Doctoral Dissertation

Computational Mechanistic Studies of C–H Bond Functionalization

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Table of contents

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Abbreviations

The following abbreviations are used throughout this report.

AcOH	acetic acid
ASA	activation strain analysis
ASM	activation strain model
α	alpha
AMLA	ambiphilic metal-ligand activation
Å	angstrom
β	beta
BX	benziodoxolone
BE	bromide elimination
cat.	catalytic
CMD	concerted metalation-deprotonation
CCSD(T)	coupled cluster single-double and triple
°C	degree(s) Celsius
Δ	delta
DFT	density functional theory
DCE	1,2-dichloroethane
DMAP	4-dimethylaminopyridine
BHT	3,5-di-*tert*-4-butylhydroxytoluene
DG	directing group
ECP	effective core potential
eV	electron volt
S_EAr	electrophilic aromatic substitution

EIE	equilibrium isotope effect
FAB-MS	fast atom bombardment mass spectrometry
FG	functional group
G09	Gaussian 09
GC	gas chromatography
GGA	generalized gradient approximation
HOMO	highest occupied molecular orbital
h	hours
IR	infrared spectroscopy
IRC	intrinsic reaction coordinate
I_2	iodine
^{i}Pr	isopropyl
kcal	kilocalorie
KIE	kinetic isotope effect
LSF	late-stage functionalization
LLHT	ligand-to-ligand hydrogen transfer
LDA	local density approximation
LUMO	lowest unoccupied molecular orbital
MS	mass spectrometry
OMe	methoxy
Me	methyl
MI	migratory insertion
MECP	minimum energy crossing point
mol	mole
MM	molecular mechanics
NBO	natural bond orbital

$Ni(OAc)_2$	nickel(II) acetate
$Ni(OTf)_2$	nickel(II) trifluoromethanesulfonate
NMR	nuclear magnetic resonance
OA	oxidative addition
Ph	phenyl
φ	phi
PCM	Polarizable Continuum Model
KO^tBu	potassium *tert*-butoxide
PES	potential energy surface
QM	quantum mechanics
Q	8-quinolyl
RE	reductive elimination
σBM	sigma-bond metathesis
SET	single electron transfer
SMD	Solvation Model based on Density
^{t}Bu	*tert*-butyl
^{t}BuOH	*tert*-butyl alcohol
TEMPO	(2,2,6,6-tetramethylpiperidin-1-yl)oxyl
PhMe	toluene
TS	transition state
CF_3	trifluoromethyl
TIPS	triisopropylsilyl
TMS	trimethylsilyl
PPh_3	triphenylphosphine

List of Publications

[1] Yamazaki, K.; Obata, A.; Sasagawa, A.; Ano, Y.; Chatani, N. Computational Mechanistic Study on the Nickel-Catalyzed C-H/N-H Oxidative Annulation of Aromatic Amides with Alkynes: The Role of the Nickel(0) Ate Complex. *Organometallics* **2019**, *38*, 248.

[2] Yamazaki, K.; Kommagalla, Y.; Ano, Y.; Chatani, N. A Computational Study of Cobalt-Catalyzed C-H Iodination Reactions Using a Bidentate Directing Group with Molecular Iodine. *Org. Chem. Front.* **2019**, 6, 537.

[3] Yamazaki, K.; Rej, S.; Ano, Y.; Chatani, N. Mechanism and Origins of Regiochemical Control in Rh(III)-Catalyzed Oxidative C–H Alkenylation and Coupling Sequence of Unprotected 1-Naphthylamines with *α,β*-Unsaturated Esters. *Organometallics* **2021**, *40*, 1371.

[4] Yamazaki, K.; Rej, S.; Ano, Y.; Chatani, N. An Unusual Perpendicular Metallacycle Intermediate is the Origin of Branch Selectivity in the Rh(II)-Catalyzed C–H Alkylation of Aryl Sulfonamides with Vinylsilanes. *Organometallics* **2021**, *40*, 3935.

[5] Yamazaki, K.; Rej, S.; Ano, Y.; Chatani, N. Origin of the Enhanced Reactivity in the ortho C–H Borylation of Benzaldehydes with BBr_3. *Org. Lett.* **2022**, *24*, 213.

[6] Yamazaki, K.; Mahato, S. K.; Ano, Y.; Chatani, N. Double 1,2-Migration of Bromine and Silicon in Directed C–H Alkynylation Reactions with Silyl-Substituted Alkynyl Bromides through an Iridium Vinylidene Intermediate. *Organometallics* **2022**, *41*, 20.

Supplementary Publications

[1] Kommagalla, Y.; Yamazaki, K.; Yamaguchi, T.; Chatani, N. Cobalt(II)-Catalyzed Chelation-Assisted C-H Iodination of Aromatic Amides with I_2. *Chem. Commun.* **2018**, *54*, 1359.

[2] Obata, A.; Sasagawa, A.; Yamazaki, K.; Ano, Y.; Chatani, N. Nickel-Catalyzed Oxidative C-H/N-H Annulation of *N*-Heteroaromatic Compounds with Alkynes. *Chem. Sci.* **2019**, *10*, 3242.

[3] Yamaguchi, T.; Natsui, S.; Shibata, K.; Yamazaki, K.; Rej, S.; Ano, Y.; Chatani, N. Rhodium-Catalyzed Alkylation of C-H Bonds in Aromatic Amides with Non-activated 1-Alkenes: The Possible Generation of Carbene Intermediates from Alkenes. *Chem. Eur. J.* **2019**, *25*, 6915.

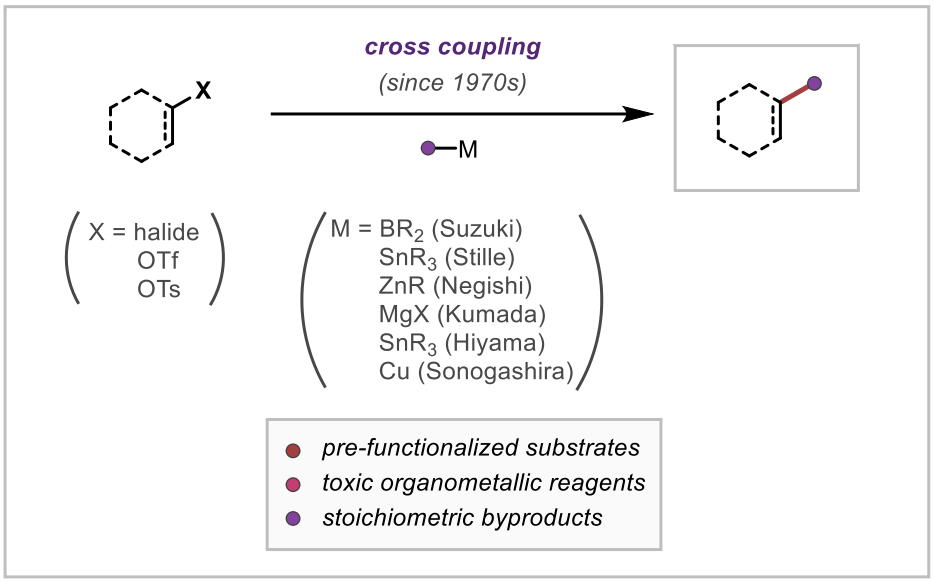
[4] Iyori, Y.; Takahashi, K.; Yamazaki, K.; Ano, Y.; Chatani, N. Nickel-Catalyzed Reductive Defunctionalization of Esters in the absence of an External Reductant: Activation of C-O Bonds. *Chem. Commun.* **2019**, *55*, 13610.

[5] Khake, S. M.; Yamazaki, K.; Ano, Y.; Chatani, N. Iridium(III)-Catalyzed Branch-Selective C-H Alkenylation of Aniline Derivatives with Alkenes. *ACS Catal.* **2021**, *11*, 5463.

[6] He, Q.; Yamazaki, K.; Ano, Y.; Chatani, N. Palladium-Catalyzed Site-Selective [5+1] Annulation of Aromatic Amides with Alkenes: Acceleration of β-Hydride Elimination by Maleic Anhydride from Six-Membered Palladacycle. *ACS Catal.* **2022**, *12*, 1595.

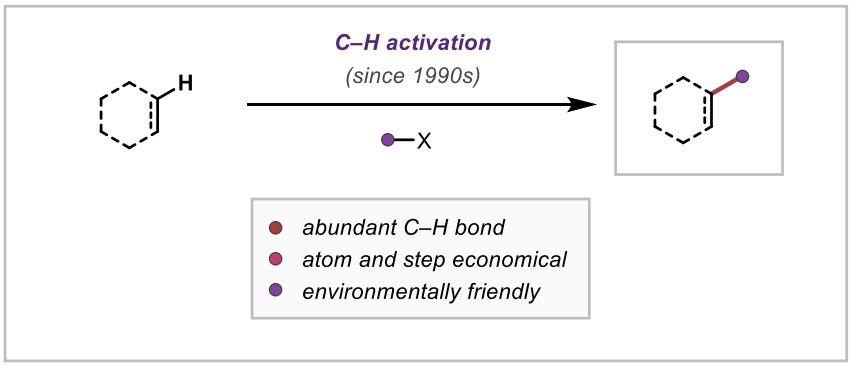
General Introduction

The discovery that transition metals can function as active catalysts in molecular synthesis is one of the greatest findings of the 20th century and has allowed tremendous progress to be made in academic and industrial design as well and producing engineered functional molecules.[1] Since Bury first used the term "transition metal" in 1921, the field of organic synthesis research has been thriving for over a century by continuously expanding our capabilities to achieve complex molecular transformations.[2] Transition metals usually have partially filled *d* orbitals, and the small energy gaps between these orbitals confer unique characteristic properties and reactivity to these metals. The major use of transition metal catalysis is for the cross-coupling reactions between organic electrophiles and organometallic nucleophiles for the construction of C–C bonds (Scheme 1).[3-7] The foundations of cross-coupling reactions were laid in the 1970s by several research groups. Representative examples among them include the Suzuki-Miyaura reaction that utilizes organoborane reagents, the Negishi reaction that utilizes organozinc reagents, and the Heck reaction that affords *trans*-substituted alkenes. These remarkable discoveries were recognized when the Nobel Prize in Chemistry was awarded for the development of Pd-catalyzed cross-coupling reactions in 2010.[8-10] The extensive development and applications of these methods are now fully acknowledged as a successful research field that has accelerated progress in a wide range of basic science.



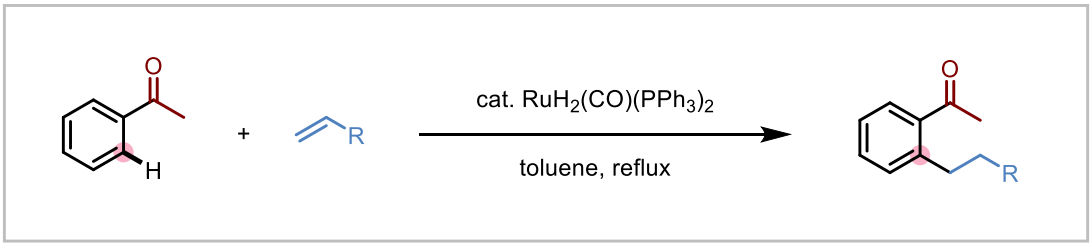
Scheme 1. Cross-coupling reactions.

While these cross-coupling reactions are generally highly reliable and reproducible, the pre-functionalization of substrates is required and the generation of undesired stoichiometric amounts of byproducts is unavoidable. Furthermore, even though it is well known that several transition metals have catalytic activities for a wide range of cross-coupling reactions, the use of rare and expensive palladium salts dominates the choice of a catalyst, which potentially limits industrial applications.



Scheme 2. Catalytic C–H activation.

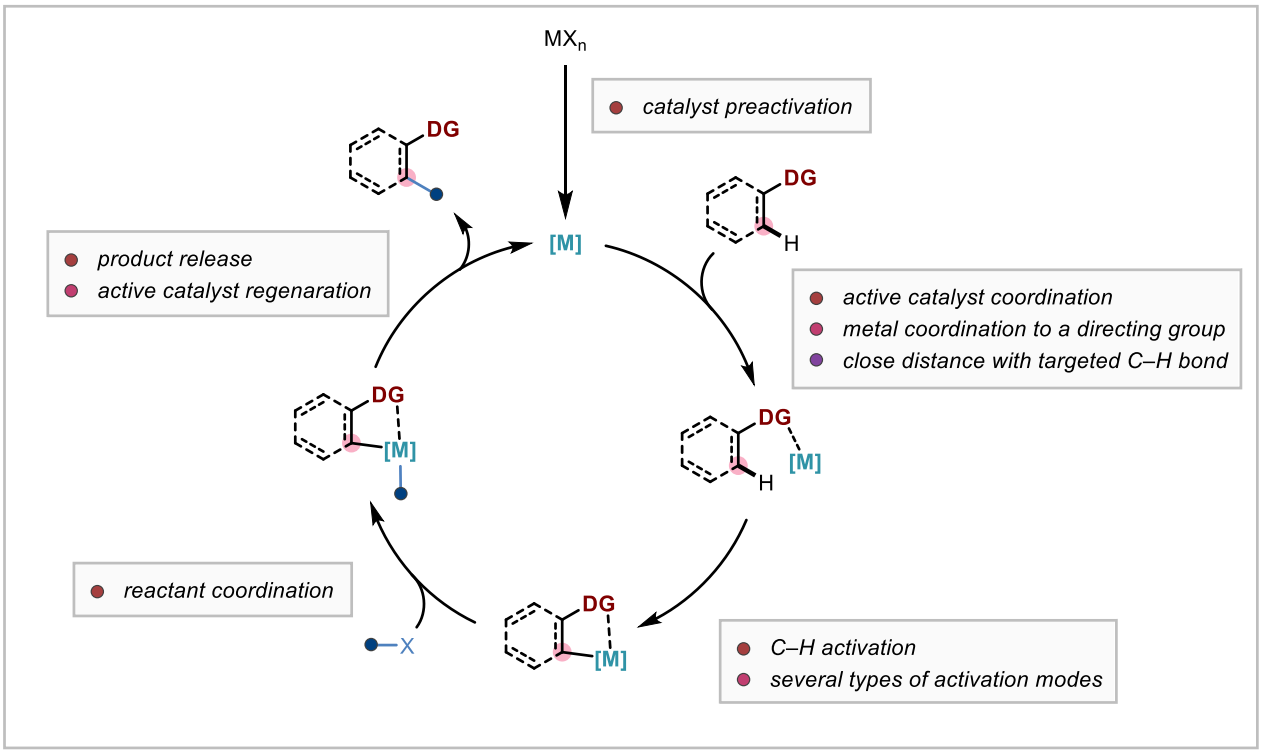
In contrast, the direct functionalization of naturally abundant and thermodynamically stable C–H bonds enables atom- and step-economic transformations in organic synthesis (Scheme 2).[11-13] Since the first example of the ruthenium-catalyzed C–H alkylation of aromatic ketones by Murai in 1993,[14] a large number of C–H activation reactions have subsequently been developed (Scheme 3).[15-17] In this reaction, the ketone functions as a directing group that initially coordinates to the transition metal, and the C–H bond adjacent to the metal center is then activated by an oxidative addition mechanism. The most common strategy for selective C–H functionalization involves the use of a suitable directing group, and the C–H bonds can be converted to new C–C or C–heteroatom bonds for use in the construction of complex molecules.[18-21]



Scheme 3. The Murai reaction.

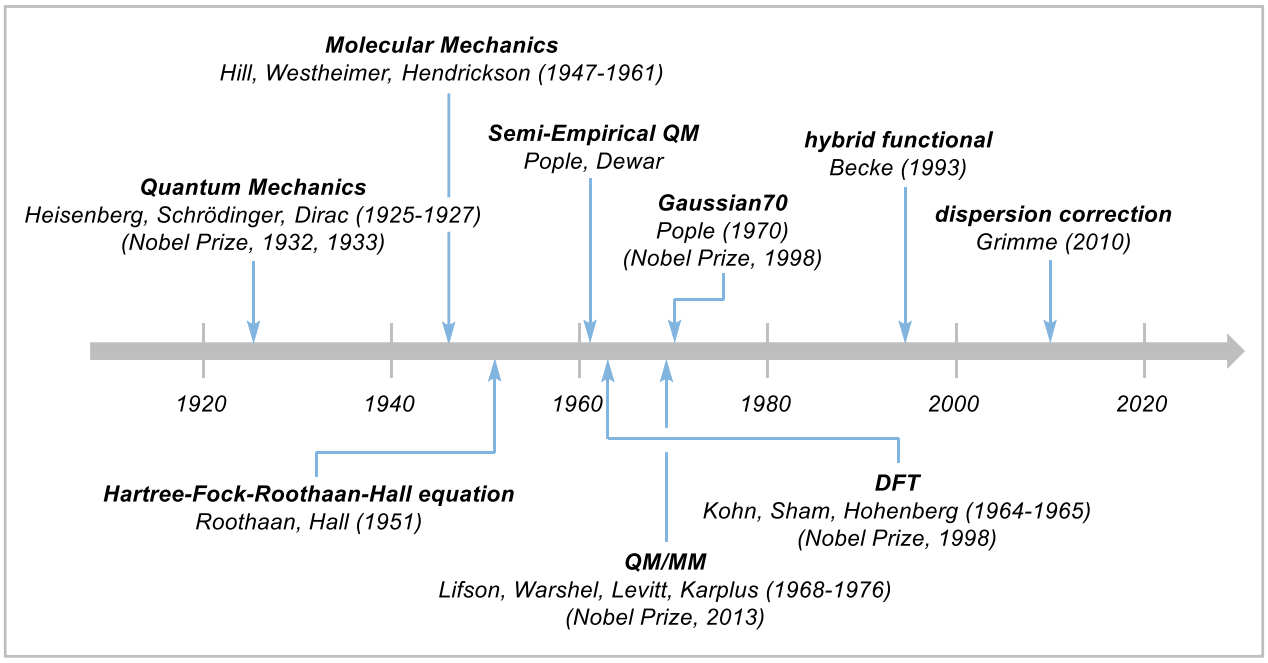
One of the major efforts driving the development of novel C–H activation reactions is the discovery of an appropriate transition metal catalysis and directing groups that are suitable for the selective targeting of a particular C–H bond. The major goal for C–H activation is to selectively convert any C–H bond in a complex molecule into a desired functional group. In order to accomplish this, fully understanding the reaction mechanisms that are responsible is crucial.

The generally accepted catalytic cycle for C–H activation reactions is shown in Scheme 4.[18,22] Initially, a transition metal catalyst is activated to initiate the catalytic cycle. The activated catalyst is then coordinated to the substrate, in which the targeted C–H bond is positioned in relatively close proximity to the metal center. There are several types of C–H activation mechanisms (oxidative addition (OA), electrophilic aromatic substitution (S_EAr), σ-bond metathesis (σBM), single electron transfer (SET), concerted metalation-deprotonation (CMD), etc.). After the C–H activation, which proceeds through any of the above mechanisms, a cyclic metallacycle is obtained. After C–H activation, the generated metallacycle reacts with a reactant, the final product is then released and the active catalyst is regenerated to initiate another catalytic cycle. Since monitoring such chemical reactions is often difficult, especially when multiple steps are involved in the catalytic cycle or a transition metal catalysis is used, computational methods, in conjunction with experimental mechanistic studies, are frequently used to gain insights into reaction mechanisms.[23,24]



Scheme 4. General mechanism for directed C–H activation.

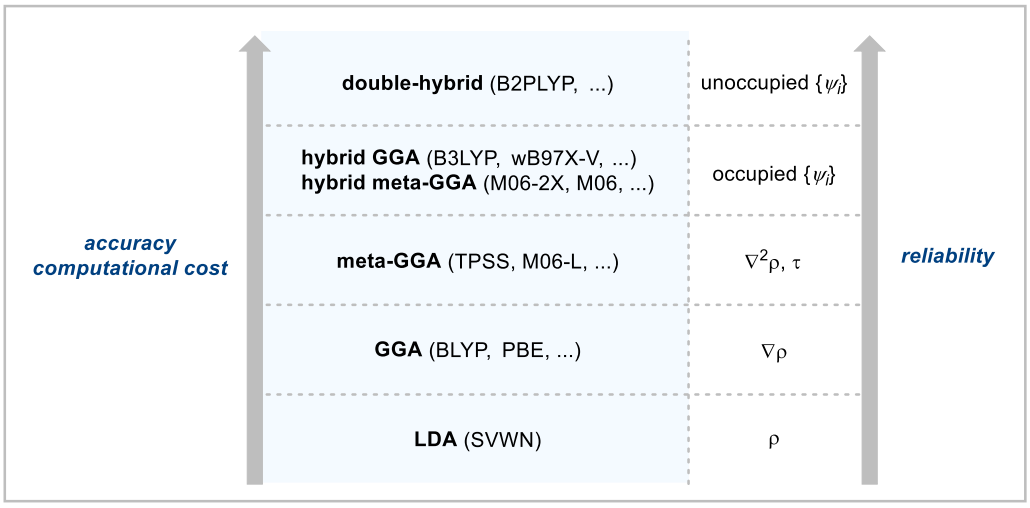
Tremendous advances have been made in computational organic chemistry since the late 1960s along with the development of computational resources and, like the commonly used nuclear magnetic resonance (NMR) spectroscopy, mass spectrometry (MS), and infrared (IR) spectroscopy it has become an essential research tool (Scheme 5).[25-29] The computational modeling of chemical reactions has contributed in a wide variety of research areas, and such computations are carried out not only by theoretical chemists, but also by experimental chemists in order to rationalize their observations.[30-32] All of the discoveries of mathematical theories, evolution of algorithms and computer programs, and benchmark studies for the demonstration of accuracy have enabled outstanding improvements to be made in computational chemistry.



Scheme 5. Milestones in computational organic chemistry.

