183702	-2.107838	1	-5.649185	-2.488709	1.109955
6	-0.484406	1.399078	-2.195353	1	-3.256048	-5.245973	-1.180066
1	0.311947	1.368328	-2.947824	6	0.082659	3.076685	-1.306841
1	-0.960093	0.414170	-2.204630	1	-0.491012	-1.505768	2.636696
1	-1.221292	2.163388	-2.481713	6	0.786466	2.414524	-0.257323
34	-0.342575	-2.325204	-1.107121	6	0.042198	2.546619	0.928713
34	0.427226	-1.028892	2.093571	6	1.998876	1.681164	-0.455784
7	-2.487504	0.294594	-0.083067	6	2.833587	1.964112	-1.659429
1	-1.822602	-0.354489	-0.513651	1	2.763131	3.017198	-1.951243
6	-3.832407	-0.098468	-0.177336	1	3.881506	1.676584	-1.519124

1	2.414933	1.340561	-2.468742	1	-5.379145	-4.698266	-0.002671
8	-1.691794	0.400965	0.566864	N,O-W10			
6	-1.082637	3.559306	-0.761643	15	-2.041931	-0.951958	0.960501
6	-2.208312	4.257820	-1.290945	6	-3.376512	-1.240958	-0.223534
7	-1.076030	3.242277	0.607515	6	-4.143352	-0.137426	-0.617344
6	-3.248584	4.584786	-0.477542	6	-3.637612	-2.510990	-0.747794
1	-2.209219	4.504012	-2.353387	6	-5.172812	-0.310931	-1.539051
6	-2.154858	3.541480	1.417709	1	-3.923406	0.844589	-0.193411
6	-3.217718	4.207521	0.907328	6	-4.665366	-2.674196	-1.672377
1	-4.117820	5.112200	-0.872717	1	-3.033139	-3.362849	-0.426693
1	-2.102480	3.189851	2.445807	6	-5.430860	-1.575957	-2.067435
1	-4.062425	4.429848	1.559578	1	-5.776136	0.545566	-1.847063
6	0.299544	2.095072	2.321600	1	-4.870109	-3.663065	-2.087349
1	-0.300740	1.193969	2.523995	6	1.399501	3.227319	-1.023223
1	1.359322	1.856794	2.475678	1	-0.386792	0.831032	-1.435174
1	0.030724	2.874039	3.050742	6	1.848839	2.210359	-0.139865
34	-0.070999	-0.861220	-1.912090	6	0.969220	2.135143	0.941207
34	0.358885	-1.798906	1.471243	6	3.007812	1.329307	-0.364628
7	2.356112	0.716916	0.360778	6	4.249704	1.956126	-0.940189
1	1.641498	0.308260	0.985376	1	4.670849	2.671027	-0.216946
6	3.550160	-0.069601	0.247267	1	5.011415	1.210160	-1.196899
6	4.713729	0.356456	0.886882	1	3.991605	2.532295	-1.840839
6	3.514788	-1.265480	-0.468893	8	-2.038747	0.463144	1.427901
6	5.865852	-0.421944	0.797667	6	0.234313	3.748547	-0.484446
1	4.710732	1.293046	1.448493	6	-0.684214	4.757341	-0.890113
6	4.671728	-2.038630	-0.545845	7	-0.007698	3.072964	0.721201
1	2.584545	-1.566344	-0.960533	6	-1.763902	5.049119	-0.108466
6	5.843894	-1.619423	0.082680	1	-0.497582	5.281119	-1.828781
1	6.781511	-0.093688	1.293235	6	-1.107378	3.361391	1.500758
1	4.652894	-2.977378	-1.102695	6	-1.976126	4.330165	1.111280
1	6.746632	-2.230363	0.017717	1	-2.472414	5.822480	-0.409591
1	0.351707	3.118079	-2.357892	1	-1.242037	2.747851	2.388940

1	-2.845237	4.539029	1.735276
6	1.008684	1.324462	2.190387
1	0.079402	0.749729	2.315350
1	1.844582	0.617647	2.150951
1	1.130426	1.970137	3.076598
34	-1.217525	-2.593150	1.886713
34	-0.222193	-0.622417	-1.288192
7	2.875181	0.085238	-0.086659
1	1.041660	-0.451775	-0.497957
6	3.913262	-0.848453	-0.233826
6	4.944705	-0.939015	0.709478
6	3.878450	-1.754038	-1.302302
6	5.931653	-1.913145	0.575019
1	4.959970	-0.241494	1.549881
6	4.871914	-2.720949	-1.431556
1	3.066848	-1.687003	-2.030121
6	5.902066	-2.806736	-0.494907
1	6.730517	-1.973829	1.317525
1	4.837815	-3.418268	-2.271665
1	6.676164	-3.569917	-0.595931
1	1.846390	3.530655	-1.966770
1	-6.235776	-1.707938	-2.793990

N,O-W11

15	-0.760435	0.790491	0.267
6	0.934145	0.186164	0.130
6	1.961123	1.141372	-0.343
6	1.234948	-1.182045	0.477
6	3.287752	0.721480	-0.522
1	1.706529	2.203006	-0.526
6	2.564871	-1.590959	0.380
1	0.425564	-1.915802	0.810
6	3.587777	-0.641196	-0.151

1	4.090698	1.460898	-0.923
1	2.804165	-2.656024	0.750
8	-0.820520	2.271410	0.496
34	-2.267947	-0.587121	-0.225
1	4.630213	-0.967487	-0.282

N,O-W12

6	3.769705	2.153476	0.331803
6	2.702601	1.318564	0.650400
6	2.581228	0.077104	0.014298
6	3.526843	-0.323152	-0.937557
6	4.591067	0.516939	-1.247605
6	4.712589	1.754518	-0.614917
1	3.863631	3.121999	0.826442
1	1.960054	1.626013	1.389674
1	3.421380	-1.290879	-1.432357
1	5.328249	0.204581	-1.989611
15	1.177756	-1.267	0.388597
15	-1.078091	0.985637	-0.610262
34	-0.069164	-0.353085	1.949799
34	1.265517	-2.920264	-0.342971
34	-1.114603	2.996267	-0.277101
6	-2.597532	0.046657	-0.521303
6	-2.567487	-1.286354	-0.957090
6	-3.781202	0.611264	-0.028790
6	-3.728862	-2.049447	-0.897200
1	-1.636971	-1.716055	-1.332809
6	-4.935591	-0.161979	0.025969
1	-3.789710	1.650243	0.308633
6	-4.908602	-1.489217	-0.406976
1	-3.710715	-3.087926	-1.232777
1	-5.860725	0.271236	0.410563
8	0.029035	0.191207	-1.259465

1	5.547495	2.413603	-0.862935
1	-5.817993	-2.092476	-0.361037
N,O-W13			
WR sub			
6	3.791459	2.191044	-0.593607
6	2.600165	1.487611	-0.450186
6	2.636106	0.102282	-0.240884
6	3.861479	-0.568775	-0.173904
6	5.049153	0.145943	-0.312230
6	5.014620	1.523283	-0.522594
1	3.761470	3.269033	-0.762804
1	1.648181	2.020785	-0.505430
1	3.881113	-1.650283	-0.021708
1	6.005098	-0.378425	-0.259170
15	1.095428	-0.822803	-0.033909
15	-1.095513	0.823001	-0.033763
34	0.066	0.099	1.802503
34	1.205678	-2.867414	-0.301081
34	-1.206043	2.867620	-0.300873
6	-2.636018	-0.102345	-0.240724
6	-2.599737	-1.487778	-0.449257
6	-3.861523	0.568545	-0.174577
6	-3.790845	-2.191502	-0.592768
1	-1.647607	-2.020787	-0.503832
6	-5.049016	-0.146461	-0.312995
1	-3.881399	1.650126	-0.022944
6	-5.014154	-1.523907	-0.522609
1	-3.760603	-3.269576	-0.761380
1	-6.005074	0.377769	-0.260605
8	-0.064	0.154	-0.989773
1	-5.946762	-2.081060	-0.634803
1	5.947373	2.080209	-0.634716

Acid			
1	0.	1.051074	-0.967908
1	0.	-1.051074	-0.967908
34	0.	0.	0.056936
Indolizine			
6	5.128981	0.895505	-0.570
6	5.368585	-0.515622	-0.066
6	4.312860	-1.381334	0.357
6	2.980491	-0.883551	0.311
7	2.789383	0.507256	-0.156
6	3.858699	1.377955	-0.611
6	1.726257	-1.467199	0.647
6	0.765165	-0.420686	0.360
6	1.450481	0.799784	-0.114
6	0.976893	2.212235	-0.549
6	-0.698142	-0.626356	0.496
6	-1.164617	-2.063820	0.001252
1	5.960448	1.600801	-0.932
1	6.393171	-0.890623	-0.030
1	4.461109	-2.462317	0.747
1	3.618796	2.440411	-0.001015
1	1.540749	-2.537787	0.001040
1	-0.117813	2.218836	-0.056
1	1.334750	2.756360	0.889823
1	1.333862	2.755521	-0.891795
1	-0.773504	-2.586202	-0.884491
1	-0.772545	-2.585576	0.886934
1	-2.258292	-2.137879	0.001850
7	-1.485013	0.380974	0.036
6	-2.877677	0.254942	-0.065
6	-3.589396	0.228687	1.208005
6	-3.588945	0.225536	-1.208323

6	-4.980270	0.155930	1.202951
1	-3.036023	0.266837	2.148729
6	-4.979825	0.152821	-1.203612
1	-3.035221	0.261232	-2.148940
6	-5.684186	0.116365	-0.415
1	-5.519220	0.130534	2.153075
1	-5.518405	0.124954	-2.153875
1	-6.774578	0.060126	-0.544

Figure 43

O,O-D1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771

16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051

6	-3.574545	-1.136383	0.056104	16	-0.205101	1.508974	-1.234888
1	-1.995603	-2.616824	0.099871	6	-3.097789	0.153494	-0.508821
6	-2.769395	1.109466	-0.122320	6	-3.889132	-0.922113	-0.109355
6	-3.846604	0.226048	-0.023242	6	-3.699798	1.314177	-1.008793
1	-4.384517	-1.864961	0.130790	6	-5.276459	-0.845663	-0.194787
1	-2.942230	2.188329	-0.193797	1	-3.426514	-1.835521	0.273028
1	-4.870163	0.603990	-0.011555	6	-5.078447	1.393851	-1.104500
6	1.239675	2.194562	-0.935888	1	-3.075359	2.152559	-1.324932
1	1.074718	3.239890	-0.646013	6	-5.879444	0.316561	-0.694373
1	2.245811	2.082825	-1.369636	1	-5.872665	-1.698832	0.127300
1	0.497232	1.881452	-1.682557	1	-5.568735	2.287098	-1.493857
O,O-D2				8	-7.206993	0.485865	-0.818062
6	3.677967	-1.204578	-0.819587	6	-8.072842	-0.536092	-0.398682
6	2.295766	-1.332889	-0.724402	1	-7.954385	-0.752426	0.676831
6	1.723587	-2.497279	-0.203752	1	-9.092371	-0.175092	-0.578698
6	2.557954	-3.537920	0.227884	1	-7.916494	-1.466349	-0.971206
6	3.935813	-3.412694	0.144971	6	1.994141	2.084050	1.322953
6	4.508095	-2.245525	-0.381555	1	2.770531	1.645428	1.956591
1	4.088772	-0.292510	-1.250945	6	0.733083	1.898234	1.758743
1	1.668162	-0.507183	-1.072938	6	-0.604966	2.306008	1.163125
1	2.111740	-4.452564	0.625482	6	0.560250	1.296315	3.141306
1	4.598572	-4.213913	0.475015	6	1.578694	0.295689	3.646765
8	5.851812	-2.210210	-0.431633	1	1.893483	-0.405217	2.861534
6	6.489068	-1.081379	-0.965245	1	2.469171	0.820279	4.027777
1	7.567282	-1.268911	-0.899066	1	1.127362	-0.249877	4.484307
1	6.218075	-0.918393	-2.022529	8	-1.537747	1.485571	1.204803
1	6.252214	-0.167998	-0.391297	8	-0.359652	1.661159	3.832808
15	-0.078793	-2.669774	-0.062429	6	2.565934	2.721533	0.125260
15	-1.298266	0.054418	-0.424253	6	3.874044	2.361718	-0.238247
16	-0.692510	-1.083267	1.262516	7	1.869216	3.622415	-0.575006
16	-0.927604	-1.670414	-1.732357	6	4.439576	2.915519	-1.380746
16	-0.709161	-4.438325	0.384459	1	4.429634	1.646449	0.371374

6	2.415629	4.154676	-1.661250	6	1.695256	2.854300	0.520219
6	3.692978	3.829225	-2.118520	1	2.221844	3.272	1.374704
1	5.451818	2.643017	-1.688056	6	0.232990	2.580377	0.464362
1	1.804485	4.883689	-2.203254	6	-0.016529	2.148153	-1.021318
1	4.091241	4.292738	-3.022283	6	-0.719994	3.629303	1.036283
6	-0.883657	3.763018	1.008893	6	-0.215886	4.410958	2.222636
1	-1.847115	3.907861	0.506043	1	0.562656	5.112659	1.886125
1	-0.947588	4.163525	2.035815	1	-1.046468	4.968416	2.670648
1	-0.059553	4.257383	0.480505	1	0.242460	3.745281	2.969096
O,O-D3				8	-0.987585	1.175268	-1.147922
6	3.686977	-0.808271	1.612083	8	-1.826745	3.805762	0.584303
6	2.409009	-1.361495	1.520336	6	2.290576	2.191036	-0.513963
6	2.058657	-2.176344	0.448052	6	3.667113	1.939386	-0.843881
6	3.024865	-2.472274	-0.528796	7	1.341453	1.651974	-1.375319
6	4.290377	-1.922656	-0.451218	6	3.975934	1.228549	-1.962376
6	4.626306	-1.068175	0.611914	1	4.440463	2.314308	-0.173373
1	3.922193	-0.163005	2.457925	6	1.654608	0.994532	-2.521876
1	1.672480	-1.135585	2.292493	6	2.953659	0.745703	-2.843072
1	2.772866	-3.136992	-1.358928	1	5.022963	1.015819	-2.188801
1	5.046070	-2.130603	-1.210189	1	0.808530	0.665260	-3.126328
15	0.366584	-2.791382	0.195903	1	3.198061	0.183510	-3.742603
15	-1.119988	-0.104547	-0.014699	6	-0.370309	3.301879	-1.952221
6	-2.926758	-0.134712	-0.009791	1	-0.360164	2.936290	-2.988096
6	-3.630255	-1.333253	-0.123385	1	-1.367460	3.684067	-1.713495
6	-3.628156	1.076602	0.086229	1	0.371790	4.106	-1.847346
6	-5.022121	-1.339044	-0.135859	8	-7.062831	-0.033512	0.001697
1	-3.091929	-2.279963	-0.200104	8	5.866789	-0.543079	0.577287
6	-5.012651	1.073809	0.095302	6	6.282676	0.289966	1.625232
1	-3.091636	2.025196	0.155132	1	6.264081	-0.233775	2.596301
6	-5.722856	-0.131675	-0.015443	1	7.314666	0.585959	1.401569
1	-5.542986	-2.290906	-0.233487	1	5.657586	1.197151	1.699372
1	-5.574991	2.004438	0.182359	6	-7.839700	-1.197869	-0.101445

1	-7.671972	-1.715771	-1.061284	6	-0.180285	-2.446875	0.687895
1	-7.635636	-1.899558	0.725312	6	-0.065786	-2.449337	-0.852119
1	-8.887878	-0.880552	-0.047371	6	0.811380	-3.294342	1.448109
16	0.225718	-4.674528	-0.203590	6	0.443871	-3.635610	2.870358
16	-0.908680	-1.893714	1.577910	1	-0.362165	-4.385707	2.862979
16	-0.285869	-1.471575	-1.403009	1	1.320147	-4.045329	3.385918
16	-0.138446	1.013521	1.463604	1	0.067095	-2.749961	3.403080
O,O-D4				8	0.968779	-1.616230	-1.315875
6	-3.875052	0.901114	1.414838	8	1.860676	-3.654226	0.958897
6	-2.559214	1.356687	1.467151	6	-2.295736	-2.179495	-0.183284
6	-2.045550	2.170107	0.456732	6	-3.681313	-1.933923	-0.477328
6	-2.870748	2.528096	-0.622287	7	-1.395233	-1.924896	-1.218215
6	-4.168966	2.061202	-0.693792	6	-4.041046	-1.446573	-1.695405
6	-4.680958	1.239206	0.323946	1	-4.418009	-2.125809	0.302564
1	-4.247364	0.267385	2.219251	6	-1.759300	-1.469836	-2.446206
1	-1.922751	1.074879	2.307658	6	-3.064117	-1.197508	-2.717030
1	-2.479834	3.177751	-1.408825	1	-5.091856	-1.226760	-1.895702
1	-4.820120	2.319772	-1.529976	1	-0.945499	-1.308335	-3.155049
15	-0.338323	2.753655	0.510051	1	-3.349154	-0.790451	-3.685452
15	1.193159	-0.173719	-0.582264	6	0.139301	-3.814596	-1.492001
6	2.967187	-0.032914	-0.451392	1	0.064104	-3.715064	-2.583701
6	3.583426	1.208209	-0.616700	1	1.125324	-4.207766	-1.225034
6	3.738021	-1.159924	-0.112460	1	-0.641609	-4.502077	-1.138115
6	4.960275	1.339044	-0.458204	8	7.060291	0.235018	0.037769
1	2.983034	2.085391	-0.869028	8	-5.950103	0.819613	0.160264
6	5.105784	-1.034355	0.037911	6	-6.570664	0.096392	1.189318
1	3.260106	-2.131353	0.037829	1	-6.581762	0.663485	2.135649
6	5.729629	0.214865	-0.132387	1	-7.603745	-0.083692	0.868950
1	5.416	2.319542	-0.590217	1	-6.078134	-0.875628	1.364095
1	5.726873	-1.893413	0.295409	6	7.753916	1.449141	-0.094005
6	-1.635972	-2.598693	0.935503	1	7.647319	1.871575	-1.107656
1	-2.099353	-2.778259	1.901613	1	7.411266	2.194462	0.643611

1	8.811621	1.226733	0.089313	6	-0.490662	3.278237	1.606209
16	-0.030912	4.521454	-0.179015	6	-0.635	3.477311	3.018353
16	0.746578	1.824492	1.861938	1	0.827847	4.202617	3.005207
16	0.353051	1.303298	-1.609871	1	-0.816855	3.871268	3.634887
16	0.294215	-0.592997	1.272581	1	0.383480	2.540528	3.447012
O,O-D5				8	-0.928444	1.816788	-1.293876
6	3.456397	-1.046303	1.734491	8	-1.526006	3.763646	1.215099
6	2.244100	-1.724074	1.644629	6	2.420102	2.151074	-0.350772
6	1.919271	-2.460613	0.503758	6	3.768669	1.885919	-0.761585
6	2.824829	-2.497915	-0.571127	7	1.444071	2.010379	-1.329358
6	4.023	-1.815062	-0.496260	6	4.019386	1.487047	-2.039825
6	4.353284	-1.090045	0.661319	1	4.569181	1.981480	-0.029708
1	3.684615	-0.487895	2.641705	6	1.693738	1.632995	-2.608754
1	1.536186	-1.681613	2.474478	6	2.966282	1.345607	-2.999428
1	2.572814	-3.067499	-1.467854	1	5.046072	1.258821	-2.334612
1	4.735311	-1.827239	-1.322068	1	0.820218	1.544331	-3.256613
15	0.358117	-3.347254	0.409437	1	3.163756	1.004470	-4.014040
15	-1.157877	0.286785	-0.703534	6	-0.993	3.981546	-1.319186
6	-2.930276	0.231150	-0.441388	1	0.012207	3.981297	-2.417648
6	-3.634038	-0.943687	-0.702578	1	-0.950013	4.393949	-0.963067
6	-3.605910	1.346412	0.084603	1	0.831964	4.594414	-0.947740
6	-5.002258	-1.021558	-0.450465	8	-6.988729	0.120389	0.344580
1	-3.107530	-1.810717	-1.108057	8	5.547922	-0.471394	0.651617
6	-4.964412	1.277021	0.328857	6	5.981231	0.195871	1.807465
1	-3.062217	2.269337	0.301454	1	6.045726	-0.488243	2.670537
6	-5.674882	0.091673	0.067012	1	6.980684	0.589673	1.587704
1	-5.524329	-1.954523	-0.659617	1	5.315465	1.037073	2.069685
1	-5.510365	2.131208	0.731637	6	-7.764996	-1.026908	0.117162
6	1.859717	2.507005	0.846255	1	-7.762459	-1.315301	-0.948001
1	2.398547	2.584883	1.786248	1	-7.415686	-1.881396	0.721469
6	0.388072	2.412768	0.707698	1	-8.790054	-0.775862	0.414584
6	0.158900	2.548814	-0.828181	16	0.278132	-4.750488	-0.892157

16	-0.935204	-2.885025	1.755246	1	0.669479	3.865541	3.293008
16	-0.438778	-1.119352	-1.830436	1	-1.054546	3.652073	3.761945
16	-0.215531	0.627252	1.155499	1	0.019273	2.232144	3.544360
O,O-D6				8	-0.925389	1.621735	-1.345247
6	3.853283	-1.233763	1.502964	8	-1.754047	3.539924	1.370803
6	2.521505	-1.637042	1.443083	6	2.385091	2.131048	-0.097454
6	2.003802	-2.199919	0.277466	6	3.712784	1.726656	-0.462955
6	2.835608	-2.360826	-0.843508	7	1.486994	2.426215	-1.154274
6	4.151900	-1.948487	-0.796272	6	4.067500	1.636663	-1.768941
6	4.670606	-1.373302	0.376416	1	4.416919	1.491	0.334184
1	4.231317	-0.795786	2.426140	6	1.858939	2.330914	-2.477788
1	1.883602	-1.506749	2.319052	6	3.112178	1.944725	-2.809118
1	2.439594	-2.801817	-1.760988	1	5.075041	1.315229	-2.039472
1	4.808889	-2.047306	-1.661081	1	1.081467	2.544954	-3.210295
15	0.302977	-2.775023	0.187885	1	3.384693	1.854830	-3.860201
15	-1.211086	0.244396	-0.720278	6	-0.439791	3.978361	-1.292734
6	-2.972923	0.048707	-0.467346	1	-0.556518	3.855023	-2.376560
6	-3.641073	-1.135145	-0.773011	1	-1.422351	4.128674	-0.837317
6	-3.682599	1.135875	0.075997	1	0.188442	4.860611	-1.094066
6	-5.012406	-1.250542	-0.552312	8	-7.040585	-0.176785	0.231658
1	-3.088927	-1.980453	-1.189737	8	5.951681	-0.972901	0.318693
6	-5.042495	1.024077	0.295812	6	6.562796	-0.451985	1.471056
1	-3.160987	2.061034	0.341832	1	6.556576	-1.182448	2.297480
6	-5.720459	-0.167624	-0.017614	1	7.601173	-0.227058	1.201206
1	-5.509888	-2.187685	-0.799490	1	6.073471	0.477495	1.809994
1	-5.614572	1.851585	0.717617	6	-7.787525	-1.328406	-0.060080
6	1.734121	2.299096	1.083995	1	-7.748723	-1.576714	-1.134660
1	2.153469	2.099146	2.066502	1	-7.439733	-2.198844	0.522179
6	0.339425	2.603927	0.785777	1	-8.825448	-1.107543	0.215802
6	0.228416	2.779329	-0.667772	16	-0.026783	-4.600875	-0.283051
6	-0.640632	3.171086	1.717030	16	-0.874861	-1.885359	1.613527
6	-0.227340	3.239506	3.172335	16	-0.419985	-1.269278	-1.827908

16	-0.305033	0.282174	1.239992	1	-5.711727	1.858825	0.824664
O,O-D7				8	-6.580377	-0.469640	0.366375
LR pentacycle				6	-7.016273	-1.774587	0.080708
6	4.410798	0.764260	-0.080292	1	-6.500645	-2.521577	0.707554
6	3.075444	0.423965	-0.277757	1	-8.089150	-1.801310	0.304100
6	2.674579	-0.914343	-0.258307	1	-6.865225	-2.028166	-0.982178
6	3.635809	-1.921564	-0.060060	8	0.809950	-2.857590	-0.919134
6	4.964094	-1.589477	0.131897	16	-0.036240	-1.245385	1.435220
6	5.363430	-0.241781	0.130187	Indolizine			
1	4.693312	1.816218	-0.102854	6	-3.314580	0.544323	-0.058
1	2.349157	1.218682	-0.458594	6	-3.369348	-0.887307	-0.111
1	3.328275	-2.969620	-0.070183	6	-2.211924	-1.609901	-0.039
1	5.725388	-2.356308	0.281646	6	-0.953112	-0.945392	0.077
8	6.670140	-0.015523	0.327953	7	-0.944977	0.460093	0.035
6	7.150407	1.304815	0.346628	6	-2.118347	1.186485	0.064
1	8.229184	1.239963	0.534	6	0.365875	-1.361996	0.179
1	6.981152	1.812754	-0.617837	6	1.178830	-0.196662	0.142
1	6.683897	1.895136	1.153367	6	0.342390	0.923968	-0.033
15	0.976038	-1.461751	-0.443708	6	0.643869	2.382512	-0.063
15	-0.950908	1.320427	-0.272496	6	2.661096	-0.167381	-0.032
16	0.045101	0.829825	1.565566	6	3.367767	-1.507089	-0.152
16	0.025739	0.020602	-1.679245	8	3.296388	0.867672	0.005
16	-0.709282	3.204553	-0.609874	1	-4.231497	1.134345	-0.047
6	-2.646023	0.711065	-0.154757	1	-4.337378	-1.390285	-0.226
6	-3.004610	-0.605538	-0.454951	1	-2.220273	-2.700963	-0.013
6	-3.630655	1.601941	0.308790	1	-2.014550	2.270881	0.222
6	-4.317759	-1.039379	-0.290892	1	0.695744	-2.397669	0.318
1	-2.263078	-1.309588	-0.835491	1	1.729765	2.520303	-0.890
6	-4.935745	1.177872	0.472585	1	0.223807	2.879683	-0.890290
1	-3.364443	2.638675	0.527003	1	0.225345	2.879394	0.891066
6	-5.292104	-0.149516	0.177943	1	3.083900	-2.092583	0.887620
1	-4.564172	-2.071707	-0.536690	1	3.082298	-2.093631	-0.886705