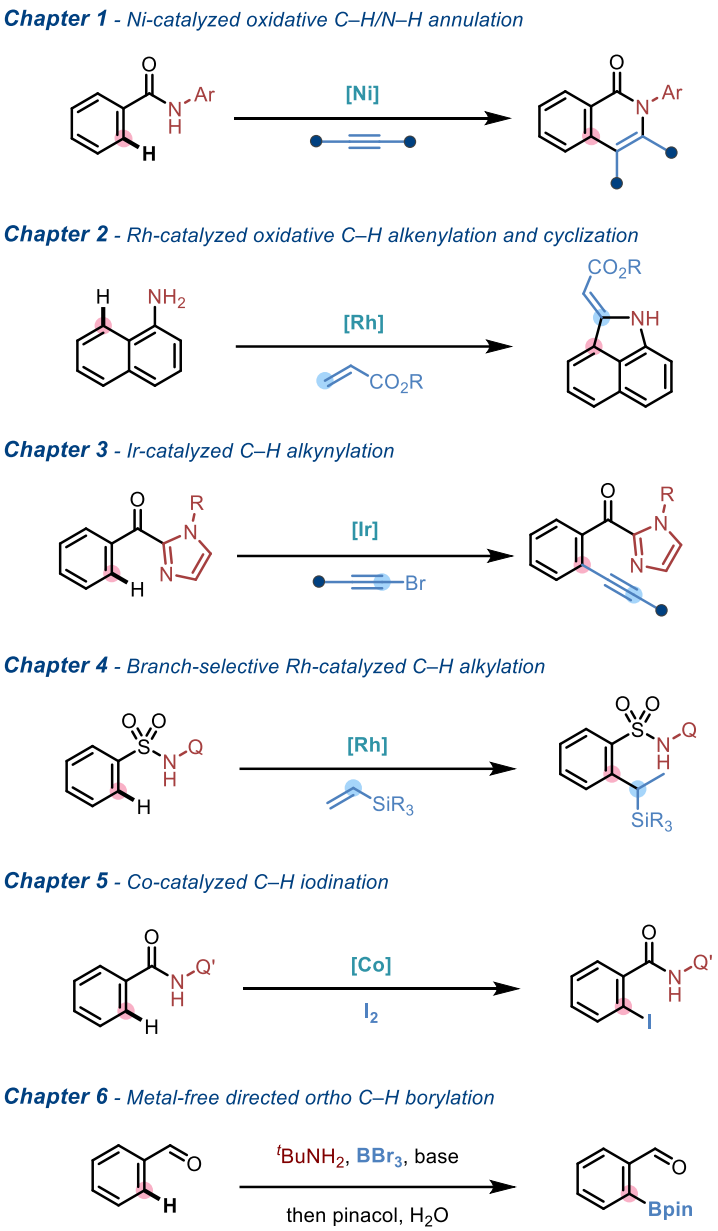
In quantum chemistry, it is well known that a coupled cluster method such as the coupled-cluster singles and doubles plus perturbative triples CCSD(T) method is the gold-standard for obtaining accurate molecular properties.[33,34] However, the application of such methodologies to a complex catalytic system is not practical since the computational cost is extremely high. On the other hand, density functional theory (DFT) methods have been significantly advanced in the last few decades with a low computational cost and high accuracy, and the use of these methods in mechanistic investigations of catalytic cycles has now become more accurate and useful for designing selective C–H activation reactions.[24,35-55] DFT-based computational methods were originally developed by Kohn, who was awarded the Nobel Prize in Chemistry in 1998 “for his development of the density-functional theory”, together with Pople “for his development of computational methods in quantum chemistry”, who initially established the popular Gaussian programs. The systematic organization of several DFT approximations was proposed by Perdew, and this is now known

as the "Jacob's ladder of DFT" (Scheme 6).[56] The higher rung of the ladder leads to high accuracy (±1 kcal mol^{-1}), but this requires increased computational costs. The hybrid functionals B3LYP, PBE0, and M06 have been the most successful functionals with a high accuracy and relatively low computational cost, and are frequently utilized in the field of organic and organometallic chemistry. DFT calculations are especially useful in providing insights into the nature of short-lived intermediates and rate-determining transition states. The objective of computational analyses of such reactions is to be able to design novel reactions that are more selective and efficient. Therefore, detailed computational studies of unique reactions where the mechanism is not yet fully understood will shed light on opportunities for the development of future novel reactions.



Scheme 6. Jacob's ladder of density functional theory methods.

In this thesis, six examples of computational studies of C–H activations are discussed (Scheme 7). In Chapter 1, the nickel-catalyzed oxidative C−H/N−H annulation of aromatic amides and *N*-heterocycles with alkynes is described. In Chapter 2, the rhodium-catalyzed oxidative C–H alkenylation and coupling sequence of unprotected 1-naphthylamines with *a,β*-unsaturated esters is described. In Chapter 3, the iridium-catalyzed C–H alkynylation of 2-acylimidazoles with alkynyl bromides is described. In Chapter 4, the dimeric rhodium-catalyzed branch-selective C–H alkylation of aryl sulfonamides with vinylsilanes is described. In Chapter 5, the cobalt-catalyzed C–H iodination with molecular iodine using the 8-aminoquinoline directing group is described. In Chapter 6, the metal-free directed *ortho* C–H borylation of benzaldehydes using an imine transient directing group is described. The aim of this thesis is to demonstrate that computational data as a powerful tool for understanding unique reactivities and has potential applications for the development of reactions in the future.



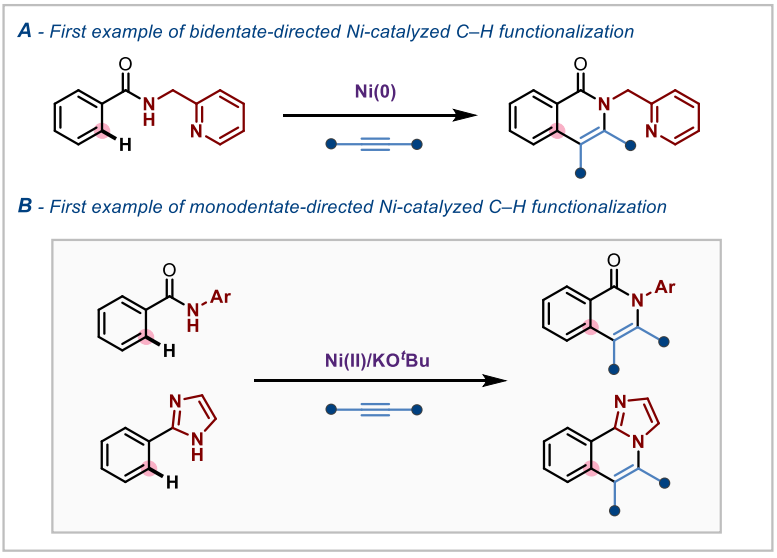
Scheme 7. Computational studies of C–H activation reactions in this thesis.

Chapter 1

Nickel-Catalyzed Oxidative C–H/N–H Annulation

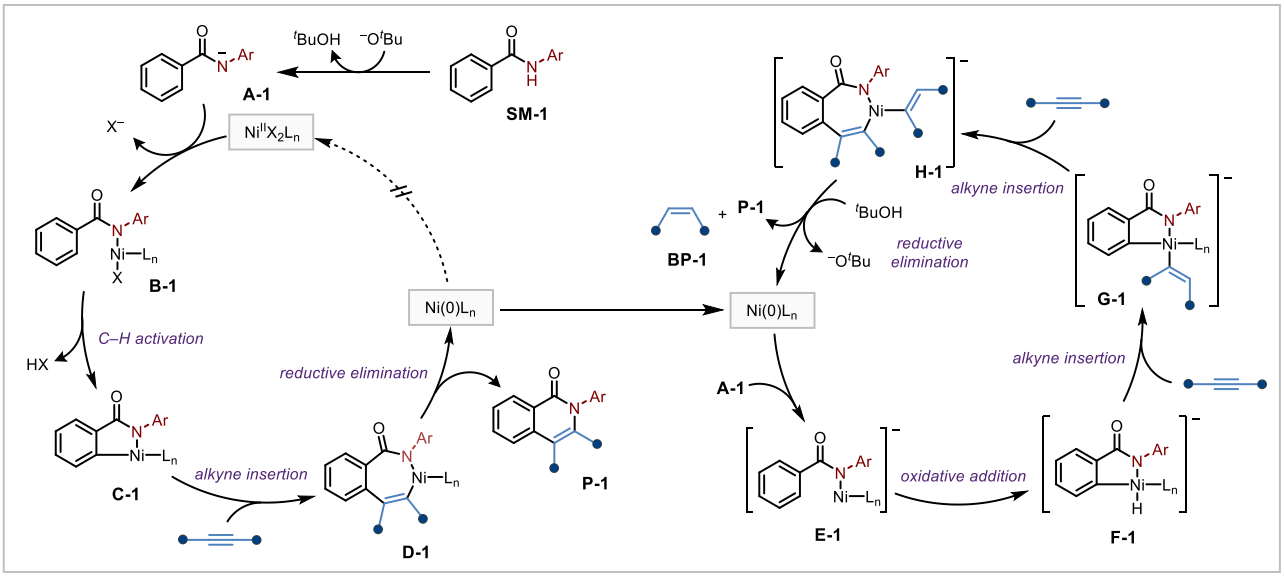
1.1. Introduction

A large effort has been made in the field of metal-catalyzed C−H functionalization, and it is now routinely used for various applications such as drug discovery and total synthesis of natural products.[57-62] A broad range of transition metal complexes are applicable for C−H functionalization, and rare and expensive second- and third-row transition metals such as Pd, Ru, Rh, and Ir are usually more reactive towards substrates with a simple weakly coordinating directing group.[63-65] However, the use of these precious metals limits the application for bulk synthesis on an industrial scale. In order to address this drawback, first-row transition metal complexes have been attracting attention as an alternative to second- and third-row transition metals.[66-77] Nickel and palladium have the same number of d-electrons, which allows Ni catalysts to be chosen as a replacement for Pd catalysts. Nickel-catalyzed C−H functionalization reactions have been reported over the past decade and have exhibited unique reactivity.[78-80] However, a large number of examples with nickel catalysts focus on transformations of a highly acidic C−H bond or require a bidentate directing group, which sometimes suffer from harsh installation/removal reaction conditions.[81,82] To overcome this limitation, the Chatani group has utilized amides and *N*-heterocycles as monodentate directing groups for nickel-catalyzed oxidative C−H/N−H annulation with alkynes (Scheme 1.1).[83,84] The use of a catalytic amount of KO^{t}Bu as a base was key to the success of the reaction.



Scheme 1.1. Bidentate- and monodentate-directed nickel-catalyzed C−H functionalization.

In the oxidative C−H/N−H annulation reaction of aromatic amides, a reaction mechanism that involves two reaction paths was initially proposed (Scheme 1.2). The initial path starts from the anion exchange with an amide on a Ni(II) center. Then the *ortho* C−H bond is cleaved through a concerted metalation-deprotonation (CMD) mechanism to generate a five-membered metallacycle **C-1**. An alkyne inserts into this metallacycle by migratory insertion, and a final reductive elimination step furnishes the cyclized product **P-1** and a Ni(0) species. Since an oxidant was not employed in this reaction, this Ni(0) initiates another catalytic cycle. The amidate anion **A-1** coordinates to the Ni(0) species and forms a nickelate complex **E-1**, which can facilitate the following oxidative addition to C−H bonds. The subsequent double migratory insertion of two alkyne molecules into the Ni−H and Ni−C bonds leads to the formation of a seven-membered metallacycle **H-1**, and the final reductive elimination furnishes the product with regeneration of the Ni(0) species. In an attempt to validate this proposed mechanism and to understand the factors that determine the mechanism of monodentate-directed nickel-catalyzed C−H activation systems, a detailed computational study on the nickel-catalyzed oxidative C−H/N−H annulation of aromatic amides and *N*-heterocycles with alkynes was performed.



Scheme 1.2. Initially proposed mechanism for the nickel-catalyzed oxidative C−H/N−H annulation of aromatic amides.

1.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional[86,87] with the 6-31+G(d) basis set for C, H, O, N, P, and F and the Lanl2dz effective core potential (ECP) for Ni.[88-90] Single

point energy calculations were performed using the B3PW91 functional[86,91] with the 6-311+G(2d,p) basis set for C, H, O, N, P, and F and the SDD ECP for Ni.[92-94] The polarizable continuum model (PCM) solvent effects were incorporated for all calculations with toluene as the solvent.[95-97] Each reported minimum has zero imaginary frequency, and each transition state (TS) has only one imaginary frequency. From the TSs, the reaction paths were traced by the intrinsic reaction coordinate (IRC) method to obtain the energy-minimum geometries.[98,99] A Mulliken population analysis using the B3LYP functional with the STO-3G basis set for C, H, O, N, P, and F, and the Lanl2mb ECP for Ni was used to reveal the atomic charges.[100] Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using CYLview20.[101]

1.3. Results and Discussion

1.3.1. Initial Path

In this computational study, $Ni(OAc)_2$ was chosen as a catalyst instead of $Ni(OTf)_2$ for simplification, since the product was also obtained with $Ni(OAc)_2$ in moderate yield. Initially, the acidic amide N−H bond is deprotonated by *tert*-butoxide anion to give the **2a** (Figure 1.1). Since a catalytic amount of potassium *tert*-butoxide was used, 20 mol% of the aromatic amide is deprotonated instantly. This process is highly exergonic because of the p*K*a difference between the amide and *tert*-butoxide. Then, this anionic species and PPh_3 coordinate to $Ni(OAc)_2$ and the intermediate **Int1_1** is generated. The acetate ligand promotes the CMD process and gives the nickelacycle **Int2_1** through the transition state **TS1_1** ($\Delta G^{\ddagger}$ = 24.6 kcal mol^{-1}).[102-105] The dihedral angle around the cleaving C−H bond is far more strained (36° as opposed to the ideal angle of 90°), indicating there are severe geometric constraints on the substrate and the energy barrier of the CMD process is increased.[106] After ligand exchange, the migratory insertion of alkyne proceeds selectively into the Ni−C bond through the transition state **TS2_1** with a small energy barrier ($\Delta G^{\ddagger}$ = 5.8 kcal mol^{-1}). The migratory insertion into the Ni−N bond through **TS3_1** requires a significantly larger energy barrier due to the loss of stabilization from the negatively charged nitrogen atom. Finally, the reductive elimination proceeds through the transition state **TS4_1** ($\Delta G^{\ddagger}$ = 14.1 kcal mol^{-1}), and the residual deprotonated amide **2a** coordinates to the nickel(0) species to generate a stable nickelate species **Int5_1**. Since there is no oxidant in the reaction mixture, this anionic species initiates the main catalytic cycle.

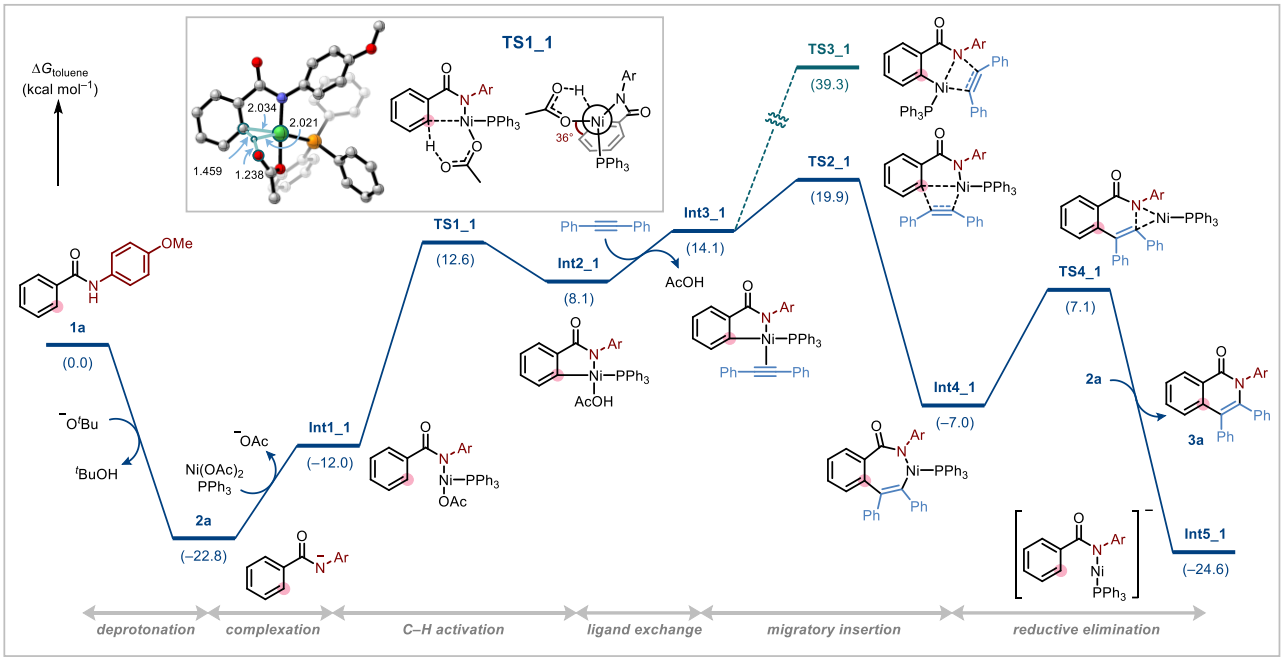


Figure 1.1. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the initial path. Ar = *p*-methoxyphenyl. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

1.3.2. Main Catalytic Cycle

To evaluate the role of nickelate complexes, the potential energy surface of the main catalytic cycle was computed from **Int5_1** (Figure 1.2). The initially proposed oxidative addition of the *ortho* C−H bond proceeds through **TS5_1** ($\Delta G^{\ddagger}$ = 13.1 kcal mol^{-1}), and the nickel hydride species **Int6_1** is generated. After ligand exchange, the migratory insertion of alkyne into the Ni−H bond is facile through the transition state **TS6_1** to furnish the stable intermediate **Int8_1** that has an interaction between nickel and hydrogen. During the migratory insertion process, the Ni−H bond is more reactive than the Ni−C bond (**TS6_1** vs. **TS7_1**).

An alternative pathway from **Int5_1** that involves the initial ligand exchange was also investigated. Interestingly, all our attempts to optimize the oxidative addition of Ni−H bond from the alkyne coordinated nickelate species **Int9_1** converged to the transition state **TS8_1**, which is a concerted process that involves both C−H bond cleavage and formation ($\Delta G^{\ddagger}$ = 20.5 kcal mol^{-1}). This process is also known as a ligand-to-ligand hydrogen transfer (LLHT), and a nickel hydride species is not formed during this process.[107,108] Surprisingly, the LLHT requires much lower energy than the previously mentioned oxidative addition-migratory insertion sequence, indicating the reaction proceeds through this mechanism. In addition, the coordination of the C−H bond to the nickel in the precursor **Int9_1** facilitates the LLHT, and the mechanism that involves this agostic interaction is known as an "ambiphilic metal-ligand activation (AMLA)".[109,110] This is the first example that computationally proves that the LLHT mechanism with Ni(0) and a non-acidic C−H bond is operative.

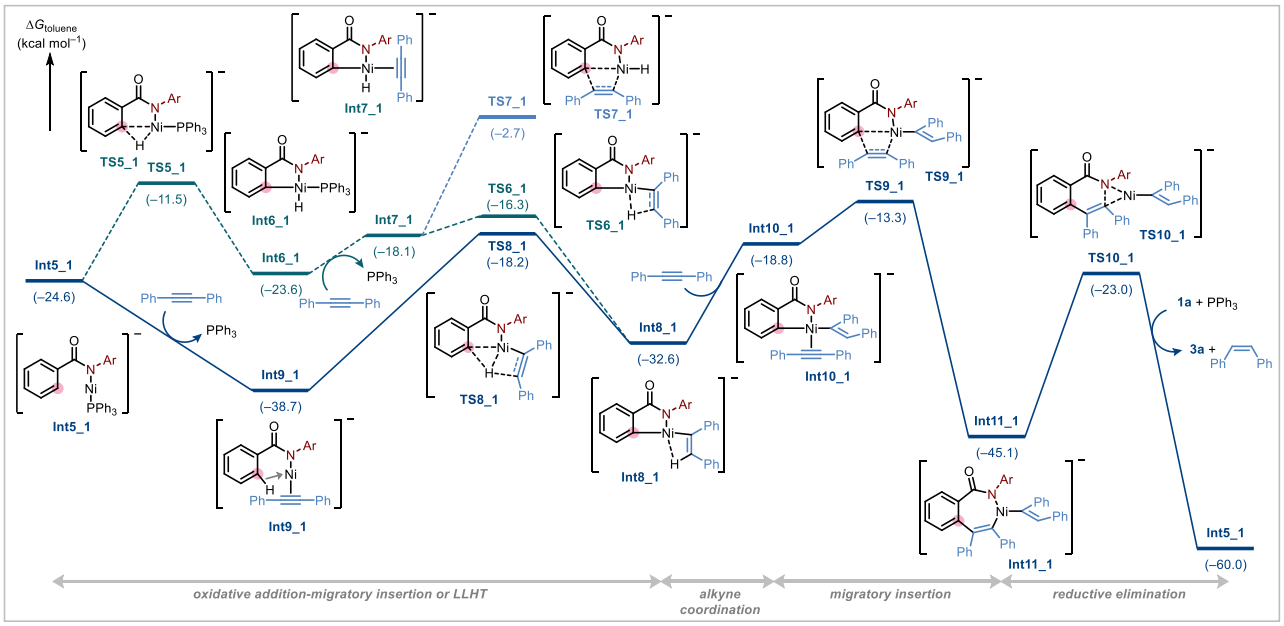


Figure 1.2. Computed reaction energy profile (Δ*G* [kcal mol^{-1}]) for the main catalytic cycle. Energies (kcal mol^{-1}) are provided in the insert.

Once the LLHT process is complete, another alkyne molecule coordinates for the next migratory insertion step. This process through the transition state **TS9_1** is highly exergonic and generates a seven-membered nickelacycle **Int11_1** (Δ*G* = 26.3 kcal mol^{-1}). The alkyne insertion into the Ni–N bond was not considered due to the selectivity shown in the initial path (**TS2_1** vs. **TS3_1**). Finally, the reductive elimination through **TS10_1** and the protonation with **1a** provide the product and *cis*-stilbene along with the regenerated active intermediate **Int5_1**. A mixture of *cis*- and *trans*-stilbene was experimentally detected by GC, and the isomerization is presumably due to the high temperature reaction conditions.[83] These results are consistent with the experimental results that only a catalytic amount of KO^{t}Bu (20 mol%) is required to promote both the initial path and the main catalytic cycle with 10 mol% of the nickel catalyst.

A C–H bond cleavage process from a neutral species was also considered (Figure 1.3). The coordination of neutral amide **1a** instead of the deprotonated form **2a** gave an unstable intermediate **Int12_1**. Moreover, the oxidative addition from **Int12_1** preferably takes place through the N–H bond cleaving transition state **TS12_1** (Δ$G^{‡}$ = 11.5 kcal mol^{-1}) than the C–H bond cleaving transition state **TS11_1** (Δ$G^{‡}$ = 12.1 kcal mol^{-1}). Overall, the formation of nickelate complexes is energetically favored and plays an important role during the C–H bond activation event.

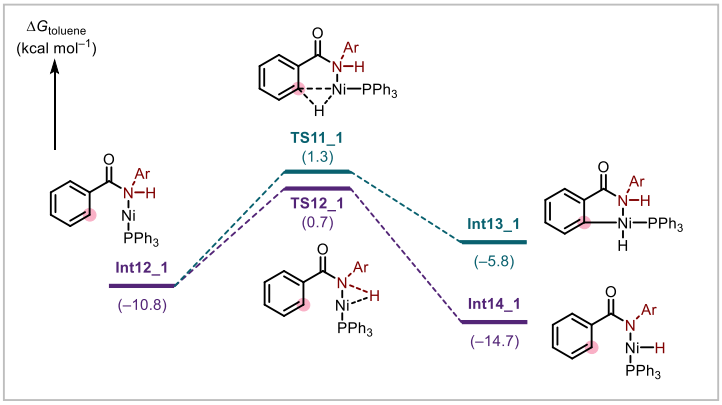


Figure 1.3. Computed reaction energy profile (Δ*G* [kcal mol^{-1}]) for the oxidative addition of neutral species. Energies (kcal mol^{-1}) are provided in the insert.

Another alternative pathway for the main catalytic cycle initiated from **Int5_1** was investigated (Figure 1.4). This mechanism involves the initial migratory insertion of alkyne into the Ni−N bond, and then the C−H bond is cleaved by an oxidative addition. The migratory insertion requires extremely high energy to overcome the energy of **TS13_1**, and the following oxidative addition TS also has an even higher energy. The results clearly indicate that this pathway is not involved, and the migratory insertion into the Ni−N bond is always unfavorable due to the loss of stabilizing interaction by the more negatively charged nitrogen atom. Therefore, the monodentate directed C−H activation could be achieved by the formation of nickelate species that can increase the negative charge of the nitrogen atom.

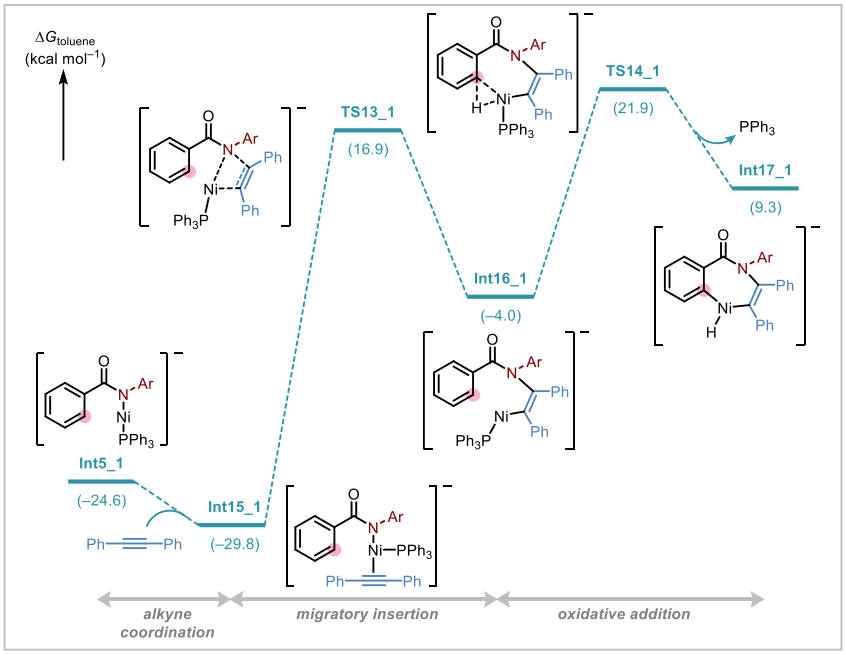
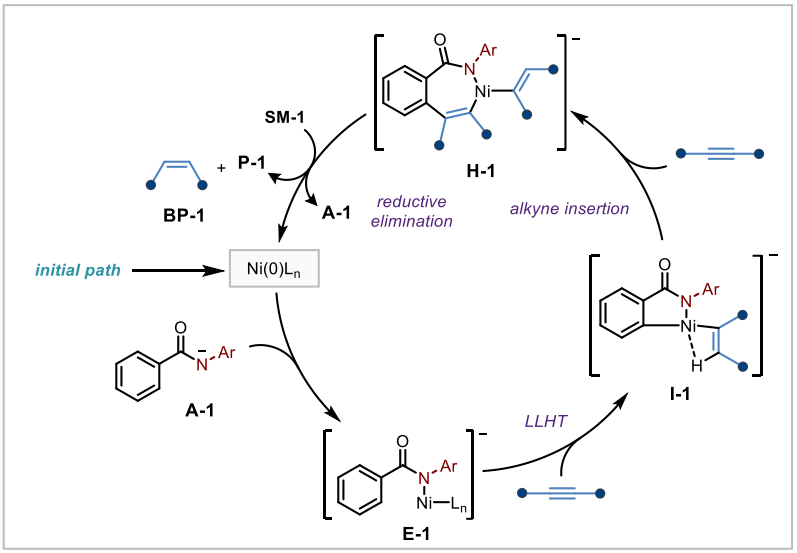


Figure 1.4. Computed reaction energy profile (Δ*G* [kcal mol^{-1}]) for the alternative pathway in the main catalytic cycle. Energies (kcal mol^{-1}) are provided in the insert.

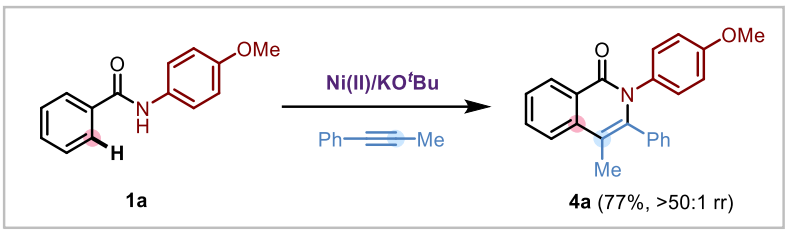
A summary of the revised catalytic cycle is shown in Scheme 1.3. The main catalytic cycle is initiated after Ni(II) species are reduced to Ni(0) in the initial path. The main features are as follows: (i) C−H bond activation by the LLHT mechanism, (ii) alkyne insertion into a five-membered nickelacycle **I-1**, and (iii) reductive elimination of C−N bond to generate the annulated product. The presence of a strong base promotes the reaction by forming nickelate complexes.



Scheme 1.3. Summary of the revised catalytic cycle of the nickel-catalyzed oxidative C−H/N−H annulation of benzamides.

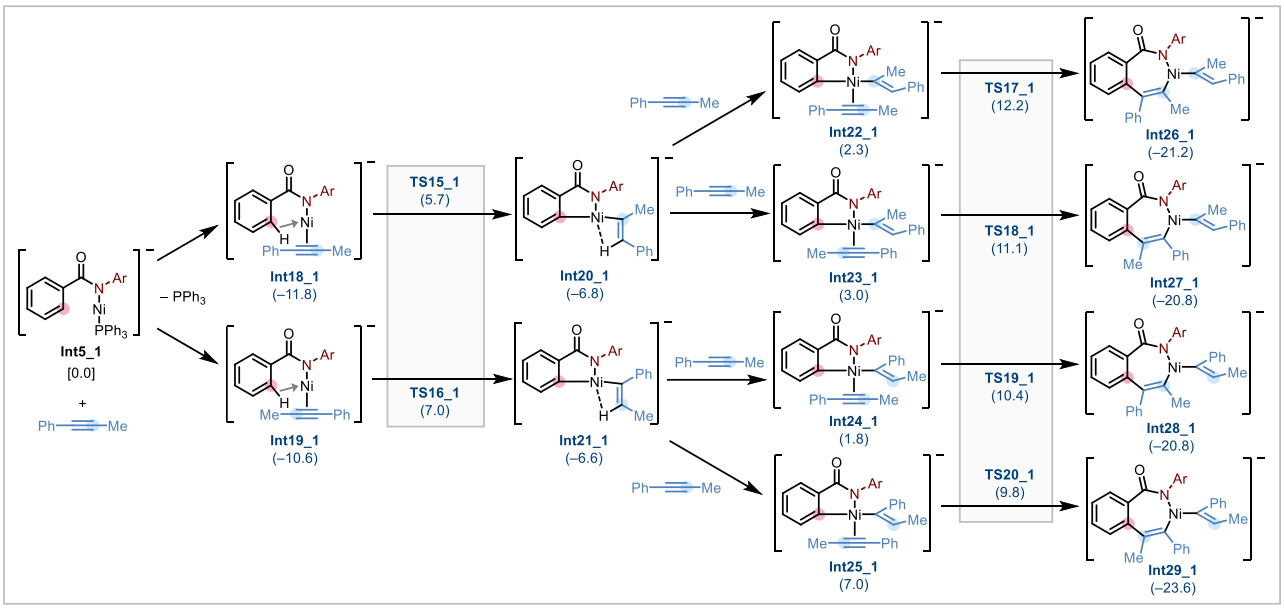
1.3.3. Rationalization of Regioselectivity with Asymmetric Alkynes

When an asymmetric alkyne such as 1-phenyl-1-propyne was used under the reaction condition, very high regioselectivity was observed (Scheme 1.4).[83] The newly formed C−C bond in the major product **4a** is between the *ortho*-carbon atom of the substrate and the alkyne carbon next to the Ph ring.



Scheme 1.4. Regioselectivity with asymmetric alkynes.

In order to reveal the origin of the regioselectivity, processes involving the alkynes in the main catalytic cycle were computed (Scheme 1.5). The first process is the LLHT for the formation of nickelacycle, and the second process is the migratory insertion that ultimately determines the regioselectivity. The LLHT step preferably proceeds through **TS15_1** that forms a bond between the nickel and the carbon next to the methyl group ($\Delta\Delta G^{\ddagger}$ = 1.3 kcal mol^{-1}). The transition state **TS15_1** is favored because of the presence of a stabilizing CH–π interaction between the methyl group and the *para*-methoxyphenyl group (Figure 1.5). There are four possible transition states for the following regioselectivity-determining migratory insertion step (Figure 1.6). All of them have higher energies than the LLHT step, and the migratory insertion step is the rate-determining step with 1-phenyl-1-propyne. The most preferred transition state was **TS20_1**, and the regioselectivity is consistent with the experimental results. In addition, the relatively destabilized intermediate **Int29_1** compared to the regioisomers, with steric repulsion between aromatic rings, decreases the activation energy barrier to promote the facile migratory insertion process.



Scheme 1.5. Regioselectivity of asymmetric alkynes. All energies (kcal mol^{-1}) are relative to **Int5_1**.

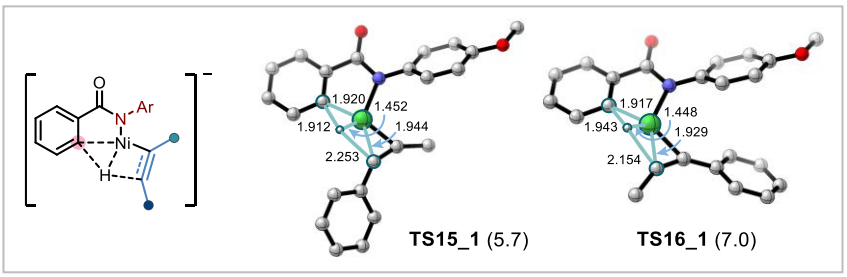


Figure 1.5. Transition state structures of LLHT with 1-phenyl-1-propyne. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

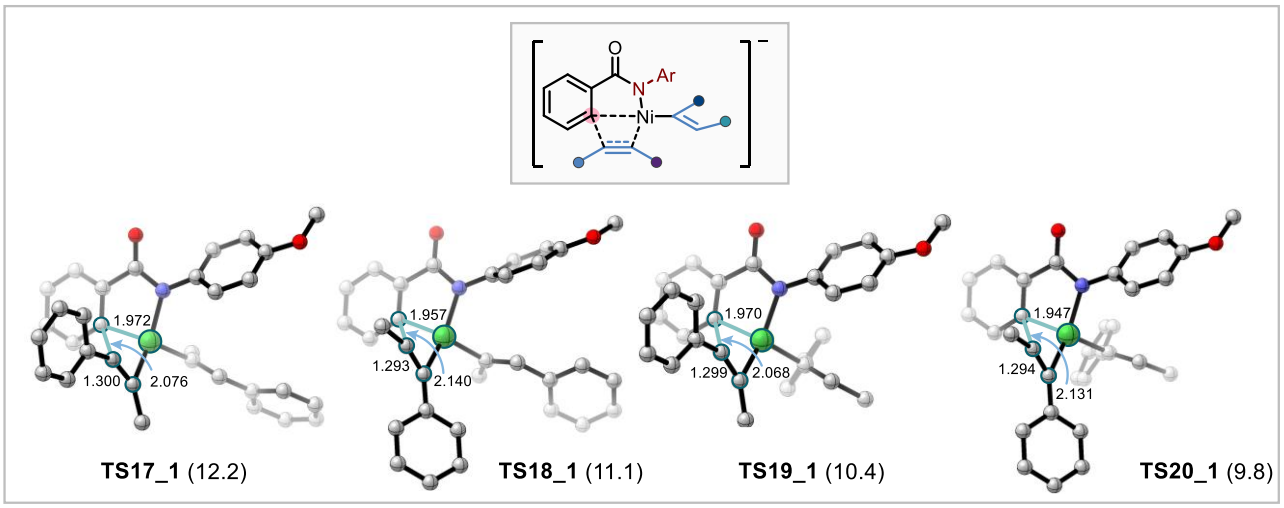
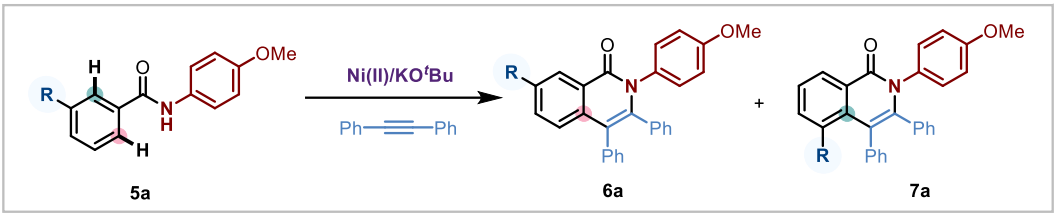


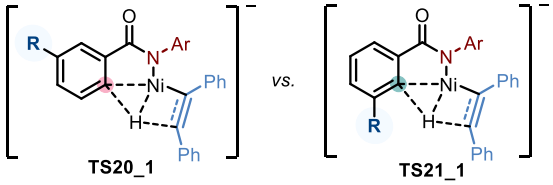
Figure 1.6. Transition state structures of migratory insertion with 1-phenyl-1-propyne. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

1.3.4. Rationalization of Regioselectivity with *meta*-Substituted Benzamides

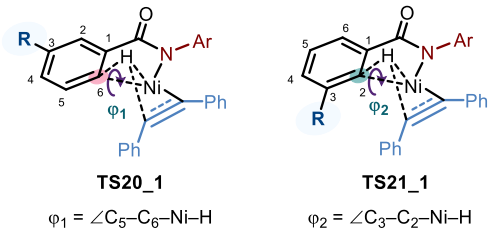
Another unique feature of this reaction is that the substituent at the *meta* position of amides influences the regioselectivity in the C−H cleavage step (Scheme 1.6). Only a single product was formed with *meta*-CF_3 substituted amide. On the other hand, mixtures of regioisomers were obtained with *meta*-methyl or methoxy substituted amides. To understand this trend and the role of substituents, the LLHT transition states leading to both isomers were computed. The large energy difference with CF_3 of 5.5 kcal mol^{-1} agrees with the observed perfect selectivity that the LLHT occurs only at the less hindered C−H bond. In addition, the *meta*-methoxy amide substrate gave much smaller $\Delta\Delta G^{\ddagger}$, and these computational trends are in agreement with the experimental observation. Analysis of both transition state structures revealed that the dihedral angles φ_1 around the forming Ni−C bond are identical in **TS20_1** for the less-hindered C−H bond activation, while the dihedral angles φ_2 in **TS21_1** for the hindered C−H bond activation change in a wide range depending on the adjacent substituent (Figure 1.7). Interestingly, the presence of intramolecular hydrogen bonding between the CF_3 group and the C(2)−H bond decreases the agostic interaction with the nickel atom and reduces the reactivity. Therefore, the steric factor mainly contributes to the regioselectivity, and the intramolecular interaction also plays a key role in the case of the reaction with *meta*-CF_3 substituted amide.



R	*yield (%)*	*product ratio (6a : 7a)*	*calculated ΔΔG‡*
CF_3	91	100 : 0	5.5
Me	81	67 : 33	3.7
OMe	86	44 : 56	1.2



Scheme 1.6. Regioselectivity with *meta*-substituted benzamides. Energies (kcal mol^{-1}) are provided in the insert.

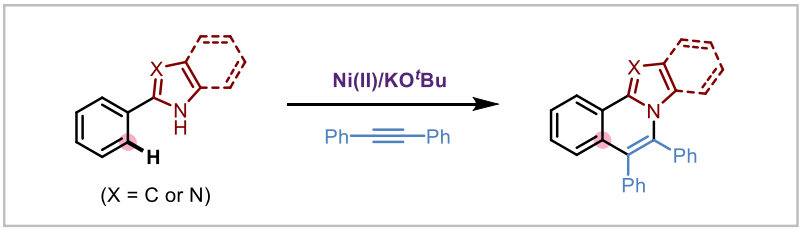


R	φ_1 (°)	φ_2 (°)
CF_3	44.6	54.8
Me	42.6	43.0
OMe	41.3	39.7

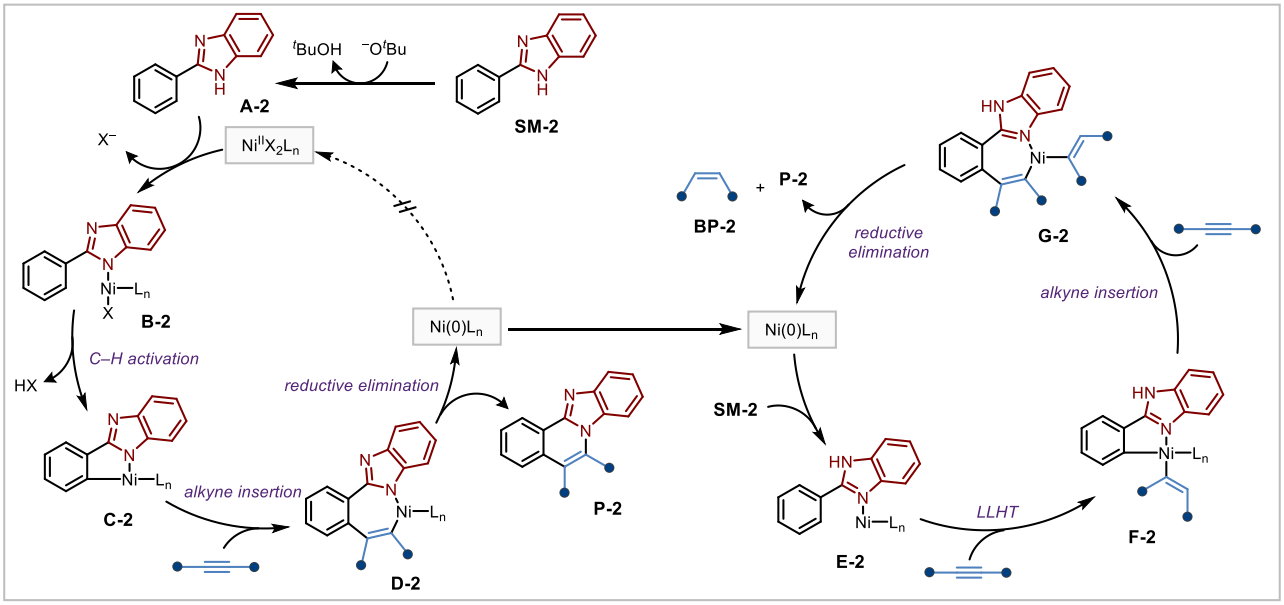
Figure 1.7. Regioselectivity with *meta*-substituted benzamides.

1.3.5. Catalytic Cycle with *N*-heterocyclic Compounds

The reaction proceeds efficiently with 2-aryl pyrrole, benzimidazole, imidazole, indole, and pyrazole derivatives (Scheme 1.7).[84] Based on our new insights into the nickel-catalyzed oxidative C−H/N−H annulation of aromatic amides with alkynes, the findings were extended to the reaction with *N*-heterocyclic compounds. Interestingly, detailed experimental mechanistic studies suggested that KO^{t}Bu is not crucial in the main catalytic cycle for the annulation reaction with 2-phenyl benzimidazole, and a nickelate species is not likely to form under the reaction conditions. The following mechanism is proposed instead, and the computational analysis on the main catalytic cycle was performed using DFT calculations (Scheme 1.8).



Scheme 1.7. Nickel-catalyzed oxidative C−H/N−H annulation of *N*-heterocyclic compounds.



Scheme 1.8. Proposed mechanism for the nickel-catalyzed oxidative C−H/N−H annulation of imidazoles.

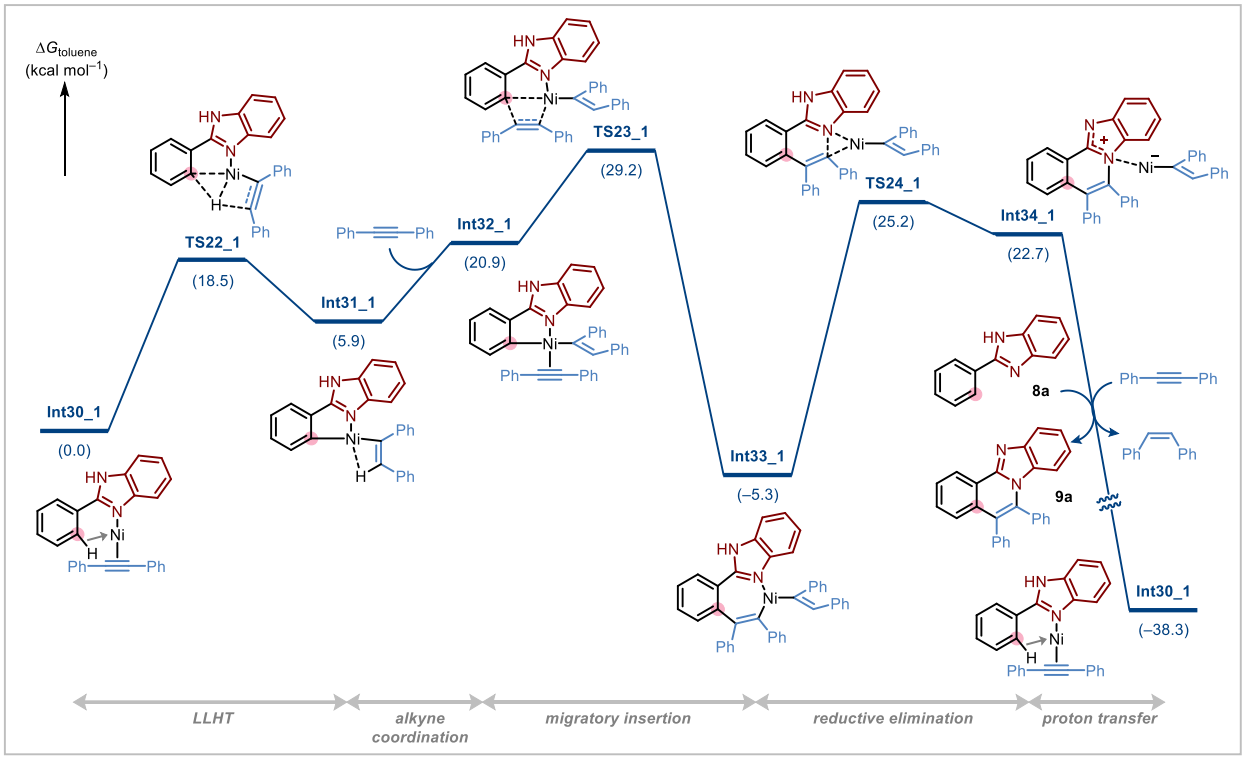


Figure 1.8. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the main catalytic cycle. Energies (kcal mol^{-1}) are provided in the insert.

The initial step of the main catalytic cycle is the LLHT from the neutral nickel complex **Int30_1** (Figure 1.8). This process requires an energy barrier of 18.5 kcal mol^{-1} through **TS22_1**, and the five-membered nickelacycle **Int31_1** is generated. After the coordination of another alkyne molecule, migratory insertion of the alkyne into the Ni–C bond through **TS23_1** is the irreversible and highly exergonic step. The reductive elimination of C–N bond proceeds with a large energy barrier through the transition state **TS24_1**, and the formed zwitterionic intermediate **Int34_1** is then immediately transformed into the annulated product and *cis*-stilbene by the proton shift. Although the detailed mechanism of proton shift is not studied, the large energy release indicates that this process is the driving force for the reaction.