1 4.451489 -1.340867 -0.001188

Figure 44

O,O-E1

LR

6 4.399900 -0.931020 0.078

6 3.051574 -0.594451 0.074

6 2.652608 0.746089 0.098

6 3.625607 1.755391 0.006

6 4.971010 1.427326 0.027

6 5.371218 0.082184 0.079

1 4.679398 -1.984067 0.068

1 2.307030 -1.395415 0.071

1 3.315697 2.802948 -0.108

1 5.741782 2.198979 -0.020

8 6.693580 -0.140809 0.086

6 7.174688 -1.460847 0.183

1 8.268794 -1.392340 0.326

1 6.850105 -2.011894 0.899028

1 6.850302 -2.011911 -0.898728

15 0.901258 1.184195 -0.247

15 -0.901144 -1.183693 -0.071

16 -0.184 0.609 -1.552090

16 -0.116 0.185 1.553327

16 0.492940 3.068803 -0.771

16 -0.492242 -3.068189 -0.603

6 -2.652613 -0.746168 -0.150

6 -3.051857 0.594301 0.287

6 -3.625394 -1.755670 -0.493

6 -4.400241 0.930604 0.362

1 -2.307453 1.395396 0.536

6 -4.970864 -1.427866 -0.432

1 -3.315267 -2.803163 -0.809

6 -5.371350 -0.082808 0.013

1 -4.679935 1.983600 0.725

1 -5.741489 -2.199662 -0.707

8 -6.693755 0.139912 0.103

6 -7.175115 1.459861 0.447

1 -6.850662 2.011249 -0.898237

1 -8.269204 1.391129 0.340

1 -6.850803 2.010720 0.899507

Preindolizine

6 0.178997 -1.007094 -0.061471

1 0.344103 -2.083841 -0.158607

6 1.241723 -0.189608 0.035834

6 1.157013 1.312645 0.278992

6 2.649285 -0.701640 -0.049454

6 2.902049 -2.193470 -0.049733

1 2.462099 -2.668778 0.839244

1 2.458138 -2.665040 -0.939439

1 3.985338 -2.360717 -0.058901

8 1.125 1.721883 1.410299

8 3.564577 0.088276 -0.125556

6 -1.233616 -0.593404 -0.052625

6 -2.248065 -1.556404 0.038139

7 -1.504383 0.713443 -0.139051

6 -3.574545 -1.136383 0.056104

1 -1.995603 -2.616824 0.099871

6 -2.769395 1.109466 -0.122320

6 -3.846604 0.226048 -0.023242

1 -4.384517 -1.864961 0.130790

1 -2.942230 2.188329 -0.193797

1 -4.870163 0.603990 -0.011555

6 1.239675 2.194562 -0.935888

1	1.074718	3.239890	-0.646013	6	5.239282	-0.503636	-0.127213
1	2.245811	2.082825	-1.369636	1	5.008365	1.456113	0.793375
1	0.497232	1.881452	-1.682557	1	5.155828	-2.472745	-0.988319
O,O-E2				8	6.554046	-0.461539	-0.378351
6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	O,O-E3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	O,O-E4			
6	4.518843	0.533126	0.484738	6	-3.334661	0.397287	-0.108530
1	2.590010	1.198244	1.169247	1	-4.118597	0.841972	-0.722543
6	4.574104	-1.679850	-0.516320	6	-2.413161	1.137904	0.523965
1	2.700275	-2.728593	-0.606940	6	-1.331402	0.469811	1.339344

6	-2.423406	2.642127	0.573366	1	4.751288	2.038421	0.583111
6	-3.226687	3.371879	-0.471469	1	2.366028	2.293570	-0.127409
1	-2.942736	3.028651	-1.475901	1	2.137963	-1.937187	-0.842338
1	-4.301678	3.184930	-0.320741	1	4.497353	-2.202090	-0.158553
1	-3.035202	4.446410	-0.371560	1	7.772680	-1.129256	0.989940
8	-0.181966	0.303263	0.873581	1	6.291452	-2.066358	1.350436
8	-1.840026	3.212329	1.466614	1	6.791949	-1.791956	-0.352023
6	-3.262443	-1.057243	0.047002	O,O-E5			
6	-4.026569	-1.984634	-0.659766	6	-3.140294	1.584731	-0.280793
7	-2.344662	-1.437919	0.937046	1	-3.709346	2.314968	-0.851029
6	-3.781158	-3.337644	-0.441352	6	-1.835213	1.665546	0.090194
1	-4.772442	-1.650062	-1.381820	6	-1.480183	0.491734	1.008572
6	-2.094447	-2.720682	1.142669	6	-0.930	2.850856	-0.038497
6	-2.797807	-3.718820	0.469015	6	-1.271552	3.857357	-1.106844
1	-4.347532	-4.093322	-0.989262	1	-1.458073	3.363216	-2.069440
1	-1.306134	-2.962164	1.861521	1	-2.182418	4.403799	-0.811958
1	-2.572631	-4.769972	0.652262	1	-0.445870	4.572077	-1.201154
6	-1.475502	0.477469	2.828198	8	-0.317280	-0.179641	0.828175
1	-0.772198	-0.234987	3.276436	8	-0.016499	3.007072	0.741074
1	-1.221252	1.499873	3.148804	6	-3.641042	0.282075	0.068685
1	-2.506781	0.258154	3.129696	6	-4.848867	-0.366933	-0.195334
6	4.776332	-0.086964	0.264722	7	-2.680203	-0.390818	0.748746
6	4.160975	1.175118	0.271815	6	-4.992672	-1.686546	0.211374
6	2.839920	1.309386	-0.118334	1	-5.639784	0.157630	-0.730794
6	2.099257	0.186979	-0.519755	6	-2.779272	-1.671388	1.127676
6	2.712662	-1.064653	-0.522233	6	-3.951747	-2.354049	0.871303
6	4.044366	-1.211129	-0.135774	1	-5.923496	-2.216349	-0.626
8	6.065983	-0.118937	0.651254	1	-1.897723	-2.106604	1.599296
6	6.750251	-1.342013	0.655008	1	-4.039900	-3.400726	1.158560
15	0.365113	0.365313	-1.020351	6	-1.536444	0.938450	2.474250
16	-0.395518	-1.250449	-1.791788	1	-1.392286	0.061315	3.119785
16	-0.068646	2.175	-1.599652	1	-0.715143	1.646720	2.632687

1	-2.495026	1.423241	2.705257	6	-2.972923	0.048707	-0.467346
6	4.722340	-0.478309	0.214403	6	-3.641073	-1.135145	-0.773011
6	4.147210	-1.725998	-0.061687	6	-3.682599	1.135875	0.075997
6	2.789598	-1.825263	-0.329545	6	-5.012406	-1.250542	-0.552312
6	1.981623	-0.683022	-0.334273	1	-3.088927	-1.980453	-1.189737
6	2.557916	0.559332	-0.060484	6	-5.042495	1.024077	0.295812
6	3.917767	0.669611	0.217513	1	-3.160987	2.061034	0.341832
8	6.048008	-0.475075	0.464652	6	-5.720459	-0.167624	-0.017614
6	6.684189	0.737929	0.757572	1	-5.509888	-2.187685	-0.799490
15	0.206411	-0.789886	-0.700188	1	-5.614572	1.851585	0.717617
16	-0.436380	-2.634319	-0.905621	6	1.734121	2.299096	1.083995
16	-0.346921	0.608717	-2.010456	1	2.153469	2.099146	2.066502
1	4.791428	-2.606844	-0.058579	6	0.339425	2.603927	0.785777
1	2.335118	-2.797119	-0.537347	6	0.228416	2.779329	-0.667772
1	1.938599	1.459807	-0.058644	6	-0.640632	3.171086	1.717030
1	4.336146	1.653318	0.429602	6	-0.227340	3.239506	3.172335
1	7.743047	0.506438	0.926120	1	0.669479	3.865541	3.293008
1	6.605952	1.456258	-0.077134	1	-1.054546	3.652073	3.761945
1	6.272880	1.206956	1.668523	1	0.019273	2.232144	3.544360
O,O-E6				8	-0.925389	1.621735	-1.345247
6	3.853283	-1.233763	1.502964	8	-1.754047	3.539924	1.370803
6	2.521505	-1.637042	1.443083	6	2.385091	2.131048	-0.097454
6	2.003802	-2.199919	0.277466	6	3.712784	1.726656	-0.462955
6	2.835608	-2.360826	-0.843508	7	1.486994	2.426215	-1.154274
6	4.151900	-1.948487	-0.796272	6	4.067500	1.636663	-1.768941
6	4.670606	-1.373302	0.376416	1	4.416919	1.491	0.334184
1	4.231317	-0.795786	2.426140	6	1.858939	2.330914	-2.477788
1	1.883602	-1.506749	2.319052	6	3.112178	1.944725	-2.809118
1	2.439594	-2.801817	-1.760988	1	5.075041	1.315229	-2.039472
1	4.808889	-2.047306	-1.661081	1	1.081467	2.544954	-3.210295
15	0.302977	-2.775023	0.187885	1	3.384693	1.854830	-3.860201
15	-1.211086	0.244396	-0.720278	6	-0.439791	3.978361	-1.292734

1	-0.556518	3.855023	-2.376560	1	-4.231497	1.134345	-0.047
1	-1.422351	4.128674	-0.837317	1	-4.337378	-1.390285	-0.226
1	0.188442	4.860611	-1.094066	1	-2.220273	-2.700963	-0.013
8	-7.040585	-0.176785	0.231658	1	-2.014550	2.270881	0.222
8	5.951681	-0.972901	0.318693	1	0.695744	-2.397669	0.318
6	6.562796	-0.451985	1.471056	1	1.729765	2.520303	-0.890
1	6.556576	-1.182448	2.297480	1	0.223807	2.879683	-0.890290
1	7.601173	-0.227058	1.201206	1	0.225345	2.879394	0.891066
1	6.073471	0.477495	1.809994	1	3.083900	-2.092583	0.887620
6	-7.787525	-1.328406	-0.060080	1	3.082298	-2.093631	-0.886705
1	-7.748723	-1.576714	-1.134660	1	4.451489	-1.340867	-0.001188
1	-7.439733	-2.198844	0.522179	LR 5 Cycle Carbonyl			
1	-8.825448	-1.107543	0.215802	6	4.410798	0.764260	-0.080292
16	-0.026783	-4.600875	-0.283051	6	3.075444	0.423965	-0.277757
16	-0.874861	-1.885359	1.613527	6	2.674579	-0.914343	-0.258307
16	-0.419985	-1.269278	-1.827908	6	3.635809	-1.921564	-0.060060
16	-0.305033	0.282174	1.239992	6	4.964094	-1.589477	0.131897
O,O-E7				6	5.363430	-0.241781	0.130187
Indolizine				1	4.693312	1.816218	-0.102854
6	-3.314580	0.544323	-0.058	1	2.349157	1.218682	-0.458594
6	-3.369348	-0.887307	-0.111	1	3.328275	-2.969620	-0.070183
6	-2.211924	-1.609901	-0.039	1	5.725388	-2.356308	0.281646
6	-0.953112	-0.945392	0.077	8	6.670140	-0.015523	0.327953
7	-0.944977	0.460093	0.035	6	7.150407	1.304815	0.346628
6	-2.118347	1.186485	0.064	1	8.229184	1.239963	0.534
6	0.365875	-1.361996	0.179	1	6.981152	1.812754	-0.617837
6	1.178830	-0.196662	0.142	1	6.683897	1.895136	1.153367
6	0.342390	0.923968	-0.033	15	0.976038	-1.461751	-0.443708
6	0.643869	2.382512	-0.063	15	-0.950908	1.320427	-0.272496
6	2.661096	-0.167381	-0.032	16	0.045101	0.829825	1.565566
6	3.367767	-1.507089	-0.152	16	0.025739	0.020602	-1.679245
8	3.296388	0.867672	0.005	16	-0.709282	3.204553	-0.609874

6	-2.646023	0.711065	-0.154757
6	-3.004610	-0.605538	-0.454951
6	-3.630655	1.601941	0.308790
6	-4.317759	-1.039379	-0.290892
1	-2.263078	-1.309588	-0.835491
6	-4.935745	1.177872	0.472585
1	-3.364443	2.638675	0.527003
6	-5.292104	-0.149516	0.177943
1	-4.564172	-2.071707	-0.536690
1	-5.711727	1.858825	0.824664
8	-6.580377	-0.469640	0.366375
6	-7.016273	-1.774587	0.080708
1	-6.500645	-2.521577	0.707554
1	-8.089150	-1.801310	0.304100
1	-6.865225	-2.028166	-0.982178
8	0.809950	-2.857590	-0.919134
16	-0.036240	-1.245385	1.435220

Figure 45

O,O-F1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086

6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454

6	2.902049	-2.193470	-0.049733	6	-0.781222	2.506295	0.638182
1	2.462099	-2.668778	0.839244	6	-2.064570	2.175195	0.187164
1	2.458138	-2.665040	-0.939439	7	-0.494089	2.590175	1.938503
1	3.985338	-2.360717	-0.058901	6	-3.048382	1.870302	1.119582
8	1.125	1.721883	1.410299	1	-2.272592	2.120794	-0.882030
8	3.564577	0.088276	-0.125556	6	-1.432633	2.289552	2.827111
6	-1.233616	-0.593404	-0.052625	6	-2.726870	1.910706	2.472928
6	-2.248065	-1.556404	0.038139	1	-4.050359	1.586240	0.791747
7	-1.504383	0.713443	-0.139051	1	-1.143772	2.358421	3.881197
6	-3.574545	-1.136383	0.056104	1	-3.463096	1.664213	3.239498
1	-1.995603	-2.616824	0.099871	6	2.909039	2.945097	2.327286
6	-2.769395	1.109466	-0.122320	1	3.232588	2.214953	3.078721
6	-3.846604	0.226048	-0.023242	1	3.771321	3.449618	1.870101
1	-4.384517	-1.864961	0.130790	1	2.265282	3.708576	2.789543
1	-2.942230	2.188329	-0.193797	6	-4.385864	-0.179300	-1.481444
1	-4.870163	0.603990	-0.011555	6	-3.159213	-0.771994	-1.190223
6	1.239675	2.194562	-0.935888	6	-3.004504	-1.578180	-0.061162
1	1.074718	3.239890	-0.646013	6	-4.105603	-1.785792	0.785020
1	2.245811	2.082825	-1.369636	6	-5.324482	-1.190109	0.510875
1	0.497232	1.881452	-1.682557	6	-5.477669	-0.381598	-0.627284
O,O-F2				1	-4.473572	0.435122	-2.377165
6	0.317856	2.850112	-0.317751	1	-2.315384	-0.591926	-1.859685
1	-0.022750	3.390829	-1.203079	1	-4.327	-2.432210	1.659287
6	1.611126	3.041250	0.093034	1	-6.187979	-1.342972	1.159785
6	2.121586	2.259814	1.257895	8	-6.693870	0.156341	-0.811309
6	2.604331	3.713242	-0.765059	6	-6.922347	0.984506	-1.922205
6	2.132535	4.354970	-2.057675	1	-7.968641	1.305916	-1.861418
1	1.723775	3.591252	-2.738685	1	-6.272911	1.876762	-1.905215
1	1.349037	5.106064	-1.878635	1	-6.767916	0.445613	-2.872268
1	2.994905	4.833997	-2.536013	15	-1.418333	-2.342929	0.376950
8	1.907185	1.031745	1.301212	15	0.714384	-0.612354	-0.710404
8	3.790063	3.735531	-0.479004	16	-0.268786	-2.388419	-1.436140

16	-0.178988	-0.802854	1.216327	7	2.282696	1.315431	0.916161
16	-1.542105	-3.962304	1.413516	6	2.344603	0.967133	3.678258
16	0.282459	0.990907	-1.754625	1	0.581840	2.222565	3.680182
6	2.453144	-1.050141	-0.632080	6	3.224933	0.568969	1.492784
6	2.845980	-2.251472	-0.040477	6	3.296205	0.352636	2.864648
6	3.423748	-0.156867	-1.106027	1	2.365659	0.832735	4.761914
6	4.194460	-2.573634	0.071281	1	3.957354	0.109789	0.822096
1	2.096446	-2.947507	0.344906	1	4.081223	-0.279853	3.281756
6	4.765540	-0.469871	-0.997941	6	0.228663	2.441582	-2.922841
1	3.120041	0.794189	-1.547343	1	-0.255262	1.623381	-3.469323
6	5.163886	-1.680883	-0.408348	1	-0.199895	3.407486	-3.218539
1	4.474876	-3.516957	0.538522	1	1.294100	2.493586	-3.185847
1	5.533915	0.218604	-1.351227	6	3.623025	-1.073707	-1.583669
8	6.486060	-1.898764	-0.344533	6	2.283273	-1.271242	-1.260205
6	6.965977	-3.080567	0.242289	6	1.903778	-2.263479	-0.354868
1	6.611827	-3.976203	-0.296086	6	2.893342	-3.062517	0.237279
1	8.059626	-3.037250	0.179094	6	4.229269	-2.867890	-0.070820
1	6.671621	-3.158015	1.302758	6	4.606499	-1.874033	-0.988499
O,O-F3				1	3.883590	-0.288388	-2.292385
6	0.259825	2.678820	1.006588	1	1.523732	-0.639604	-1.724355
1	0.161646	3.627424	1.553659	1	2.600282	-3.852106	0.933227
6	0.516020	2.988640	-0.445602	1	5.010087	-3.484425	0.377032
6	0.062995	2.204497	-1.453174	8	5.924311	-1.757179	-1.227549
6	1.353244	4.179938	-0.770950	6	6.373350	-0.787747	-2.138285
6	1.988342	4.930030	0.385741	1	7.463956	-0.888083	-2.189349
1	1.223625	5.449285	0.984493	1	5.952193	-0.948444	-3.145275
1	2.537541	4.251938	1.055215	1	6.122430	0.233764	-1.804074
1	2.675147	5.677158	-0.028585	15	0.157232	-2.533573	0.067554
8	-0.590961	1.017066	-1.275267	15	-1.293572	0.205457	-0.021263
8	1.553621	4.556161	-1.908516	16	-0.302398	-0.902973	1.455351
6	1.359151	1.876416	1.688914	16	-1.001451	-1.682408	-1.427039
6	1.362252	1.745847	3.083690	16	-0.250119	-4.291862	0.765234

16	-1.414959	1.966159	1.273192	1	-3.644007	-1.325230	-2.367714
6	-3.095051	0.059568	-0.155199	6	-3.229851	-1.425642	1.451011
6	-3.741678	-1.106855	0.254300	6	-4.042703	-2.380286	0.853845
6	-3.843467	1.120745	-0.683041	1	-4.835094	-3.081568	-1.029089
6	-5.125056	-1.217005	0.157461	1	-3.021732	-1.412433	2.523583
1	-3.165607	-1.948903	0.645084	1	-4.523150	-3.148173	1.460383
6	-5.218113	1.005283	-0.807377	6	-1.648428	1.344548	2.492802
1	-3.350631	2.043893	-0.994642	1	-1.495468	0.513691	3.195792
6	-5.872483	-0.161489	-0.383555	1	-0.916373	2.134788	2.704142
1	-5.603536	-2.135914	0.494261	1	-2.642081	1.792131	2.600798
1	-5.817303	1.814353	-1.227050	15	0.323193	-0.898372	-0.122791
8	-7.206476	-0.179928	-0.534617	16	-0.067343	-2.778665	0.108002
6	-7.929194	-1.315641	-0.134499	16	-0.396793	-0.029011	-1.923830
1	-7.816373	-1.509191	0.945788	6	2.055064	-0.419632	-0.063038
1	-8.983725	-1.107511	-0.350109	6	3.056866	-1.384501	0.003512
1	-7.619325	-2.213826	-0.695370	6	2.402218	0.942799	-0.075444
O,O-F4				6	4.404	-1.012679	0.054810
6	-1.971670	0.724965	-1.192629	1	2.781784	-2.442175	0.020403
1	-2.455461	1.175796	-2.066819	6	3.730141	1.320071	-0.020799
6	-1.733297	1.642982	-0.060218	1	1.620547	1.705136	-0.130563
6	-1.432475	0.865602	1.094567	6	4.742016	0.344664	0.043443
6	-2.139016	3.019091	-0.007577	1	5.163567	-1.788185	0.105510
6	-2.574531	3.661827	-1.323831	1	4.022654	2.371050	-0.026381
1	-1.833248	3.504899	-2.122796	8	6.001584	0.808426	0.089880
1	-3.536238	3.246559	-1.667518	6	7.068399	-0.101418	0.151946
1	-2.702005	4.737644	-1.153387	1	7.092753	-0.761614	-0.731964
8	-0.297854	0.048572	1.073749	1	7.988081	0.495126	0.175382
8	-2.134952	3.701981	1.014513	1	7.021784	-0.722461	1.062963
6	-2.798031	-0.412620	-0.608643	Indolizine			
6	-3.568424	-1.355001	-1.280223	6	-3.314580	0.544323	-0.058
7	-2.669868	-0.470924	0.717530	6	-3.369348	-0.887307	-0.111
6	-4.211147	-2.336759	-0.531113	6	-2.211924	-1.609901	-0.039

6	-0.953112	-0.945392	0.077	8	6.670140	-0.015523	0.327953
7	-0.944977	0.460093	0.035	6	7.150407	1.304815	0.346628
6	-2.118347	1.186485	0.064	1	8.229184	1.239963	0.534
6	0.365875	-1.361996	0.179	1	6.981152	1.812754	-0.617837
6	1.178830	-0.196662	0.142	1	6.683897	1.895136	1.153367
6	0.342390	0.923968	-0.033	15	0.976038	-1.461751	-0.443708
6	0.643869	2.382512	-0.063	15	-0.950908	1.320427	-0.272496
6	2.661096	-0.167381	-0.032	16	0.045101	0.829825	1.565566
6	3.367767	-1.507089	-0.152	16	0.025739	0.020602	-1.679245
8	3.296388	0.867672	0.005	16	-0.709282	3.204553	-0.609874
1	-4.231497	1.134345	-0.047	6	-2.646023	0.711065	-0.154757
1	-4.337378	-1.390285	-0.226	6	-3.004610	-0.605538	-0.454951
1	-2.220273	-2.700963	-0.013	6	-3.630655	1.601941	0.308790
1	-2.014550	2.270881	0.222	6	-4.317759	-1.039379	-0.290892
1	0.695744	-2.397669	0.318	1	-2.263078	-1.309588	-0.835491
1	1.729765	2.520303	-0.890	6	-4.935745	1.177872	0.472585
1	0.223807	2.879683	-0.890290	1	-3.364443	2.638675	0.527003
1	0.225345	2.879394	0.891066	6	-5.292104	-0.149516	0.177943
1	3.083900	-2.092583	0.887620	1	-4.564172	-2.071707	-0.536690
1	3.082298	-2.093631	-0.886705	1	-5.711727	1.858825	0.824664
1	4.451489	-1.340867	-0.001188	8	-6.580377	-0.469640	0.366375
LR 5 Cycle Carbonyl				6	-7.016273	-1.774587	0.080708
6	4.410798	0.764260	-0.080292	1	-6.500645	-2.521577	0.707554
6	3.075444	0.423965	-0.277757	1	-8.089150	-1.801310	0.304100
6	2.674579	-0.914343	-0.258307	1	-6.865225	-2.028166	-0.982178
6	3.635809	-1.921564	-0.060060	8	0.809950	-2.857590	-0.919134
6	4.964094	-1.589477	0.131897	16	-0.036240	-1.245385	1.435220
6	5.363430	-0.241781	0.130187				
1	4.693312	1.816218	-0.102854				
1	2.349157	1.218682	-0.458594				
1	3.328275	-2.969620	-0.070183				
1	5.725388	-2.356308	0.281646				

Figure 46

O,O-G1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103

6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013
1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557

O,O-G2

6	-4.040100	-0.995309	-0.715057	6	7.292017	0.681090	-0.023996
6	-2.806060	-0.380074	-0.894362	1	7.259570	0.862974	1.063412
6	-2.537931	0.861547	-0.308140	1	8.328884	0.487145	-0.321802
6	-3.531311	1.490869	0.464960	1	6.928185	1.578435	-0.551917
6	-4.758656	0.886153	0.643939	O,O-G3			
6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	O,O-G4			
6	4.518843	0.533126	0.484738	6	-3.334661	0.397287	-0.108530
1	2.590010	1.198244	1.169247	1	-4.118597	0.841972	-0.722543
6	4.574104	-1.679850	-0.516320	6	-2.413161	1.137904	0.523965
1	2.700275	-2.728593	-0.606940	6	-1.331402	0.469811	1.339344
6	5.239282	-0.503636	-0.127213	6	-2.423406	2.642127	0.573366
1	5.008365	1.456113	0.793375	6	-3.226687	3.371879	-0.471469
1	5.155828	-2.472745	-0.988319	1	-2.942736	3.028651	-1.475901
8	6.554046	-0.461539	-0.378351	1	-4.301678	3.184930	-0.320741

1	-3.035202	4.446410	-0.371560
8	-0.181966	0.303263	0.873581
8	-1.840026	3.212329	1.466614
6	-3.262443	-1.057243	0.047002
6	-4.026569	-1.984634	-0.659766
7	-2.344662	-1.437919	0.937046
6	-3.781158	-3.337644	-0.441352
1	-4.772442	-1.650062	-1.381820
6	-2.094447	-2.720682	1.142669
6	-2.797807	-3.718820	0.469015
1	-4.347532	-4.093322	-0.989262
1	-1.306134	-2.962164	1.861521
1	-2.572631	-4.769972	0.652262
6	-1.475502	0.477469	2.828198
1	-0.772198	-0.234987	3.276436
1	-1.221252	1.499873	3.148804
1	-2.506781	0.258154	3.129696
6	4.776332	-0.086964	0.264722
6	4.160975	1.175118	0.271815
6	2.839920	1.309386	-0.118334
6	2.099257	0.186979	-0.519755
6	2.712662	-1.064653	-0.522233
6	4.044366	-1.211129	-0.135774
8	6.065983	-0.118937	0.651254
6	6.750251	-1.342013	0.655008
15	0.365113	0.365313	-1.020351
16	-0.395518	-1.250449	-1.791788
16	-0.068646	2.175	-1.599652
1	4.751288	2.038421	0.583111
1	2.366028	2.293570	-0.127409
1	2.137963	-1.937187	-0.842338
1	4.497353	-2.202090	-0.158553

1	7.772680	-1.129256	0.989940
1	6.291452	-2.066358	1.350436
1	6.791949	-1.791956	-
0.352023O,O-G5			
6	-3.140294	1.584731	-0.280793
1	-3.709346	2.314968	-0.851029
6	-1.835213	1.665546	0.090194
6	-1.480183	0.491734	1.008572
6	-0.930	2.850856	-0.038497
6	-1.271552	3.857357	-1.106844
1	-1.458073	3.363216	-2.069440
1	-2.182418	4.403799	-0.811958
1	-0.445870	4.572077	-1.201154
8	-0.317280	-0.179641	0.828175
8	-0.016499	3.007072	0.741074
6	-3.641042	0.282075	0.068685
6	-4.848867	-0.366933	-0.195334
7	-2.680203	-0.390818	0.748746
6	-4.992672	-1.686546	0.211374
1	-5.639784	0.157630	-0.730794
6	-2.779272	-1.671388	1.127676
6	-3.951747	-2.354049	0.871303
1	-5.923496	-2.216349	-0.626
1	-1.897723	-2.106604	1.599296
1	-4.039900	-3.400726	1.158560
6	-1.536444	0.938450	2.474250
1	-1.392286	0.061315	3.119785
1	-0.715143	1.646720	2.632687
1	-2.495026	1.423241	2.705257
6	4.722340	-0.478309	0.214403
6	4.147210	-1.725998	-0.061687
6	2.789598	-1.825263	-0.329545

6	1.981623	-0.683022	-0.334273	6	3.966562	1.004552	-2.023042
6	2.557916	0.559332	-0.060484	1	4.958379	2.825119	-1.352980
6	3.917767	0.669611	0.217513	1	2.656864	-0.640521	-2.524288
8	6.048008	-0.475075	0.464652	1	4.872664	0.508551	-2.365661
6	6.684189	0.737929	0.757572	6	-0.057917	-0.034670	-3.147397
15	0.206411	-0.789886	-0.700188	1	0.656846	-0.798366	-3.481747
16	-0.436380	-2.634319	-0.905621	1	-1.068541	-0.449509	-3.177617
16	-0.346921	0.608717	-2.010456	1	-0.013292	0.833877	-3.818854
1	4.791428	-2.606844	-0.058579	6	3.812707	0.218558	1.473852
1	2.335118	-2.797119	-0.537347	6	2.597345	-0.237475	0.976598
1	1.938599	1.459807	-0.058644	6	2.511311	-1.453529	0.289332
1	4.336146	1.653318	0.429602	6	3.676317	-2.220588	0.125408
1	7.743047	0.506438	0.926120	6	4.890180	-1.774825	0.618295
1	6.605952	1.456258	-0.077134	6	4.972215	-0.545091	1.290224
1	6.272880	1.206956	1.668523	1	3.837215	1.177471	1.994
O,O-G6				1	1.717909	0.387901	1.122667
6	0.306553	2.640231	-0.879918	1	3.624138	-3.167214	-0.417095
1	0.030761	3.612120	-0.483296	1	5.802817	-2.358336	0.489225
6	-0.583843	1.554435	-1.135761	8	6.192795	-0.178626	1.712662
6	0.268844	0.394935	-1.725109	6	6.347120	1.043198	2.387467
6	-1.979749	1.820591	-1.631583	1	7.413615	1.138405	2.622819
6	-2.603770	3.124043	-1.194718	1	6.041936	1.896613	1.757551
1	-2.167876	3.947493	-1.782037	1	5.768596	1.066371	3.326359
1	-3.683215	3.076344	-1.379757	15	0.970537	-2.041050	-0.458141
1	-2.404902	3.333811	-0.132571	15	-1.355941	0.836546	1.031403
8	-2.578003	1.038466	-2.336445	16	-0.480702	-0.695371	2.248747
6	1.604713	2.248099	-1.151370	8	0.134384	-0.681969	-0.827986
6	2.855900	2.925262	-1.025538	16	-0.960542	2.334366	2.247109
7	1.632173	0.969886	-1.673378	6	-3.103154	0.382828	0.871373
6	3.999877	2.310597	-1.450882	6	-3.454973	-0.679428	0.034340
1	2.865526	3.924458	-0.590598	6	-4.108526	1.088154	1.547742
6	2.765009	0.367697	-2.120100	6	-4.787138	-1.050071	-0.121897

1	-2.682320	-1.228112	-0.509210	1	1.922491	-0.449062	-2.938357
6	-5.437337	0.730842	1.390794	1	4.309786	0.262162	-3.032075
1	-3.832372	1.916845	2.204635	6	-0.698323	0.208108	-2.570824
6	-5.787947	-0.343258	0.557536	1	-0.269208	-0.725190	-2.961283
1	-5.030729	-1.880714	-0.783434	1	-1.758999	0.043455	-2.356886
1	-6.234213	1.264073	1.911665	1	-0.618282	0.997651	-3.328693
8	-7.101500	-0.619575	0.470414	6	4.220588	-0.237343	1.189424
6	-7.525919	-1.690723	-0.330147	6	2.866565	-0.491939	1.006748
1	-7.091296	-2.647886	0.005737	6	2.444702	-1.581044	0.236963
1	-8.616750	-1.742732	-0.230815	6	3.403760	-2.428705	-0.338612
1	-7.270538	-1.533485	-1.392133	6	4.752913	-2.175776	-0.166904
16	1.199599	-3.349066	-1.867223	6	5.173725	-1.071706	0.591287
16	-0.373547	-2.702225	1.009118	1	4.516575	0.626424	1.783257
O,O-G7				1	2.134717	0.181014	1.457964
6	0.696265	2.487157	0.046973	1	3.075865	-3.285101	-0.932101
1	0.697030	3.281839	0.786629	1	5.511879	-2.819288	-0.613938
6	-0.545297	1.785667	-0.427822	8	6.500584	-0.890140	0.686190
6	0.032482	0.607727	-1.302238	6	6.996367	0.201854	1.416925
6	-1.532126	2.708066	-1.211180	1	8.089013	0.159286	1.337924
6	-1.210690	4.173592	-1.277213	1	6.643559	1.161732	1.002211
1	-0.212611	4.332374	-1.709811	1	6.711853	0.143411	2.481162
1	-1.979567	4.682297	-1.870485	15	0.694411	-1.901074	-0.027215
1	-1.193824	4.576247	-0.253076	15	-1.580133	1.222572	1.082025
8	-2.516723	2.237450	-1.724206	16	-0.405316	0.019640	2.439770
6	1.760838	2.062260	-0.669050	8	0.003601	-0.482710	-0.389726
6	3.141596	2.489623	-0.711558	16	-1.922223	2.821295	2.161066
7	1.401930	1.029228	-1.548837	6	-3.062910	0.300147	0.588149
6	4.015612	1.873999	-1.545130	6	-3.050715	-0.903659	-0.125204
1	3.446263	3.308782	-0.059553	6	-4.301869	0.837688	0.975981
6	2.304419	0.386948	-2.350933	6	-4.236874	-1.554556	-0.451574
6	3.602049	0.778586	-2.386381	1	-2.119151	-1.363696	-0.442833
1	5.057162	2.202024	-1.577948	6	-5.485171	0.198666	0.652173

1	-4.325145	1.774036	1.537297	6	-0.969217	0.582818	-2.583057
6	-5.465862	-1.005891	-0.066002	1	-0.458164	-0.251964	-3.074497
1	-4.179975	-2.493201	-1.001878	1	-1.968873	0.276161	-2.269230
1	-6.449446	0.615785	0.945582	1	-1.103015	1.408022	-3.299076
8	-6.660188	-1.557948	-0.335639	6	3.988958	-0.080412	1.230057
6	-6.714388	-2.759456	-1.059307	6	2.674138	-0.397632	0.906349
1	-6.207004	-3.581405	-0.525782	6	2.394015	-1.400607	-0.027349
1	-7.776173	-3.008894	-1.171081	6	3.458707	-2.091339	-0.631384
1	-6.265149	-2.651262	-2.061370	6	4.766903	-1.777783	-0.315294
16	0.272435	-3.399757	-1.169413	6	5.044749	-0.761700	0.614482
16	-0.354488	-1.990665	1.841311	1	4.169528	0.716767	1.949810
O,O-G8				1	1.878921	0.171900	1.387941
6	0.395788	2.834581	0.033847	1	3.249723	-2.862304	-1.375968
1	0.370495	3.582799	0.819336	1	5.604010	-2.296636	-0.784276
6	-0.734086	2.048451	-0.440750	8	6.342443	-0.506969	0.842120
6	-0.197413	1.128446	-1.423900	6	6.693810	0.516553	1.737704
6	-2.102879	2.612316	-0.527556	1	7.789312	0.553908	1.756259
6	-2.402739	3.759218	0.413190	1	6.305943	1.494782	1.405568
1	-1.879807	4.665899	0.071240	1	6.324770	0.311394	2.756734
1	-3.483585	3.944810	0.412167	15	0.718841	-1.799504	-0.541031
1	-2.048320	3.533518	1.430142	15	-0.943688	0.221239	1.179363
8	-2.949703	2.201326	-1.296401	16	-0.344324	-1.533204	2.310515
6	1.507426	2.439277	-0.639576	8	-0.086792	-0.302627	-0.304885
6	2.891972	2.820884	-0.597053	16	-0.475923	1.403835	2.676291
7	1.127010	1.449211	-1.585189	6	-2.668158	-0.068984	0.772605
6	3.781034	2.257599	-1.451174	6	-3.056561	-0.946140	-0.241793
1	3.193389	3.570234	0.136099	6	-3.651443	0.602296	1.515564
6	2.049961	0.880074	-2.449697	6	-4.404066	-1.144746	-0.527356
6	3.344975	1.260704	-2.403282	1	-2.315085	-1.489747	-0.828064
1	4.833838	2.544263	-1.424265	6	-4.990734	0.412653	1.232457
1	1.676266	0.110123	-3.123489	1	-3.354220	1.283205	2.315897
1	4.057393	0.797808	-3.085464	6	-5.381067	-0.456762	0.201926

1	-4.675057	-1.834315	-1.325991	1	3.083900	-2.092583	0.887620
1	-5.766867	0.934353	1.793849	1	3.082298	-2.093631	-0.886705
8	-6.701889	-0.568017	-0.009796	1	4.451489	-1.340867	-0.001188
6	-7.165228	-1.388308	-1.050668	LR pentaCycle			
1	-6.897741	-2.446158	-0.886441	6	-4.873230	0.922247	0.943235
1	-8.257651	-1.295436	-1.058443	6	-3.644647	1.358178	0.452580
1	-6.771201	-1.063835	-2.028745	6	-2.658407	0.439795	0.093137
16	0.536005	-2.551904	-2.315042	6	-2.903794	-0.938528	0.232279
16	-0.305503	-3.023008	0.822747	6	-4.119009	-1.376322	0.721976
O,O-G9				6	-5.115654	-0.450607	1.081361
Indolizine				1	-5.626347	1.659923	1.218013
6	-3.314580	0.544323	-0.058	1	-3.447016	2.428104	0.352361
6	-3.369348	-0.887307	-0.111	1	-2.132813	-1.666170	-0.036277
6	-2.211924	-1.609901	-0.039	1	-4.328538	-2.439448	0.846374
6	-0.953112	-0.945392	0.077	8	-6.259435	-0.971697	1.547917
7	-0.944977	0.460093	0.035	6	-7.303213	-0.115108	1.935281
6	-2.118347	1.186485	0.064	1	-8.120520	-0.757725	2.282648
6	0.365875	-1.361996	0.179	1	-6.996732	0.552303	2.758466
6	1.178830	-0.196662	0.142	1	-7.662176	0.496250	1.089986
6	0.342390	0.923968	-0.033	15	-1.086296	1.017265	-0.544484
6	0.643869	2.382512	-0.063	15	1.086300	-1.016866	-0.545057
6	2.661096	-0.167381	-0.032	16	1.038550	-0.121873	-2.511642
6	3.367767	-1.507089	-0.152	8	0.405	0.329	0.172602
8	3.296388	0.867672	0.005	16	0.659623	-2.881768	-0.374579
1	-4.231497	1.134345	-0.047	6	2.658719	-0.439912	0.092317
1	-4.337378	-1.390285	-0.226	6	3.644845	-1.358439	0.451617
1	-2.220273	-2.700963	-0.013	6	2.904128	0.938378	0.232012
1	-2.014550	2.270881	0.222	6	4.873365	-0.922745	0.942674
1	0.695744	-2.397669	0.318	1	3.447162	-2.428317	0.350945
1	1.729765	2.520303	-0.890	6	4.119262	1.375935	0.722091
1	0.223807	2.879683	-0.890290	1	2.133243	1.666151	-0.036454
1	0.225345	2.879394	0.891066	6	5.115778	0.450039	1.081398

1	5.626450	-1.660519	1.217281
1	4.328813	2.439007	0.846931
8	6.259488	0.970918	1.548355
6	7.303030	0.114141	1.935903
1	7.662361	-0.496934	1.090560
1	8.120201	0.756591	2.283896
1	6.996124	-0.553570	2.758689
16	-0.659933	2.882211	-0.373649
16	-1.038924	0.122658	-2.511284

Figure 47

O,O-WE1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072
6	2.817837	0.280772	-0.094
6	4.093206	-0.289717	-0.218
6	5.218069	0.534573	-0.176
6	5.069304	1.919305	-0.011
1	3.674106	3.572726	0.245
1	1.671888	2.128423	0.172
1	4.199989	-1.376962	-0.346
1	6.213736	0.086979	-0.273
15	1.349546	-0.804254	-0.147
15	-1.349549	0.804259	0.157
6	-2.817832	-0.280777	0.091
6	-2.666465	-1.674016	-0.013
6	-4.093205	0.289704	0.128
6	-3.793899	-2.487737	-0.074
1	-1.671870	-2.128420	-0.047
6	-5.218063	-0.534594	0.061
1	-4.199996	1.376948	0.207
6	-5.069288	-1.919326	-0.038

1	-3.674079	-3.572737	-0.154
1	-6.213733	-0.087007	0.087
34	0.079	-0.183	1.668777
34	-0.077	0.194	-1.668768
34	1.718838	-2.850294	-0.372
34	-1.718852	2.850296	0.392
1	5.952123	2.562719	0.021
1	-5.952103	-2.562746	-0.087

Preindolizine

6	0.178997	-1.007094	-0.061471
1	0.344103	-2.083841	-0.158607
6	1.241723	-0.189608	0.035834
6	1.157013	1.312645	0.278992
6	2.649285	-0.701640	-0.049454
6	2.902049	-2.193470	-0.049733
1	2.462099	-2.668778	0.839244
1	2.458138	-2.665040	-0.939439
1	3.985338	-2.360717	-0.058901
8	1.125	1.721883	1.410299
8	3.564577	0.088276	-0.125556
6	-1.233616	-0.593404	-0.052625
6	-2.248065	-1.556404	0.038139
7	-1.504383	0.713443	-0.139051
6	-3.574545	-1.136383	0.056104
1	-1.995603	-2.616824	0.099871
6	-2.769395	1.109466	-0.122320
6	-3.846604	0.226048	-0.023242
1	-4.384517	-1.864961	0.130790
1	-2.942230	2.188329	-0.193797
1	-4.870163	0.603990	-0.011555
6	1.239675	2.194562	-0.935888
1	1.074718	3.239890	-0.646013

1	2.245811	2.082825	-1.369636
1	0.497232	1.881452	-1.682557
O,O-WE2			
6	-4.298518	-1.963420	-0.528116
6	-3.071957	-1.342369	-0.742646
6	-2.849875	-0.055080	-0.237604
6	-3.852878	0.602052	0.486252
6	-5.075471	-0.028108	0.696660
6	-5.299179	-1.308838	0.189851
1	-4.471791	-2.965818	-0.924006
1	-2.281363	-1.850636	-1.298863
1	-3.671442	1.605768	0.877116
1	-5.859036	0.485695	1.257006
15	-1.249960	0.753638	-0.511858
15	1.447068	-1.018601	0.481954
6	2.450864	0.477482	0.344280
6	2.171597	1.588598	1.149129
6	3.511477	0.516787	-0.572830
6	2.952875	2.736757	1.030735
1	1.353496	1.549383	1.870424
6	4.282064	1.666040	-0.683251
1	3.723975	-0.354289	-1.196789
6	4.001653	2.777575	0.116699
1	2.733472	3.603363	1.656848
1	5.103962	1.698888	-1.400837
34	-0.237548	-0.828342	1.742395
34	-0.026076	-0.175282	-1.963588
34	-1.127504	2.747712	0.001490
34	2.347861	-2.793628	-0.023433
1	-6.260687	-1.799511	0.355688
1	4.607957	3.681126	0.023607

O,O-WE3			
15	-0.591699	-0.001	0.018
6	1.224915	-0.033	0.037
6	1.925949	-1.213933	0.362
6	1.925953	1.213872	-0.263
6	3.317418	-1.209159	0.309
1	1.375344	-2.157190	0.621
6	3.317417	1.209103	-0.330
1	1.375330	2.157122	-0.465
6	4.013078	-0.031	-0.054
1	3.860472	-2.156115	0.558
1	3.860482	2.156052	-0.594
34	-1.486067	-1.854380	-0.121
34	-1.485986	1.854417	0.102
1	5.105294	-0.023	-0.108
O,O-WE4			
6	2.695433	1.018354	0.001450
1	3.297182	1.648364	0.657541
6	1.645099	1.495935	-0.682255
6	0.834143	0.582414	-1.569883
6	1.268927	2.951804	-0.743133
6	1.819942	3.867777	0.319346
1	1.647624	3.450991	1.321069
1	2.903371	4.001897	0.171029
1	1.327791	4.842820	0.227317
8	-0.260120	0.106849	-1.192684
8	0.598330	3.354099	-1.666174
6	3.029651	-0.398133	-0.161404
6	3.979480	-1.094542	0.584505
7	2.299416	-0.998270	-1.102949
6	4.126750	-2.458764	0.347707
1	4.565176	-0.582330	1.348982

6	2.424055	-2.296107	-1.328964	1	-3.142577	-2.153305	-1.163977
6	3.336980	-3.076230	-0.619671	1	-2.198318	-4.436952	-0.911970
1	4.846709	-3.041770	0.925358	15	-3.125119	0.179343	0.585897
1	1.770506	-2.730272	-2.091073	15	0.913032	1.003490	-0.788182
1	3.418562	-4.145197	-0.819166	6	1.294505	2.771898	-0.746079
6	1.074302	0.653154	-3.044896	6	0.301428	3.705440	-1.053851
1	0.638	-0.219448	-3.538919	6	2.571410	3.194542	-0.353340
1	0.567997	1.569027	-3.387635	6	0.586742	5.067074	-0.969672
1	2.144179	0.733922	-3.271484	1	-0.689449	3.362264	-1.360835
6	-4.911833	-1.564594	-1.263134	6	2.847441	4.556029	-0.280468
6	-3.950759	-2.475159	-0.825414	1	3.342384	2.463284	-0.099924
6	-2.769773	-2.019709	-0.243045	6	1.857260	5.491695	-0.585847
6	-2.549068	-0.647417	-0.094700	1	-0.188914	5.797392	-1.207787
6	-3.514701	0.265314	-0.531913	1	3.843018	4.888171	0.020862
6	-4.692569	-0.195223	-1.115133	34	-2.345808	1.598133	1.869110
15	-0.988664	-0.040532	0.641049	34	-0.758688	0.480561	-1.923093
1	-4.121680	-3.548195	-0.935496	34	-4.672039	0.379609	-0.755959
1	-2.013075	-2.724719	0.109513	34	1.069992	0.183901	1.296140
1	-3.339971	1.335920	-0.402116	1	-1.016467	-5.071885	1.183540
1	-5.444576	0.521218	-1.452372	1	2.077946	6.559537	-0.521034
34	0.147576	-1.535561	1.563652	6	2.679307	-2.264283	1.084402
34	-1.130216	1.919886	1.367340	1	2.754419	-2.723929	2.065706
1	-5.838047	-1.924217	-1.717281	6	2.826718	-0.823182	0.794408
O,O-WE5				6	2.889384	-0.770970	-0.761585
6	-1.275641	-3.136525	2.099	6	3.881204	-0.029037	1.549595
6	-1.789431	-1.850588	1.955050	6	4.097523	-0.410671	2.993546
6	-2.464577	-1.496948	0.781787	1	3.145883	-0.587846	3.515018
6	-2.617686	-2.434413	-0.248835	1	4.673106	-1.348978	3.027264
6	-2.091180	-3.711940	-0.102923	1	4.664709	0.380472	3.497429
6	-1.424330	-4.065104	1.071347	8	2.346794	0.374326	-1.334359
1	-0.754923	-3.410382	3.018590	8	4.513969	0.859433	1.027114
1	-1.665725	-1.112398	2.749900	6	2.167413	-2.875287	-0.028405

6	1.697360	-4.206175	-0.287343	1	2.736049	2.815475	0.027184
7	2.107071	-1.983625	-1.092758	6	0.691339	5.412937	-0.793889
6	1.204027	-4.518248	-1.518897	1	-1.402461	5.244381	-1.311195
1	1.738949	-4.940450	0.517109	1	2.778119	5.276319	-0.243591
6	1.630710	-2.298112	-2.324092	34	-1.514183	1.154481	1.766510
6	1.149762	-3.548212	-2.570664	34	-0.914990	-0.213039	-1.408632
1	0.835279	-5.528877	-1.709689	34	-4.232309	1.183516	-0.734114
1	1.633044	-1.488460	-3.055504	34	1.456956	-0.028322	1.554916
1	0.730613	-3.790209	-3.545655	1	-3.729386	-5.313171	1.353182
6	4.296574	-0.930658	-1.329611	1	0.715283	6.497629	-0.920073
1	4.223148	-1.059005	-2.418032	6	3.468105	-2.006257	0.801609
1	4.892179	-0.040836	-1.104047	1	3.828306	-2.466910	1.717199
1	4.774315	-1.817679	-0.891302	6	3.227873	-0.555725	0.603884
O,O-WE6				6	2.923903	-0.437351	-0.923945
6	-2.392583	-3.646771	1.673185	6	4.227193	0.439075	1.172888
6	-2.131513	-2.306700	1.404407	6	4.945601	0.025877	2.432460
6	-3.007775	-1.574458	0.594774	1	4.247323	-0.387991	3.175351
6	-4.144504	-2.188562	0.062986	1	5.670544	-0.765797	2.188335
6	-4.401057	-3.531316	0.337197	1	5.471325	0.891418	2.851431
6	-3.526588	-4.261274	1.139486	8	1.973483	0.532593	-1.258853
1	-1.707731	-4.215052	2.306075	8	4.424019	1.514897	0.654937
1	-1.246861	-1.822664	1.824583	6	2.901819	-2.683393	-0.239817
1	-4.827007	-1.605656	-0.560386	6	2.699039	-4.083485	-0.501666
1	-5.292425	-4.006134	-0.078141	7	2.433055	-1.800200	-1.208786
15	-2.646217	0.180959	0.193693	6	2.110069	-4.474356	-1.664266
15	0.661549	0.862614	-0.294468	1	3.025009	-4.805512	0.247104
6	0.626951	2.658536	-0.470884	6	1.889475	-2.197423	-2.392453
6	-0.536433	3.333169	-0.851582	6	1.693770	-3.517248	-2.650294
6	1.824591	3.348924	-0.253809	1	1.950024	-5.537547	-1.856099
6	-0.495535	4.714215	-1.015485	1	1.606262	-1.397495	-3.079145
1	-1.474620	2.795553	-1.009203	1	1.221424	-3.830481	-3.579619
6	1.847191	4.732223	-0.413773	6	4.157133	-0.163166	-1.777828

1	3.889211	-0.265649	-2.838109
1	4.524623	0.850397	-1.591121
1	4.941130	-0.893673	-1.533536
O,O-WE7			
WR-5 Members Ring			
6	4.597558	1.564036	0.429939
6	3.326379	1.030518	0.244937
6	3.189169	-0.236512	-0.335227
6	4.315429	-0.964525	-0.732809
6	5.584266	-0.417622	-0.548851
6	5.724579	0.841358	0.032378
1	4.710486	2.550771	0.883056
1	2.442809	1.599266	0.545661
1	4.185223	-1.949446	-1.186270
1	6.466959	-0.978649	-0.862295
15	1.579430	-1.028933	-0.569150
15	-1.438019	0.794239	-0.195095
6	-2.472572	-0.697637	-0.348141
6	-2.041441	-1.868612	-0.980653
6	-3.747860	-0.639120	0.231010
6	-2.886452	-2.976589	-1.027093
1	-1.053449	-1.936456	-1.440486
6	-4.581608	-1.750836	0.181174
1	-4.088102	0.282093	0.709629
6	-4.151543	-2.920184	-0.447625
1	-2.545070	-3.887876	-1.521266
1	-5.574653	-1.700941	0.631840
8	1.656308	-2.339997	-1.273244
34	-2.391534	2.635100	-0.382352
34	-0.387203	0.679928	1.826467
34	0.329924	0.586077	-1.616694
34	0.597005	-1.401132	1.466947

1	6.719926	1.267744	0.174937
1	-4.809690	-3.790857	-0.487926
Indolizine			
6	-0.365870	-1.361970	0.088
1	-0.695716	-2.397652	0.040
6	-1.178876	-0.196643	-0.018
6	-0.342441	0.923957	-0.009
6	-2.661141	-0.167383	-0.019
6	-3.367656	-1.507171	0.048
1	-3.082728	-2.093244	-0.887011
1	-3.082879	-2.093030	0.887300
1	-4.451396	-1.341153	-0.057
8	-3.296455	0.867652	-0.095
6	0.953126	-0.945392	0.064
6	2.211959	-1.609874	-0.087
7	0.944975	0.460109	0.105
6	3.369384	-0.887272	-0.147
1	2.220364	-2.700938	-0.058
6	2.118353	1.186500	0.139
6	3.314600	0.544356	0.003
1	4.337411	-1.390256	-0.263
1	2.014543	2.270894	0.387
1	4.231517	1.134385	0.063
6	-0.643958	2.382504	-0.076
1	-0.224751	2.879452	-0.890839
1	-1.729855	2.520292	0.026
1	-0.224580	2.879609	0.890516

Figure 48

O,O-WF1

WR

6	3.793919	2.487725	0.113
6	2.666479	1.674012	0.072

6	2.817837	0.280772	-0.094	6	2.902049	-2.193470	-0.049733
6	4.093206	-0.289717	-0.218	1	2.462099	-2.668778	0.839244
6	5.218069	0.534573	-0.176	1	2.458138	-2.665040	-0.939439
6	5.069304	1.919305	-0.011	1	3.985338	-2.360717	-0.058901
1	3.674106	3.572726	0.245	8	1.125	1.721883	1.410299
1	1.671888	2.128423	0.172	8	3.564577	0.088276	-0.125556
1	4.199989	-1.376962	-0.346	6	-1.233616	-0.593404	-0.052625
1	6.213736	0.086979	-0.273	6	-2.248065	-1.556404	0.038139
15	1.349546	-0.804254	-0.147	7	-1.504383	0.713443	-0.139051
15	-1.349549	0.804259	0.157	6	-3.574545	-1.136383	0.056104
6	-2.817832	-0.280777	0.091	1	-1.995603	-2.616824	0.099871
6	-2.666465	-1.674016	-0.013	6	-2.769395	1.109466	-0.122320
6	-4.093205	0.289704	0.128	6	-3.846604	0.226048	-0.023242
6	-3.793899	-2.487737	-0.074	1	-4.384517	-1.864961	0.130790
1	-1.671870	-2.128420	-0.047	1	-2.942230	2.188329	-0.193797
6	-5.218063	-0.534594	0.061	1	-4.870163	0.603990	-0.011555
1	-4.199996	1.376948	0.207	6	1.239675	2.194562	-0.935888
6	-5.069288	-1.919326	-0.038	1	1.074718	3.239890	-0.646013
1	-3.674079	-3.572737	-0.154	1	2.245811	2.082825	-1.369636
1	-6.213733	-0.087007	0.087	1	0.497232	1.881452	-1.682557
34	0.079	-0.183	1.668777	O,O-WF2			
34	-0.077	0.194	-1.668768	6	-3.048117	2.698855	-2.081817
34	1.718838	-2.850294	-0.372	6	-2.556867	1.470678	-1.644891
34	-1.718852	2.850296	0.392	6	-3.129766	0.844898	-0.533006
1	5.952123	2.562719	0.021	6	-4.189092	1.461995	0.142744
1	-5.952103	-2.562746	-0.087	6	-4.667493	2.696002	-0.292275
Preindolizine				6	-4.102213	3.313898	-1.407698
6	0.178997	-1.007094	-0.061471	1	-2.603867	3.173961	-2.958929
1	0.344103	-2.083841	-0.158607	1	-1.726260	1.002476	-2.176845
6	1.241723	-0.189608	0.035834	1	-4.649404	0.963920	0.999196
6	1.157013	1.312645	0.278992	1	-5.497711	3.169127	0.236045
6	2.649285	-0.701640	-0.049454				