Since substrates such as 2-phenylindole and 2-phenylpyrrole also gave the cyclized product, an alternative pathway initiated by the oxidative addition of N–H bond was also investigated (Figure 1.9). Substrate coordination at the nitrogen of N–H bond is energetically unfavorable (ΔG = 17.8 kcal mol^{-1}). The LLHT transition state from **Int35_1** could not be found, and instead the oxidative addition occurs through the transition state **TS25_1** ($\Delta G^{\ddagger}$ = 12.5 kcal mol^{-1}). A migratory insertion of alkyne to the generated Ni–H bond proceeds smoothly through **TS26_1**, and then the *ortho* C–H bond is cleaved by σ-bond metathesis to furnish the metallacycle **Int38_1**. The slightly higher Gibbs free energy of **TS27_1** compared to **TS23_1** suggests that the pathway in Figure 1.8 is preferred in the case of 2-phenylimidazole, while the pathway in Figure 1.9 is operative with 2-phenylindole and 2-phenylpyrrole.

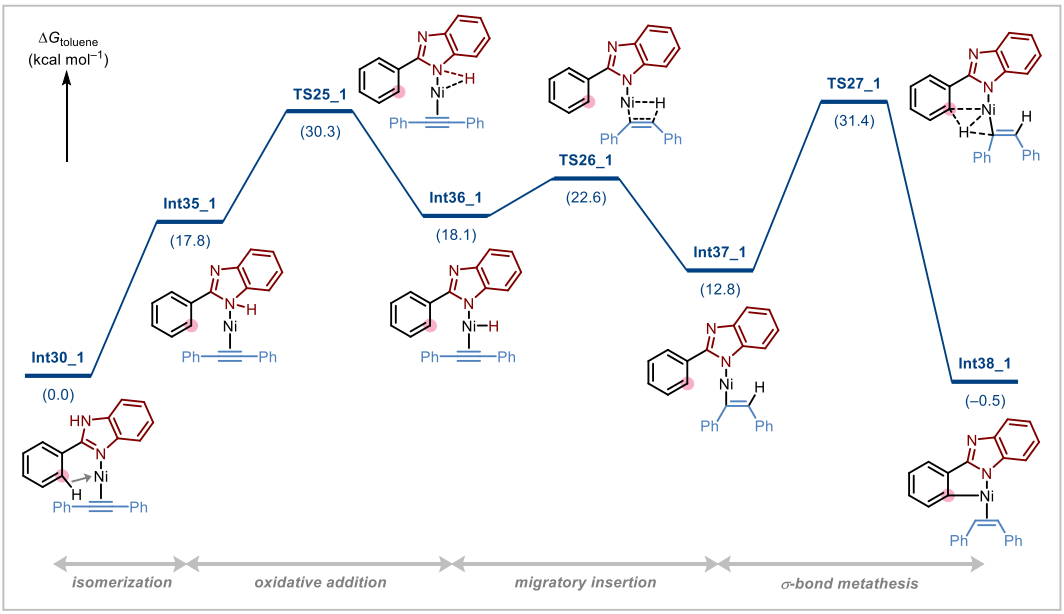


Figure 1.9. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the alternative pathway in the main catalytic cycle. Energies (kcal mol^{-1}) are provided in the insert.

1.4. Conclusion

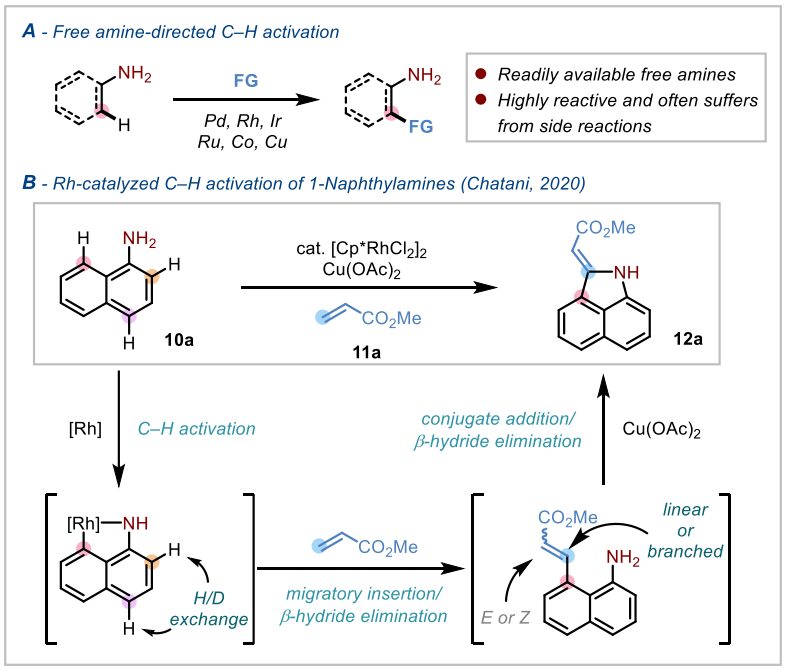
In summary, a detailed computational mechanistic study of the nickel-catalyzed oxidative C−H/N−H annulation of aromatic amides and *N*-heterocyclic compounds with alkynes was performed using DFT calculations. The catalytic cycle is initiated from a Ni(II) species, and the rate-determining step was found to be the CMD process. Severe geometric constraints on the substrate arene during the CMD process creates a high energy barrier. Since the oxidation of Ni(0) to Ni(II) is difficult under the reaction condition, a main catalytic cycle starts from a Ni(0) species, and the formation of nickelate complexes accelerates the reaction through the revised LLHT mechanism. The computed model can be extended for explaining the experimentally observed regioselectivities with asymmetrical alkynes and *meta*-substituted aromatic amides. Furthermore, the computation with 2-phenylimidazole was performed to validate the notion that the computed catalytic cycle with amides can be applied for other substrates. These findings have the potential to promote development of efficient reaction conditions for the synthesis of complex molecules.

Chapter 2

Rhodium-Catalyzed Oxidative C–H Alkenylation and Cyclization

2.1. Introduction

The research field of C–H bond activation has been extensively studied due to its potential as a selective and atom-economical strategy for the construction of new functional groups.[12,15-17,21,62,66,111-114] A wide variety of molecules have been successfully utilized for site-selective C–H functionalization using a transition-metal catalyst with or without directing groups.[14,18,19,21,63,115] One of the most desired transformations in C–H functionalization is the use of primary amines without protecting groups, since amines are well known as highly important and useful building blocks in both academia and industry for the synthesis of bioactive compounds or fluorescent materials.[116-118] However, high reactivity and ability to release protons limits the use of readily available free amines in synthetic chemistry. Instead, amines are protected after installation, or other functional groups are installed before amines are used.[20,119-121] In order to address these drawbacks, several strategies for the selective C–H activation of unprotected amines have been reported (Scheme 2.1A).[122-131] These methods have shown usefulness and can suppress undesired N–H functionalization or less selective Friedel-Crafts reactions in the case of aniline derivatives. In contrast to aniline derivatives, 1-naphthylamines have more reactive sites at the *ortho*-, *para*- and *peri*-positions that make it difficult to perform site-selective C–H activation. The Chatani group recently achieved the *peri*-selective C–H activation of unprotected 1-naphthylamines for the formation of synthetically useful benzoindole scaffolds (Scheme 2.1B).[132] In particular, the transformation is extremely diastereoselective, and the reaction mechanism is fascinating because there are several selective steps throughout the catalytic cycle. Detailed experimental mechanistic studies have been performed, however we were unable to obtain a full explanation for such high selectivity during the catalytic cycle. In order to explore the selectivity further, a detailed computational approach was used in this study in order to better understand the complex nature of such novel catalytic C–H activation reactions.



Scheme 2.1. (A) Transition metal-catalyzed free amine-directed C–H activation, and (B) Rh-catalyzed oxidative C–H alkenylation and coupling sequence of unprotected 1-naphthylamines with acrylates.

2.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional[86,87] with the 6-31G(d) basis set for C, H, O, N and the Lanl2dz effective core potential (ECP) for Rh.[88-90] Single point energy calculations were performed using the M06 functional[133] with the 6-311+G(d,p) basis set for C, H, O, N and the SDD ECP for Rh.[92-94] The solvation model based on density (SMD) solvent effects were incorporated into all calculations with toluene as the solvent.[134] Each reported minimum has a zero imaginary frequency and each transition state (TS) has only one imaginary frequency. Energy changes are shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using the CYLview program.[101]

Quantitative analyses of the activation barriers associated with the migratory insertion were obtained by means of the activation strain model (ASM), which involves decomposing the electronic energy of the transition structure $\Delta E^{\ddagger}$ into the strain $\Delta E^{\ddagger}_{\text{strain}}$ associated with the structural deformation of the reactants from their equilibrium geometry and the interaction $\Delta E^{\ddagger}_{\text{int}}$ between the deformed reactants [Eq. 1].[135-141] The $\Delta E^{\ddagger}_{\text{strain}}$ is determined by the rigidity of the reactants and by the extent to which they must deform to achieve the geometry of the transition structure. The $\Delta E^{\ddagger}_{\text{int}}$ is usually stabilizing and is related to the electronic structure of the reactants and how they are mutually oriented over the course of the reaction.

$$\Delta E^{\ddagger} = \Delta E^{\ddagger}_{\text{strain}} + \Delta E^{\ddagger}_{\text{int}} \quad (1)$$

2.3. Results and Discussion

The initial step of the reaction is the substrate coordination to the rhodium center. The *in situ* generation of Cp*Rh(OAc)$_2$ from [Cp*RhCl$_2$]$_2$ and Cu(OAc)$_2$ was hypothesized, and used it as an active species in our calculation.[142-144] As described above, there are several steps to determine the selectivity towards product formation: (i) *peri*-selective C–H activation of 1-naphthylamine, (ii) linear-selective migratory insertion of methyl acrylate, and (iii) *Z*-selective oxidative cyclization. In this computational study, all of these experimentally observed selectivities were successfully illustrated in the DFT calculations (*vide infra*).

2.3.1. C–H Activation

A significant amount of H/D exchange was confirmed at the *ortho*-, *para*- and *peri*-positions of the 1-naphthylamine substrate in the absence of methyl acrylate.[132] Transition states for the C–H activation at each position were computed, and the energy barrier for the *peri* C–H activation through **TS1_2** was found to be the most feasible process compared to the *ortho* and *para* C–H activation transition states (Figure 2.1). Analysis of the cleaving C–H bonds in each transition state revealed that **TS1_2** has the shortest bond length and is the earliest TS. The transition state **TS2_2** for *ortho* C–H activation is highly strained, and the reverse process from the formed four-membered intermediate **Int4_2** is rapid and barrierless (Figure 2.2). The *para* C–H activation may occur through **TS3_2** but with a higher energy barrier than **TS1_2**. Overall, the *peri* C–H bond reacts under kinetic control after complexation and acetic acid elimination to furnish the five-membered rhodacycle **Int3_2**.

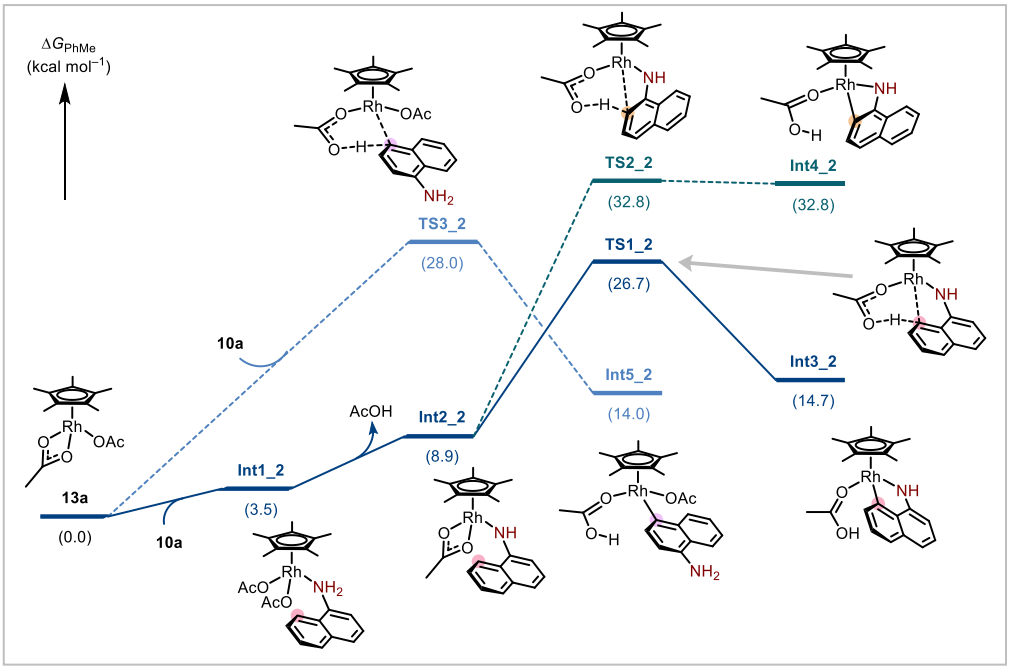


Figure 2.1. Computed reaction energy profile for the C–H activation step.

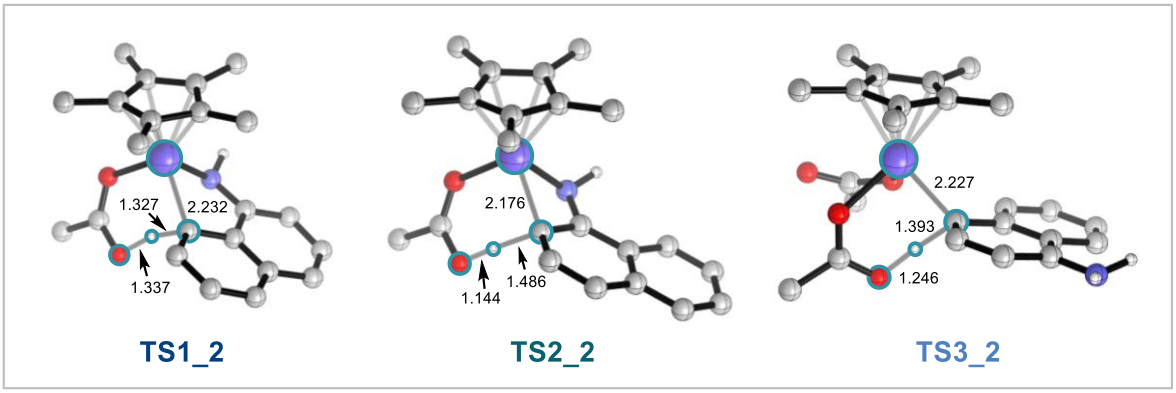
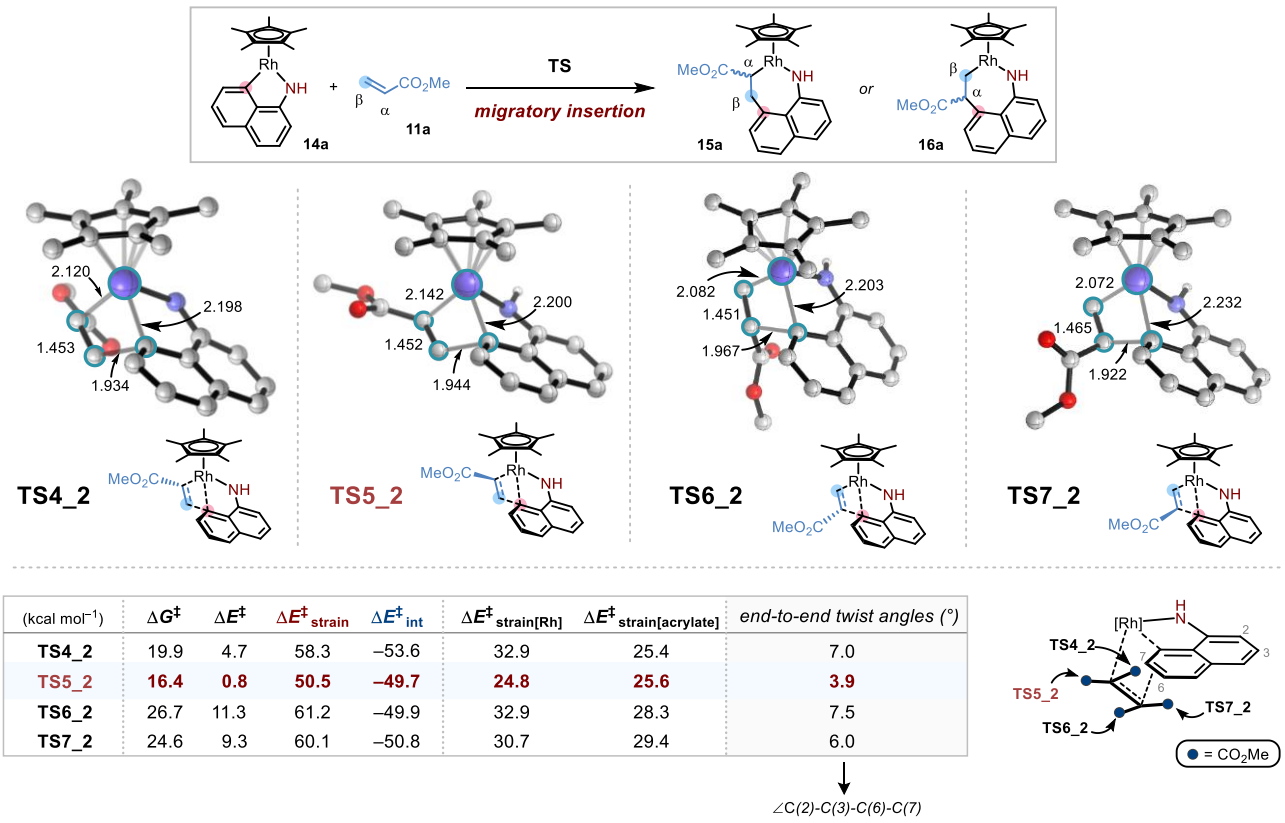


Figure 2.2. Transition structures for the C–H activation of 1-naphthylamine. Bond lengths (Å) are provided in the insert.

2.3.2. Migratory Insertion and C–H Alkenylation

The next step in the catalytic cycle after the *peri*-selective C–H activation is the migratory insertion of methyl acrylate into the Rh–C bond. There are four possible migratory insertion transition states that form different isomers of seven-membered rhodacycle, and all of them were computed (Figure 2.3). The most favorable transition structure with the lowest energy barrier was **TS5_2**, and it is preferred by more than 3.5 kcal mol^{-1}. The new C–C bond is formed between the *peri* position of the substrate and the *β*-carbon of methyl acrylate. In order to elucidate the origin of this selectivity and the kinetic preference for the migratory insertion step, an activation strain model (ASM) was used.[135-141] The ASM involves the decomposition of the electronic activation barrier ($\Delta E^{\ddagger}$) into two distinct energy terms, namely, the strain energy ($\Delta E^{\ddagger}_{strain}$) that results from the deformation of the individual reactants and the interaction energy ($\Delta E^{\ddagger}_{int}$) between the deformed reactants. The results of ASM on the migratory insertion transition states are shown in Figure 2.3, and the strain energy is found to be decisive for the selectivity in the migratory insertion step, while the interaction energy is similar in all cases. The most favorable transition state **TS5_2** has the least destabilizing strain energy ($\Delta E^{\ddagger}_{strain}$ = 50.5 kcal mol^{-1}), and this trend mainly derives from the strain energy in the rhodacycle fragment ($\Delta E^{\ddagger}_{strain[Rh]}$). When the rhodacycle is strained and loses planarity of the naphthyl moiety, the TS structure is destabilized with a higher $\Delta E^{\ddagger}_{strain[Rh]}$. This is evidenced by the linear correlation between the $\Delta E^{\ddagger}_{strain[Rh]}$ and the end-to-end twist angles, defined as the dihedral angles of C(2)–C(3)–C(6)–C(7) in the naphthalene scaffold (Figure 2.4). The **TS5_2** has the smallest end-to-end angle (3.9°) with a more planar naphthyl ring because the ester group avoids close contact with the naphthyl ring.[145,146] Therefore, the transition state that minimizes the steric repulsion between the naphthyl ring and the ester group benefits from a lower activation barrier.



(kcal mol^{-1})	$\Delta G^{\ddagger}$	$\Delta E^{\ddagger}$	$\Delta E^{\ddagger}_{strain}$	$\Delta E^{\ddagger}_{int}$	$\Delta E^{\ddagger}_{strain[Rh]}$	$\Delta E^{\ddagger}_{strain[acrylate]}$	*end-to-end twist angles (°)*
TS4_2	19.9	4.7	58.3	–53.6	32.9	25.4	7.0
TS5_2	**16.4**	**0.8**	**50.5**	**–49.7**	**24.8**	**25.6**	**3.9**
TS6_2	26.7	11.3	61.2	–49.9	32.9	28.3	7.5
TS7_2	24.6	9.3	60.1	–50.8	30.7	29.4	6.0

Figure 2.3. Transition structures for the migratory insertion of methyl acrylate. Energies (kcal mol^{-1}), bond lengths (Å), and angles (°) of TS geometries are provided in the insert.

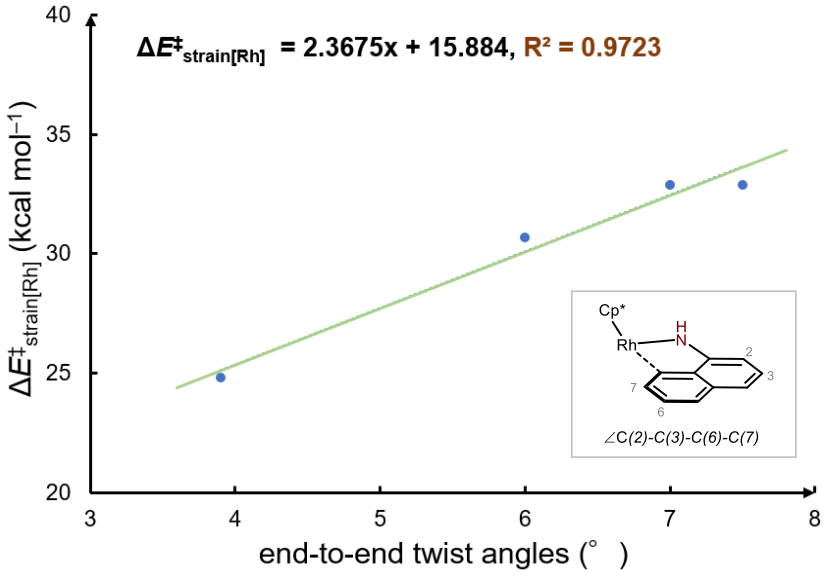


Figure 2.4. Correlation between $\Delta E^{\ddagger}_{strain[Rh]}$ (kcal mol^{-1}) and the end-to-end twist angles (°) of the rhodacycle fragment.

The reaction energy profile after the C–H activation process was computed as shown in Figure 2.5. Initially, a replacement of acetic acid with methyl acrylate is exergonic, and the intermediate **Int6_2** is obtained. The following step is the migratory insertion step which selectively proceeds through **TS5_2** that can minimize the destabilizing strain energy of the rhodacycle fragment. Then, the selectively formed seven-membered rhodacycle **Int7_2** undergoes either intramolecular proton shift or *β*-hydride elimination to generate a proposed *α,β*-unsaturated ester intermediate. The intramolecular proton shift proceeds only on one of the benzylic protons to furnish the (*Z*)-*α,β*-unsaturated ester intermediate **Int10_2**, however the energy of the transition state **TS8_2** is high ($\Delta G^{\ddagger}$ = 36.5 kcal mol^{-1}).

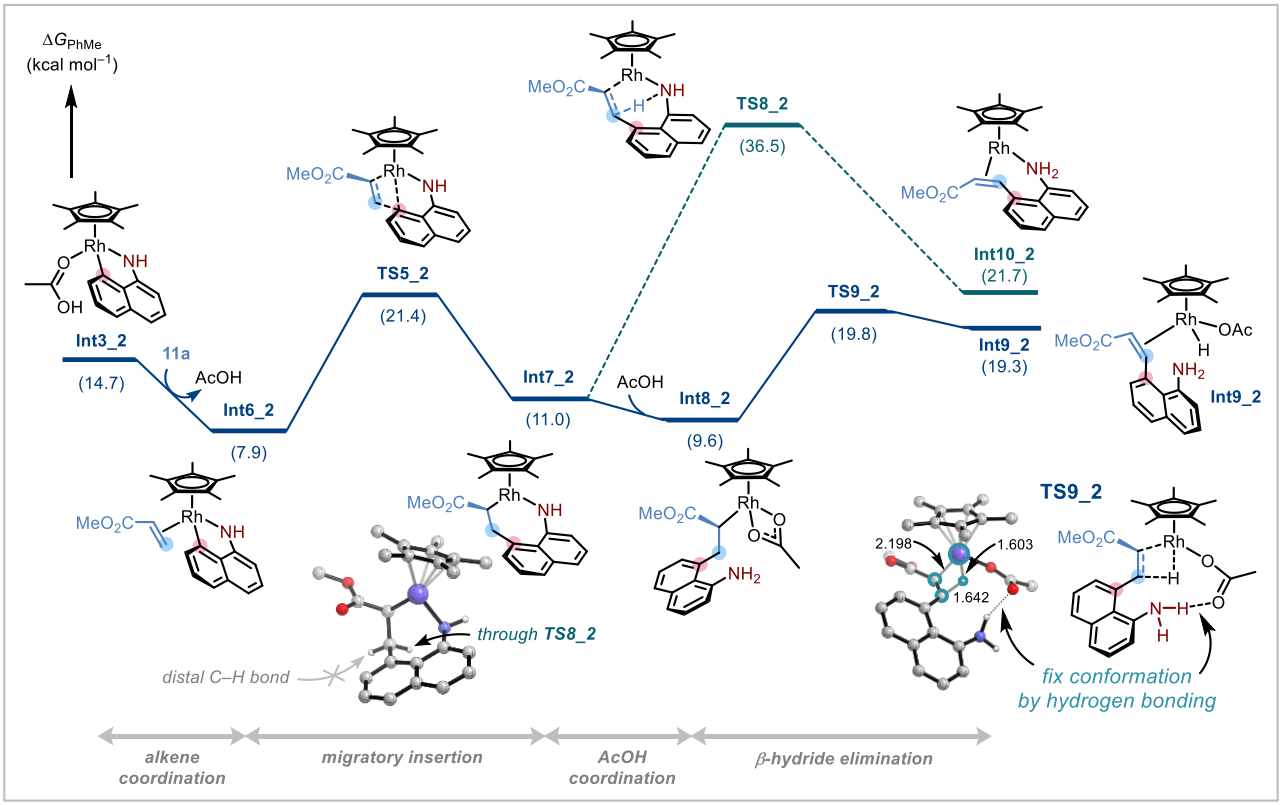


Figure 2.5. Reaction energy profile (ΔG [kcal mol^{-1}]) for the migratory insertion and the *β*-hydride elimination processes. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

In contrast, the *β*-hydride elimination begins after the acetic acid incorporation to **Int7_2**. The Rh–N bond is replaced with the η^2-acetate ligand, and the intermediate **Int8_2** with the free amine moiety is energetically more stable. The significantly lower energy barrier for the *β*-hydride elimination through transition state **TS9_2** suggests that this is a more favorable pathway. Again, the intermediate after the *β*-hydride elimination is the (*Z*)-*α,β*-*α*unsaturated ester due to the existence of hydrogen bonding between the acetate and the N–H bond of the substrate. In addition, the migratory insertion step is irreversible and the key C–C bond formation event occurs under kinetic control.

2.3.3. Conjugate Addition and *β*-Hydride Elimination

Since copper(II) acetate was used as an external oxidant for the reaction, the rhodium hydride species **Int9_2** is rapidly oxidized by the Cu(II) species. A dimeric copper(II) species $Cu_2(OAc)_4$ was used in this calculation because copper(II) acetate exists as a dimeric form, and also the use of a less stable monomeric $Cu(OAc)_2$ artificially lowers the activation barrier.[147,148] This oxidation process from **Int9_2** to **Int11_2** is extremely exergonic, and a dimeric copper(I) complex $Cu_2(OAc)_2$ and acetic acid is released (Figure 2.6). The final process of the catalytic cycle is the intramolecular conjugate addition and *β*-hydride elimination. After N–H bond activation occurs by one of the acetate ligands on rhodium center to increase the nucleophilicity of nitrogen, the intermediate **Int12_2** is formed with the unsaturated ester moiety that is pointing away. The conjugate addition transition state **TS10_2** gives a zwitterionic intermediate **Int13_2**, which then proceeds to the *β*-hydride elimination through the transition state **TS12_2** with a small activation energy barrier to furnish the product and Cp*RhH(OAc) species. During this process, the hydrogen bonding between the N–H bond and the ester group stabilizes intermediates and transition states to control the *E*/*Z* selectivity.

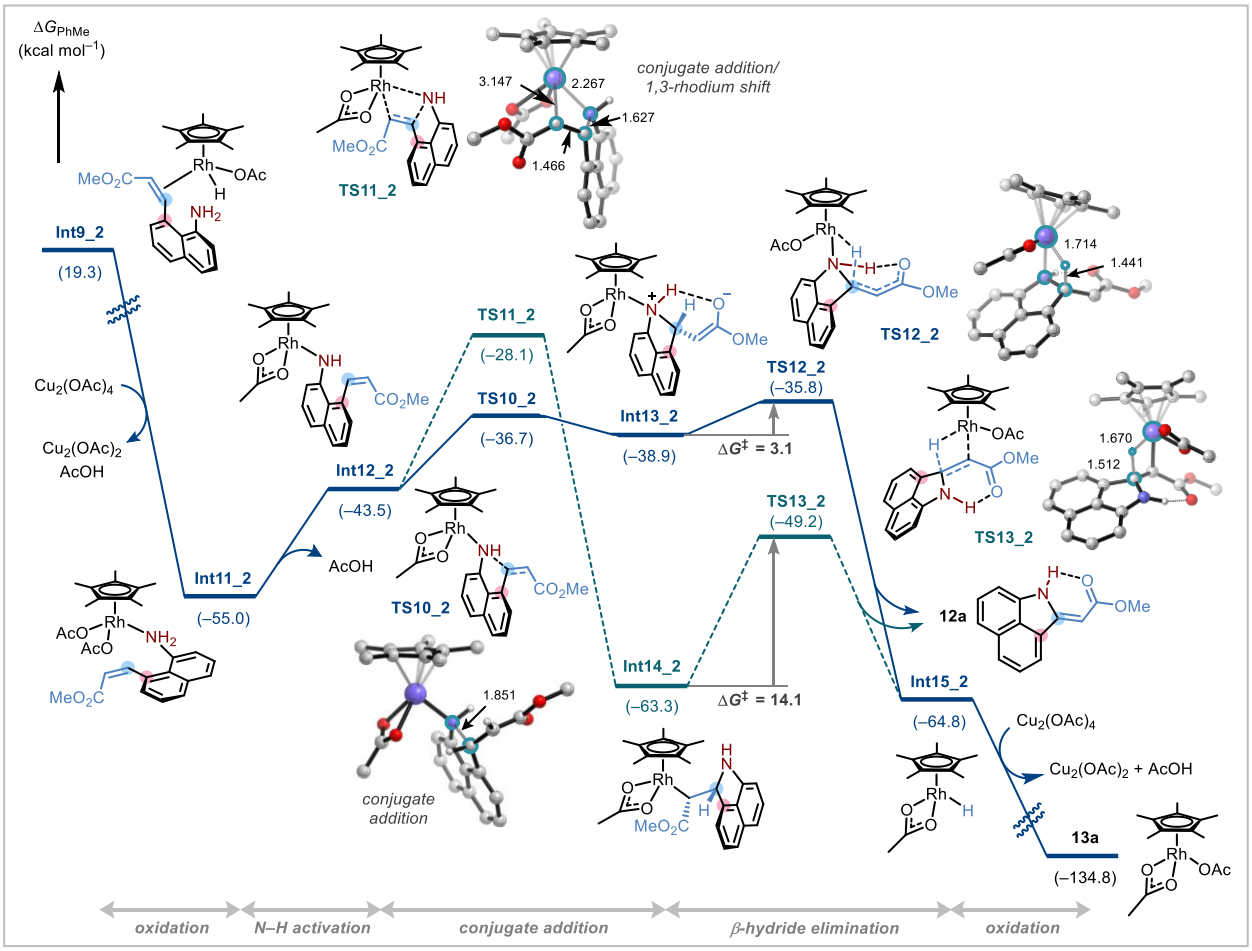
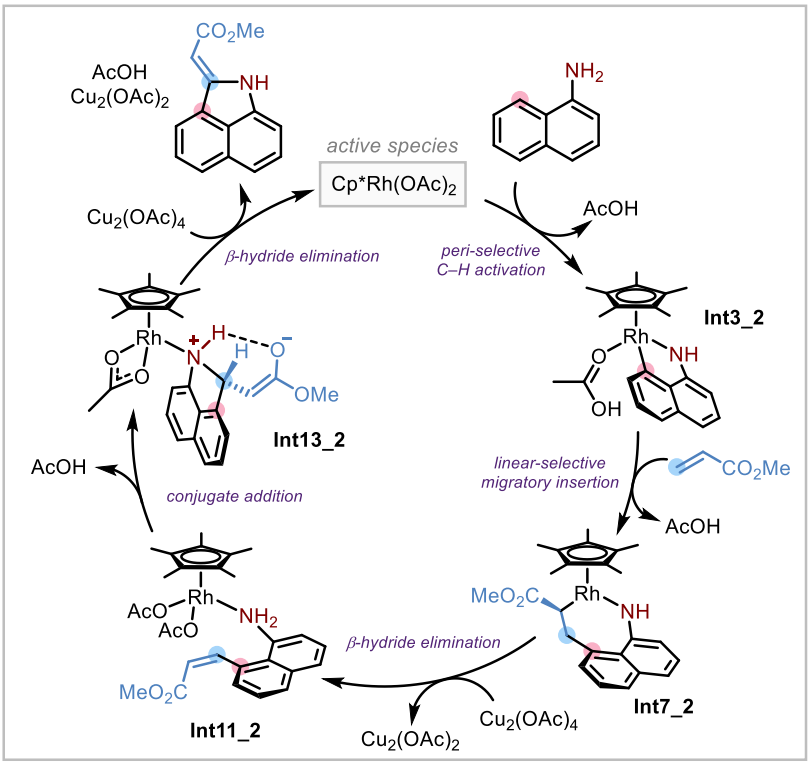


Figure 2.6. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the conjugate addition and the *β*-hydride elimination processes. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

On the other hand, the diastereomeric transition state **TS11_2** is a concerted process of conjugate addition and 1,3-rhodium shift due to the close contact distance between the rhodium atom and the ester *α*-carbon atom as a result of charge transfer from nitrogen. The energy barrier for this process is much higher, but the intermediate formation is highly exergonic. The *β*-hydride elimination from the neutral species **Int14_2** requires relatively high energy to overcome compared to **TS13_2**. The difference in the activation energy barrier for **TS12_2** and **TS13_2** originates from the nucleophilicity of the *β*-hydride in the precursors. Although the process through **TS13_2** is unfavorable, the obtained product has the same configuration due to the existence of hydrogen bonding. Therefore, the final conjugate addition/*β*-hydride elimination sequence is controlled by the key hydrogen bonding to furnish the experimentally observed cyclized product. Finally, the rhodium hydride species **Int15_2** is oxidized by $Cu_2(OAc)_4$ to regenerate the active species $Cp^*Rh(OAc)_2$.

Our overall computed catalytic cycle is summarized in Scheme 2.2. An active species $Cp^*Rh(OAc)_2$ is formed to initiate the cycle. The C–H activation process selectively proceeds at the *peri* position and gives a five-membered rhodacycle **Int3_2**. Then, the migratory insertion of methyl acrylate is a regio- and diastereoselective process through a transition state that minimizes steric repulsion between the aromatic ring and ester group. A stabilizing hydrogen bonding fixes the confirmation during the *β*-hydride elimination step, and the subsequent oxidation furnishes the *Z*-olefin intermediate **Int11_2**. Finally, sequential conjugate addition and *β*-hydride elimination process generates the experimentally observed cyclized product. The current calculations showed that each step is highly selective to produce only a single product.



Scheme 2.2. Summary of the computed catalytic cycle for the rhodium(III)-catalyzed oxidative C–H alkenylation and coupling sequence of unprotected 1-naphthylamines with *α*,*β*-unsaturated esters.

2.4. Conclusion

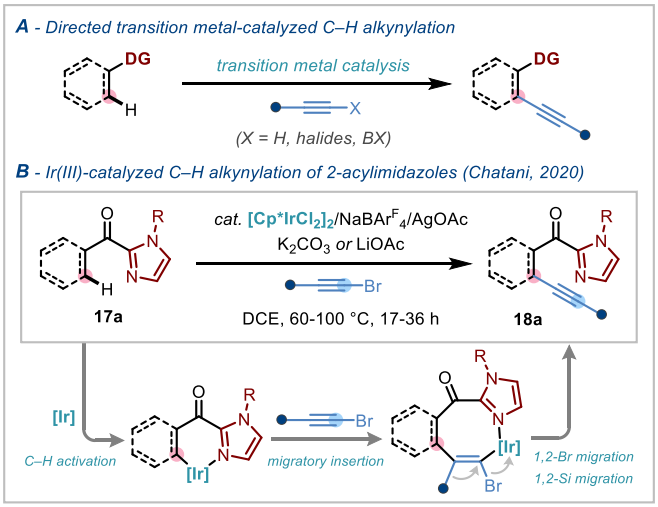
In conclusion, a mechanistic study of the rhodium(III)-catalyzed oxidative C–H alkenylation and coupling sequence of unprotected 1-naphthylamines with *α*,*β*-unsaturated esters was performed using state-of-the-art DFT calculations. Several steps in the catalytic cycle determine the regioselectivities of the product; (i) *peri*-selective C–H activation, (ii) linear-selective migratory insertion, and (iii) hydrogen-bonding-assisted *β*-hydride elimination, and our calculations agree with the experimentally observed selectivity. The key C–C bond forming migratory insertion was quantified using the activation strain analysis, and the selectivity originates from the steric repulsion between the aromatic ring and ester group. These mechanistic insights can facilitate the development of more efficient and selective reaction conditions.

Chapter 3

Iridium-Catalyzed C–H Alkynylation with Alkynyl Bromides

3.1. Introduction

Transition metal-catalyzed C–H functionalization has been recognized as an atom economical and useful method for complex molecule syntheses in medicinal and material sciences by forming new C–C and C–heteroatom bonds.[12,15-17,21,62,66,111-114,149] The potential for selective C–H bond transformation has allowed the late-stage functionalization (LSF) strategies to the reshape chemical space of pharmaceutically important functionalities.[150-152] In particular, a C–H alkynylation reaction can provide rigid structures with stable C(sp)–C(sp^2) or C(sp)–C(sp^3) bond selectively.[153-155] Many types of functional groups have been known as a directing group in transition metal-catalyzed C–H alkynylation reactions, and a wide variety of chemicals such as terminal alkynes, alkynyl halides, and hyper-valent iodine alkynylation reagents can be utilized as a coupling partner (Scheme 3.1A).[106,156-162] Recently, the Chatani group discovered an iridium(III)-catalyzed C(sp^2)–H and C(sp^3)–H alkynylation of 2-acylimidazoles with alkynyl bromides (Scheme 3.1B).[163] The 2-acylimidazole derivatives are synthetically useful in organic chemistry as a building block, and the use of this functionality as a directing group enables the LSF of complex molecules.[164-168] Previously, several experimental mechanistic studies were performed for better understanding the reaction mechanism including X-ray crystallography, NMR, and FAB-MS studies.[163] In order to validate the proposed mechanism and the generation of intermediates, state-of-the-art computational studies were performed.



Scheme 3.1. Transition metal-catalyzed C–H alkynylation with alkynes. BX = benziodoxolone.

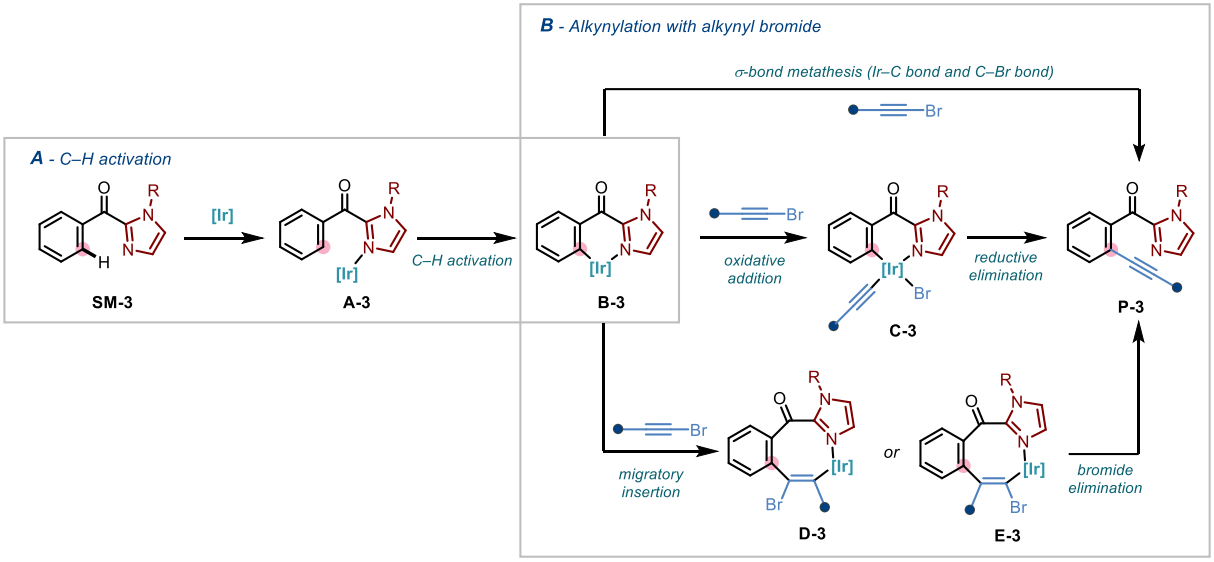
3.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional[86,87] with the 6-31G(d) basis set for C, H, O, N, Si, Br and the Lanl2dz effective core potential (ECP) for Ir.[88-90] Single point energy calculations were performed using the M06 functional[133] with the 6-311+G(d,p) basis set for C, H, O, N, Si, Br and the SDD ECP for Ir.[92-94] The solvation model based on density (SMD) solvent effects were incorporated into all calculations with dichloroethane (DCE) as the solvent.[134] Each reported minimum has zero imaginary frequency and each transition state (TS) has only one imaginary frequency. Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using CYLview20.[101] Natural bond orbital (NBO) analyses were performed on the optimized geometries.[169] The NBO interactions were visualized using Jmol.[170]

Quantitative analyses of the activation barriers associated with the migratory insertion were performed using the activation strain model (ASM). ASM involves the decomposition of the electronic energy ($\Delta E^{\ddagger}$) of the transition structure into the strain energy ($\Delta E^{\ddagger}_{\text{strain}}$) associated with the structural deformation of the iridacycle and an alkynyl bromide and the interaction energy ($\Delta E^{\ddagger}_{\text{int}}$) between the deformed reactants [Eq. 1] (see Chapter 2).[135-141] The $\Delta E^{\ddagger}_{\text{strain}}$ value is the penalty required to deform the fragments from the transition structure. Since $\Delta E^{\ddagger}_{\text{int}}$ is related to the electronic structure of the deformed reactants, it accounts for the mutual interaction between these fragments.

3.3. Results and Discussion

The previous detailed experimental mechanistic studies indicated the existence of several reaction intermediates using X-ray crystallography, NMR and FAB-MS.[163] Based on these results, the following mechanisms were proposed, and each pathway was computed and compared using DFT calculations in this study (Scheme 3.2). Initially, a six-membered iridacycle **B-3** is formed from the iridium-substrate complex **A-3** by C–H activation at the *ortho* position (Scheme 3.2A). Then, the intermediate **B-3** reacts with an alkynyl bromide by either an oxidative addition-reductive elimination sequence (OA/RE) through an iridium(V) intermediate **C-3** formation, a migratory insertion-bromide elimination sequence (MI/BE) through eight-membered iridacycle **D-3** or **E-3** formation, or a direct σ-bond metathesis (σBM) between Ir–C and C–Br bonds (Scheme 3.2B). These plausible pathways were thoroughly studied and analyzed using a computational method.



Scheme 3.2. Plausible mechanisms.

3.3.1. C–H Activation

A cationic active species Cp*Ir(OAc)$^{+}$ is proposed to be generated *in situ* under the reaction conditions, and the catalytic cycle is initiated from **Int1_3** after the coordination of the 2-acylimidazole substrate to the active species (Figure 3.1).[171] The *ortho* C–H bond activation is promoted by the acetate ligand by an ambiphilic metal-ligand activation/concerted metalation deprotonation (AMLA/CMD) mechanism through **TS1_3** ($\Delta G^{\ddagger}$ = 17.3 kcal mol^{-1}).[43] After the AMLA/CMD process, the coordinating acetic acid is easily dissociated to furnish a more stable intermediate **Int3_3**.