15	-2.515436	-0.763093	0.099844	6	-1.003671	3.579409	0.771536
15	0.569729	-0.838178	-0.466065	1	-0.072660	3.120295	-1.120791
6	1.564655	-2.347160	-0.245910	6	0.342886	3.007248	2.657905
6	1.008943	-3.434684	0.432444	6	-0.851878	3.519378	2.153682
6	2.869071	-2.406330	-0.740978	1	-1.917910	3.973022	0.322199
6	1.768560	-4.586546	0.616065	1	0.512735	2.960363	3.739026
1	-0.011819	-3.383394	0.819440	1	-1.634847	3.867824	2.829178
6	3.618250	-3.565978	-0.557675	6	4.172357	-0.248706	2.147502
1	3.299914	-1.546218	-1.258792	1	3.652764	-0.900738	2.860555
6	3.070324	-4.654342	0.120148	1	4.886688	-0.838773	1.553910
1	1.337341	-5.436727	1.147815	1	4.763364	0.519476	2.660821
1	4.637335	-3.615500	-0.946017	O ₂ O-WF3			
34	-1.278155	-1.707436	-1.566563	6	-2.491801	3.739786	-1.002694
34	-0.652263	-0.275252	1.342935	6	-2.222387	2.398571	-0.755904
34	-3.949158	-1.932087	1.052570	6	-3.239945	1.554554	-0.293048
34	1.357475	0.631390	-1.848570	6	-4.525341	2.059502	-0.087547
1	-4.489870	4.273548	-1.756724	6	-4.790224	3.405785	-0.340214
1	3.660801	-5.561628	0.263412	6	-3.776773	4.245792	-0.794706
6	2.341497	2.093901	-0.260930	1	-1.693910	4.393027	-1.361696
1	2.591005	2.821635	-1.038970	1	-1.216139	2.010029	-0.928914
6	3.446265	1.433548	0.333739	1	-5.312928	1.392212	0.270887
6	3.153342	0.356756	1.229750	1	-5.796715	3.797182	-0.179091
6	4.822975	1.717838	-0.099776	15	-2.891018	-0.209454	0.066985
6	5.032838	2.741929	-1.207664	15	0.304474	-0.772207	-0.029776
1	4.514817	2.443029	-2.133165	6	0.723442	-2.547115	-0.099787
1	4.660053	3.735587	-0.915874	6	0.148145	-3.421894	0.826459
1	6.108775	2.808422	-1.407332	6	1.668094	-3.010753	-1.018583
8	2.011406	-0.168927	1.219102	6	0.528252	-4.760799	0.833643
8	5.796778	1.165843	0.384617	1	-0.601390	-3.061726	1.534982
6	1.172568	2.574546	0.565959	6	2.044002	-4.353172	-1.055
6	0.024880	3.107273	-0.034605	1	2.117174	-2.327782	-1.742284
7	1.326928	2.554667	1.889609	6	1.479112	-5.227446	-0.074316

1	0.076768	-5.444285	1.555384	1	4.285571	-1.588714	2.382879
1	2.787722	-4.712375	-1.713826	O,O-WF4			
34	-1.604635	-1.042193	-1.574103	6	-3.467113	3.417377	-1.024305
34	-1.134791	-0.095625	1.563353	6	-2.864100	2.198134	-0.736157
34	-4.531423	-1.320733	0.712185	6	-3.632032	1.141828	-0.229494
34	1.235333	0.523299	-1.592595	6	-5.001278	1.314029	-0.019343
1	-3.986002	5.299815	-0.989955	6	-5.600874	2.539341	-0.311973
1	1.777060	-6.277833	-0.061467	6	-4.836706	3.590095	-0.812827
6	2.909704	1.052520	-0.682991	1	-2.864688	4.237805	-1.419707
1	3.540751	1.288211	-1.548565	1	-1.792787	2.067023	-0.907839
6	3.555658	-0.067125	0.107504	1	-5.592013	0.482770	0.373447
6	2.825141	-0.719734	1.051256	1	-6.672324	2.669252	-0.146730
6	4.991240	-0.404954	-0.119045	15	-2.848061	-0.472995	0.158903
6	5.803452	0.489678	-1.031664	15	0.413242	-0.400898	-0.026100
1	5.505203	0.330951	-2.081327	6	1.091085	-2.098888	-0.067995
1	5.645634	1.552906	-0.796509	6	1.040422	-2.868352	1.096317
1	6.860344	0.217627	-0.927625	6	1.666867	-2.613854	-1.231342
8	1.517978	-0.398547	1.186520	6	1.558810	-4.163154	1.089089
8	5.507350	-1.372419	0.404919	1	0.585353	-2.465346	2.004081
6	2.799089	2.353965	0.101388	6	2.192612	-3.901819	-1.225781
6	1.680642	2.722820	0.855882	1	1.739704	-1.999410	-2.131463
7	3.890489	3.119482	0.034349	6	2.136207	-4.679761	-0.068908
6	1.714909	3.922260	1.558801	1	1.507653	-4.768888	1.996195
1	0.798036	2.086609	0.897532	1	2.660319	-4.294012	-2.130552
6	3.919308	4.264362	0.711898	34	-1.476763	-0.990333	-1.537463
6	2.856855	4.716025	1.490629	34	-1.113243	0.103503	1.559933
1	0.852388	4.230880	2.153546	34	-4.156991	-1.919714	0.900620
1	4.837194	4.855212	0.626049	34	1.081883	0.925302	-1.702154
1	2.925270	5.665725	2.023428	1	-5.307989	4.548682	-1.040900
6	3.280728	-1.785201	1.993765	1	2.548771	-5.690713	-0.070164
1	2.547602	-1.866535	2.806501	6	2.977338	1.190710	-1.016953
1	3.332216	-2.750827	1.465417	1	3.580814	1.289244	-1.929633

6	3.443937	0.068742	-0.181239	1	-5.527245	0.393486	0.406016
6	2.875950	0.199329	1.122462	1	-6.640704	2.556885	-0.142940
6	4.433012	-0.823676	-0.713018	15	-2.777692	-0.544077	0.152940
6	4.961144	-1.963183	0.146750	15	0.508829	-0.382782	0.010573
1	5.621981	-1.589929	0.943948	6	1.200592	-2.071604	-0.031317
1	4.142620	-2.531148	0.613768	6	1.186056	-2.823838	1.146526
1	5.541411	-2.632558	-0.499971	6	1.738627	-2.603627	-1.204156
8	1.501252	0.176394	1.220539	6	1.695384	-4.121105	1.140836
8	4.821558	-0.721525	-1.876205	1	0.762620	-2.404910	2.062098
6	2.992991	2.397983	-0.116619	6	2.262846	-3.892806	-1.195002
6	2.983049	3.744920	-0.471777	1	1.791658	-2.002569	-2.114315
7	3.016505	2.048494	1.172008	6	2.235244	-4.655652	-0.028073
6	3.013352	4.700253	0.539897	1	1.669778	-4.714405	2.057226
1	2.951185	4.030789	-1.524135	1	2.706769	-4.295777	-2.106811
6	3.003524	2.938576	2.157974	34	-1.391783	-1.062107	-1.522156
6	3.020154	4.299225	1.878056	34	-1.066427	0.086529	1.561395
1	3.026852	5.762772	0.288473	34	-4.074426	-1.995574	0.912089
1	2.987656	2.547107	3.178613	34	1.080846	0.916170	-1.726657
1	3.036764	5.027423	2.689250	1	-5.315388	4.425722	-1.115002
6	3.489519	-0.325213	2.386342	1	2.643004	-5.668624	-0.028107
1	2.965348	0.100297	3.253369	6	3.048776	1.322976	-1.067767
1	3.343109	-1.414103	2.419899	1	3.593938	1.456336	-2.008289
1	4.561180	-0.100704	2.442534	6	3.544786	0.291131	-0.171599
O,O-WF5				6	2.929520	0.555524	1.145309
6	-3.463450	3.312069	-1.109964	6	4.280670	-0.807868	-0.707442
6	-2.842250	2.105977	-0.805068	6	4.841391	-1.883382	0.212211
6	-3.587844	1.055417	-0.255122	1	5.519394	-1.460876	0.969012
6	-4.953544	1.220995	-0.018752	1	4.036006	-2.424098	0.733608
6	-5.571660	2.433111	-0.327768	1	5.397512	-2.597548	-0.407072
6	-4.829575	3.477972	-0.872259	8	1.542593	0.219238	1.253189
1	-2.878760	4.127269	-1.541535	8	4.481787	-0.894891	-1.921985
1	-1.774184	1.978752	-0.998922	6	2.879238	2.506438	-0.194936

6	2.737210	3.861020	-0.481299	1	-1.411114	-2.094727	1.953815
7	2.852732	2.094868	1.089039	6	-0.989127	-4.713423	-0.180636
6	2.568327	4.751435	0.570966	1	-0.295575	-4.565972	-2.222200
1	2.755266	4.194004	-1.519106	1	-1.649263	-4.553206	1.873677
6	2.636038	2.923776	2.117758	34	1.557235	-0.446081	1.877179
6	2.506831	4.279977	1.888364	34	1.052741	0.714130	-1.314341
1	2.471188	5.820323	0.371656	34	3.466096	-2.047399	-0.867713
1	2.575393	2.475428	3.109079	34	-1.334801	0.866383	1.723237
1	2.355717	4.958723	2.727249	1	6.382071	4.061282	0.164115
6	3.595986	0.077027	2.414675	1	-1.092190	-5.800155	-0.212067
1	3.018772	0.380502	3.299756	6	-3.344245	0.858147	1.104742
1	3.604929	-1.018520	2.400400	1	-3.891808	0.804994	2.052415
1	4.628790	0.443538	2.484871	6	-3.616179	-0.214984	0.144796
O,O-WF6				6	-3.151084	0.271796	-1.158802
6	4.491711	3.288612	0.870125	6	-4.047964	-1.489745	0.619325
6	3.598460	2.221962	0.845065	6	-4.323436	-2.625297	-0.355850
6	3.891343	1.084607	0.083038	1	-5.094686	-2.356359	-1.093010
6	5.080649	1.020142	-0.646672	1	-3.408329	-2.912357	-0.898797
6	5.972645	2.091829	-0.616495	1	-4.669163	-3.489369	0.224291
6	5.679352	3.225234	0.139105	8	-1.693642	0.274241	-1.328911
1	4.262511	4.173264	1.468280	8	-4.196989	-1.687816	1.827669
1	2.672083	2.257306	1.424119	6	-3.484332	2.092443	0.304909
1	5.303495	0.120970	-1.226870	6	-3.653399	3.425498	0.669205
1	6.904550	2.035615	-1.183175	7	-3.410311	1.769320	-1.004998
15	2.701462	-0.317220	0.028451	6	-3.740202	4.385539	-0.329208
15	-0.622344	-0.144767	-0.137569	1	-3.712326	3.686914	1.725713
6	-0.725781	-1.950522	-0.094981	6	-3.435799	2.682845	-1.986717
6	-0.419279	-2.637698	-1.273700	6	-3.620946	4.014667	-1.675740
6	-1.155750	-2.637475	1.042295	1	-3.893457	5.434021	-0.066982
6	-0.550028	-4.024551	-1.309210	1	-3.311014	2.318021	-3.005673
1	-0.058040	-2.099117	-2.152374	1	-3.665892	4.754735	-2.474027
6	-1.294378	-4.019172	0.990880	6	-3.707113	-0.279747	-2.449418

1	-3.241667	0.204627	-3.319202	6	3.364840	-0.154150	1.295464
1	-3.455082	-1.344051	-2.505734	1	3.636120	0.138384	2.314434
1	-4.798604	-0.166611	-2.485257	6	3.493653	0.871171	0.274120
O,O-WF7				6	3.480100	0.176067	-1.027083
6	-4.475578	-3.537180	0.152322	6	3.460309	2.248416	0.659070
6	-3.872052	-2.386107	0.648676	6	3.589112	3.347981	-0.383788
6	-4.001508	-1.177500	-0.046423	1	4.537302	3.278133	-0.937723
6	-4.734791	-1.128806	-1.238162	1	2.759423	3.306305	-1.107105
6	-5.336468	-2.284363	-1.727168	1	3.550706	4.311756	0.137886
6	-5.207156	-3.488084	-1.034303	8	2.178172	-0.302639	-1.482798
1	-4.368538	-4.479749	0.692641	8	3.328221	2.561745	1.843704
1	-3.289930	-2.417383	1.572064	6	4.041865	-1.331576	0.703390
1	-4.823720	-0.183938	-1.778528	6	4.535876	-2.503771	1.268299
1	-5.905799	-2.244485	-2.657928	7	4.143611	-1.145204	-0.628958
15	-3.189024	0.319919	0.581068	6	5.111980	-3.453478	0.436020
15	0.806979	-0.223127	-0.568447	1	4.450086	-2.656253	2.343980
6	0.433839	1.556122	-0.545407	6	4.637570	-2.071670	-1.461893
6	0.204427	2.162052	-1.790153	6	5.154524	-3.244409	-0.948658
6	0.359621	2.311145	0.624583	1	5.522399	-4.372095	0.859652
6	-0.083312	3.520754	-1.855634	1	4.609450	-1.845011	-2.527144
1	0.238071	1.563628	-2.703903	1	5.579093	-3.987538	-1.622939
6	0.070035	3.672731	0.550507	6	4.131561	0.797272	-2.239433
1	0.559118	1.849409	1.592061	1	4.046270	0.137334	-3.114035
6	-0.149165	4.277476	-0.683383	1	3.594094	1.720567	-2.481473
1	-0.262124	3.991369	-2.824701	1	5.184438	1.036164	-2.039264
1	0.026701	4.258914	1.469615	O,O-WF8			
34	-2.270993	0.135253	2.418015	6	-1.802925	-3.837599	0.496542
34	-0.685776	-1.406227	-1.411946	6	-1.607180	-2.505061	0.139981
34	-3.429690	2.022048	-0.549251	6	-2.634944	-1.576144	0.341145
34	1.381365	-0.896520	1.499441	6	-3.850780	-1.990449	0.900962
1	-5.676968	-4.394042	-1.423570	6	-4.034011	-3.322602	1.258906
1	-0.374405	5.344846	-0.736446	6	-3.010936	-4.248005	1.056526

1	-0.999759	-4.555168	0.322688	8	4.316957	1.108910	1.041901
1	-0.656142	-2.207238	-0.304897	6	2.294124	-2.903565	0.027729
1	-4.656179	-1.266407	1.043347	6	1.734663	-4.207137	-0.209455
1	-4.985123	-3.638776	1.691862	7	2.447666	-2.062737	-1.104614
15	-2.457350	0.206101	-0.025531	6	1.404102	-4.592287	-1.468459
15	0.876584	0.945174	-0.600510	1	1.594078	-4.868283	0.647134
6	1.002072	2.737079	-0.590344	6	2.131588	-2.473636	-2.377582
6	-0.079875	3.564362	-0.904895	6	1.605918	-3.702044	-2.591202
6	2.242822	3.273977	-0.217411	1	0.979299	-5.582609	-1.644379
6	0.085167	4.946274	-0.854510	1	2.292069	-1.741268	-3.169515
1	-1.045652	3.136270	-1.183287	1	1.334502	-4.006036	-3.601326
6	2.390250	4.656685	-0.173634	6	4.331282	-0.507319	-1.508121
1	3.075650	2.616022	0.053664	1	4.146855	-0.447168	-2.588911
6	1.316695	5.490111	-0.492697	1	4.735202	0.445231	-1.152019
1	-0.755431	5.598314	-1.098576	1	5.060349	-1.307481	-1.310984
1	3.351759	5.084908	0.115666	O,O-WF9			
34	-1.408095	1.189859	1.687870	6	4.597558	1.564036	0.429939
34	-0.903308	0.269462	-1.764716	6	3.326379	1.030518	0.244937
34	-4.211425	1.202717	-0.560057	6	3.189169	-0.236512	-0.335227
34	0.801575	0.067208	1.466092	6	4.315429	-0.964525	-0.732809
1	-3.159130	-5.295272	1.328658	6	5.584266	-0.417622	-0.548851
1	1.441139	6.574538	-0.453628	6	5.724579	0.841358	0.032378
6	2.716135	-2.238918	1.133742	1	4.710486	2.550771	0.883056
1	2.667938	-2.620399	2.150551	1	2.442809	1.599266	0.545661
6	3.075791	-0.877088	0.736655	1	4.185223	-1.949446	-1.186270
6	3.061009	-0.835632	-0.750554	1	6.466959	-0.978649	-0.862295
6	3.886721	0.058254	1.507405	15	1.579430	-1.028933	-0.569150
6	4.149101	-0.298897	2.956097	15	-1.438019	0.794239	-0.195095
1	4.729668	-1.231709	3.022602	6	-2.472572	-0.697637	-0.348141
1	4.701591	0.518620	3.434202	6	-2.041441	-1.868612	-0.980653
1	3.202182	-0.464038	3.494720	6	-3.747860	-0.639120	0.231010
8	2.133648	0.387518	-1.337904	6	-2.886452	-2.976589	-1.027093

1	-1.053449	-1.936456	-1.440486
6	-4.581608	-1.750836	0.181174
1	-4.088102	0.282093	0.709629
6	-4.151543	-2.920184	-0.447625
1	-2.545070	-3.887876	-1.521266
1	-5.574653	-1.700941	0.631840
8	1.656308	-2.339997	-1.273244
34	-2.391534	2.635100	-0.382352
34	-0.387203	0.679928	1.826467
34	0.329924	0.586077	-1.616694
34	0.597005	-1.401132	1.466947
1	6.719926	1.267744	0.174937
1	-4.809690	-3.790857	-0.487926

Indolizine

6	-3.314580	0.544323	-0.058
6	-3.369348	-0.887307	-0.111
6	-2.211924	-1.609901	-0.039
6	-0.953112	-0.945392	0.077
7	-0.944977	0.460093	0.035
6	-2.118347	1.186485	0.064
6	0.365875	-1.361996	0.179
6	1.178830	-0.196662	0.142
6	0.342390	0.923968	-0.033
6	0.643869	2.382512	-0.063
6	2.661096	-0.167381	-0.032
6	3.367767	-1.507089	-0.152
8	3.296388	0.867672	0.005
1	-4.231497	1.134345	-0.047
1	-4.337378	-1.390285	-0.226
1	-2.220273	-2.700963	-0.013
1	-2.014550	2.270881	0.222
1	0.695744	-2.397669	0.318

1	1.729765	2.520303	-0.890
1	0.223807	2.879683	-0.890290
1	0.225345	2.879394	0.891066
1	3.083900	-2.092583	0.887620
1	3.082298	-2.093631	-0.886705
1	4.451489	-1.340867	-0.001188

Figure 49

N,O-B1

6	-1.930290	0.408578	-1.367349
1	-1.689527	-0.219937	-2.237521
6	-0.670027	0.957777	-0.728202
6	-0.661971	2.309311	-0.178057
6	0.448768	0.142603	-0.608671
6	0.412915	-1.291340	-1.070791
1	1.197865	-1.888977	-0.592444
1	-0.554921	-1.746003	-0.826527
1	0.548861	-1.363429	-2.161532
8	0.320394	2.796580	0.394728
6	-2.829272	-0.375414	-0.429555
6	-3.333834	-1.633406	-0.781114
7	-3.122863	0.193842	0.742669
6	-4.155681	-2.311521	0.115318
1	-3.081530	-2.073296	-1.748706
6	-3.909095	-0.454993	1.594845
6	-4.451567	-1.713437	1.336515
1	-4.557872	-3.295573	-0.136339
1	-4.121709	0.052896	2.542020
1	-5.087973	-2.205476	2.073792
6	-1.909145	3.160048	-0.292752
1	-2.758714	2.642232	0.175015
1	-1.723006	4.114851	0.212788
1	-2.160851	3.355870	-1.346914

7	1.589	0.608752	-0.028432	15	-0.901144	-1.183693	-0.071
1	1.442024	1.561599	0.355050	16	-0.184	0.609	-1.552090
6	2.837381	0.001943	0.106181	16	-0.116	0.185	1.553327
6	3.464265	-0.685960	-0.941875	16	0.492940	3.068803	-0.771
6	3.517384	0.149321	1.323508	16	-0.492242	-3.068189	-0.603
6	4.726894	-1.245524	-0.758146	6	-2.652613	-0.746168	-0.150
1	2.971318	-0.761556	-1.911971	6	-3.051857	0.594301	0.287
6	4.786073	-0.395952	1.493279	6	-3.625394	-1.755670	-0.493
1	3.031530	0.691116	2.137866	6	-4.400241	0.930604	0.362
6	5.394161	-1.105380	0.457483	1	-2.307453	1.395396	0.536
1	5.200807	-1.780062	-1.584507	6	-4.970864	-1.427866	-0.432
1	5.300129	-0.272304	2.448964	1	-3.315267	-2.803163	-0.809
1	6.386079	-1.540296	0.594635	6	-5.371350	-0.082808	0.013
1	-2.527440	1.237618	-1.774861	1	-4.679935	1.983600	0.725
LR				1	-5.741489	-2.199662	-0.707
6	4.399900	-0.931020	0.078	8	-6.693755	0.139912	0.103
6	3.051574	-0.594451	0.074	6	-7.175115	1.459861	0.447
6	2.652608	0.746089	0.098	1	-6.850662	2.011249	-0.898237
6	3.625607	1.755391	0.006	1	-8.269204	1.391129	0.340
6	4.971010	1.427326	0.027	1	-6.850803	2.010720	0.899507
6	5.371218	0.082184	0.079	N,O-B2			
1	4.679398	-1.984067	0.068	6	-4.040100	-0.995309	-0.715057
1	2.307030	-1.395415	0.071	6	-2.806060	-0.380074	-0.894362
1	3.315697	2.802948	-0.108	6	-2.537931	0.861547	-0.308140
1	5.741782	2.198979	-0.020	6	-3.531311	1.490869	0.464960
8	6.693580	-0.140809	0.086	6	-4.758656	0.886153	0.643939
6	7.174688	-1.460847	0.183	6	-5.024024	-0.367057	0.059747
1	8.268794	-1.392340	0.326	1	-4.217340	-1.963686	-1.181138
1	6.850105	-2.011894	0.899028	1	-2.040794	-0.873401	-1.495921
1	6.850302	-2.011911	-0.898728	1	-3.326587	2.460132	0.924601
15	0.901258	1.184195	-0.247	1	-5.542149	1.356584	1.239391
				8	-6.239018	-0.877646	0.295638

6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	N,O-B4			
6	4.518843	0.533126	0.484738	15	-0.031410	-1.175269	-0.460215
1	2.590010	1.198244	1.169247	6	-1.839669	-1.370891	-0.352772
6	4.574104	-1.679850	-0.516320	6	-2.413751	-1.939466	0.785931
1	2.700275	-2.728593	-0.606940	6	-2.673950	-0.960591	-1.399535
6	5.239282	-0.503636	-0.127213	6	-3.796091	-2.066929	0.905314
1	5.008365	1.456113	0.793375	1	-1.766431	-2.286246	1.594500
1	5.155828	-2.472745	-0.988319	6	-4.050904	-1.098678	-1.300855
8	6.554046	-0.461539	-0.378351	1	-2.226581	-0.512056	-2.289429
6	7.292017	0.681090	-0.023996	6	-4.625294	-1.642873	-0.143371
1	7.259570	0.862974	1.063412	1	-4.212558	-2.508772	1.810499
1	8.328884	0.487145	-0.321802	1	-4.712367	-0.787629	-2.111225
1	6.928185	1.578435	-0.551917	6	0.748570	3.206621	0.472065
N,O-B3				1	1.372913	3.661579	-0.305523
6	-2.563014	-0.295727	0.078	6	1.208495	1.809727	0.817421
6	-1.761443	-1.451863	-0.463	6	0.192527	0.984556	1.474134
6	-0.384385	-1.344393	-0.361	6	2.453676	1.311534	0.503333
6	0.230510	-0.078248	0.234	6	3.498285	2.170523	-0.155808
6	-0.571133	1.069674	0.902	1	4.483735	2.010269	0.298899
6	-1.957541	0.970024	0.948	1	3.577856	1.878160	-1.214674

1	3.267094	3.237489	-0.099520	6	6.442852	-1.697585	-0.591433
8	0.022801	-0.252040	1.194807	1	7.302263	-1.040606	1.279430
6	-0.679651	3.137631	-0.021047	1	5.315501	-2.241849	-2.351822
6	-1.281146	4.069735	-0.867564	1	7.368871	-2.154596	-0.947228
7	-1.360960	2.096844	0.440637	1	0.774150	3.900601	1.335136
6	-2.613077	3.877870	-1.224613	N,O-B5			
1	-0.711497	4.919826	-1.246911	15	0.726542	-0.389811	1.131278
6	-2.636977	1.905013	0.123732	6	2.296530	-1.119739	0.536765
6	-3.310819	2.779919	-0.721033	6	3.503120	-0.433995	0.652092
1	-3.106513	4.581597	-1.898511	6	2.292642	-2.379644	-0.081688
1	-3.125265	1.023316	0.548801	6	4.693260	-0.976107	0.159951
1	-4.353706	2.595968	-0.981681	1	3.509361	0.538701	1.151321
6	-0.310217	1.368038	2.839957	6	3.463300	-2.924886	-0.581564
1	-0.349027	2.455499	2.975508	1	1.353720	-2.934410	-0.149536
1	-1.297298	0.924995	3.023739	6	4.676401	-2.227966	-0.463048
1	0.402128	0.951809	3.570770	1	5.622545	-0.419354	0.283376
8	-5.970426	-1.722537	-0.126185	1	3.474304	-3.905158	-1.061047
6	-6.610010	-2.282509	0.988639	6	-1.385475	3.026706	0.428002
1	-6.316272	-3.334872	1.144234	1	-1.314063	3.125795	1.525243
1	-6.400181	-1.714044	1.911596	6	-1.663905	1.612561	-0.003592
1	-7.687045	-2.241607	0.786117	6	-0.540804	1.075322	-0.875029
16	0.470521	0.018979	-1.922244	6	-2.785367	0.924624	0.296398
16	0.941610	-2.788691	0.043941	6	-3.896934	1.585987	1.075265
7	2.858582	0.042937	0.787496	1	-4.391453	2.384249	0.499837
1	2.154353	-0.650873	1.032698	1	-4.659127	0.860431	1.382417
6	4.076164	-0.533059	0.313130	1	-3.479036	2.042449	1.985803
6	5.222123	-0.496750	1.110019	8	0.159913	-0.030331	-0.475733
6	4.108041	-1.163777	-0.932847	6	-0.039158	3.312964	-0.147918
6	6.406809	-1.072624	0.654768	6	0.771392	4.433634	-0.015
1	5.171911	-0.014079	2.088522	7	0.412468	2.270405	-0.855593
6	5.293117	-1.744735	-1.379839	6	2.047979	4.409836	-0.544592
1	3.194046	-1.195515	-1.530131	1	0.408780	5.287538	0.571820