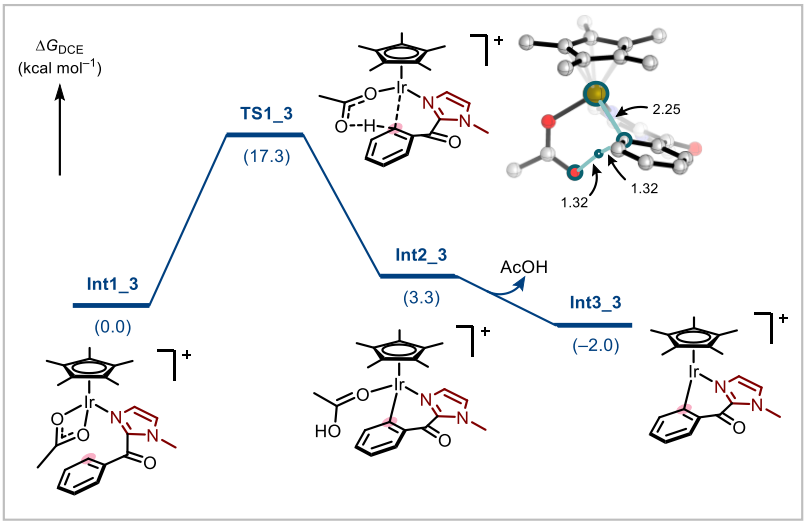


Figure 3.1. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the C–H activation step of the Ir(III)-catalyzed C–H alkynylation of 2-acylimidazoles with alkynyl bromides. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

3.3.2. Reaction between Iridacycle and Alkynyl Bromide

Three reaction mechanisms are plausible between the iridacycle **Int3_3** and alkynyl bromide, and the computed pathways are shown in Figure 3.2. Originally proposed oxidative addition proceeds through the transition state **TS2_3** to give the iridium(V) intermediate **Int4_3**, and the following reductive elimination through **TS3_3** gives a new C(sp)–C(sp^2) bond. Although the Cp*Ir(V) species was previously observed experimentally,[172] the activation energy barrier is high ($\Delta G^{\ddagger}$ = 33.9 kcal mol^{-1}) and this process is energetically unfavorable. The σ-bond metathesis between Ir–C(sp^2) and C(sp)–Br bonds requires even higher energy to overcome the four-membered transition state **TS4_3** ($\Delta G^{\ddagger}$ = 44.2 kcal mol^{-1}), indicating the direct formation of C(sp)–C(sp^2) bond is not possible. In contrast, the migratory insertion process is more facile, and the activation energy barriers for the transition states **TS5_3** and **TS6_3** are much lower ($\Delta G^{\ddagger}$ = 15.8 and 18.1 kcal mol^{-1}, respectively). The energy difference between the regioisomeric TSs is relatively large ($\Delta\Delta G^{\ddagger}$ = 2.3 kcal mol^{-1}), and this suggests that the migratory insertion is regioselective towards **TS5_3**, and the C–C bond is formed between the *ortho* C(sp^2) atom and the C(sp) atom next to the TMS group. In order to quantify the origin of the regioselective migratory insertion, the activation strain model (ASM) was performed using the six-membered iridacycle and the alkynyl bromide as the fragments (Figure 3.3).[135-141] The ASM revealed that the trend of regioselectivity is solely determined by the strain energy, and the interaction energies were identical. Further decomposition of $\Delta E^{\ddagger}_{strain}$ into the strain energies of each fragments ($\Delta E^{\ddagger}_{strain[Ir]}$ and $\Delta E^{\ddagger}_{strain[alkyne]}$) showed that both fragments contribute to the more destabilized $\Delta E^{\ddagger}_{strain}$ in **TS6_3**. The bend angle of TMS group in alkynyl bromide is larger in the disfavored transition state **TS6_3** (∠Ir–C–C = 137.5°) than the one in the favored transition state **TS5_3** (∠Ir–C–C = 145.7°). In other words, **TS5_3** can benefit from the more linear-like geometry of the alkynyl bromide at the transition state. This is evidenced by the closer distance between the H atoms of TMS group and Cp* ring in **TS6_3** (2.33 Å). The computational study on the *meta*-selective Pd-catalyzed C–H alkynylation with alkynyl bromides reported by Maiti and Paton indicated that there was almost no regioselectivity in the migratory insertion step.[161] The difference of the computed selectivity between their Pd-catalyzed system and this Ir-catalyzed system can be attributed to the flexibility of the metallacycles that arise from the ring size of metallacycle intermediates. Therefore, difference in the degree of steric clash between the bulky TMS group and the iridacycle leads to the regioselective migratory insertion of alkynyl bromide for the formation of the eight-membered iridacycle **Int5_3**.

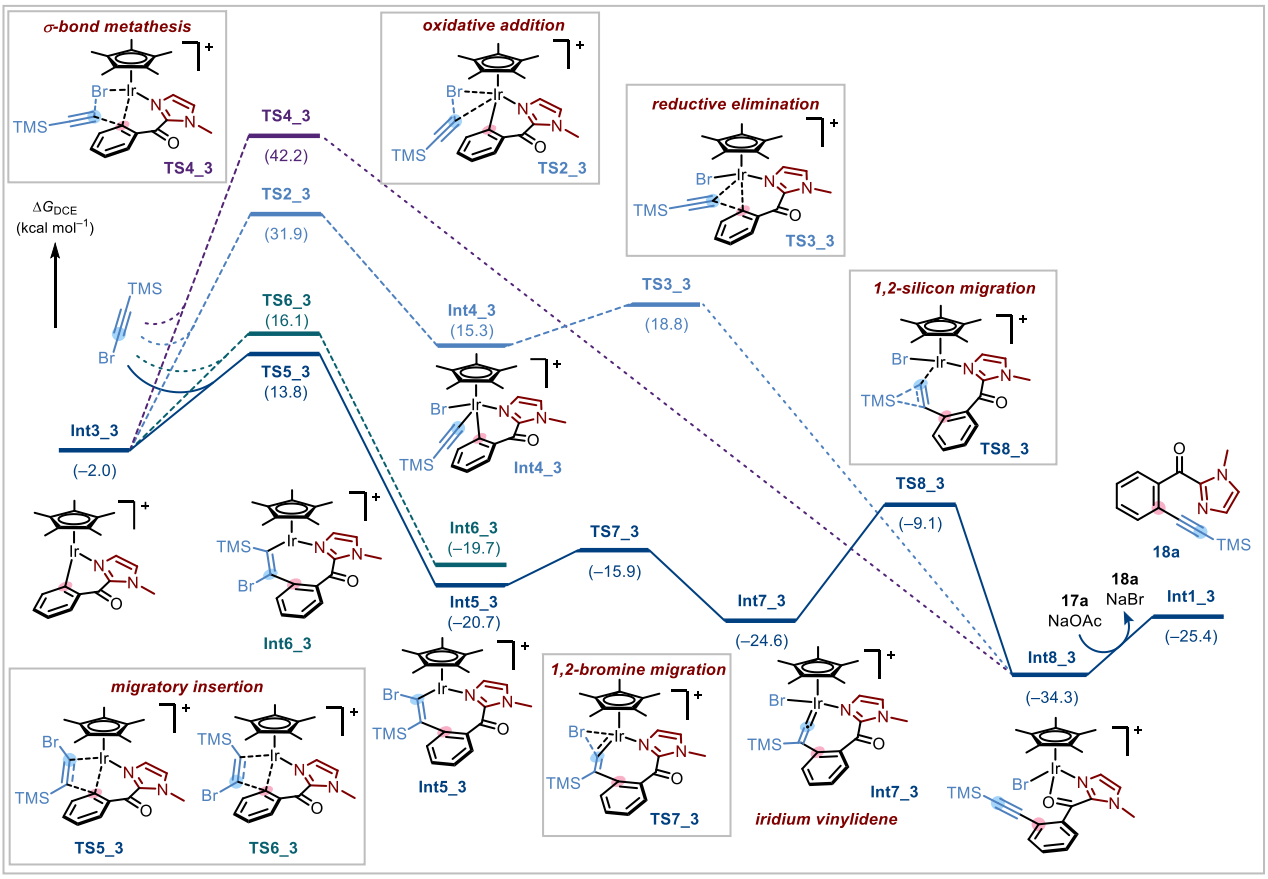


Figure 3.2. Computed potential energy surface (Δ*G* [kcal mol^{-1}]) of the Ir(III)-catalyzed C–H alkynylation of 2-acylimidazoles with alkynyl bromides from **Int3_3**. Energies (kcal mol^{-1}) are provided in the insert.

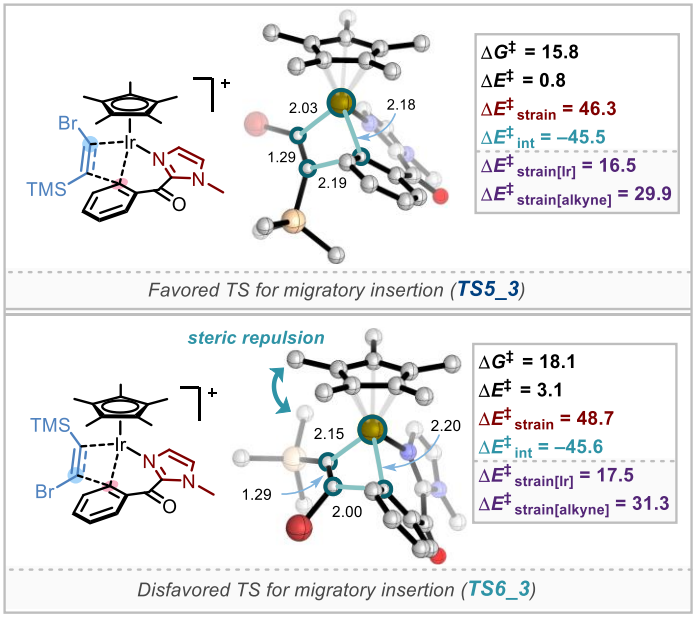


Figure 3.3. Activation strain analysis of migratory insertion transition states. Energies (kcal mol^{-1}) and bond lengths (Å) of TS geometries are provided in the insert.

After the migratory insertion step, the TMS group in **Int5_3** is required to migrate to the adjacent carbon atom by a consecutive 1,2-bromine migration and 1,2-silicon migration in order to obtain an alkynylated product. The second migration is known as the Fritsch-Buttenberg-Wiechell rearrangement, and a carbene intermediate is involved.[173-176] The 1,2-bromine migration process is facile through **TS7_3**, and the iridium vinylidene intermediate **Int7_3** is generated (∠Ir–C–C = 171.9°). Interestingly, this process has a low activation energy barrier ($\Delta G^{\ddagger}$ = 4.8 kcal mol^{-1}) and is exergonic (ΔG = –3.9 kcal mol^{-1}), even though only a few iridium vinylidene species are known to date.[177-183] Finally, the TMS group migrates to the adjacent carbon atom through the transition state **TS8_3** ($\Delta G^{\ddagger}$ = 15.5 kcal mol^{-1}) to give the alkynylated intermediate **Int8_3**. The product **18a** is exchanged with the starting material to regenerate **Int1_3** to complete the catalytic cycle. This study demonstrates the first computational evidence that both bromine and silicon atoms can migrate smoothly by a 1,2-migration mechanism with an iridium catalyst.[161,184-190]

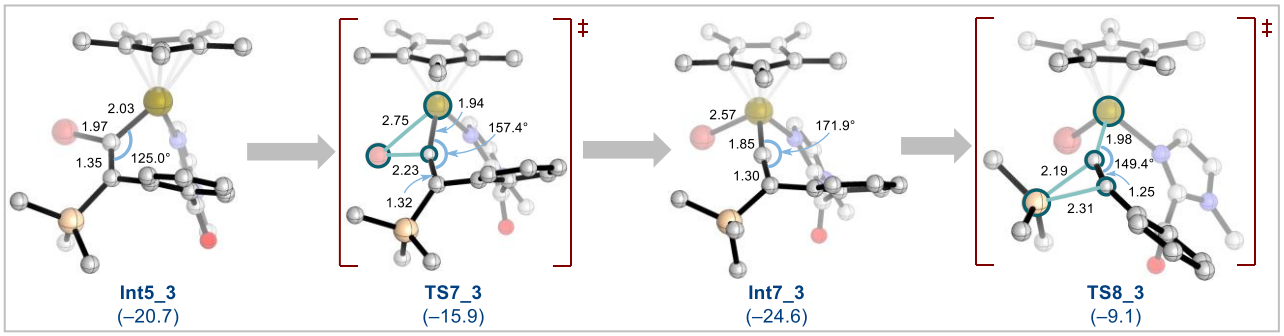
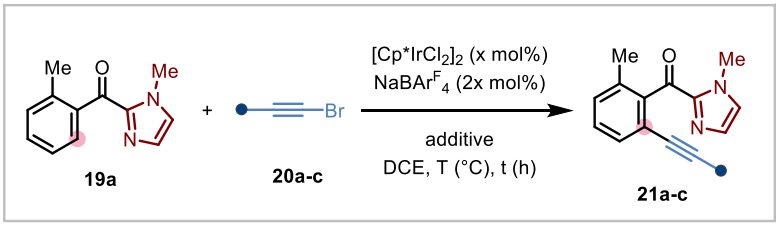


Figure 3.4. Intermediate and transition state structures (ΔG [kcal mol^{-1}]) for the double 1,2-migration. Energies (kcal mol^{-1}), bond lengths (Å), and angles (°) of computed geometries are provided in the insert.

During the 1,2-migration of bromine atom, both Br and Ir atoms gain negative charges, and *α*-C atom gains positive charge. The charge in Br atom changes from +0.013 in **Int5_3** to –0.031 in **TS7_3** to –0.253 in **Int7_3**, and the charge in Ir atom changes from +0.372 in **Int5_3** to +0.128 in **TS7_3** to 0.000 in **Int7_3**. On the other hand, the charge in *α*-C atom changes from –0.155 in **Int5_3** to +0.076 in **TS7_3** to +0.361 in **Int7_3**. Furthermore, the Ir–C bond length shortens during the 1,2-bromine migration process from 2.03 Å in **Int5_3** to 1.94 Å in **TS7_3** to 1.85 Å in **Int7_3**) (Figure 3.4). Therefore, a significant amount of charge is transferred to form a cyclic iridium vinylidene intermediate (*vide infra*). Overall, the most favorable pathway in the catalytic cycle is the sequential *ortho* C–H activation, migratory insertion, 1,2-bromine migration, and 1,2-silicon migration.

3.3.3. Various Alkynyl Bromide Coupling Partners

A dramatic reactivity change depending on the substituent on the alkynyl bromide was observed in the previous experimental study (Figure 3.5).[183] The reaction proceeded smoothly with a triisopropylsilyl (TIPS)-substituted alkynyl bromide and gave the corresponding product in excellent yield. An aryl-substituted alkynyl bromide also furnished the corresponding product, but more harsh conditions were required. A *tert*-butyl-substituted alkynyl bromide failed to give the product even at higher temperature. In an attempt to explain the reactivity difference, the reaction pathways with various alkynyl bromides were computed (Figure 3.6).

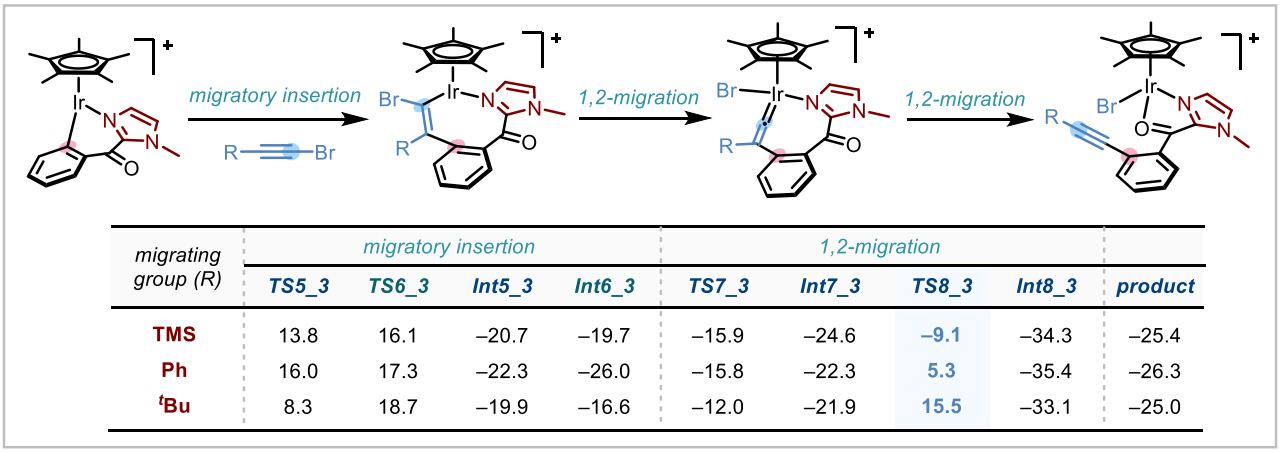


entry	alkyne (**20**)	x	T (°C)	t (h)	**3** (%)	**1** (%)
1[c]	TIPS—≡—Br	2.5	60	17	**97**[a]	**0**[a]
2[d]	Me—C6H4—≡—Br	5	120	36	**46**[a]	**17**[a]
3[d]		5	120	36	**0**[b]	**91**[b]

Figure 3.5. Reaction with different alkynyl bromides.[163] [a] Isolated yields. [b] ^{1}H NMR yields. [c] K_2CO_3 (1.5 equiv.) and AgOAc (5 mol%) were used as additives. [d] LiOAc (3 equiv.) and AgOAc (1 equiv.) were used as additives.

When the TMS group is replaced with a Ph group, the energy barrier for the migratory insertion process was increased ($\Delta G^{\ddagger}$ = 18.0 kcal mol^{-1}). The regioselectivity for this step is the same, and the C–C bond formation occurs between the *ortho* C(sp^2) atom and the C(sp) atom next to the Ph group ($\Delta\Delta G^{\ddagger}$ = 1.3 kcal mol^{-1}). The eight-membered iridacycle intermediate **Int5_3_Ph** after the migratory insertion then proceeds to facile 1,2-bromine migration ($\Delta G^{\ddagger}$ = 6.5 kcal mol^{-1}), however a higher activation energy barrier for the final 1,2-aryl migration transition state **TS8_3_Ph** is required ($\Delta G^{\ddagger}$ = 27.6 kcal mol^{-1}). This trend is in line with the requirement of more harsh reaction conditions and increased amount of catalyst and coupling partner to obtain the product. A *tert*-butyl-substituted alkynyl bromide undergoes a facile migratory insertion, and the energy barrier is lower ($\Delta G^{\ddagger}$ = 10.3 kcal mol^{-1}) and the regioselectivity is higher ($\Delta\Delta G^{\ddagger}$ = 10.4 kcal mol^{-1}) due to the size difference between the ^{t}Bu group and the TMS group, which leads to a shorter interatomic distance between the Cp* ring and the ^{t}Bu group. The 1,2-bromine migration is facile and exergonic through **TS7_3_^{t}Bu**, however a significant amount of energy is needed to achieve this transformation through the transition state **TS8_3_^{t}Bu** ($\Delta G^{\ddagger}$ = 37.4 kcal mol^{-1}), and the product cannot be

formed. Therefore, these computational results suggested that the second 1,2-migration process solely determines the reactivity of various alkynyl bromide coupling partners.



migrating group (R)	migratory insertion				1,2-migration				
	TS5_3	**TS6_3**	**Int5_3**	**Int6_3**	**TS7_3**	**Int7_3**	**TS8_3**	**Int8_3**	**product**
TMS	13.8	16.1	–20.7	–19.7	–15.9	–24.6	**–9.1**	–34.3	–25.4
Ph	16.0	17.3	–22.3	–26.0	–15.8	–22.3	**5.3**	–35.4	–26.3
^{t}Bu	8.3	18.7	–19.9	–16.6	–12.0	–21.9	**15.5**	–33.1	–25.0

Figure 3.6. Gibbs free energies (ΔG [kcal mol^{-1}]) for the migratory insertion and double 1,2-migration sequence with various alkynyl bromide derivatives.

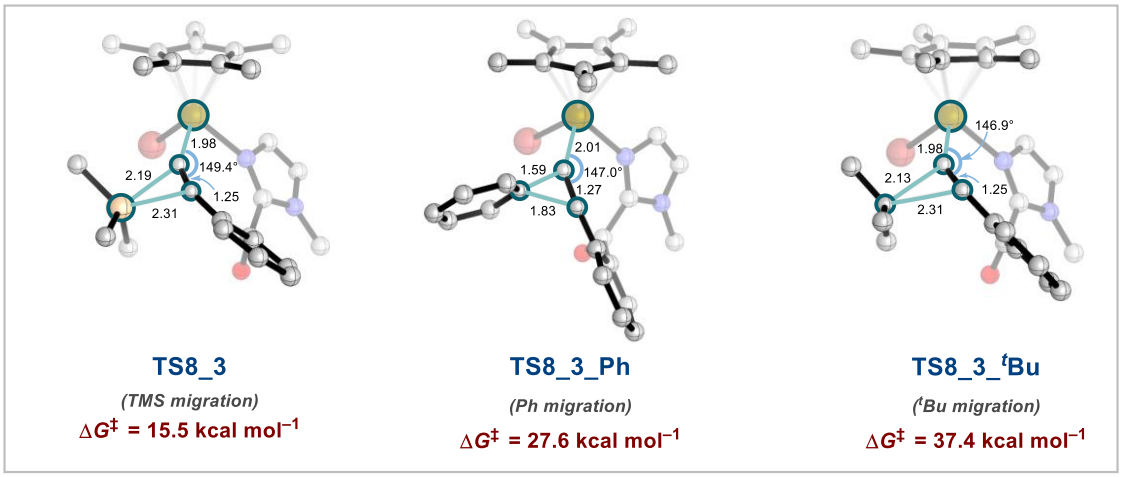


Figure 3.7. Transition state structures for the second 1,2-migration with various alkynyl bromide derivatives. Energies (kcal mol^{-1}), bond lengths (Å), and angles (°) of TS geometries are provided in the insert.

The 1,2-migration transition state structures with various substituents are shown in Figure 3.7. The activation energy barriers for the 1,2-migration step increase from TMS, Ph, and ^{t}Bu groups ($\Delta G^‡$ = 15.5, 27.6, and 37.4 kcal mol^{-1}, respectively). All newly forming C–C or C–Si bonds are consistently shorter than the breaking bonds. The migrating Ph group in **TS8_3_Ph** has closer contact to the C=C bond compared to **TS8_3** and **TS8_3_^{t}Bu**, indicating that the aromatic π orbital and the vacant *p** orbital of *α*-C atom are

overlapped leading to a stabilizing interaction. The origin of the highly stabilized 1,2-silicon migration TS is due to the existence of the *β*-silicon effect, and the electron donation from the σ_{C-Si} occupied orbital to the adjacent vacant *p** orbital of *α*-C atom can stabilize the transition state (Figure 3.8). The second-order perturbation interaction energy $E^{(2)}$ obtained from NBO calculations supports the presence of a strong interaction originating from donor-acceptor bonding ($E^{(2)}$ = 19.1 kcal mol^{-1}) from the σ_{C-Si} occupied orbital and the adjacent vacant *p** orbital of the *α*-C atom. The similar interaction from the ^{t}Bu σ_{C-C} occupied orbital is significantly reduced ($E^{(2)}$ = 3.5 kcal mol^{-1}), and this leads to a destabilized transition state. Overall, the computed trend for the second 1,2-migration process is in agreement with the experimental results, and the reactivity with various alkynyl bromides is mainly determined by the migration ability of each substituent.

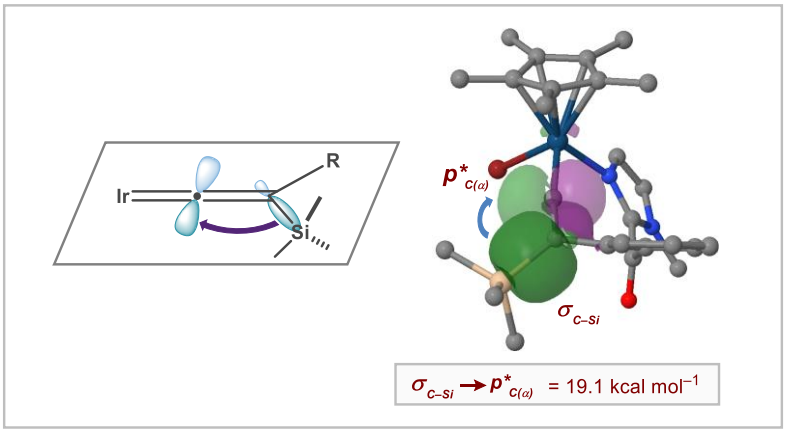


Figure 3.8. Schematic representation of 1,2-silicon migration and the NBO $\sigma_{C-Si} \rightarrow p^*_{C(a)}$ perturbative donor-acceptor interaction of **Int7_3**.