6	1.653853	2.194787	-1.353224	6	2.394225	-1.156947	0.485632
6	2.503903	3.272159	-1.220751	6	3.380709	-0.231036	0.139314
1	2.708676	5.270118	-0.421831	6	2.673881	-2.523745	0.363902
1	1.930048	1.244649	-1.813599	6	4.624999	-0.649030	-0.326437
1	3.514789	3.214561	-1.622782	1	3.185038	0.837810	0.256663
6	-0.985656	0.834950	-2.316166	6	3.909001	-2.951757	-0.097397
1	-0.143415	0.478042	-2.926108	1	1.906491	-3.250419	0.640970
1	-1.757714	0.055891	-2.300413	6	4.895188	-2.018947	-0.448557
1	-1.406944	1.750518	-2.754143	1	5.375534	0.099608	-0.579556
8	5.766843	-2.842429	-0.969055	1	4.139907	-4.013563	-0.195158
6	7.019530	-2.234630	-0.822228	6	-1.136895	2.654603	0.971350
1	7.071481	-1.264378	-1.347555	1	-0.104094	1.940577	1.786103
1	7.275348	-2.075807	0.239943	6	-1.632244	1.423370	0.335035
1	7.755213	-2.916615	-1.266013	6	-0.629377	1.033602	-0.750162
16	-0.487238	-1.774318	1.833767	6	-2.713430	0.688853	0.675848
16	1.068152	1.289601	2.125055	6	-3.657356	1.122124	1.766847
7	-2.873306	-0.424308	-0.015126	1	-3.763058	2.213880	1.822863
1	-2.064809	-0.984450	0.283048	1	-4.654338	0.683869	1.627906
6	-4.044151	-1.127479	-0.273595	1	-3.271859	0.760571	2.734868
6	-5.145514	-0.524357	-0.900568	8	0.217269	-0.049421	-0.463593
6	-4.113555	-2.492071	0.054084	6	-0.151398	3.194373	0.127155
6	-6.296801	-1.263527	-1.163473	6	0.591614	4.402780	0.178861
1	-5.090223	0.524115	-1.200998	7	0.218952	2.266502	-0.807868
6	-5.260724	-3.223327	-0.231485	6	1.663699	4.568021	-0.659225
1	-3.254704	-2.963260	0.538157	1	0.305084	5.166279	0.901759
6	-6.364704	-2.615498	-0.832907	6	1.299589	2.400370	-1.610272
1	-7.146321	-0.775894	-1.647710	6	2.045329	3.544826	-1.569615
1	-5.296250	-4.283700	0.029178	1	2.241987	5.493612	-0.619834
1	-7.266477	-3.192251	-1.046992	1	1.527665	1.550777	-2.255218
1	-2.129613	3.758445	0.067288	1	2.910573	3.657307	-2.221096
N,O-B6				6	-1.247705	0.771270	-2.117157
15	0.752995	-0.599143	1.028289	1	-0.468028	0.503392	-2.844049

1	-1.949466	-0.065340	-2.034576	6	4.772042	-2.210406	-0.357919
1	-1.787044	1.662836	-2.463588	1	5.150751	-0.308226	-1.345898
8	6.064020	-2.524796	-0.885105	1	4.131805	-3.950290	0.727315
6	7.103365	-1.651249	-1.233552	6	-1.620903	2.846098	0.659890
1	6.817841	-0.986725	-2.067611	1	0.326980	2.055524	2.135032
1	7.422677	-1.032399	-0.377032	6	-1.835359	1.464543	0.257536
1	7.945767	-2.277029	-1.551994	6	-0.739626	1.103708	-0.753466
16	-0.381915	-2.038024	1.710391	6	-2.835471	0.627961	0.623141
16	1.097604	1.019444	2.260389	6	-3.933401	1.059259	1.558404
7	-2.885386	-0.590090	0.130902	1	-4.158642	2.130125	1.465384
1	-2.145285	-1.258909	0.364102	1	-4.858410	0.496129	1.373238
6	-4.085030	-1.104546	-0.331127	1	-3.633109	0.856698	2.600807
6	-5.095888	-0.266832	-0.832272	8	0.196059	0.089922	-0.358333
6	-4.287251	-2.495644	-0.357130	6	-0.560386	3.350247	-0.037389
6	-6.282495	-0.810011	-1.319225	6	0.101482	4.628899	-0.038086
1	-4.937037	0.813846	-0.854937	7	-0.018779	2.376107	-0.878780
6	-5.469123	-3.025035	-0.862175	6	1.211051	4.819175	-0.800472
1	-3.504241	-3.153711	0.027844	1	-0.299259	5.420821	0.595484
6	-6.480632	-2.189292	-1.340143	6	1.097788	2.567261	-1.627951
1	-7.057327	-0.140460	-1.700662	6	1.741730	3.764653	-1.622545
1	-5.605615	-4.109042	-0.874395	1	1.714578	5.788307	-0.788242
1	-7.409059	-2.610627	-1.729980	1	1.432604	1.708007	-2.211646
1	-1.729983	3.276415	1.641139	1	2.633689	3.913204	-2.228854
N,O-B7				6	-1.280505	0.645740	-2.101799
15	0.863804	-0.251673	1.096794	1	-0.453729	0.443980	-2.797762
6	2.404668	-1.010574	0.541364	1	-1.862792	-0.272541	-1.969838
6	3.294538	-0.301722	-0.270765	1	-1.925961	1.429887	-2.518843
6	2.711732	-2.328716	0.903124	8	5.878743	-2.867391	-0.741185
6	4.474046	-0.888537	-0.719185	6	6.815326	-2.223142	-1.564376
1	3.078154	0.731831	-0.552440	1	6.371900	-1.925134	-2.529883
6	3.880656	-2.923496	0.457723	1	7.245042	-1.332344	-1.075130
1	2.019328	-2.884943	1.539402	1	7.616870	-2.947580	-1.750608

16	-0.229957	-1.328804	2.287654	6	-2.658611	0.823069	0.657560
16	1.572281	1.564589	1.917565	6	-3.534343	1.126638	1.845383
7	-2.779819	-0.730682	0.267064	1	-3.992198	2.122925	1.766212
1	-1.992012	-1.250919	0.652430	1	-4.324202	0.380423	1.981552
6	-3.833416	-1.461773	-0.248815	1	-2.905276	1.118087	2.748539
6	-4.882383	-0.842201	-0.950868	8	0.672707	0.545402	-0.468853
6	-3.845021	-2.862744	-0.121848	6	-0.190929	3.432471	0.614556
6	-5.919513	-1.604400	-1.482968	6	0.584975	4.602185	0.932839
1	-4.868071	0.241060	-1.091263	7	0.020161	2.840286	-0.655458
6	-4.877898	-3.612229	-0.672484	6	1.503111	5.071071	0.052998
1	-3.031683	-3.353723	0.418829	1	0.414370	5.086137	1.895468
6	-5.929102	-2.991965	-1.350678	6	0.998226	3.296039	-1.512380
1	-6.727434	-1.102006	-2.020811	6	1.727662	4.392177	-1.204855
1	-4.865428	-4.699185	-0.560999	1	2.090209	5.959745	0.292834
1	-6.742182	-3.584129	-1.774473	1	1.145817	2.726554	-2.428565
1	-2.217907	3.405927	1.374108	1	2.484850	4.747020	-1.903200
N,O-B8				6	-1.110539	1.188005	-2.125187
15	0.728350	-0.953167	-0.009945	1	-0.326110	1.379609	-2.866592
6	2.503019	-1.305901	-0.006939	1	-1.319457	0.114665	-2.162415
6	3.430419	-0.267738	-0.088619	1	-2.013614	1.748672	-2.406936
6	2.961499	-2.627622	0.100598	8	6.547512	-2.209786	0.096927
6	4.800378	-0.530776	-0.068	6	7.535649	-1.219575	0.005401
1	3.077028	0.760919	-0.184593	1	7.478211	-0.673065	-0.951942
6	4.317881	-2.897896	0.134669	1	7.468542	-0.494661	0.835086
1	2.240272	-3.447152	0.147134	1	8.502318	-1.734120	0.062639
6	5.250726	-1.850721	0.056221	16	-0.339618	-2.291202	-0.976953
1	5.502196	0.300127	-0.130792	16	0.128471	-1.008532	2.037263
1	4.692220	-3.919426	0.217219	7	-2.917437	-0.295622	-0.072440
6	-1.144305	2.729319	1.276295	1	-2.120197	-0.792349	-0.482685
1	0.775980	0.132343	2.364289	6	-4.135675	-0.989200	-0.160036
6	-1.572030	1.635484	0.417774	6	-5.354137	-0.311394	-0.294244
6	-0.668421	1.624725	-0.751537	6	-4.121693	-2.390318	-0.163215

6	-6.543773	-1.028133	-0.396310	6	-0.595224	4.716500	1.297645
1	-5.363319	0.779893	-0.335395	7	-1.048708	3.214840	-0.558390
6	-5.314062	-3.096616	-0.289088	6	0.156093	5.489738	0.467241
1	-3.166562	-2.910537	-0.062532	1	-0.737164	4.970186	2.348921
6	-6.530679	-2.422389	-0.396339	6	-0.244359	3.976472	-1.382116
1	-7.488836	-0.489732	-0.496228	6	0.341069	5.099440	-0.901382
1	-5.291044	-4.188578	-0.292474	1	0.636609	6.396181	0.838555
1	-7.464658	-2.980316	-0.487021	1	-0.094912	3.601896	-2.392382
1	-1.530349	2.971084	2.262085	1	0.978851	5.686809	-1.561856
N,O-B9				6	-1.711597	1.528788	-2.250392
15	1.042001	-0.221214	-0.238197	1	-0.743872	1.066917	-2.502395
6	2.751486	-0.825441	-0.098950	1	-2.484538	0.759472	-2.366096
6	3.782339	0.109130	-0.157607	1	-1.929965	2.337856	-2.964690
6	3.069549	-2.181459	0.063643	8	6.678902	-2.127153	0.238244
6	5.118156	-0.285744	-0.050383	6	7.761313	-1.241330	0.182365
1	3.528096	1.162394	-0.296477	1	7.811295	-0.713909	-0.786497
6	4.388877	-2.585383	0.174666	1	7.721978	-0.491624	0.992078
1	2.267768	-2.923159	0.092660	1	8.669875	-1.844112	0.303183
6	5.425356	-1.638846	0.120120	16	-0.011435	-1.479654	-1.403223
1	5.901739	0.470178	-0.103757	16	0.229779	-0.567413	1.751018
1	4.653408	-3.636466	0.301801	7	-2.783911	-0.672999	-0.205885
6	-1.993549	2.549467	1.363105	1	-1.878656	-0.734455	-0.761513
1	0.746729	0.570040	2.262444	6	-3.492143	-1.908207	-0.145171
6	-2.266229	1.595711	0.336030	6	-4.853633	-1.956304	-0.452957
6	-1.678885	2.048764	-0.858063	6	-2.790466	-3.070250	0.179212
6	-2.990087	0.374176	0.552285	6	-5.524781	-3.175182	-0.404528
6	-3.907839	0.299540	1.731351	1	-5.378184	-1.040440	-0.734417
1	-4.562813	1.178829	1.773619	6	-3.470692	-4.285378	0.214257
1	-4.501852	-0.618760	1.756993	1	-1.719642	-3.006167	0.380322
1	-3.263811	0.314557	2.625663	6	-4.834696	-4.340325	-0.069614
8	1.056476	1.256145	-0.525898	1	-6.590174	-3.215936	-0.639732
6	-1.213723	3.531732	0.798298	1	-2.926284	-5.197308	0.466668

1	-5.361405	-5.296127	-0.037530
1	-2.279283	2.495936	2.409513
N,O-B10			
15	1.114303	-0.007919	-0.150396
6	2.813902	-0.624507	-0.068678
6	3.837010	0.308736	-0.227568
6	3.141638	-1.968382	0.163785
6	5.175580	-0.077369	-0.153613
1	3.575757	1.352390	-0.416643
6	4.466667	-2.361817	0.241284
1	2.349088	-2.712848	0.272834
6	5.495608	-1.418478	0.084694
1	5.952923	0.675228	-0.284852
1	4.740467	-3.402902	0.418972
6	-2.306753	2.383860	1.321049
1	0.009037	1.131220	1.869372
6	-2.435968	1.413351	0.286119
6	-1.859263	1.927847	-0.878426
6	-3.047065	0.136	0.462876
6	-4.086093	-0.025450	1.542173
1	-4.595308	-0.994911	1.526668
1	-3.577416	0.080127	2.513667
1	-4.821836	0.786353	1.466542
8	1.062986	1.420532	-0.602990
6	-1.618066	3.456091	0.786577
6	-1.152622	4.698860	1.304850
7	-1.365430	3.161360	-0.559402
6	-0.460862	5.553984	0.499614
1	-1.357635	4.934070	2.350159
6	-0.632310	4.011657	-1.357468
6	-0.190	5.193862	-0.860072
1	-0.095796	6.505963	0.888544

1	-0.419978	3.664180	-2.366414
1	0.395066	5.851990	-1.502389
6	-1.772110	1.405887	-2.268691
1	-0.727379	1.164441	-2.519558
1	-2.360958	0.487758	-2.373029
1	-2.151071	2.146772	-2.991384
8	6.752389	-1.894981	0.176175
6	7.830444	-1.010801	0.032616
1	7.838228	-0.531744	-0.961799
1	7.820505	-0.224464	0.807134
1	8.744017	-1.606964	0.145271
16	0.081794	-1.426493	-1.234677
16	0.387023	-0.165498	1.870140
7	-2.644325	-0.902937	-0.243560
1	-1.336558	-1.009227	-0.768952
6	-3.226526	-2.189611	-0.159148
6	-4.439484	-2.463604	-0.799434
6	-2.542398	-3.208566	0.510481
6	-4.976800	-3.747225	-0.746049
1	-4.953722	-1.662955	-1.335733
6	-3.086975	-4.490236	0.556054
1	-1.589086	-2.980355	0.990250
6	-4.303746	-4.763449	-0.067817
1	-5.927111	-3.954883	-1.242532
1	-2.552826	-5.282774	1.084494
1	-4.727053	-5.769091	-0.028777
1	-2.644535	2.301852	2.350696
N,O-B11			
15	-1.438623	0.293821	0.167592
6	-3.217206	0.107063	0.210089
6	-3.943240	0.200752	1.397348
6	-3.892032	-0.101103	-1.005850

6	-5.329904	0.090844	1.387501	6	-8.131880	-0.180307	1.213591
1	-3.424301	0.348095	2.346449	1	-7.875795	-0.982015	1.926681
6	-5.269471	-0.208726	-1.020374	1	-8.043839	0.795702	1.720869
1	-3.336085	-0.211208	-1.938598	1	-9.167744	-0.316753	0.881631
6	-6.001196	-0.115513	0.174298	16	-1.167600	2.177640	-0.608945
1	-5.872278	0.157567	2.329934	16	-0.589311	0.175116	2.049801
1	-5.808981	-0.387334	-1.950918	7	1.622491	3.491690	-0.199740
6	2.815974	1.719230	2.734431	1	0.203880	2.406317	-0.395923
1	-0.750741	-1.206628	1.973581	6	1.414243	4.717079	-0.859773
6	2.608207	2.018546	1.362569	6	2.310287	5.165483	-1.838350
6	2.578080	0.821874	0.642592	6	0.255749	5.458007	-0.595046
6	2.428258	3.357325	0.790396	6	2.054964	6.347478	-2.529302
6	3.196752	4.487254	1.420402	1	3.205471	4.577105	-2.051565
1	2.990884	4.516816	2.500361	6	0.008509	6.639218	-1.291361
1	4.276283	4.307563	1.306950	1	-0.444772	5.102454	0.163798
1	2.942787	5.459279	0.981424	6	0.904954	7.089389	-2.259409
8	-0.795025	-0.789712	-0.773480	1	2.762293	6.690138	-3.287755
6	2.874323	0.340352	2.844112	1	-0.896248	7.211079	-1.073947
6	3.003451	-0.570587	3.930412	1	0.707434	8.014782	-2.803816
7	2.743649	-0.186464	1.551991	1	2.867469	2.419232	3.564336
6	2.990989	-1.915350	3.698224	6	3.225873	-3.827748	-1.810292
1	3.103500	-0.164048	4.937878	6	2.566424	-2.861472	-2.589444
6	2.732853	-1.543451	1.320619	6	1.265845	-2.493272	-2.290816
6	2.850563	-2.407295	2.361294	6	0.601866	-3.048844	-1.186031
1	3.080314	-2.621171	4.525484	6	1.254567	-4.014365	-0.424106
1	2.602438	-1.859975	0.287415	6	2.556548	-4.415672	-0.731517
1	2.820324	-3.477412	2.157595	8	4.487311	-4.123602	-2.176016
6	2.465038	0.536283	-0.815220	6	5.204005	-5.080372	-1.442924
1	1.520618	0.022262	-1.054518	15	-1.120203	-2.589573	-0.821568
1	2.494215	1.471200	-1.385689	16	-1.623090	-3.072524	1.034665
1	3.284757	-0.114994	-1.159421	16	-2.274159	-2.886291	-2.352257
8	-7.331962	-0.237930	0.061231	1	3.099357	-2.426847	-3.436673

1	0.749856	-1.763872	-2.919409	1	3.306	0.792120	5.444097
1	0.739285	-4.448288	0.436236	6	3.070030	-1.295987	2.173256
1	3.034699	-5.179617	-0.118398	6	3.373335	-1.912314	3.345272
1	6.191513	-5.161199	-1.912747	1	3.704502	-1.663357	5.493982
1	5.332710	-4.775639	-0.389645	1	2.954632	-1.817599	1.225051
1	4.713736	-6.068600	-1.472205	1	3.526504	-2.991914	3.350612
N,O-B12				6	2.435064	0.273849	-0.297064
15	-1.623419	-0.919177	0.400966	1	1.539190	-0.358207	-0.399189
6	-3.397432	-0.624101	0.523021	1	2.353795	1.077832	-1.035052
6	-3.999760	-0.500440	1.770913	1	3.310441	-0.350818	-0.539061
6	-4.165569	-0.509288	-0.645082	8	-7.463008	0.097029	0.694607
6	-5.370573	-0.260359	1.870103	6	-8.147278	0.232843	1.911694
1	-3.402829	-0.593544	2.681393	1	-8.080749	-0.684857	2.521272
6	-5.523573	-0.266652	-0.549192	1	-7.766156	1.084361	2.501354
1	-3.703752	-0.622914	-1.629359	1	-9.198949	0.416920	1.662196
6	-6.139279	-0.137918	0.707516	16	-1.239068	1.468526	0.787120
1	-5.819865	-0.169864	2.858499	16	-0.502871	-1.185404	2.081155
1	-6.142853	-0.175283	-1.442532	7	1.427142	3.164364	-0.363521
6	2.653525	2.149754	2.948430	1	-0.096885	1.674453	0.077524
1	-0.576281	0.450033	1.896417	6	1.154	4.208430	-1.238535
6	2.393580	2.155898	1.551758	6	2.089685	4.878972	-1.971593
6	2.536696	0.850155	1.071343	6	-0.246443	4.535889	-1.451216
6	2.038148	3.338934	0.749175	6	1.736817	5.868259	-2.886917
6	2.387300	4.683720	1.336303	1	3.137733	4.610423	-1.820153
1	1.872047	4.803372	2.301415	6	-0.588943	5.530951	-2.362364
1	3.467201	4.747031	1.535702	1	-1.016647	3.999364	-0.893003
1	2.090584	5.508798	0.678633	6	0.397937	6.201856	-3.085508
8	-1.633	-0.689239	-1.100728	1	2.518867	6.381599	-3.451382
6	2.931090	0.843285	3.310974	1	-1.642029	5.778361	-2.514135
6	3.245042	0.190416	4.535584	1	0.123581	6.975700	-3.805066
7	2.859389	0.065040	2.145602	1	2.624857	2.994674	3.631305
6	3.466430	-1.156571	4.557582	6	3.637213	-2.961436	-1.880950

6	3.020987	-2.315761	-2.966369	6	0.976893	2.212235	-0.549
6	1.651093	-2.126003	-2.979603	6	-0.698142	-0.626356	0.496
6	0.862570	-2.556762	-1.899005	6	-1.164617	-2.063820	0.001252
6	1.475044	-3.213027	-0.830795	1	5.960448	1.600801	-0.932
6	2.851704	-3.429326	-0.820274	1	6.393171	-0.890623	-0.030
8	4.972253	-3.080336	-1.942190	1	4.461109	-2.462317	0.747
6	5.661431	-3.662871	-0.865746	1	3.618796	2.440411	-0.001015
15	-0.906768	-2.194459	-1.900947	1	1.540749	-2.537787	0.001040
16	-1.784001	-3.102744	-0.239653	1	-0.117813	2.218836	-0.056
16	-1.749141	-2.174611	-3.626482	1	1.334750	2.756360	0.889823
1	3.648920	-1.972056	-3.789462	1	1.333862	2.755521	-0.891795
1	1.176544	-1.636135	-3.832842	1	-0.773504	-2.586202	-0.884491
1	0.872486	-3.554191	0.013554	1	-0.772545	-2.585576	0.886934
1	3.296791	-3.960622	0.020695	1	-2.258292	-2.137879	0.001850
1	6.728486	-3.606387	-1.110369	7	-1.485013	0.380974	0.036
1	5.481402	-3.115730	0.075767	6	-2.877677	0.254942	-0.065
1	5.382376	-4.721128	-0.726709	6	-3.589396	0.228687	1.208005
N,O-B13				6	-3.588945	0.225536	-1.208323
Acid				6	-4.980270	0.155930	1.202951
1	0.	-0.973735	-0.828280	1	-3.036023	0.266837	2.148729
1	0.	0.973735	-0.828280	6	-4.979825	0.152821	-1.203612
16	0.	0.	0.103535	1	-3.035221	0.261232	-2.148940
Indolizine				6	-5.684186	0.116365	-0.415
6	5.128981	0.895505	-0.570	1	-5.519220	0.130534	2.153075
6	5.368585	-0.515622	-0.066	1	-5.518405	0.124954	-2.153875
6	4.312860	-1.381334	0.357	1	-6.774578	0.060126	-0.544
6	2.980491	-0.883551	0.311	LR-Substituted			
7	2.789383	0.507256	-0.156	6	4.305405	0.899139	-0.213571
6	3.858699	1.377955	-0.611	6	2.954360	0.605738	-0.070665
6	1.726257	-1.467199	0.647	6	2.517319	-0.721821	-0.004248
6	0.765165	-0.420686	0.360	6	3.457540	-1.760747	-0.078879
6	1.450481	0.799784	-0.114	6	4.804457	-1.475674	-0.217267

6	5.241729	-0.143139	-0.287336
1	4.613880	1.942601	-0.268695
1	2.239764	1.431187	-0.015062
1	3.118688	-2.798112	-0.033058
1	5.549083	-2.270318	-0.278238
8	6.562862	0.037852	-0.425215
6	7.079190	1.342052	-0.510688
1	8.164420	1.239123	-0.625662
1	6.675697	1.881645	-1.383961
1	6.868076	1.922787	0.403120
15	0.772537	-1.096982	0.173845
15	-0.772523	1.096903	0.175282
16	-0.056	-0.652	1.856818
16	0.265562	-2.938220	-0.020532
16	-0.265734	2.938333	-0.018391
6	-2.517295	0.721728	-0.003248
6	-2.954693	-0.605799	-0.067517
6	-3.457173	1.760787	-0.080646
6	-4.305688	-0.899093	-0.211098
1	-2.240362	-1.431335	-0.009700
6	-4.804047	1.475841	-0.219691
1	-3.118035	2.798127	-0.036427
6	-5.241652	0.143308	-0.287685
1	-4.614423	-1.942573	-0.264459
1	-5.548387	2.270594	-0.282760
8	-6.562706	-0.037575	-0.426382
6	-7.079239	-1.341792	-0.510494
1	-6.869497	-1.921122	0.404516
1	-8.164289	-1.238770	-0.627059
1	-6.674708	-1.882853	-1.382376
8	0.126	0.431	-0.816553

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6	-1.930290	0.408578	-1.367349
1	-1.689527	-0.219937	-2.237521
6	-0.670027	0.957777	-0.728202
6	-0.661971	2.309311	-0.178057
6	0.448768	0.142603	-0.608671
6	0.412915	-1.291340	-1.070791
1	1.197865	-1.888977	-0.592444
1	-0.554921	-1.746003	-0.826527
1	0.548861	-1.363429	-2.161532
8	0.320394	2.796580	0.394728
6	-2.829272	-0.375414	-0.429555
6	-3.333834	-1.633406	-0.781114
7	-3.122863	0.193842	0.742669
6	-4.155681	-2.311521	0.115318
1	-3.081530	-2.073296	-1.748706
6	-3.909095	-0.454993	1.594845
6	-4.451567	-1.713437	1.336515
1	-4.557872	-3.295573	-0.136339
1	-4.121709	0.052896	2.542020
1	-5.087973	-2.205476	2.073792
6	-1.909145	3.160048	-0.292752
1	-2.758714	2.642232	0.175015
1	-1.723006	4.114851	0.212788
1	-2.160851	3.355870	-1.346914
7	1.589	0.608752	-0.028432
1	1.442024	1.561599	0.355050
6	2.837381	0.001943	0.106181
6	3.464265	-0.685960	-0.941875
6	3.517384	0.149321	1.323508

6	4.726894	-1.245524	-0.758146
1	2.971318	-0.761556	-1.911971
6	4.786073	-0.395952	1.493279
1	3.031530	0.691116	2.137866
6	5.394161	-1.105380	0.457483
1	5.200807	-1.780062	-1.584507
1	5.300129	-0.272304	2.448964
1	6.386079	-1.540296	0.594635
1	-2.527440	1.237618	-1.774861

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6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603

6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493
6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

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6	-4.040100	-0.995309	-0.715057
6	-2.806060	-0.380074	-0.894362
6	-2.537931	0.861547	-0.308140
6	-3.531311	1.490869	0.464960
6	-4.758656	0.886153	0.643939
6	-5.024024	-0.367057	0.059747
1	-4.217340	-1.963686	-1.181138
1	-2.040794	-0.873401	-1.495921
1	-3.326587	2.460132	0.924601
1	-5.542149	1.356584	1.239391
8	-6.239018	-0.877646	0.295638
6	-6.575757	-2.137635	-0.229085
1	-7.598145	-2.349814	0.104217
1	-6.550899	-2.137520	-1.331831
1	-5.902560	-2.925468	0.148168
15	-0.937468	1.631443	-0.512316

15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	N,O-C4			
6	4.518843	0.533126	0.484738	15	-0.031410	-1.175269	-0.460215
1	2.590010	1.198244	1.169247	6	-1.839669	-1.370891	-0.352772
6	4.574104	-1.679850	-0.516320	6	-2.413751	-1.939466	0.785931
1	2.700275	-2.728593	-0.606940	6	-2.673950	-0.960591	-1.399535
6	5.239282	-0.503636	-0.127213	6	-3.796091	-2.066929	0.905314
1	5.008365	1.456113	0.793375	1	-1.766431	-2.286246	1.594500
1	5.155828	-2.472745	-0.988319	6	-4.050904	-1.098678	-1.300855
8	6.554046	-0.461539	-0.378351	1	-2.226581	-0.512056	-2.289429
6	7.292017	0.681090	-0.023996	6	-4.625294	-1.642873	-0.143371
1	7.259570	0.862974	1.063412	1	-4.212558	-2.508772	1.810499
1	8.328884	0.487145	-0.321802	1	-4.712367	-0.787629	-2.111225
1	6.928185	1.578435	-0.551917	6	0.748570	3.206621	0.472065
N,O-C3				1	1.372913	3.661579	-0.305523
6	-2.563014	-0.295727	0.078	6	1.208495	1.809727	0.817421
6	-1.761443	-1.451863	-0.463	6	0.192527	0.984556	1.474134
6	-0.384385	-1.344393	-0.361	6	2.453676	1.311534	0.503333
6	0.230510	-0.078248	0.234	6	3.498285	2.170523	-0.155808
6	-0.571133	1.069674	0.902	1	4.483735	2.010269	0.298899
6	-1.957541	0.970024	0.948	1	3.577856	1.878160	-1.214674
8	-3.885436	-0.498129	-0.230	1	3.267094	3.237489	-0.099520
6	-4.759250	0.603778	-0.315	8	0.022801	-0.252040	1.194807
15	2.021612	0.066269	-0.039	6	-0.679651	3.137631	-0.021047
16	2.707743	1.856016	-0.605	6	-1.281146	4.069735	-0.867564
16	2.982996	-1.591296	0.363	7	-1.360960	2.096844	0.440637

6	-2.613077	3.877870	-1.224613	N,O-C5			
1	-0.711497	4.919826	-1.246911	15	0.726542	-0.389811	1.131278
6	-2.636977	1.905013	0.123732	6	2.296530	-1.119739	0.536765
6	-3.310819	2.779919	-0.721033	6	3.503120	-0.433995	0.652092
1	-3.106513	4.581597	-1.898511	6	2.292642	-2.379644	-0.081688
1	-3.125265	1.023316	0.548801	6	4.693260	-0.976107	0.159951
1	-4.353706	2.595968	-0.981681	1	3.509361	0.538701	1.151321
6	-0.310217	1.368038	2.839957	6	3.463300	-2.924886	-0.581564
1	-0.349027	2.455499	2.975508	1	1.353720	-2.934410	-0.149536
1	-1.297298	0.924995	3.023739	6	4.676401	-2.227966	-0.463048
1	0.402128	0.951809	3.570770	1	5.622545	-0.419354	0.283376
8	-5.970426	-1.722537	-0.126185	1	3.474304	-3.905158	-1.061047
6	-6.610010	-2.282509	0.988639	6	-1.385475	3.026706	0.428002
1	-6.316272	-3.334872	1.144234	1	-1.314063	3.125795	1.525243
1	-6.400181	-1.714044	1.911596	6	-1.663905	1.612561	-0.003592
1	-7.687045	-2.241607	0.786117	6	-0.540804	1.075322	-0.875029
16	0.470521	0.018979	-1.922244	6	-2.785367	0.924624	0.296398
16	0.941610	-2.788691	0.043941	6	-3.896934	1.585987	1.075265
7	2.858582	0.042937	0.787496	1	-4.391453	2.384249	0.499837
1	2.154353	-0.650873	1.032698	1	-4.659127	0.860431	1.382417
6	4.076164	-0.533059	0.313130	1	-3.479036	2.042449	1.985803
6	5.222123	-0.496750	1.110019	8	0.159913	-0.030331	-0.475733
6	4.108041	-1.163777	-0.932847	6	-0.039158	3.312964	-0.147918
6	6.406809	-1.072624	0.654768	6	0.771392	4.433634	-0.015
1	5.171911	-0.014079	2.088522	7	0.412468	2.270405	-0.855593
6	5.293117	-1.744735	-1.379839	6	2.047979	4.409836	-0.544592
1	3.194046	-1.195515	-1.530131	1	0.408780	5.287538	0.571820
6	6.442852	-1.697585	-0.591433	6	1.653853	2.194787	-1.353224
1	7.302263	-1.040606	1.279430	6	2.503903	3.272159	-1.220751
1	5.315501	-2.241849	-2.351822	1	2.708676	5.270118	-0.421831
1	7.368871	-2.154596	-0.947228	1	1.930048	1.244649	-1.813599
1	0.774150	3.900601	1.335136	1	3.514789	3.214561	-1.622782

6	-0.985656	0.834950	-2.316166	6	3.909001	-2.951757	-0.097397
1	-0.143415	0.478042	-2.926108	1	1.906491	-3.250419	0.640970
1	-1.757714	0.055891	-2.300413	6	4.895188	-2.018947	-0.448557
1	-1.406944	1.750518	-2.754143	1	5.375534	0.099608	-0.579556
8	5.766843	-2.842429	-0.969055	1	4.139907	-4.013563	-0.195158
6	7.019530	-2.234630	-0.822228	6	-1.136895	2.654603	0.971350
1	7.071481	-1.264378	-1.347555	1	-0.104094	1.940577	1.786103
1	7.275348	-2.075807	0.239943	6	-1.632244	1.423370	0.335035
1	7.755213	-2.916615	-1.266013	6	-0.629377	1.033602	-0.750162
16	-0.487238	-1.774318	1.833767	6	-2.713430	0.688853	0.675848
16	1.068152	1.289601	2.125055	6	-3.657356	1.122124	1.766847
7	-2.873306	-0.424308	-0.015126	1	-3.763058	2.213880	1.822863
1	-2.064809	-0.984450	0.283048	1	-4.654338	0.683869	1.627906
6	-4.044151	-1.127479	-0.273595	1	-3.271859	0.760571	2.734868
6	-5.145514	-0.524357	-0.900568	8	0.217269	-0.049421	-0.463593
6	-4.113555	-2.492071	0.054084	6	-0.151398	3.194373	0.127155
6	-6.296801	-1.263527	-1.163473	6	0.591614	4.402780	0.178861
1	-5.090223	0.524115	-1.200998	7	0.218952	2.266502	-0.807868
6	-5.260724	-3.223327	-0.231485	6	1.663699	4.568021	-0.659225
1	-3.254704	-2.963260	0.538157	1	0.305084	5.166279	0.901759
6	-6.364704	-2.615498	-0.832907	6	1.299589	2.400370	-1.610272
1	-7.146321	-0.775894	-1.647710	6	2.045329	3.544826	-1.569615
1	-5.296250	-4.283700	0.029178	1	2.241987	5.493612	-0.619834
1	-7.266477	-3.192251	-1.046992	1	1.527665	1.550777	-2.255218
1	-2.129613	3.758445	0.067288	1	2.910573	3.657307	-2.221096
N,O-C6				6	-1.247705	0.771270	-2.117157
15	0.752995	-0.599143	1.028289	1	-0.468028	0.503392	-2.844049
6	2.394225	-1.156947	0.485632	1	-1.949466	-0.065340	-2.034576
6	3.380709	-0.231036	0.139314	1	-1.787044	1.662836	-2.463588
6	2.673881	-2.523745	0.363902	8	6.064020	-2.524796	-0.885105
6	4.624999	-0.649030	-0.326437	6	7.103365	-1.651249	-1.233552
1	3.185038	0.837810	0.256663	1	6.817841	-0.986725	-2.067611

1	7.422677	-1.032399	-0.377032	6	-1.835359	1.464543	0.257536
1	7.945767	-2.277029	-1.551994	6	-0.739626	1.103708	-0.753466
16	-0.381915	-2.038024	1.710391	6	-2.835471	0.627961	0.623141
16	1.097604	1.019444	2.260389	6	-3.933401	1.059259	1.558404
7	-2.885386	-0.590090	0.130902	1	-4.158642	2.130125	1.465384
1	-2.145285	-1.258909	0.364102	1	-4.858410	0.496129	1.373238
6	-4.085030	-1.104546	-0.331127	1	-3.633109	0.856698	2.600807
6	-5.095888	-0.266832	-0.832272	8	0.196059	0.089922	-0.358333
6	-4.287251	-2.495644	-0.357130	6	-0.560386	3.350247	-0.037389
6	-6.282495	-0.810011	-1.319225	6	0.101482	4.628899	-0.038086
1	-4.937037	0.813846	-0.854937	7	-0.018779	2.376107	-0.878780
6	-5.469123	-3.025035	-0.862175	6	1.211051	4.819175	-0.800472
1	-3.504241	-3.153711	0.027844	1	-0.299259	5.420821	0.595484
6	-6.480632	-2.189292	-1.340143	6	1.097788	2.567261	-1.627951
1	-7.057327	-0.140460	-1.700662	6	1.741730	3.764653	-1.622545
1	-5.605615	-4.109042	-0.874395	1	1.714578	5.788307	-0.788242
1	-7.409059	-2.610627	-1.729980	1	1.432604	1.708007	-2.211646
1	-1.729983	3.276415	1.641139	1	2.633689	3.913204	-2.228854
N,O-C7				6	-1.280505	0.645740	-2.101799
15	0.863804	-0.251673	1.096794	1	-0.453729	0.443980	-2.797762
6	2.404668	-1.010574	0.541364	1	-1.862792	-0.272541	-1.969838
6	3.294538	-0.301722	-0.270765	1	-1.925961	1.429887	-2.518843
6	2.711732	-2.328716	0.903124	8	5.878743	-2.867391	-0.741185
6	4.474046	-0.888537	-0.719185	6	6.815326	-2.223142	-1.564376
1	3.078154	0.731831	-0.552440	1	6.371900	-1.925134	-2.529883
6	3.880656	-2.923496	0.457723	1	7.245042	-1.332344	-1.075130
1	2.019328	-2.884943	1.539402	1	7.616870	-2.947580	-1.750608
6	4.772042	-2.210406	-0.357919	16	-0.229957	-1.328804	2.287654
1	5.150751	-0.308226	-1.345898	16	1.572281	1.564589	1.917565
1	4.131805	-3.950290	0.727315	7	-2.779819	-0.730682	0.267064
6	-1.620903	2.846098	0.659890	1	-1.992012	-1.250919	0.652430
1	0.326980	2.055524	2.135032	6	-3.833416	-1.461773	-0.248815

6	-4.882383	-0.842201	-0.950868	8	0.672707	0.545402	-0.468853
6	-3.845021	-2.862744	-0.121848	6	-0.190929	3.432471	0.614556
6	-5.919513	-1.604400	-1.482968	6	0.584975	4.602185	0.932839
1	-4.868071	0.241060	-1.091263	7	0.020161	2.840286	-0.655458
6	-4.877898	-3.612229	-0.672484	6	1.503111	5.071071	0.052998
1	-3.031683	-3.353723	0.418829	1	0.414370	5.086137	1.895468
6	-5.929102	-2.991965	-1.350678	6	0.998226	3.296039	-1.512380
1	-6.727434	-1.102006	-2.020811	6	1.727662	4.392177	-1.204855
1	-4.865428	-4.699185	-0.560999	1	2.090209	5.959745	0.292834
1	-6.742182	-3.584129	-1.774473	1	1.145817	2.726554	-2.428565
1	-2.217907	3.405927	1.374108	1	2.484850	4.747020	-1.903200
N ₂ O-C8				6	-1.110539	1.188005	-2.125187
15	0.728350	-0.953167	-0.009945	1	-0.326110	1.379609	-2.866592
6	2.503019	-1.305901	-0.006939	1	-1.319457	0.114665	-2.162415
6	3.430419	-0.267738	-0.088619	1	-2.013614	1.748672	-2.406936
6	2.961499	-2.627622	0.100598	8	6.547512	-2.209786	0.096927
6	4.800378	-0.530776	-0.068	6	7.535649	-1.219575	0.005401
1	3.077028	0.760919	-0.184593	1	7.478211	-0.673065	-0.951942
6	4.317881	-2.897896	0.134669	1	7.468542	-0.494661	0.835086
1	2.240272	-3.447152	0.147134	1	8.502318	-1.734120	0.062639
6	5.250726	-1.850721	0.056221	16	-0.339618	-2.291202	-0.976953
1	5.502196	0.300127	-0.130792	16	0.128471	-1.008532	2.037263
1	4.692220	-3.919426	0.217219	7	-2.917437	-0.295622	-0.072440
6	-1.144305	2.729319	1.276295	1	-2.120197	-0.792349	-0.482685
1	0.775980	0.132343	2.364289	6	-4.135675	-0.989200	-0.160036
6	-1.572030	1.635484	0.417774	6	-5.354137	-0.311394	-0.294244
6	-0.668421	1.624725	-0.751537	6	-4.121693	-2.390318	-0.163215
6	-2.658611	0.823069	0.657560	6	-6.543773	-1.028133	-0.396310
6	-3.534343	1.126638	1.845383	1	-5.363319	0.779893	-0.335395
1	-3.992198	2.122925	1.766212	6	-5.314062	-3.096616	-0.289088
1	-4.324202	0.380423	1.981552	1	-3.166562	-2.910537	-0.062532
1	-2.905276	1.118087	2.748539	6	-6.530679	-2.422389	-0.396339

1	-7.488836	-0.489732	-0.496228	6	0.341069	5.099440	-0.901382
1	-5.291044	-4.188578	-0.292474	1	0.636609	6.396181	0.838555
1	-7.464658	-2.980316	-0.487021	1	-0.094912	3.601896	-2.392382
1	-1.530349	2.971084	2.262085	1	0.978851	5.686809	-1.561856
N,O-C9				6	-1.711597	1.528788	-2.250392
15	1.042001	-0.221214	-0.238197	1	-0.743872	1.066917	-2.502395
6	2.751486	-0.825441	-0.098950	1	-2.484538	0.759472	-2.366096
6	3.782339	0.109130	-0.157607	1	-1.929965	2.337856	-2.964690
6	3.069549	-2.181459	0.063643	8	6.678902	-2.127153	0.238244
6	5.118156	-0.285744	-0.050383	6	7.761313	-1.241330	0.182365
1	3.528096	1.162394	-0.296477	1	7.811295	-0.713909	-0.786497
6	4.388877	-2.585383	0.174666	1	7.721978	-0.491624	0.992078
1	2.267768	-2.923159	0.092660	1	8.669875	-1.844112	0.303183
6	5.425356	-1.638846	0.120120	16	-0.011435	-1.479654	-1.403223
1	5.901739	0.470178	-0.103757	16	0.229779	-0.567413	1.751018
1	4.653408	-3.636466	0.301801	7	-2.783911	-0.672999	-0.205885
6	-1.993549	2.549467	1.363105	1	-1.878656	-0.734455	-0.761513
1	0.746729	0.570040	2.262444	6	-3.492143	-1.908207	-0.145171
6	-2.266229	1.595711	0.336030	6	-4.853633	-1.956304	-0.452957
6	-1.678885	2.048764	-0.858063	6	-2.790466	-3.070250	0.179212
6	-2.990087	0.374176	0.552285	6	-5.524781	-3.175182	-0.404528
6	-3.907839	0.299540	1.731351	1	-5.378184	-1.040440	-0.734417
1	-4.562813	1.178829	1.773619	6	-3.470692	-4.285378	0.214257
1	-4.501852	-0.618760	1.756993	1	-1.719642	-3.006167	0.380322
1	-3.263811	0.314557	2.625663	6	-4.834696	-4.340325	-0.069614
8	1.056476	1.256145	-0.525898	1	-6.590174	-3.215936	-0.639732
6	-1.213723	3.531732	0.798298	1	-2.926284	-5.197308	0.466668
6	-0.595224	4.716500	1.297645	1	-5.361405	-5.296127	-0.037530
7	-1.048708	3.214840	-0.558390	1	-2.279283	2.495936	2.409513
6	0.156093	5.489738	0.467241	N,O-C10			
1	-0.737164	4.970186	2.348921	15	-1.364035	-0.301616	1.220968
6	-0.244359	3.976472	-1.382116	6	-2.977001	-0.746872	0.548938

6	-3.814432	0.272559	0.094110	1	2.384804	2.032860	2.737566
6	-3.409019	-2.079025	0.472429	8	-6.682349	-1.741251	-1.010721
6	-5.069655	-0.019731	-0.436668	6	-7.574678	-0.772668	-1.492421
1	-3.475706	1.308448	0.166113	1	-7.873508	-0.062126	-0.702633
6	-4.652135	-2.379746	-0.055656	1	-7.145947	-0.207789	-2.338199
1	-2.756861	-2.874516	0.840954	1	-8.464631	-1.310828	-1.840090
6	-5.493020	-1.352586	-0.515711	16	-0.528031	-1.644031	2.327353
1	-5.706014	0.795977	-0.779443	16	-0.171802	-0.613132	-0.986892
1	-5.008441	-3.408812	-0.123586	7	2.755995	-0.738097	-0.337291
6	2.400851	2.597333	-1.489615	1	1.221527	-0.690144	-0.488713
1	-0.090457	0.702086	-1.281964	6	3.369148	-2.007001	-0.361017
6	2.599455	1.602947	-0.495408	6	4.392580	-2.331835	0.536051
6	1.891663	1.959835	0.652180	6	2.892753	-2.975345	-1.251954
6	3.356144	0.354021	-0.655100	6	4.946779	-3.609482	0.525331
6	4.753844	0.436379	-1.197234	1	4.738447	-1.580977	1.249766
1	5.431665	0.792476	-0.405771	6	3.456698	-4.248333	-1.259155
1	5.119402	-0.530181	-1.566386	1	2.083408	-2.718567	-1.938412
1	4.791529	1.184696	-2.001206	6	4.484742	-4.570222	-0.373462
8	-1.237967	1.182004	1.360874	1	5.742488	-3.857133	1.231090
6	1.542567	3.540029	-0.946247	1	3.085738	-4.996678	-1.962674
6	0.951550	4.741967	-1.429198	1	4.921404	-5.570725	-0.378802
7	1.249711	3.135967	0.364493	1	2.795690	2.609584	-2.502742
6	0.126548	5.466581	-0.619615	N,O-C11			
1	1.177712	5.058538	-2.448432	15	-1.438623	0.293821	0.167592
6	0.397311	3.858808	1.171215	6	-3.217206	0.107063	0.210089
6	-0.157436	5.007537	0.706559	6	-3.943240	0.200752	1.397348
1	-0.328951	6.390361	-0.980099	6	-3.892032	-0.101103	-1.005850
1	0.181097	3.428712	2.146980	6	-5.329904	0.090844	1.387501
1	-0.837118	5.563463	1.352302	1	-3.424301	0.348095	2.346449
6	1.877599	1.367570	2.018292	6	-5.269471	-0.208726	-1.020374
1	0.848810	1.195506	2.362307	1	-3.336085	-0.211208	-1.938598
1	2.387194	0.397188	2.018686	6	-6.001196	-0.115513	0.174298

1	-5.872278	0.157567	2.329934	16	-0.589311	0.175116	2.049801
1	-5.808981	-0.387334	-1.950918	7	1.622491	3.491690	-0.199740
6	2.815974	1.719230	2.734431	1	0.203880	2.406317	-0.395923
1	-0.750741	-1.206628	1.973581	6	1.414243	4.717079	-0.859773
6	2.608207	2.018546	1.362569	6	2.310287	5.165483	-1.838350
6	2.578080	0.821874	0.642592	6	0.255749	5.458007	-0.595046
6	2.428258	3.357325	0.790396	6	2.054964	6.347478	-2.529302
6	3.196752	4.487254	1.420402	1	3.205471	4.577105	-2.051565
1	2.990884	4.516816	2.500361	6	0.008509	6.639218	-1.291361
1	4.276283	4.307563	1.306950	1	-0.444772	5.102454	0.163798
1	2.942787	5.459279	0.981424	6	0.904954	7.089389	-2.259409
8	-0.795025	-0.789712	-0.773480	1	2.762293	6.690138	-3.287755
6	2.874323	0.340352	2.844112	1	-0.896248	7.211079	-1.073947
6	3.003451	-0.570587	3.930412	1	0.707434	8.014782	-2.803816
7	2.743649	-0.186464	1.551991	1	2.867469	2.419232	3.564336
6	2.990989	-1.915350	3.698224	6	3.225873	-3.827748	-1.810292
1	3.103500	-0.164048	4.937878	6	2.566424	-2.861472	-2.589444
6	2.732853	-1.543451	1.320619	6	1.265845	-2.493272	-2.290816
6	2.850563	-2.407295	2.361294	6	0.601866	-3.048844	-1.186031
1	3.080314	-2.621171	4.525484	6	1.254567	-4.014365	-0.424106
1	2.602438	-1.859975	0.287415	6	2.556548	-4.415672	-0.731517
1	2.820324	-3.477412	2.157595	8	4.487311	-4.123602	-2.176016
6	2.465038	0.536283	-0.815220	6	5.204005	-5.080372	-1.442924
1	1.520618	0.022262	-1.054518	15	-1.120203	-2.589573	-0.821568
1	2.494215	1.471200	-1.385689	16	-1.623090	-3.072524	1.034665
1	3.284757	-0.114994	-1.159421	16	-2.274159	-2.886291	-2.352257
8	-7.331962	-0.237930	0.061231	1	3.099357	-2.426847	-3.436673
6	-8.131880	-0.180307	1.213591	1	0.749856	-1.763872	-2.919409
1	-7.875795	-0.982015	1.926681	1	0.739285	-4.448288	0.436236
1	-8.043839	0.795702	1.720869	1	3.034699	-5.179617	-0.118398
1	-9.167744	-0.316753	0.881631	1	6.191513	-5.161199	-1.912747
16	-1.167600	2.177640	-0.608945	1	5.332710	-4.775639	-0.389645

1	4.713736	-6.068600	-1.472205	1	4.951068	0.670826	2.265237
N,O-C12				6	1.372978	3.304205	-0.106658
15	-0.735449	-1.506613	-1.284910	1	2.001269	2.700921	-0.778570
6	-1.996604	-2.490382	-0.455429	1	0.487742	3.634288	-0.660123
6	-3.298249	-2.003511	-0.368846	1	1.964672	4.192438	0.175503
6	-1.685260	-3.762536	0.048289	8	-4.885416	-4.863236	1.303947
6	-4.300911	-2.772379	0.221978	6	-6.219263	-4.449180	1.437556
1	-3.546122	-1.012288	-0.755774	1	-6.303785	-3.535881	2.051295
6	-2.680035	-4.529519	0.625125	1	-6.690188	-4.266701	0.456197
1	-0.662614	-4.146842	0.008226	1	-6.750877	-5.265872	1.940121
6	-3.995493	-4.043699	0.719771	16	-1.465682	-1.852616	-3.280088
1	-5.309422	-2.364846	0.284727	16	-1.039961	0.559926	-1.377863
1	-2.462874	-5.519715	1.027543	7	-1.721779	3.337529	0.056172
6	-0.122449	1.725358	2.950500	1	-0.416578	-1.271805	-3.901415
1	-0.491047	0.896084	-0.183261	6	-2.874832	3.946842	-0.453949
6	-0.297777	2.467977	1.753418	6	-3.139814	5.304522	-0.221023
6	0.940769	2.544346	1.100484	6	-3.743388	3.217092	-1.277750
6	-1.574395	3.049823	1.295601	6	-4.258887	5.910575	-0.787743
6	-2.646474	3.212257	2.345667	1	-2.453676	5.879844	0.404674
1	-2.906452	2.224424	2.755730	6	-4.864054	3.828610	-1.833182
1	-2.273668	3.820513	3.182625	1	-3.523024	2.166828	-1.478136
1	-3.555202	3.670033	1.938594	6	-5.129122	5.177026	-1.593148
8	0.711778	-2.184560	-1.533849	1	-4.454	6.969299	-0.597556
6	1.203708	1.334057	3.004825	1	-5.534034	3.243850	-2.467793
6	1.963515	0.526680	3.895379	1	-6.005126	5.654441	-2.036564
7	1.840131	1.855571	1.872366	1	-0.881131	1.454454	3.679353
6	3.282313	0.285859	3.642874	6	5.150592	0.601418	-1.496972
1	1.460281	0.117	4.763789	6	3.822126	0.872313	-1.867411
6	3.178118	1.627316	1.631069	6	2.800241	0.023358	-1.479546
6	3.899175	0.856459	2.484809	6	3.078817	-1.129518	-0.729288
1	3.869619	-0.343605	4.312869	6	4.399310	-1.403621	-0.379428
1	3.596144	2.071342	0.729064	6	5.435680	-0.545483	-0.748178