3.4. Conclusion

In conclusion, a mechanistic study of the iridium(III)-catalyzed C–H alkynylation of 2-acylimidazoles with alkynyl bromides was performed using state-of-the-art DFT calculations. The calculations suggest that the key steps in the catalytic cycle are the following: (i) *ortho* C–H activation by an ambiphilic metal-ligand activation/concerted metalation deprotonation (AMLA/CMD), (ii) strain-controlled regioselective migratory insertion of alkynyl bromide, (iii) 1,2-bromine migration for the formation of iridium vinylidene intermediate, and (iv) reactivity-determining 1,2-migration. The reactivity difference with various alkynyl bromides originates from the second 1,2-migration step, and the transition state with a TMS group is stabilized by the *β*-silicon effect ($\sigma_{C-Si} \rightarrow p^*_{C(a)}$). Experimental support for the 1,2-migration by an isotopic labelling experiment is currently in progress. These computational insights can potentially accelerate further development of efficient reaction conditions.

Chapter 4

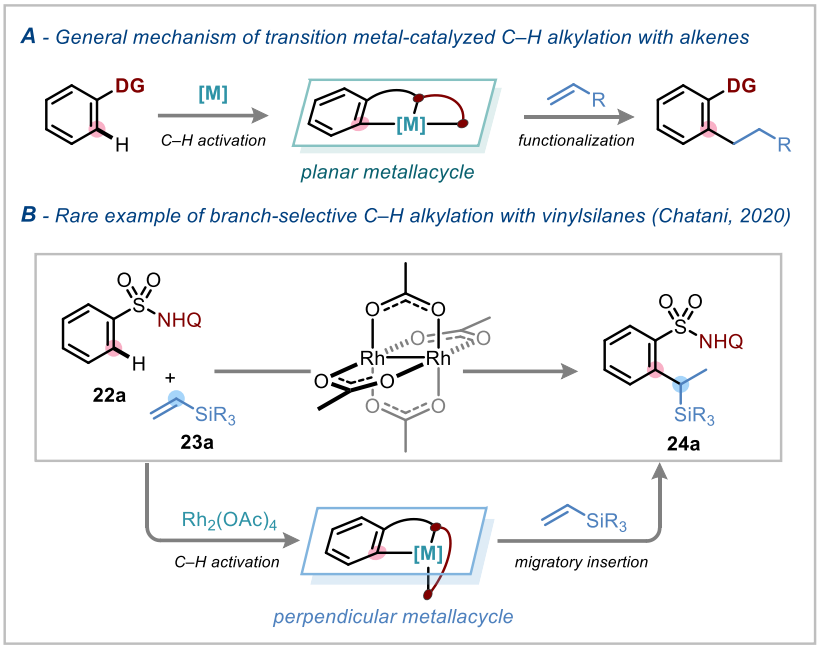
Rhodium-Catalyzed C–H Alkylation with Vinylsilanes

4.1. Introduction

The area of transition-metal-catalyzed C–H activation has been extensively studied as a selective, powerful, and atom-economical strategy for the construction of new C–C and C–heteroatom bonds which can be applied for complex molecule syntheses.[12,15-17,21,62,66,111-114,149,191] A large number of directing groups and coupling partners have been employed in various synthetic methods.[18-21] A directed transition-metal-catalyzed C–H alkylation with alkene coupling partners has been attracting attention as it offers atom-economic reactions (Scheme 4.1A).[192-196] Since the first report on the directed Ru-catalyzed *ortho*-C–H alkylation of aromatic ketones with alkenes,[14] many reactions on directed C–H alkylation have been developed. Most of these reactions were linear-selective C–H alkylation, and only a few have achieved branch-selective C–H alkylation.[197-217] Furthermore, the use of activated alkenes such as styrenes, acrylate esters and vinyl esters were required to perform those branch-selective alkylation reactions. Recently, the Chatani group reported the first example of branch-selective *ortho*-C–H alkylation of sulfonamides with vinylsilanes (Scheme 4.1B).[218] The reaction can be achieved using the dirhodium complex $Rh_2(OAc)_4$ combined with the 8-aminoquinolyl directing group in toluene at 160 °C for 24 h. In order to elucidate the origin of the branch selectivity of such novel catalytic C–H alkylation reactions, a detailed investigation was performed utilizing a computational approach.

4.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional[86,87] with the 6-31G(d) basis set for C, H, O, N, S and the Lanl2dz effective core potential (ECP) for Rh.[88-90] Single point energy calculations were performed using the M06 functional[133] with the 6-311+G(d,p) basis set for C, H, O, N, S and the SDD ECP for Rh.[92-94] The solvation model based on density (SMD) solvent effects were incorporated into all calculations with toluene as the solvent.[134] Each reported minimum has a zero imaginary frequency and each transition state (TS) has only one imaginary frequency. Energy changes were determined from the Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using CYLview20.[101] Molecular orbitals were visualized using the Gaussview 5.0.8 program.[219]



Scheme 4.1. (A) General mechanism for transition-metal-catalyzed C–H alkylation with alkenes using bidentate directing groups, and (B) Rh(II)-catalyzed branch-selective C–H alkylation of aryl sulfonamides with vinylsilanes. Q = 8-quinolyl.

Quantitative analyses of the activation barriers associated with the migratory insertion were performed using the activation strain model (ASM). ASM involves the decomposition of the electronic energy ($\Delta E^{\ddagger}$) of the transition structure into the strain energy ($\Delta E^{\ddagger}_{strain}$) associated with the structural deformation of the metallacycle and the alkene and the interaction energy ($\Delta E^{\ddagger}_{int}$) between the deformed reactants [Eq. 1] (see Chapter 2).[135-141] The $\Delta E^{\ddagger}_{strain}$ value is the penalty required to deform the fragments from the transition structure. Since $\Delta E^{\ddagger}_{int}$ is related to the electronic structure of the deformed reactants, it accounts for the mutual interaction between these fragments.

4.3. Results and Discussion

The previous experimental mechanistic study of the catalytic branch-selective C–H alkylation of aryl sulfonamides with vinylsilanes revealed that the novel twisted paddlewheel-shaped dirhodium complex **26a** was isolated as a catalytically active species (Figure 4.1).[218,220] Interestingly, X-ray diffraction analysis showed that each sulfonamide substrate coordinates to each rhodium atom by the amino-quinoline moiety. Based on both experimental and computational analysis of dimeric rhodium(II) complexes in C–H functionalization reactions,[24,221-227] in-depth computational studies of the stability and reactivity of the isolated species, and the branch-selectivity of this reaction were carried out.

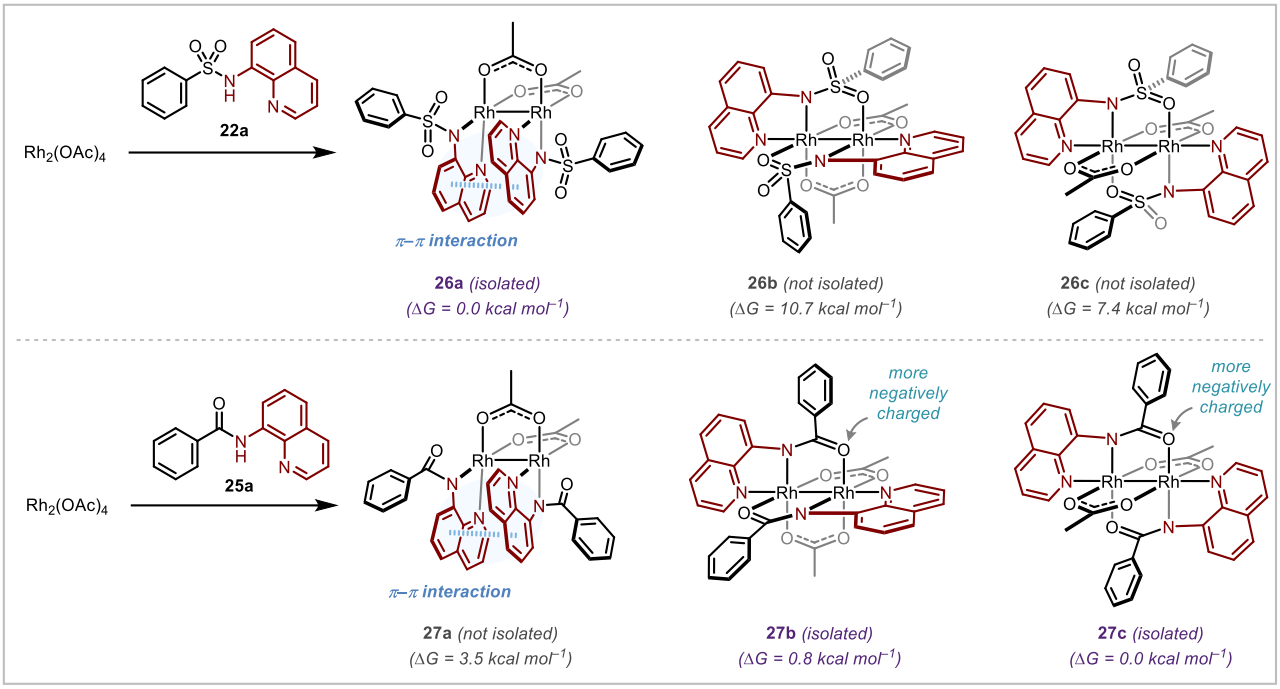
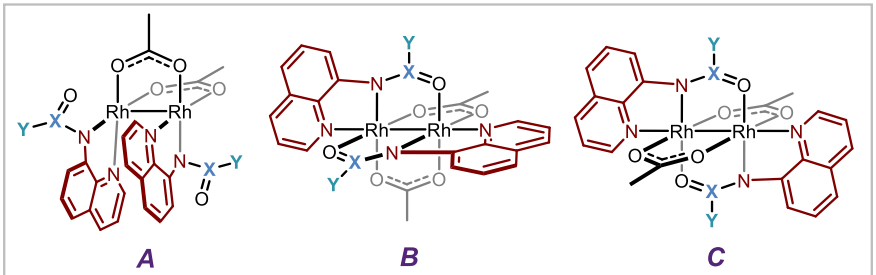


Figure 4.1. Structures and observed interactions of paddlewheel dirhodium complexes with sulfonamide and amide substrates. Relative stability (ΔG in kcal mol^{-1}) of dirhodium paddlewheel complexes are provided in the insert.

4.3.1. Complexation of Sulfonamides and Amides with Rhodium Dimer

Two coordination modes exist to generate isomeric paddlewheel-shaped dirhodium complexes. One is "twisted paddlewheel complex" where each substrate chelates to each rhodium center, and the second is a "tethered paddlewheel complex" with a substrate binds as a bridging ligand with an extra tethered axial coordination. Initially, the difference in coordination modes in the dirhodium paddlewheel complexes with suldonamides or amides were compared (Figure 4.1). As described above, only the twisted paddlewheel complex **26a** was observed when sulfonamide substrate was used, and the *cis*- or *trans*-oriented tethered paddlewheel complexes **26b** and **26c** could not be obtained.[220] The calculations suggest that the complexes **26b** and **26c** were energetically unstable compared to **26a** (10.7 and 7.4 kcal mol^{-1}, respectively). The phenyl group in **26a** is positioned away from rhodium because of the tetrahedral geometry of the sulfonamide moiety, the axial site becomes vacant. Moreover, both sulfonamide ligands are aligned to each other and stabilizes the dirhodium complex by π-π interaction between the quinoline rings. On the other hand, the twisted paddlewheel complex **27a** with *N*-(quinoline-8-yl)benzamide is relatively more unstable than *cis*- and *trans*-oriented tethered paddlewheel complexes **27b** and **27c**. Comparison between these calculated complexes and the model system in Figure 4.2 suggests that the steric bulk of the Ph group is not relevant, and the strain around the sulfur atom and the electronegativity of oxygen are the controlling factors for this trend.



		ΔG (kcal mol^{-1})		
X	Y	A	B	C
S=O	Ph	0.0	10.7	7.4
S=O	H	0.0	12.7	10.0
C	Ph	3.5	0.8	0.0
C	H	4.0	0.8	0.0

Figure 4.2. Relative stability (ΔG in kcal mol^{-1}) of dirhodium paddlewheel complexes with sulfonamide or amide substrates.

Generally, the Rh–Rh bond lengths of tethered paddlewheel complexes are shorter than those of twisted paddlewheel complexes (Table 4.1). The HOMO-LUMO energy gaps in the twisted paddlewheel complexes **26a** and **27a** are smaller, indicating that these complexes are more reactive. The LUMO is Rh–Rh σ* antibonding molecular orbital from the overlap of two d_{z2} orbitals, and the existence of vacant axial sites increases the reactivity to allow C–H activation to occur at this position (Figure 4.3).

Table 4.1. Relative Gibbs free energies (kcal mol^{-1}), molecular orbitals (eV), and Rh–Rh bond lengths (Å) of dirhodium complexes.

	ΔΔG	HOMO (eV)	LUMO (eV)	HOMO–LUMO (eV)	Rh–Rh (Å)
26a	***0.0***	–5.70	***–3.55***	***2.15***	***2.548***
26b	10.7	–5.56	–1.86	3.70	2.460
26c	7.4	–5.61	–1.95	3.66	2.465
27a	***3.5***	–5.53	***–3.21***	***2.31***	***2.543***
27b	0.8	–5.26	–1.84	3.43	2.430
27c	0.0	–5.24	–1.79	3.45	2.431

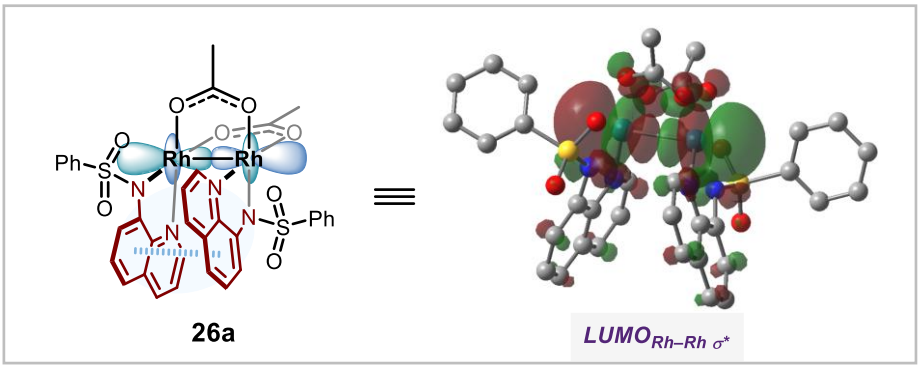


Figure 4.3. Lowest unoccupied molecular orbital (LUMO) of the dirhodium complex **26a**.

4.3.2. C–H Activation

The *ortho* C–H activation of the phenyl group is enabled by the dirhodium complex formation and the presence of a vacant axial site (Figure 4.4). For the simplicity of calculations, only the C–H activation of one sulfonamide in the dirhodium complex **26a** was considered throughout the catalytic cycle. Initially, rhodium(II) acetate $Rh_2(OAc)_4$ and two molecules of sulfonamide substrate **22a** react rapidly to generate a twisted paddlewheel complex **Int1_4**. Two acetic acid molecules coordinate on the axial sites, and the dissociation of these ligands gives more stable dirhodium complex **26a**. The Ph group of sulfonamide is pointing away from the rhodium atoms, and this is originating from the tetrahedral geometry of the sulfonamide group. When the Ph group approaches to the rhodium center, the *ortho* C–H bond is activated with the assistance of a bridged acetate ligand. This process occurs through the transition state **TS1_4**, and this is also known as the concerted-metalation-deprotonation (CMD) mechanism.[102-105] The C–H activation process leads to the formation of a perpendicular metallacycle **Int2_4**. It is worth noting that the Rh–Rh bond is elongated during the C–H activation process (**26a**: 2.548 Å, **TS1_4**: 2.621 Å, **Int2_4**: 2.702 Å). This is caused by the orbital overlap between the vacant Rh–Rh σ* molecular orbital and the π orbital of the Ph group. The formation of a perpendicular metallacycle is particularly rare compared to the commonly observed or hypothesized planar metallacycle because of its highly strained geometry. Nevertheless, it is possible to form such structure when sulfonamide and rhodium(II) acetate react to generate twisted paddlewheel complex with vacant axial sites. Consideration of other possible C–H activation transition states confirmed that **TS1_4** is the most reasonable TS in this step.

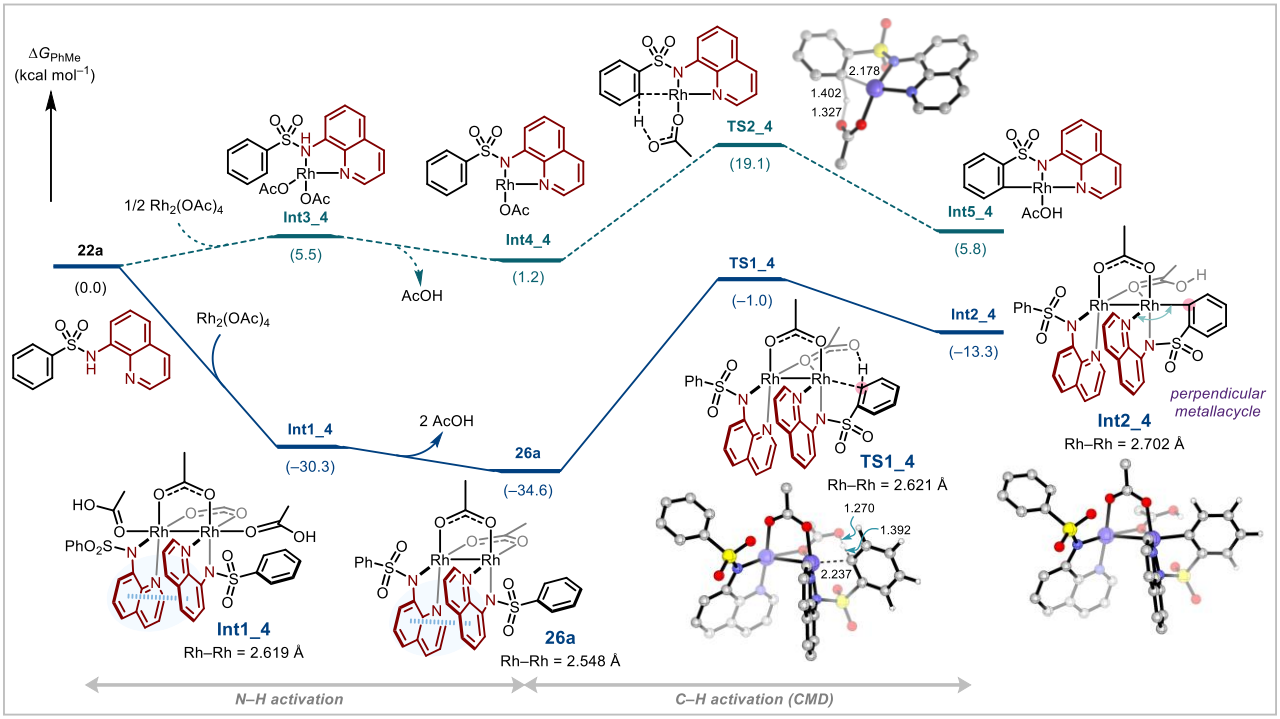


Figure 4.4. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the C–H activation step of monomeric and dimeric Rh(II)-catalyzed C–H alkylation of sulfonamides with vinylsilanes. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

In order to study the effect of the dirhodium complex for the C–H activation step, a homolytic dissociation of Rh–Rh bond for the formation of a monomeric rhodium(II) complex was calculated (green line in Figure 4.4). The rhodium complex **Int3_4** is initially formed, and the N–H bond activation and acetic acid dissociation give the Rh(II) species **Int4_4**. The *ortho* C–H bond is then cleaved by the CMD mechanism through **TS2_4** to furnish the planar metallacycle **Int5_4**. The energies of all monorhodium intermediate and transition state structures are much higher compared to the dirhodium species, which indicates the monomeric pathway is not involved.

4.3.3. Migratory Insertion

The perpendicular metallacycle **Int2_4** is then coordinated by vinylsilane to give **Int6_4** prior to the following C–C bond forming migratory insertion. Four possible transition states for the migratory insertion can be drawn, and the branch selectivity is ultimately determined by this step (Figure 4.5). Interestingly, the linear-selective migratory insertion transition states (**TS5_4**, **TS6_4**) are more destabilized than the branch-selective migratory insertion TSs (**TS3_4**, **TS4_4**). This selectivity trend agrees with experimental data, where branched products are obtained preferably.

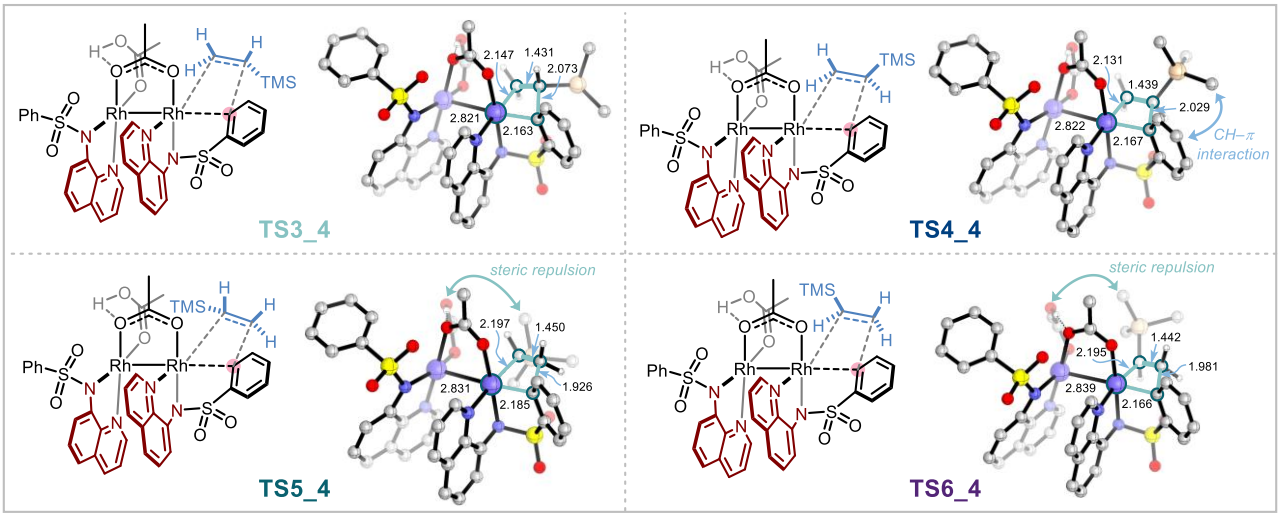


Figure 4.5. Transition state structures for the migratory insertion. Bond lengths (Å) of TS geometries are provided in the insert.

The rare branch selectivity originates from the steric clash between the trimethylsilyl group and the equatorial AcOH molecule on the non-participating rhodium atom.[228] The TMS group in linear-selective migratory insertion TSs has close contact with the methyl group of AcOH, and the acid ligand is forced to distort from the preferred geometry. Then, the distance between two rhodium atoms is elongated, which leads to destabilize the transition state structures by reduced orbital overlap between those atoms. As proof, a strong correlation between the Rh–Rh bond length and the Gibbs free energy ($\Delta G^{\ddagger}$) of transition states is observed (Figure 4.6). In addition, **TS4_4** is slightly more preferred over **TS3_4** due to the additional stabilizing CH–π interactions between TMS and Ph groups. The migratory insertion step was further examined using the activation strain analysis (ASA), and indeed, the origin of regioselectivity is the reduced strain energies in the branch-selective migratory insertion transition states (Figure 4.7).[135-141] Therefore, the steric repulsion between the perpendicular metallacycle and vinylsilane controls the branch selectivity.