8	6.070915	1.494135	-1.903146	1	0.450688	1.374049	2.177516
6	7.419952	1.285321	-1.577850	1	-0.342333	3.559584	-1.392468
15	1.749948	-2.218007	-0.150982	6	5.298774	-0.580708	0.391769
16	0.430132	-1.209494	1.019299	6	4.793052	-1.794546	-0.098410
16	2.332057	-4.008805	0.281909	6	3.444760	-1.923976	-0.386834
1	3.622427	1.764208	-2.464157	6	2.570636	-0.845281	-0.193243
1	1.773132	0.265235	-1.759255	6	3.077366	0.362463	0.294613
1	4.621369	-2.309784	0.189224	6	4.429874	0.503158	0.587507
1	6.456943	-0.789502	-0.456109	8	6.617250	-0.546472	0.643465
1	7.978185	2.125950	-2.006537	6	7.198360	0.638062	1.122998
1	7.579070	1.270524	-0.485722	15	0.813888	-1.012194	-0.564963
1	7.803281	0.344507	-2.008576	16	0.299487	0.656500	-1.860596
N,O-C13				16	0.219079	-2.766820	-1.066845
15	-0.804015	1.214402	-0.140111	1	5.486844	-2.623908	-0.243107
6	-2.444417	0.463724	0.037370	1	3.048643	-2.869079	-0.765991
6	-2.777268	-0.186578	1.226113	1	2.412959	1.216574	0.445239
6	-3.374621	0.493380	-1.011518	1	4.793767	1.458110	0.965718
6	-4.028807	-0.771350	1.392348	1	8.266545	0.430847	1.256765
1	-2.049689	-0.247780	2.036536	1	7.082576	1.467360	0.404381
6	-4.614876	-0.102895	-0.861360	1	6.769228	0.939357	2.093800
1	-3.124380	0.980261	-1.956125	N,O-C14			
6	-4.958090	-0.732925	0.344455	15	-0.720027	0.910833	-0.094369
1	-4.260551	-1.263475	2.336338	6	-2.471515	0.505126	-0.117759
1	-5.346374	-0.095929	-1.670262	6	-2.895017	-0.743919	0.337047
8	0.037266	-0.215295	0.608734	6	-3.406250	1.432100	-0.594577
8	-6.186619	-1.271876	0.402731	6	-4.247396	-1.072170	0.319693
6	-6.603175	-1.912337	1.580277	1	-2.173150	-1.480601	0.698751
1	-5.966024	-2.780467	1.820864	6	-4.752332	1.106414	-0.615383
1	-6.608140	-1.219766	2.439395	1	-3.077245	2.409808	-0.954196
1	-7.626386	-2.262575	1.400424	6	-5.186042	-0.147272	-0.157760
16	-1.567887	3.074751	-1.098295	1	-4.553022	-2.054460	0.678663
16	-0.134932	2.380053	1.490183	1	-5.498007	1.811650	-0.984740

8	0.174564	-0.090853	0.854868
8	-6.508611	-0.373130	-0.217333
6	-7.017857	-1.607847	0.215881
1	-6.609807	-2.446490	-0.373638
1	-6.807404	-1.783282	1.284689
1	-8.103544	-1.565368	0.069654
16	-0.116753	2.733749	-0.790473
16	-1.098747	2.189809	2.060062
1	0.167562	2.027198	2.497176
1	-0.585354	3.058978	0.707617
6	5.355401	-0.255494	0.095025
6	4.909200	-1.549483	0.407199
6	3.562552	-1.860446	0.331148
6	2.631065	-0.887580	-0.060412
6	3.078187	0.398991	-0.377997
6	4.428523	0.720985	-0.299368
8	6.675863	-0.044517	0.198740
6	7.200755	1.224064	-0.099388
15	0.878779	-1.289005	-0.127022
16	-0.001933	-0.348865	-1.791002
16	0.400617	-3.088680	0.345691
1	5.646491	-2.294172	0.709637
1	3.216090	-2.866752	0.577177
1	2.369945	1.168648	-0.695096
1	4.744168	1.733226	-0.550105
1	8.284497	1.154628	0.050147
1	7.820	1.510637	-1.145763
1	6.795573	1.999933	0.572163
N,O-C15			
Acid			
1	0.	-0.973735	-0.828280
1	0.	0.973735	-0.828280

16	0.	0.	0.103535
Indolizine			
6	5.128981	0.895505	-0.570
6	5.368585	-0.515622	-0.066
6	4.312860	-1.381334	0.357
6	2.980491	-0.883551	0.311
7	2.789383	0.507256	-0.156
6	3.858699	1.377955	-0.611
6	1.726257	-1.467199	0.647
6	0.765165	-0.420686	0.360
6	1.450481	0.799784	-0.114
6	0.976893	2.212235	-0.549
6	-0.698142	-0.626356	0.496
6	-1.164617	-2.063820	0.001252
1	5.960448	1.600801	-0.932
1	6.393171	-0.890623	-0.030
1	4.461109	-2.462317	0.747
1	3.618796	2.440411	-0.001015
1	1.540749	-2.537787	0.001040
1	-0.117813	2.218836	-0.056
1	1.334750	2.756360	0.889823
1	1.333862	2.755521	-0.891795
1	-0.773504	-2.586202	-0.884491
1	-0.772545	-2.585576	0.886934
1	-2.258292	-2.137879	0.001850
7	-1.485013	0.380974	0.036
6	-2.877677	0.254942	-0.065
6	-3.589396	0.228687	1.208005
6	-3.588945	0.225536	-1.208323
6	-4.980270	0.155930	1.202951
1	-3.036023	0.266837	2.148729
6	-4.979825	0.152821	-1.203612

1	-3.035221	0.261232	-2.148940
6	-5.684186	0.116365	-0.415
1	-5.519220	0.130534	2.153075
1	-5.518405	0.124954	-2.153875
1	-6.774578	0.060126	-0.544
LR-Substituted			
6	4.305405	0.899139	-0.213571
6	2.954360	0.605738	-0.070665
6	2.517319	-0.721821	-0.004248
6	3.457540	-1.760747	-0.078879
6	4.804457	-1.475674	-0.217267
6	5.241729	-0.143139	-0.287336
1	4.613880	1.942601	-0.268695
1	2.239764	1.431187	-0.015062
1	3.118688	-2.798112	-0.033058
1	5.549083	-2.270318	-0.278238
8	6.562862	0.037852	-0.425215
6	7.079190	1.342052	-0.510688
1	8.164420	1.239123	-0.625662
1	6.675697	1.881645	-1.383961
1	6.868076	1.922787	0.403120
15	0.772537	-1.096982	0.173845
15	-0.772523	1.096903	0.175282
16	-0.056	-0.652	1.856818
16	0.265562	-2.938220	-0.020532
16	-0.265734	2.938333	-0.018391
6	-2.517295	0.721728	-0.003248
6	-2.954693	-0.605799	-0.067517
6	-3.457173	1.760787	-0.080646
6	-4.305688	-0.899093	-0.211098
1	-2.240362	-1.431335	-0.009700
6	-4.804047	1.475841	-0.219691

1	-3.118035	2.798127	-0.036427
6	-5.241652	0.143308	-0.287685
1	-4.614423	-1.942573	-0.264459
1	-5.548387	2.270594	-0.282760
8	-6.562706	-0.037575	-0.426382
6	-7.079239	-1.341792	-0.510494
1	-6.869497	-1.921122	0.404516
1	-8.164289	-1.238770	-0.627059
1	-6.674708	-1.882853	-1.382376
8	0.126	0.431	-0.816553

Figure 51

N,O-S1

LR

6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071

16	-0.184	0.609	-1.552090	7	-3.122863	0.193842	0.742669
16	-0.116	0.185	1.553327	6	-4.155681	-2.311521	0.115318
16	0.492940	3.068803	-0.771	1	-3.081530	-2.073296	-1.748706
16	-0.492242	-3.068189	-0.603	6	-3.909095	-0.454993	1.594845
6	-2.652613	-0.746168	-0.150	6	-4.451567	-1.713437	1.336515
6	-3.051857	0.594301	0.287	1	-4.557872	-3.295573	-0.136339
6	-3.625394	-1.755670	-0.493	1	-4.121709	0.052896	2.542020
6	-4.400241	0.930604	0.362	1	-5.087973	-2.205476	2.073792
1	-2.307453	1.395396	0.536	6	-1.909145	3.160048	-0.292752
6	-4.970864	-1.427866	-0.432	1	-2.758714	2.642232	0.175015
1	-3.315267	-2.803163	-0.809	1	-1.723006	4.114851	0.212788
6	-5.371350	-0.082808	0.013	1	-2.160851	3.355870	-1.346914
1	-4.679935	1.983600	0.725	7	1.589	0.608752	-0.028432
1	-5.741489	-2.199662	-0.707	1	1.442024	1.561599	0.355050
8	-6.693755	0.139912	0.103	6	2.837381	0.001943	0.106181
6	-7.175115	1.459861	0.447	6	3.464265	-0.685960	-0.941875
1	-6.850662	2.011249	-0.898237	6	3.517384	0.149321	1.323508
1	-8.269204	1.391129	0.340	6	4.726894	-1.245524	-0.758146
1	-6.850803	2.010720	0.899507	1	2.971318	-0.761556	-1.911971
Precursor				6	4.786073	-0.395952	1.493279
6	-1.930290	0.408578	-1.367349	1	3.031530	0.691116	2.137866
1	-1.689527	-0.219937	-2.237521	6	5.394161	-1.105380	0.457483
6	-0.670027	0.957777	-0.728202	1	5.200807	-1.780062	-1.584507
6	-0.661971	2.309311	-0.178057	1	5.300129	-0.272304	2.448964
6	0.448768	0.142603	-0.608671	1	6.386079	-1.540296	0.594635
6	0.412915	-1.291340	-1.070791	1	-2.527440	1.237618	-1.774861
1	1.197865	-1.888977	-0.592444	N,O-S2			
1	-0.554921	-1.746003	-0.826527	6	-4.040100	-0.995309	-0.715057
1	0.548861	-1.363429	-2.161532	6	-2.806060	-0.380074	-0.894362
8	0.320394	2.796580	0.394728	6	-2.537931	0.861547	-0.308140
6	-2.829272	-0.375414	-0.429555	6	-3.531311	1.490869	0.464960
6	-3.333834	-1.633406	-0.781114	6	-4.758656	0.886153	0.643939

6	-5.024024	-0.367057	0.059747	6	-2.563014	-0.295727	0.078
1	-4.217340	-1.963686	-1.181138	6	-1.761443	-1.451863	-0.463
1	-2.040794	-0.873401	-1.495921	6	-0.384385	-1.344393	-0.361
1	-3.326587	2.460132	0.924601	6	0.230510	-0.078248	0.234
1	-5.542149	1.356584	1.239391	6	-0.571133	1.069674	0.902
8	-6.239018	-0.877646	0.295638	6	-1.957541	0.970024	0.948
6	-6.575757	-2.137635	-0.229085	8	-3.885436	-0.498129	-0.230
1	-7.598145	-2.349814	0.104217	6	-4.759250	0.603778	-0.315
1	-6.550899	-2.137520	-1.331831	15	2.021612	0.066269	-0.039
1	-5.902560	-2.925468	0.148168	16	2.707743	1.856016	-0.605
15	-0.937468	1.631443	-0.512316	16	2.982996	-1.591296	0.363
15	0.725823	-0.944103	0.573580	1	-2.254777	-2.424604	-0.001081
16	-0.037424	0.374100	1.823646	1	0.236002	-2.243390	-0.730
16	0.299548	0.620838	-1.668058	1	-0.098402	2.054262	0.001405
16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	N,O-S4			
6	4.518843	0.533126	0.484738	15	-1.256206	-0.743597	-0.525155
1	2.590010	1.198244	1.169247	6	-3.017504	-0.364374	-0.304
6	4.574104	-1.679850	-0.516320	6	-3.850080	-1.302251	0.315997
1	2.700275	-2.728593	-0.606940	6	-3.572291	0.844938	-0.743355
6	5.239282	-0.503636	-0.127213	6	-5.204012	-1.041629	0.511088
1	5.008365	1.456113	0.793375	1	-3.434726	-2.260890	0.635790
1	5.155828	-2.472745	-0.988319	6	-4.920510	1.110471	-0.564403
8	6.554046	-0.461539	-0.378351	1	-2.930555	1.575945	-1.241315
6	7.292017	0.681090	-0.023996	6	-5.748367	0.171300	0.067849
1	7.259570	0.862974	1.063412	1	-5.824198	-1.793728	0.998510
1	8.328884	0.487145	-0.321802	1	-5.366265	2.042739	-0.914611
1	6.928185	1.578435	-0.551917	6	2.060029	2.196534	1.683009
N,O-S3				1	2.910047	2.030810	2.358341

6	1.479724	0.867294	1.220762	6	3.654612	-3.116581	1.142082
6	0.077986	0.806973	0.935528	6	2.666429	-3.045350	-1.067734
6	2.368308	-0.188340	0.967791	6	4.420506	-4.216534	0.762383
6	3.852077	0.044983	1.090129	1	3.718946	-2.718330	2.156654
1	4.427747	-0.733101	0.578124	6	3.422455	-4.156076	-1.434253
1	4.123857	1.012123	0.651441	1	1.962865	-2.581281	-1.761082
1	4.159912	0.053744	2.147589	6	4.305591	-4.738755	-0.525511
8	-0.532374	-0.436151	0.990053	1	5.100679	-4.675950	1.482736
6	2.486470	3.128303	0.565405	1	3.320358	-4.567728	-2.440455
6	3.768764	3.687736	0.518854	1	4.939	-5.606595	-0.818883
7	1.572430	3.394300	-0.370929	1	1.318698	2.730016	2.294622
6	4.102319	4.531077	-0.538241	N,O-S5			
1	4.495205	3.462992	1.303287	15	-1.256607	-0.532680	-0.623115
6	1.893690	4.195624	-1.380289	6	-2.986193	-0.114090	-0.295487
6	3.147728	4.790376	-1.516674	6	-3.879328	-1.139875	0.027913
1	5.097427	4.977798	-0.597588	6	-3.464808	1.204019	-0.358227
1	1.110626	4.373838	-2.125069	6	-5.214586	-0.866372	0.310694
1	3.364625	5.439385	-2.366579	1	-3.528218	-2.174268	0.048306
6	-0.818014	1.935849	1.371262	6	-4.794067	1.485499	-0.090024
1	-0.484417	2.885371	0.938144	1	-2.785239	2.013483	-0.634076
1	-1.853417	1.741845	1.073470	6	-5.681106	0.453816	0.253623
1	-0.790781	1.995666	2.473102	1	-5.881716	-1.689660	0.565122
8	-7.043255	0.513571	0.197976	1	-5.180332	2.504267	-0.146532
6	-7.935554	-0.387260	0.797215	6	2.424769	1.915321	1.599423
1	-7.990728	-1.339474	0.241995	1	3.315624	1.618475	2.164999
1	-7.661801	-0.599531	1.845241	6	1.742657	0.707310	0.981372
1	-8.921985	0.091331	0.779304	6	0.264547	0.823224	0.718034
16	-0.264191	0.815688	-1.374378	6	2.518232	-0.354895	0.609082
16	-0.967007	-2.610246	-0.992247	6	4.004932	-0.367800	0.912510
7	1.976483	-1.411637	0.579523	1	4.488316	-1.247075	0.472688
1	0.974820	-1.574522	0.485936	1	4.481321	0.523160	0.476596
6	2.789299	-2.519904	0.221148	1	4.216589	-0.368334	1.992083

8	-0.424087	-0.439041	0.806931	1	3.725675	-5.001714	2.202721
6	2.811880	2.959435	0.573847	1	2.674743	-5.569301	-1.934493
6	4.091650	3.523942	0.534401	1	3.566163	-6.487638	0.208408
7	1.863848	3.314082	-0.298808	1	1.769533	2.397355	2.338594
6	4.381658	4.476607	-0.438782	N,O-S6			
1	4.848125	3.215536	1.259113	15	1.614785	0.826913	0.456206
6	2.142567	4.223530	-1.226691	6	3.310932	0.320319	0.100865
6	3.387885	4.838689	-1.343655	6	3.825954	-0.822929	0.711624
1	5.374776	4.928454	-0.492450	6	4.131852	1.061053	-0.762918
1	1.332367	4.472882	-1.920379	6	5.132851	-1.242670	0.461116
1	3.570058	5.577652	-2.125475	1	3.197844	-1.383628	1.407044
6	-0.460319	1.823442	1.605190	6	5.426670	0.649367	-1.025414
1	-0.135274	2.848755	1.391036	1	3.746258	1.976174	-1.219028
1	-1.541061	1.752995	1.434445	6	5.938256	-0.509086	-0.417408
1	-0.268092	1.582379	2.662056	1	5.508962	-2.135209	0.960900
8	-6.949953	0.820098	0.500336	1	6.077591	1.213635	-1.695010
6	-7.894636	-0.159881	0.842894	6	-2.259878	-2.117110	1.399412
1	-8.019085	-0.905645	0.039150	1	-2.846118	-1.824990	2.283077
1	-7.621646	-0.680750	1.776606	6	-1.584385	-0.912197	0.763934
1	-8.847093	0.361921	0.993059	6	-0.261979	-1.050527	0.280723
16	-0.154894	1.194016	-1.120691	6	-2.348667	0.270586	0.654563
16	-1.040274	-2.193343	-1.584088	6	-3.848506	0.200657	0.756326
7	2.076167	-1.412849	-0.154410	1	-4.268404	-0.362835	-0.089660
1	1.236168	-1.293782	-0.709215	1	-4.130802	-0.340068	1.670202
6	2.483657	-2.746592	-0.032637	1	-4.309850	1.192927	0.791334
6	2.955665	-3.274822	1.176805	8	1.003020	-0.098024	1.548
6	2.385491	-3.590911	-1.149167	6	-3.143948	-2.912387	0.456858
6	3.355340	-4.607445	1.253388	6	-4.395684	-3.388055	0.864376
1	2.984647	-2.643948	2.067115	7	-2.668533	-3.145454	-0.768225
6	2.762914	-4.925634	-1.056284	6	-5.166454	-4.122563	-0.031889
1	2.001515	-3.184805	-2.087059	1	-4.760087	-3.178651	1.872600
6	3.262222	-5.441190	0.140973	6	-3.406513	-3.849086	-1.621906

6	-4.665227	-4.359951	-1.309031	6	-1.930290	0.408578	-1.367349
1	-6.147852	-4.501673	0.262199	1	-1.689527	-0.219937	-2.237521
1	-2.972693	-4.015635	-2.613898	6	-0.670027	0.957777	-0.728202
1	-5.233179	-4.927079	-2.048223	6	-0.661971	2.309311	-0.178057
6	0.418283	-2.388152	0.337040	6	0.448768	0.142603	-0.608671
1	-0.157681	-3.080674	-0.297847	6	0.412915	-1.291340	-1.070791
1	1.438106	-2.314463	-0.054842	1	1.197865	-1.888977	-0.592444
1	0.457690	-2.780105	1.361929	1	-0.554921	-1.746003	-0.826527
8	7.207961	-0.830278	-0.731784	1	0.548861	-1.363429	-2.161532
6	7.791811	-1.964108	-0.150321	8	0.320394	2.796580	0.394728
1	7.849533	-1.876279	0.948563	6	-2.829272	-0.375414	-0.429555
1	7.241922	-2.886315	-0.406884	6	-3.333834	-1.633406	-0.781114
1	8.808868	-2.035820	-0.554379	7	-3.122863	0.193842	0.742669
16	0.327378	-0.017430	-1.093863	6	-4.155681	-2.311521	0.115318
16	1.396522	2.763220	0.577929	1	-3.081530	-2.073296	-1.748706
7	-1.795787	1.478189	0.530576	6	-3.909095	-0.454993	1.594845
1	-0.789169	1.585172	0.689898	6	-4.451567	-1.713437	1.336515
6	-2.413180	2.665358	0.066764	1	-4.557872	-3.295573	-0.136339
6	-2.172043	3.861915	0.746291	1	-4.121709	0.052896	2.542020
6	-3.196036	2.660230	-1.090839	1	-5.087973	-2.205476	2.073792
6	-2.739533	5.044203	0.279587	6	-1.909145	3.160048	-0.292752
1	-1.529544	3.855398	1.628414	1	-2.758714	2.642232	0.175015
6	-3.772465	3.844767	-1.541541	1	-1.723006	4.114851	0.212788
1	-3.331892	1.728997	-1.644175	1	-2.160851	3.355870	-1.346914
6	-3.547461	5.038752	-0.857579	7	1.589	0.608752	-0.028432
1	-2.547279	5.979080	0.809742	1	1.442024	1.561599	0.355050
1	-4.384821	3.836610	-2.445699	6	2.837381	0.001943	0.106181
1	-3.991867	5.968281	-1.218822	6	3.464265	-0.685960	-0.941875
1	-1.495230	-2.802233	1.788390	6	3.517384	0.149321	1.323508
				6	4.726894	-1.245524	-0.758146
				1	2.971318	-0.761556	-1.911971
				6	4.786073	-0.395952	1.493279

Figure 52

N₂O-A1

1	3.031530	0.691116	2.137866
6	5.394161	-1.105380	0.457483
1	5.200807	-1.780062	-1.584507
1	5.300129	-0.272304	2.448964
1	6.386079	-1.540296	0.594635
1	-2.527440	1.237618	-1.774861

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6	4.399900	-0.931020	0.078
6	3.051574	-0.594451	0.074
6	2.652608	0.746089	0.098
6	3.625607	1.755391	0.006
6	4.971010	1.427326	0.027
6	5.371218	0.082184	0.079
1	4.679398	-1.984067	0.068
1	2.307030	-1.395415	0.071
1	3.315697	2.802948	-0.108
1	5.741782	2.198979	-0.020
8	6.693580	-0.140809	0.086
6	7.174688	-1.460847	0.183
1	8.268794	-1.392340	0.326
1	6.850105	-2.011894	0.899028
1	6.850302	-2.011911	-0.898728
15	0.901258	1.184195	-0.247
15	-0.901144	-1.183693	-0.071
16	-0.184	0.609	-1.552090
16	-0.116	0.185	1.553327
16	0.492940	3.068803	-0.771
16	-0.492242	-3.068189	-0.603
6	-2.652613	-0.746168	-0.150
6	-3.051857	0.594301	0.287
6	-3.625394	-1.755670	-0.493

6	-4.400241	0.930604	0.362
1	-2.307453	1.395396	0.536
6	-4.970864	-1.427866	-0.432
1	-3.315267	-2.803163	-0.809
6	-5.371350	-0.082808	0.013
1	-4.679935	1.983600	0.725
1	-5.741489	-2.199662	-0.707
8	-6.693755	0.139912	0.103
6	-7.175115	1.459861	0.447
1	-6.850662	2.011249	-0.898237
1	-8.269204	1.391129	0.340
1	-6.850803	2.010720	0.899507

N,O-A2

6	-4.040100	-0.995309	-0.715057
6	-2.806060	-0.380074	-0.894362
6	-2.537931	0.861547	-0.308140
6	-3.531311	1.490869	0.464960
6	-4.758656	0.886153	0.643939
6	-5.024024	-0.367057	0.059747
1	-4.217340	-1.963686	-1.181138
1	-2.040794	-0.873401	-1.495921
1	-3.326587	2.460132	0.924601
1	-5.542149	1.356584	1.239391
8	-6.239018	-0.877646	0.295638
6	-6.575757	-2.137635	-0.229085
1	-7.598145	-2.349814	0.104217
1	-6.550899	-2.137520	-1.331831
1	-5.902560	-2.925468	0.148168
15	-0.937468	1.631443	-0.512316
15	0.725823	-0.944103	0.573580
16	-0.037424	0.374100	1.823646
16	0.299548	0.620838	-1.668058

16	-0.803876	3.498794	-0.124871	1	-2.554405	1.881627	0.001668
16	-0.045896	-2.658290	0.185837	1	-5.775254	0.192793	-0.002410
6	2.490809	-0.781376	0.315290	1	-4.625439	1.226573	0.899941
6	3.153407	0.389017	0.699605	1	-4.622697	1.228758	-0.898633
6	3.216076	-1.815551	-0.301885	N,O-A4			
6	4.518843	0.533126	0.484738	15	-0.031410	-1.175269	-0.460215
1	2.590010	1.198244	1.169247	6	-1.839669	-1.370891	-0.352772
6	4.574104	-1.679850	-0.516320	6	-2.413751	-1.939466	0.785931
1	2.700275	-2.728593	-0.606940	6	-2.673950	-0.960591	-1.399535
6	5.239282	-0.503636	-0.127213	6	-3.796091	-2.066929	0.905314
1	5.008365	1.456113	0.793375	1	-1.766431	-2.286246	1.594500
1	5.155828	-2.472745	-0.988319	6	-4.050904	-1.098678	-1.300855
8	6.554046	-0.461539	-0.378351	1	-2.226581	-0.512056	-2.289429
6	7.292017	0.681090	-0.023996	6	-4.625294	-1.642873	-0.143371
1	7.259570	0.862974	1.063412	1	-4.212558	-2.508772	1.810499
1	8.328884	0.487145	-0.321802	1	-4.712367	-0.787629	-2.111225
1	6.928185	1.578435	-0.551917	6	0.748570	3.206621	0.472065
N,O-A3				1	1.372913	3.661579	-0.305523
6	-2.563014	-0.295727	0.078	6	1.208495	1.809727	0.817421
6	-1.761443	-1.451863	-0.463	6	0.192527	0.984556	1.474134
6	-0.384385	-1.344393	-0.361	6	2.453676	1.311534	0.503333
6	0.230510	-0.078248	0.234	6	3.498285	2.170523	-0.155808
6	-0.571133	1.069674	0.902	1	4.483735	2.010269	0.298899
6	-1.957541	0.970024	0.948	1	3.577856	1.878160	-1.214674
8	-3.885436	-0.498129	-0.230	1	3.267094	3.237489	-0.099520
6	-4.759250	0.603778	-0.315	8	0.022801	-0.252040	1.194807
15	2.021612	0.066269	-0.039	6	-0.679651	3.137631	-0.021047
16	2.707743	1.856016	-0.605	6	-1.281146	4.069735	-0.867564
16	2.982996	-1.591296	0.363	7	-1.360960	2.096844	0.440637
1	-2.254777	-2.424604	-0.001081	6	-2.613077	3.877870	-1.224613
1	0.236002	-2.243390	-0.730	1	-0.711497	4.919826	-1.246911
1	-0.098402	2.054262	0.001405	6	-2.636977	1.905013	0.123732

6	-3.310819	2.779919	-0.721033	6	3.503120	-0.433995	0.652092
1	-3.106513	4.581597	-1.898511	6	2.292642	-2.379644	-0.081688
1	-3.125265	1.023316	0.548801	6	4.693260	-0.976107	0.159951
1	-4.353706	2.595968	-0.981681	1	3.509361	0.538701	1.151321
6	-0.310217	1.368038	2.839957	6	3.463300	-2.924886	-0.581564
1	-0.349027	2.455499	2.975508	1	1.353720	-2.934410	-0.149536
1	-1.297298	0.924995	3.023739	6	4.676401	-2.227966	-0.463048
1	0.402128	0.951809	3.570770	1	5.622545	-0.419354	0.283376
8	-5.970426	-1.722537	-0.126185	1	3.474304	-3.905158	-1.061047
6	-6.610010	-2.282509	0.988639	6	-1.385475	3.026706	0.428002
1	-6.316272	-3.334872	1.144234	1	-1.314063	3.125795	1.525243
1	-6.400181	-1.714044	1.911596	6	-1.663905	1.612561	-0.003592
1	-7.687045	-2.241607	0.786117	6	-0.540804	1.075322	-0.875029
16	0.470521	0.018979	-1.922244	6	-2.785367	0.924624	0.296398
16	0.941610	-2.788691	0.043941	6	-3.896934	1.585987	1.075265
7	2.858582	0.042937	0.787496	1	-4.391453	2.384249	0.499837
1	2.154353	-0.650873	1.032698	1	-4.659127	0.860431	1.382417
6	4.076164	-0.533059	0.313130	1	-3.479036	2.042449	1.985803
6	5.222123	-0.496750	1.110019	8	0.159913	-0.030331	-0.475733
6	4.108041	-1.163777	-0.932847	6	-0.039158	3.312964	-0.147918
6	6.406809	-1.072624	0.654768	6	0.771392	4.433634	-0.015
1	5.171911	-0.014079	2.088522	7	0.412468	2.270405	-0.855593
6	5.293117	-1.744735	-1.379839	6	2.047979	4.409836	-0.544592
1	3.194046	-1.195515	-1.530131	1	0.408780	5.287538	0.571820
6	6.442852	-1.697585	-0.591433	6	1.653853	2.194787	-1.353224
1	7.302263	-1.040606	1.279430	6	2.503903	3.272159	-1.220751
1	5.315501	-2.241849	-2.351822	1	2.708676	5.270118	-0.421831
1	7.368871	-2.154596	-0.947228	1	1.930048	1.244649	-1.813599
1	0.774150	3.900601	1.335136	1	3.514789	3.214561	-1.622782
N,O-A5				6	-0.985656	0.834950	-2.316166
15	0.726542	-0.389811	1.131278	1	-0.143415	0.478042	-2.926108
6	2.296530	-1.119739	0.536765	1	-1.757714	0.055891	-2.300413

1	-1.406944	1.750518	-2.754143	1	5.375534	0.099608	-0.579556
8	5.766843	-2.842429	-0.969055	1	4.139907	-4.013563	-0.195158
6	7.019530	-2.234630	-0.822228	6	-1.136895	2.654603	0.971350
1	7.071481	-1.264378	-1.347555	1	-0.104094	1.940577	1.786103
1	7.275348	-2.075807	0.239943	6	-1.632244	1.423370	0.335035
1	7.755213	-2.916615	-1.266013	6	-0.629377	1.033602	-0.750162
16	-0.487238	-1.774318	1.833767	6	-2.713430	0.688853	0.675848
16	1.068152	1.289601	2.125055	6	-3.657356	1.122124	1.766847
7	-2.873306	-0.424308	-0.015126	1	-3.763058	2.213880	1.822863
1	-2.064809	-0.984450	0.283048	1	-4.654338	0.683869	1.627906
6	-4.044151	-1.127479	-0.273595	1	-3.271859	0.760571	2.734868
6	-5.145514	-0.524357	-0.900568	8	0.217269	-0.049421	-0.463593
6	-4.113555	-2.492071	0.054084	6	-0.151398	3.194373	0.127155
6	-6.296801	-1.263527	-1.163473	6	0.591614	4.402780	0.178861
1	-5.090223	0.524115	-1.200998	7	0.218952	2.266502	-0.807868
6	-5.260724	-3.223327	-0.231485	6	1.663699	4.568021	-0.659225
1	-3.254704	-2.963260	0.538157	1	0.305084	5.166279	0.901759
6	-6.364704	-2.615498	-0.832907	6	1.299589	2.400370	-1.610272
1	-7.146321	-0.775894	-1.647710	6	2.045329	3.544826	-1.569615
1	-5.296250	-4.283700	0.029178	1	2.241987	5.493612	-0.619834
1	-7.266477	-3.192251	-1.046992	1	1.527665	1.550777	-2.255218
1	-2.129613	3.758445	0.067288	1	2.910573	3.657307	-2.221096
N,O-A6				6	-1.247705	0.771270	-2.117157
15	0.752995	-0.599143	1.028289	1	-0.468028	0.503392	-2.844049
6	2.394225	-1.156947	0.485632	1	-1.949466	-0.065340	-2.034576
6	3.380709	-0.231036	0.139314	1	-1.787044	1.662836	-2.463588
6	2.673881	-2.523745	0.363902	8	6.064020	-2.524796	-0.885105
6	4.624999	-0.649030	-0.326437	6	7.103365	-1.651249	-1.233552
1	3.185038	0.837810	0.256663	1	6.817841	-0.986725	-2.067611
6	3.909001	-2.951757	-0.097397	1	7.422677	-1.032399	-0.377032
1	1.906491	-3.250419	0.640970	1	7.945767	-2.277029	-1.551994
6	4.895188	-2.018947	-0.448557	16	-0.381915	-2.038024	1.710391

16	1.097604	1.019444	2.260389	6	-3.933401	1.059259	1.558404
7	-2.885386	-0.590090	0.130902	1	-4.158642	2.130125	1.465384
1	-2.145285	-1.258909	0.364102	1	-4.858410	0.496129	1.373238
6	-4.085030	-1.104546	-0.331127	1	-3.633109	0.856698	2.600807
6	-5.095888	-0.266832	-0.832272	8	0.196059	0.089922	-0.358333
6	-4.287251	-2.495644	-0.357130	6	-0.560386	3.350247	-0.037389
6	-6.282495	-0.810011	-1.319225	6	0.101482	4.628899	-0.038086
1	-4.937037	0.813846	-0.854937	7	-0.018779	2.376107	-0.878780
6	-5.469123	-3.025035	-0.862175	6	1.211051	4.819175	-0.800472
1	-3.504241	-3.153711	0.027844	1	-0.299259	5.420821	0.595484
6	-6.480632	-2.189292	-1.340143	6	1.097788	2.567261	-1.627951
1	-7.057327	-0.140460	-1.700662	6	1.741730	3.764653	-1.622545
1	-5.605615	-4.109042	-0.874395	1	1.714578	5.788307	-0.788242
1	-7.409059	-2.610627	-1.729980	1	1.432604	1.708007	-2.211646
1	-1.729983	3.276415	1.641139	1	2.633689	3.913204	-2.228854
N,O-A7				6	-1.280505	0.645740	-2.101799
15	0.863804	-0.251673	1.096794	1	-0.453729	0.443980	-2.797762
6	2.404668	-1.010574	0.541364	1	-1.862792	-0.272541	-1.969838
6	3.294538	-0.301722	-0.270765	1	-1.925961	1.429887	-2.518843
6	2.711732	-2.328716	0.903124	8	5.878743	-2.867391	-0.741185
6	4.474046	-0.888537	-0.719185	6	6.815326	-2.223142	-1.564376
1	3.078154	0.731831	-0.552440	1	6.371900	-1.925134	-2.529883
6	3.880656	-2.923496	0.457723	1	7.245042	-1.332344	-1.075130
1	2.019328	-2.884943	1.539402	1	7.616870	-2.947580	-1.750608
6	4.772042	-2.210406	-0.357919	16	-0.229957	-1.328804	2.287654
1	5.150751	-0.308226	-1.345898	16	1.572281	1.564589	1.917565
1	4.131805	-3.950290	0.727315	7	-2.779819	-0.730682	0.267064
6	-1.620903	2.846098	0.659890	1	-1.992012	-1.250919	0.652430
1	0.326980	2.055524	2.135032	6	-3.833416	-1.461773	-0.248815
6	-1.835359	1.464543	0.257536	6	-4.882383	-0.842201	-0.950868
6	-0.739626	1.103708	-0.753466	6	-3.845021	-2.862744	-0.121848
6	-2.835471	0.627961	0.623141	6	-5.919513	-1.604400	-1.482968

1	-4.868071	0.241060	-1.091263	7	0.020161	2.840286	-0.655458
6	-4.877898	-3.612229	-0.672484	6	1.503111	5.071071	0.052998
1	-3.031683	-3.353723	0.418829	1	0.414370	5.086137	1.895468
6	-5.929102	-2.991965	-1.350678	6	0.998226	3.296039	-1.512380
1	-6.727434	-1.102006	-2.020811	6	1.727662	4.392177	-1.204855
1	-4.865428	-4.699185	-0.560999	1	2.090209	5.959745	0.292834
1	-6.742182	-3.584129	-1.774473	1	1.145817	2.726554	-2.428565
1	-2.217907	3.405927	1.374108	1	2.484850	4.747020	-1.903200
N,O-A8				6	-1.110539	1.188005	-2.125187
15	0.728350	-0.953167	-0.009945	1	-0.326110	1.379609	-2.866592
6	2.503019	-1.305901	-0.006939	1	-1.319457	0.114665	-2.162415
6	3.430419	-0.267738	-0.088619	1	-2.013614	1.748672	-2.406936
6	2.961499	-2.627622	0.100598	8	6.547512	-2.209786	0.096927
6	4.800378	-0.530776	-0.068	6	7.535649	-1.219575	0.005401
1	3.077028	0.760919	-0.184593	1	7.478211	-0.673065	-0.951942
6	4.317881	-2.897896	0.134669	1	7.468542	-0.494661	0.835086
1	2.240272	-3.447152	0.147134	1	8.502318	-1.734120	0.062639
6	5.250726	-1.850721	0.056221	16	-0.339618	-2.291202	-0.976953
1	5.502196	0.300127	-0.130792	16	0.128471	-1.008532	2.037263
1	4.692220	-3.919426	0.217219	7	-2.917437	-0.295622	-0.072440
6	-1.144305	2.729319	1.276295	1	-2.120197	-0.792349	-0.482685
1	0.775980	0.132343	2.364289	6	-4.135675	-0.989200	-0.160036
6	-1.572030	1.635484	0.417774	6	-5.354137	-0.311394	-0.294244
6	-0.668421	1.624725	-0.751537	6	-4.121693	-2.390318	-0.163215
6	-2.658611	0.823069	0.657560	6	-6.543773	-1.028133	-0.396310
6	-3.534343	1.126638	1.845383	1	-5.363319	0.779893	-0.335395
1	-3.992198	2.122925	1.766212	6	-5.314062	-3.096616	-0.289088
1	-4.324202	0.380423	1.981552	1	-3.166562	-2.910537	-0.062532
1	-2.905276	1.118087	2.748539	6	-6.530679	-2.422389	-0.396339
8	0.672707	0.545402	-0.468853	1	-7.488836	-0.489732	-0.496228
6	-0.190929	3.432471	0.614556	1	-5.291044	-4.188578	-0.292474
6	0.584975	4.602185	0.932839	1	-7.464658	-2.980316	-0.487021

1	-1.530349	2.971084	2.262085	1	0.978851	5.686809	-1.561856
N,O-A9				6	-1.711597	1.528788	-2.250392
15	1.042001	-0.221214	-0.238197	1	-0.743872	1.066917	-2.502395
6	2.751486	-0.825441	-0.098950	1	-2.484538	0.759472	-2.366096
6	3.782339	0.109130	-0.157607	1	-1.929965	2.337856	-2.964690
6	3.069549	-2.181459	0.063643	8	6.678902	-2.127153	0.238244
6	5.118156	-0.285744	-0.050383	6	7.761313	-1.241330	0.182365
1	3.528096	1.162394	-0.296477	1	7.811295	-0.713909	-0.786497
6	4.388877	-2.585383	0.174666	1	7.721978	-0.491624	0.992078
1	2.267768	-2.923159	0.092660	1	8.669875	-1.844112	0.303183
6	5.425356	-1.638846	0.120120	16	-0.011435	-1.479654	-1.403223
1	5.901739	0.470178	-0.103757	16	0.229779	-0.567413	1.751018
1	4.653408	-3.636466	0.301801	7	-2.783911	-0.672999	-0.205885
6	-1.993549	2.549467	1.363105	1	-1.878656	-0.734455	-0.761513
1	0.746729	0.570040	2.262444	6	-3.492143	-1.908207	-0.145171
6	-2.266229	1.595711	0.336030	6	-4.853633	-1.956304	-0.452957
6	-1.678885	2.048764	-0.858063	6	-2.790466	-3.070250	0.179212
6	-2.990087	0.374176	0.552285	6	-5.524781	-3.175182	-0.404528
6	-3.907839	0.299540	1.731351	1	-5.378184	-1.040440	-0.734417
1	-4.562813	1.178829	1.773619	6	-3.470692	-4.285378	0.214257
1	-4.501852	-0.618760	1.756993	1	-1.719642	-3.006167	0.380322
1	-3.263811	0.314557	2.625663	6	-4.834696	-4.340325	-0.069614
8	1.056476	1.256145	-0.525898	1	-6.590174	-3.215936	-0.639732
6	-1.213723	3.531732	0.798298	1	-2.926284	-5.197308	0.466668
6	-0.595224	4.716500	1.297645	1	-5.361405	-5.296127	-0.037530
7	-1.048708	3.214840	-0.558390	1	-2.279283	2.495936	2.409513
6	0.156093	5.489738	0.467241	N,O-A10			
1	-0.737164	4.970186	2.348921	15	1.114303	-0.007919	-0.150396
6	-0.244359	3.976472	-1.382116	6	2.813902	-0.624507	-0.068678
6	0.341069	5.099440	-0.901382	6	3.837010	0.308736	-0.227568
1	0.636609	6.396181	0.838555	6	3.141638	-1.968382	0.163785
1	-0.094912	3.601896	-2.392382	6	5.175580	-0.077369	-0.153613

1	3.575757	1.352390	-0.416643	1	7.838228	-0.531744	-0.961799
6	4.466667	-2.361817	0.241284	1	7.820505	-0.224464	0.807134
1	2.349088	-2.712848	0.272834	1	8.744017	-1.606964	0.145271
6	5.495608	-1.418478	0.084694	16	0.081794	-1.426493	-1.234677
1	5.952923	0.675228	-0.284852	16	0.387023	-0.165498	1.870140
1	4.740467	-3.402902	0.418972	7	-2.644325	-0.902937	-0.243560
6	-2.306753	2.383860	1.321049	1	-1.336558	-1.009227	-0.768952
1	0.009037	1.131220	1.869372	6	-3.226526	-2.189611	-0.159148
6	-2.435968	1.413351	0.286119	6	-4.439484	-2.463604	-0.799434
6	-1.859263	1.927847	-0.878426	6	-2.542398	-3.208566	0.510481
6	-3.047065	0.136	0.462876	6	-4.976800	-3.747225	-0.746049
6	-4.086093	-0.025450	1.542173	1	-4.953722	-1.662955	-1.335733
1	-4.595308	-0.994911	1.526668	6	-3.086975	-4.490236	0.556054
1	-3.577416	0.080127	2.513667	1	-1.589086	-2.980355	0.990250
1	-4.821836	0.786353	1.466542	6	-4.303746	-4.763449	-0.067817
8	1.062986	1.420532	-0.602990	1	-5.927111	-3.954883	-1.242532
6	-1.618066	3.456091	0.786577	1	-2.552826	-5.282774	1.084494
6	-1.152622	4.698860	1.304850	1	-4.727053	-5.769091	-0.028777
7	-1.365430	3.161360	-0.559402	1	-2.644535	2.301852	2.350696
6	-0.460862	5.553984	0.499614	N,O-A11			
1	-1.357635	4.934070	2.350159	15	1.236202	0.021168	-0.220767
6	-0.632310	4.011657	-1.357468	6	2.915955	-0.614668	-0.062336
6	-0.190	5.193862	-0.860072	6	3.954256	0.223077	-0.466712
1	-0.095796	6.505963	0.888544	6	3.215816	-1.880138	0.465864
1	-0.419978	3.664180	-2.366414	6	5.283438	-0.182370	-0.351303
1	0.395066	5.851990	-1.502389	1	3.713444	1.205184	-0.879998
6	-1.772110	1.405887	-2.268691	6	4.531945	-2.288786	0.588721
1	-0.727379	1.164441	-2.519558	1	2.411430	-2.551424	0.777254
1	-2.360958	0.487758	-2.373029	6	5.577872	-1.442569	0.182089
1	-2.151071	2.146772	-2.991384	1	6.073817	0.492563	-0.678786
8	6.752389	-1.894981	0.176175	1	4.786882	-3.267402	0.997888
6	7.830444	-1.010801	0.032616	6	-2.404873	2.402378	1.324533

1	-0.439642	0.934141	1.519112	6	-3.418513	-2.135789	-0.165337
6	-2.550801	1.432211	0.292158	6	-4.617236	-2.430648	-0.827185
6	-1.911550	1.908166	-0.855021	6	-2.751676	-3.147934	0.537073
6	-3.214808	0.130577	0.457552	6	-5.150575	-3.716004	-0.766077
6	-4.266828	0.042478	1.533883	1	-5.123670	-1.641432	-1.387321
1	-4.786725	-0.922252	1.526989	6	-3.293983	-4.429582	0.593612
1	-3.784382	0.166795	2.516048	1	-1.807954	-2.913007	1.034015
1	-4.996711	0.857087	1.425073	6	-4.494140	-4.720238	-0.055077
8	1.153227	1.353595	-0.892478	1	-6.088954	-3.933711	-1.281244
6	-1.652738	3.442528	0.804336	1	-2.769557	-5.210348	1.149192
6	-1.152396	4.667776	1.327382	1	-4.915313	-5.726462	-0.009373
7	-1.366060	3.121802	-0.527989	1	-2.785942	2.349669	2.341066
6	-0.403317	5.488637	0.536024	N,O-A12			
1	-1.378658	4.919984	2.364271	15	1.106312	0.153713	0.663547
6	-0.581884	3.937416	-1.312618	6	2.790217	-0.432590	0.412118
6	-0.109322	5.107432	-0.811644	6	3.658565	0.367324	-0.333329
1	-0.012302	6.428682	0.928766	6	3.252969	-1.649552	0.934675
1	-0.355193	3.571633	-2.311842	6	4.973843	-0.030367	-0.563538
1	0.515349	5.738808	-1.443520	1	3.295004	1.317830	-0.729887
6	-1.808408	1.369965	-2.239280	6	4.556553	-2.054410	0.709030
1	-0.762022	1.123598	-2.478315	1	2.578612	-2.270625	1.528670
1	-2.405878	0.456902	-2.333145	6	5.428700	-1.248699	-0.042754
1	-2.170825	2.106580	-2.975379	1	5.630486	0.616264	-1.145178
8	6.821990	-1.927194	0.341169	1	4.937695	-2.995046	1.109474
6	7.919247	-1.144105	-0.047681	6	-2.107143	2.204152	1.351387
1	7.898033	-0.920900	-1.128302	1	0.343716	-0.238	-2.184001
1	7.963607	-0.195028	0.513745	6	-2.406371	1.337221	0.270206
1	8.818277	-1.730593	0.176286	6	-2.051984	1.976628	-0.922109
16	0.238645	-1.557250	-1.190925	6	-2.942161	-0.016623	0.421819
16	0.561437	0.063717	1.794662	6	-3.733036	-0.307100	1.666397
7	-2.834923	-0.861121	-0.260887	1	-4.318441	-1.229892	1.576750
1	-1.029208	-1.114897	-0.875896	1	-3.014599	-0.435469	2.492658

1	-4.390797	0.534885	1.917735	6	-3.874525	-4.931731	-0.271646
8	0.931568	1.531757	0.128047	1	-5.512183	-4.338007	-1.548880
6	-1.542954	3.345053	0.814873	1	-2.146445	-5.217223	0.993020
6	-0.999153	4.537255	1.366356	1	-4.176854	-5.980290	-0.234621
7	-1.535372	3.193965	-0.578599	1	-2.213521	1.992271	2.411253
6	-0.496301	5.504145	0.545681	N,O-A13			
1	-0.993611	4.648758	2.451445	15	2.252970	-0.311363	0.059
6	-1.024666	4.171008	-1.403886	6	0.470387	-0.246430	0.187
6	-0.514455	5.311758	-0.872419	6	-0.225123	0.967400	-0.116
1	-0.073902	6.420152	0.961450	6	-0.247728	-1.457799	0.327
1	-1.050651	3.966727	-2.473358	6	-1.614959	0.987136	-0.333
1	-0.111839	6.072173	-1.542138	1	0.331623	1.907244	-0.257
6	-2.233909	1.596974	-2.350829	6	-1.628908	-1.445210	0.085
1	-1.270068	1.519420	-2.882309	1	0.297965	-2.403358	0.721
1	-2.734449	0.624759	-2.421283	6	-2.326275	-0.223223	-0.304
1	-2.842417	2.342801	-2.889649	1	-2.132009	1.946032	-0.551
8	6.675612	-1.723593	-0.206253	1	-2.205794	-2.371032	0.144
6	7.610776	-0.967125	-0.928388	8	2.769476	-1.699347	-0.143
1	7.293668	-0.815037	-1.974426	8	-3.661125	-0.310474	-0.781
1	7.787324	0.016597	-0.460425	6	-4.436775	0.862771	0.655
1	8.547621	-1.536853	-0.920926	1	-4.246574	1.471815	0.900148
16	0.163679	-0.694444	2.123813	1	-4.248424	1.472794	-0.898566
16	0.212994	-1.119877	-1.445801	1	-5.484946	0.542378	0.001493
7	-2.663466	-0.907543	-0.465462	16	3.192693	1.344705	0.023
1	-1.172191	-0.896279	-1.118224	N,O-A14			
6	-3.102383	-2.244802	-0.362806	6	4.318757	0.672768	0.549301
6	-4.235973	-2.673915	-1.061568	6	3.007812	0.295985	0.821227
6	-2.348110	-3.167670	0.371834	6	2.455768	-0.843743	0.229606
6	-4.621310	-4.011596	-1.007526	6	3.237891	-1.610693	-0.650214
1	-4.810300	-1.949527	-1.642894	6	4.542178	-1.244502	-0.923317
6	-2.738164	-4.504584	0.414270	6	5.095125	-0.097197	-0.328250
1	-1.463042	-2.819506	0.911326	1	4.721154	1.566358	1.025136

1	2.401279	0.898206	1.501049
1	2.807766	-2.499704	-1.116126
1	5.165970	-1.829512	-1.600446
8	6.365235	0.182217	-0.655797
6	6.989430	1.313836	-0.105382
1	8.984	1.347450	-0.526655
1	6.459284	2.242991	-0.374569
1	7.060798	1.243954	0.993366
15	0.755097	-1.302601	0.562906
15	-0.717118	1.269408	-0.482370
16	-0.118	-0.309251	2.010575
16	0.186949	-3.003177	-0.121978
16	-0.126303	3.047084	-0.177730
6	-2.437239	0.884799	-0.349828
6	-2.854727	-0.423412	-0.633898
6	-3.381814	1.849427	0.047111
6	-4.194349	-0.770818	-0.526144
1	-2.121749	-1.178159	-0.927144
6	-4.714999	1.509052	0.150939
1	-3.054727	2.866745	0.272828
6	-5.134352	0.195034	-0.133722
1	-4.492206	-1.795754	-0.743625
1	-5.466546	2.238095	0.455771
8	-6.443230	-0.040432	-0.003760
6	-6.951007	-1.327213	-0.263285
1	-6.520333	-2.077140	0.420667
1	-8.032886	-1.271210	-0.097689
1	-6.761710	-1.632839	-1.305683
8	0.080789	0.133712	-1.073399

N,O-A16

Acid

1	0.	-0.973735	-0.828280
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1	0.	0.973735	-0.828280
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16	0.	0.	0.103535
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Indolizine

6	5.128981	0.895505	-0.570
6	5.368585	-0.515622	-0.066
6	4.312860	-1.381334	0.357
6	2.980491	-0.883551	0.311
7	2.789383	0.507256	-0.156
6	3.858699	1.377955	-0.611
6	1.726257	-1.467199	0.647
6	0.765165	-0.420686	0.360
6	1.450481	0.799784	-0.114
6	0.976893	2.212235	-0.549
6	-0.698142	-0.626356	0.496
6	-1.164617	-2.063820	0.001252
1	5.960448	1.600801	-0.932
1	6.393171	-0.890623	-0.030
1	4.461109	-2.462317	0.747
1	3.618796	2.440411	-0.001015
1	1.540749	-2.537787	0.001040
1	-0.117813	2.218836	-0.056
1	1.334750	2.756360	0.889823
1	1.333862	2.755521	-0.891795
1	-0.773504	-2.586202	-0.884491
1	-0.772545	-2.585576	0.886934
1	-2.258292	-2.137879	0.001850
7	-1.485013	0.380974	0.036
6	-2.877677	0.254942	-0.065
6	-3.589396	0.228687	1.208005
6	-3.588945	0.225536	-1.208323
6	-4.980270	0.155930	1.202951
1	-3.036023	0.266837	2.148729

6	-4.979825	0.152821	-1.203612	6	2.913479	3.279251	-0.983534
1	-3.035221	0.261232	-2.148940	1	1.489593	1.705261	-1.289099
6	-5.684186	0.116365	-0.415	6	3.406480	4.250649	-0.099700
1	-5.519220	0.130534	2.153075	1	3.240363	5.141010	1.849968
1	-5.518405	0.124954	-2.153875	1	3.321511	3.169153	-1.987765
1	-6.774578	0.060126	-0.544	6	-3.053876	-0.014215	-1.043749
LR-Hexacycle Substituted				6	-3.853995	0.044008	-2.192383
15	0.131650	-1.506650	1.034386	6	-3.653510	-0.140169	0.213925
15	0.024047	1.455891	1.224303	6	-5.232593	-0.022136	-2.082678
15	-1.276146	0.068876	-1.151524	1	-3.383915	0.142661	-3.173600
8	0.790605	-0.003596	1.185630	6	-5.036296	-0.207730	0.330997
8	-0.798727	-1.244941	-0.296037	1	-3.043083	-0.187879	1.120391
8	-0.904988	1.288400	-0.123373	6	-5.835689	-0.148469	-0.821226
16	-0.820322	-2.188495	2.543900	1	-5.875133	0.021152	-2.963074
16	-0.458706	0.219246	-2.883826	1	-5.477454	-0.307584	1.321965
16	-0.956048	1.879185	2.807476	8	4.748493	-4.523314	-1.121040
6	1.510042	-2.442884	0.392144	8	-7.175928	-0.204808	-0.810455
6	2.075731	-3.461060	1.158858	8	4.399020	5.103817	-0.395352
6	2.044201	-2.151160	-0.875343	6	5.004809	5.046620	-1.661283
6	3.169379	-4.183565	0.687410	1	4.279707	5.247852	-2.467989
1	1.650880	-3.694915	2.137918	1	5.776051	5.825462	-1.673243
6	3.127568	-2.865141	-1.350467	1	5.481419	4.067803	-1.839983
1	1.594072	-1.376726	-1.502342	6	-7.852984	-0.327003	0.414434
6	3.702479	-3.886413	-0.573058	1	-7.586552	-1.262400	0.934978
1	3.591128	-4.973705	1.307841	1	-7.646464	0.527685	1.080576
1	3.552637	-2.662006	-2.334273	1	-8.923587	-0.344077	0.179067
6	1.326414	2.559475	0.697897	6	5.369606	-5.565623	-0.413690
6	1.816436	3.537414	1.575236	1	5.798888	-5.210752	0.538767
6	1.878601	2.442085	-0.581111	1	4.667621	-6.391428	-0.207750
6	2.846656	4.373889	1.181924	1	6.179094	-5.936902	-1.052952
1	1.375723	3.638210	2.569718				

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