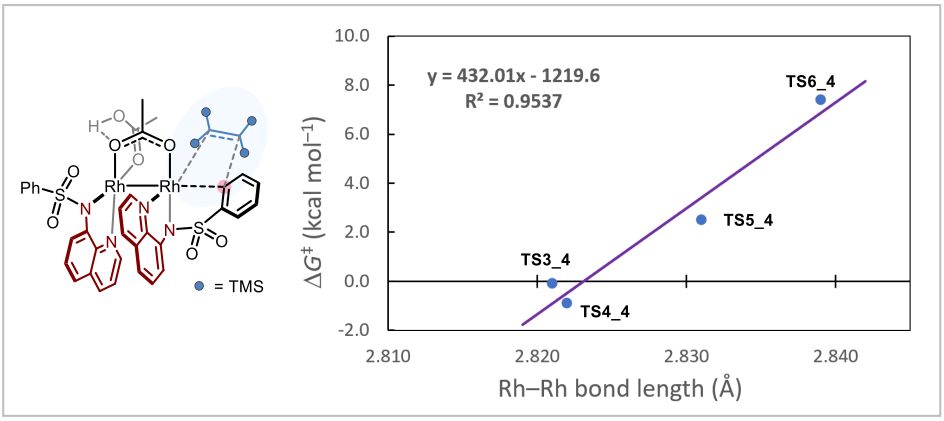


Figure 4.6. Correlation between Rh–Rh bond lengths (Å) and energies ($\Delta G^{\ddagger}$ [kcal mol^{-1}]) of the migratory insertion transition states.

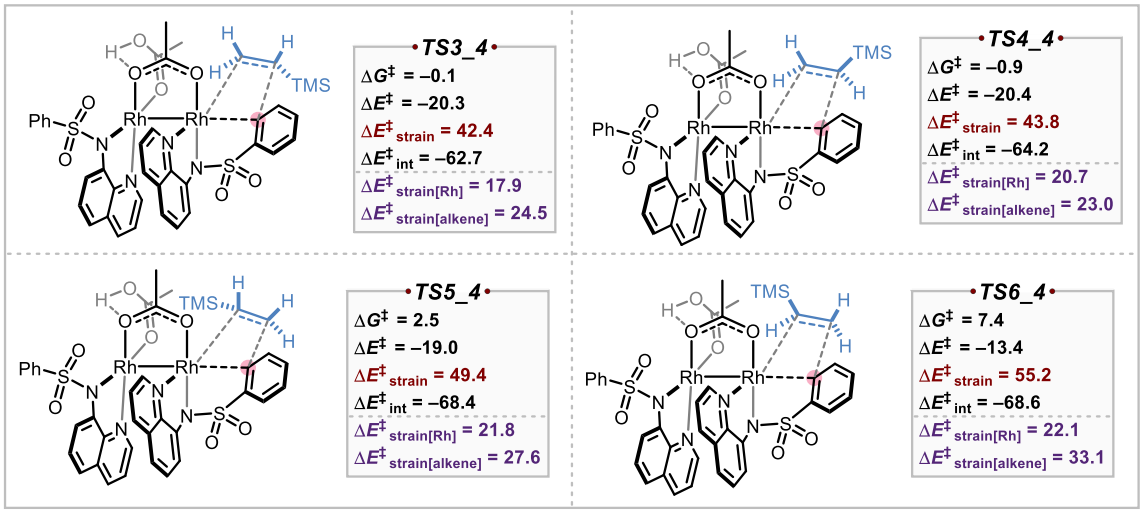


Figure 4.7. Activation strain analysis of migratory insertion transition states. Energies (kcal mol^{-1}) and bond lengths (Å) of TS geometries are provided in the insert.

In order to confirm the advantage of the dirhodium complexes, the migratory insertion of vinylsilane into the monomeric rhodium complex **Int5_4** was considered (Figure 4.8). As expected, the energy barriers are much higher than the dimeric pathway, and interestingly, the linear-selective transition states are highly preferred (**TS7_4** and **TS8_4**). This is due to the planarity of **Int5_4**, in which the Ph group is bulkier than the opposite quinolyl group. Therefore, the formation of a perpendicular metallacycle is extremely crucial for the realization of branch-selective alkylation.

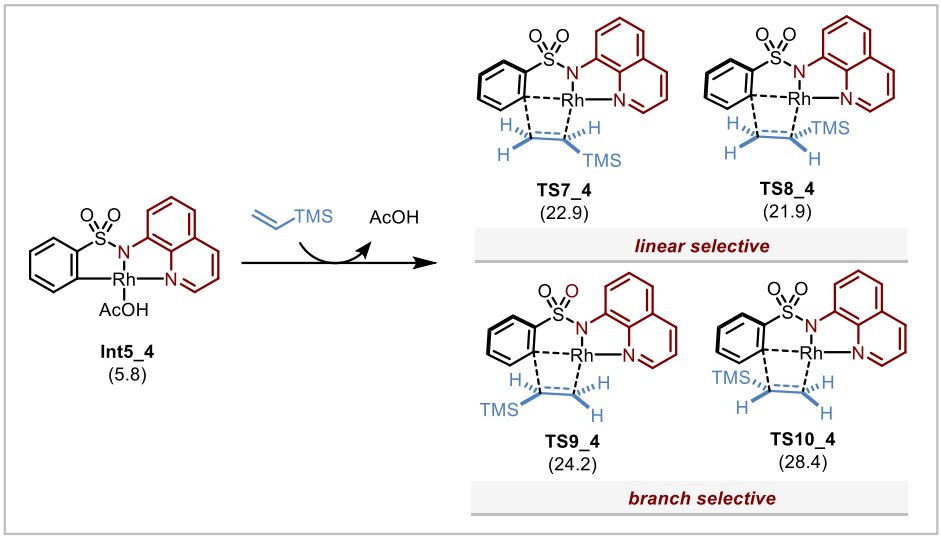


Figure 4.8. Transition state structures (Δ*G* [kcal mol^{-1}]) for the migratory insertion step of the monomeric rhodium(II)-catalyzed C–H alkylation of sulfonamides with vinylsilanes. Energies (kcal mol^{-1}) are provided in the insert.

4.3.4. Protonation and Catalyst Regeneration

Seven-membered metallacycles are formed after the migratory insertion (Figure 4.9 and 4.10), and the final protonation of the metallacycle completes the catalytic cycle. Overall, the intramolecular protonation transition states have higher energy barriers than the previous migratory insertion, and the trend is similar to the previous step, except for **TS14_4** with the lowest energy among the protonation TSs. This is because of the structural advantage of **TS14_4**, where the transition state is stabilized by the C–H bond coordination to the rhodium atom. The most favorable migratory insertion-intramolecular protonation sequence from **Int6_4** is through **TS4_4** and **TS12_4** for the formation of branch-selective product (blue line in Figure 4.9). The rate-limiting intramolecular protonation step is highly exergonic, and the branch-alkylated intermediate **Int12_4** is formed (Figure 4.11). The hydrogen-deuterium kinetic isotope effect (KIE) of 1.06 indicates that both the inverse KIE from the protonation and the normal equilibrium isotope effect (EIE) from the CMD step cancel out both effects.[218] A clear linear correlation between the relative Gibbs free energies and Rh–Rh bond lengths was again observed for the protonation TSs, indicating that the flexible sulfonamide group can change its geometry easily to minimize the Rh–Rh bond length, that ultimately increases the orbital overlap between two rhodium atoms to stabilize the transition state (Figure 4.12). Finally, the product is exchanged with the starting material to furnish the branch-alkylated product **24a**, and the catalytically active intermediate **26a** is regenerated.

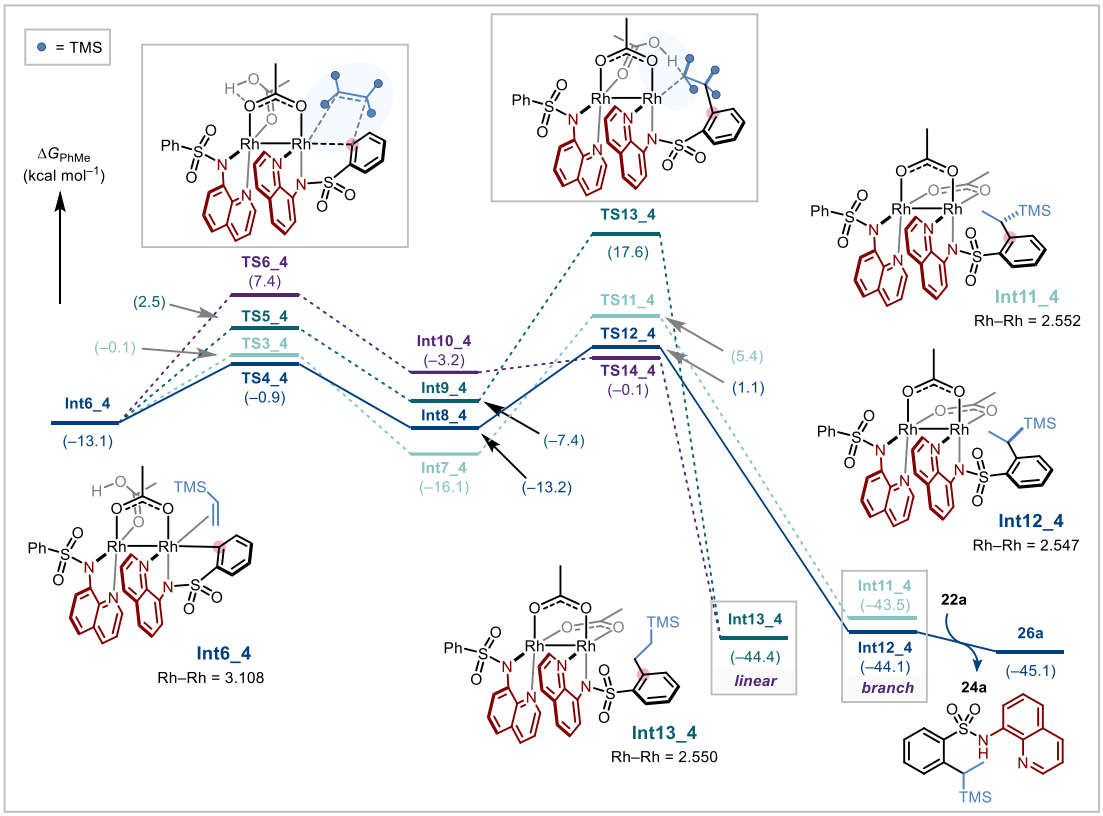


Figure 4.9. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the migratory insertion and the intramolecular protonation steps. Gibbs free energies are relative to **22a**.

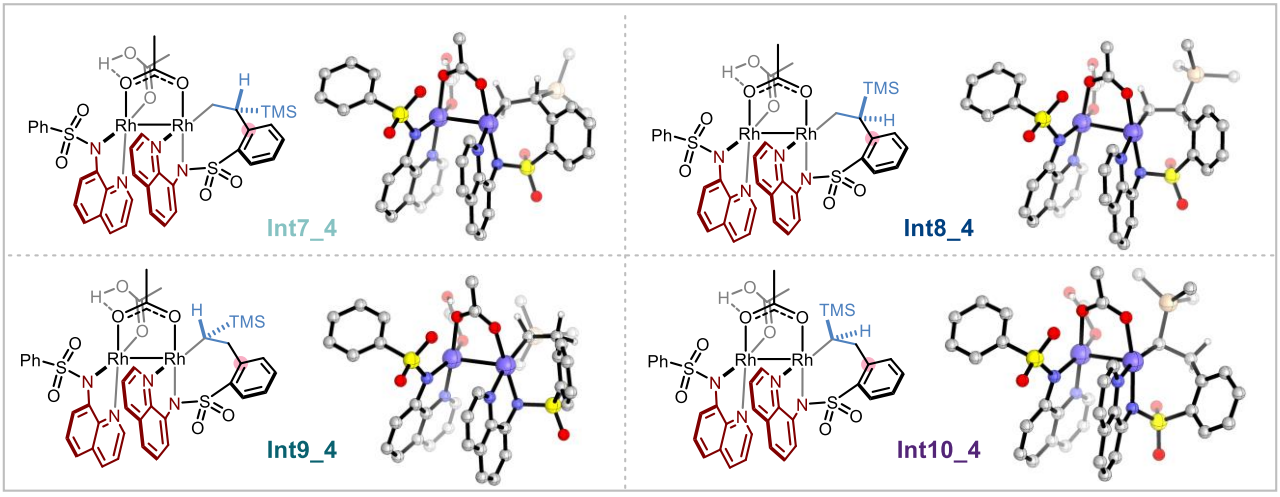


Figure 4.10. Intermediate structures after the migratory insertion.

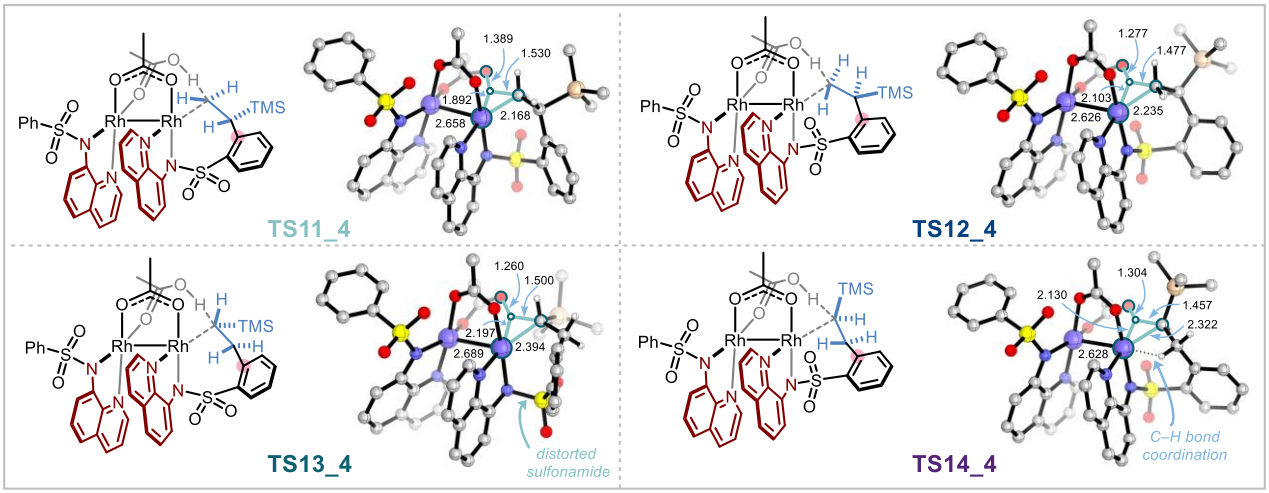


Figure 4.11. Transition state structures (ΔG [kcal mol^{-1}]) for the migratory insertion. Energies (kcal mol^{-1}) and bond lengths (Å) of TS geometries are provided in the insert.

The summary of computed catalytic cycle is described as follows. A catalytically active twisted paddlewheel dirhodium complex is initially generated from rhodium(II) acetate and sulfonamide substrate. Then, the *ortho* C–H bond is activated at the vacant axial site of the dirhodium complex to form a twisted paddlewheel complex. The following migratory insertion of vinylsilane is branch selective due to the steric clash between TMS and an adjacent acetic acid molecule. Final intramolecular protonation is highly exergonic, and the branch-alkylated product is released.

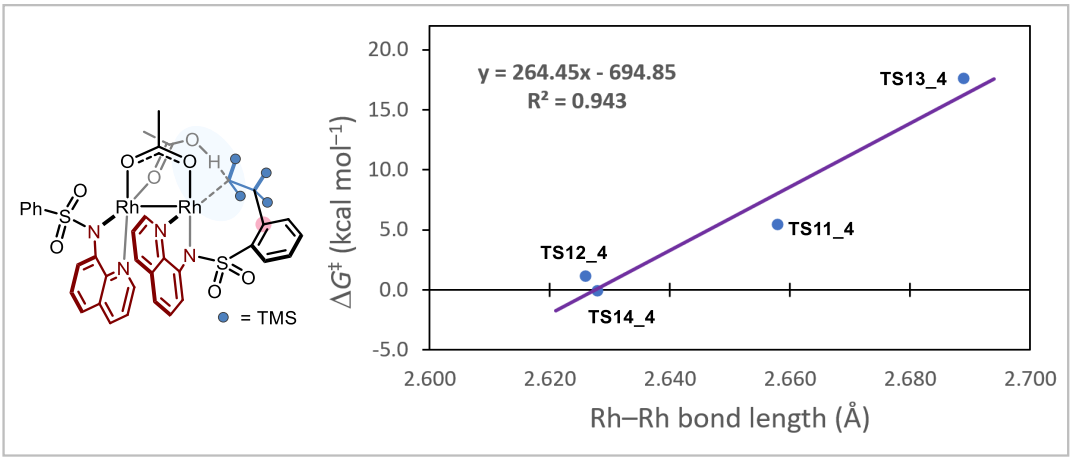


Figure 4.12. Correlation between Rh–Rh bond lengths (Å) and energies ($\Delta G^{\ddagger}$ [kcal mol^{-1}]) of the protonation transition states.

4.4. Conclusion

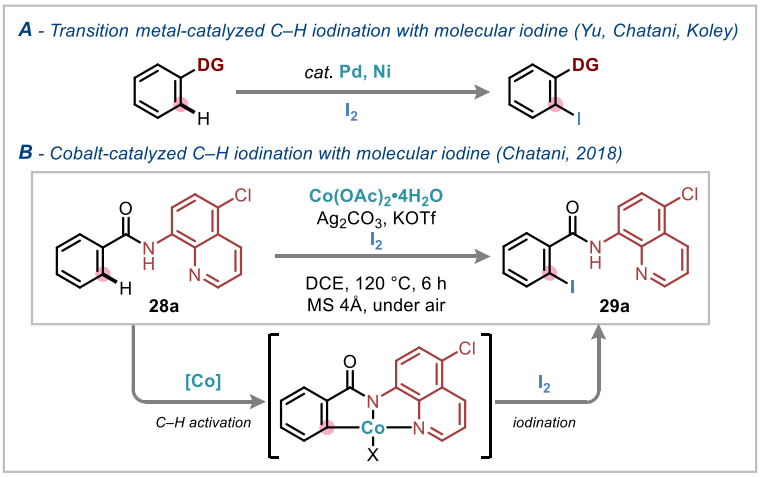
In conclusion, a detailed mechanistic study of the Rh(II)-catalyzed branch-selective C–H alkylation of aryl sulfonamides with vinylsilanes was performed using a computational approach. The formation of a catalytically active twisted paddlewheel complex leads to the generation of a rare perpendicular metallacycle. The branch selectivity originates from the steric repulsion between the perpendicular metallacycle and the vinylsilane, in which the TMS group and the acetic acid molecule cause a significant destabilization in linear-selective transition states. This state-of-the-art computational method enabled us to pinpoint the origin of this rare selectivity, and these mechanistic insights will facilitate the future development and design of more efficient reaction conditions.

Chapter 5

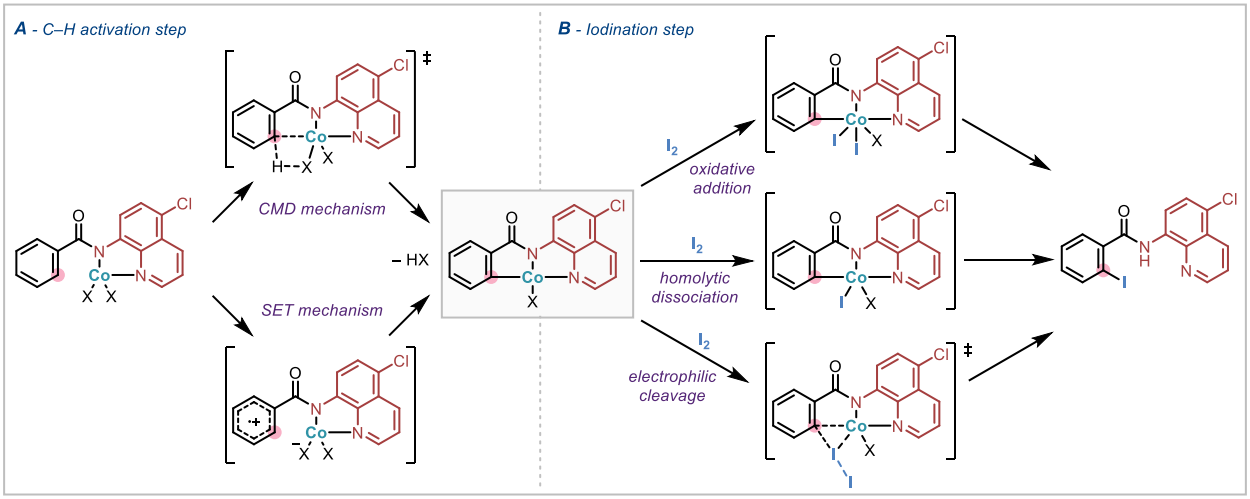
Cobalt-Catalyzed C–H Iodination with Molecular Iodine

5.1. Introduction

Transition metal-catalyzed C–H bond functionalization has been acknowledged as a powerful and economical method by synthetic and medicinal chemists.[12,15-17,21,62,66,111-114,149] Direct C–H bond modification enables an efficient construction of novel functionalized compounds from robust materials compared to the classical cross-coupling reactions, which are usually limited to the use of organoborons or organic halides. One of the most desired transformations is C–H bond halogenation for the preparation of precursors that can be used for a wide variety of applications.[229-233] Previously, the Yu, Chatani, and Koley groups reported C–H iodination reactions with palladium or nickel catalysts using molecular iodine as a mild and inexpensive iodinating reagent (Scheme 5.1A).[234-237] In addition, the Chatani group discovered that a cobalt catalyst can also be used with an appropriate directing group, and the reaction conditions are mild and not air sensitive (Scheme 5.1B).[238] Based on mechanistic investigations, the proposed mechanism involves two steps: (i) a C–H activation process and (ii) an iodination process. The initial C–H activation process can be either the CMD process through C–H bond cleavage and Co–C bond formation, or single electron transfer (SET) via a radical cation intermediate (Scheme 5.2A). On the other hand, the iodination process proceeds through either the oxidative addition of I_2, the homolytic dissociation of I–I, or an electrophilic cleavage mechanism (Scheme 5.2B). Radical trap experiments with TEMPO or BHT and the deuterium labeling experiments suggested that the C–H activation occurs by the SET mechanism.[238] Since the true nature of cobalt complexes during such C–H activation reactions is not fully understood due to their complexity, the density functional theory (DFT) method was used in this study for gaining mechanistic insights.



Scheme 5.1. Transition metal-catalyzed C–H iodination with molecular iodine.



Scheme 5.2. (A) Plausible C–H activation step, and (B) plausible iodination step.

5.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional[86,87] with the 6-31G(d) basis set for C, H, N, O, F, S, Cl and the Lanl2dz effective core potential (ECP) for Co.[88-90] Single point energy calculations were performed using the B3LYP functional[86,87] with the 6-311+G(d,p) basis set for C, H, N, O, F, S, Cl and the SDD ECP for Co.[92-94] The polarizable continuum model (PCM) solvent effects were incorporated into all calculations with dichloroethane (DCE) as the solvent.[95-97] Each reported minimum has a zero imaginary frequency and each transition state (TS) has only one imaginary frequency. Energy changes were determined from the Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using CYLview20.[101] The minimum energy crossing point (MECP) between the potential energy surfaces (PESs) of the singlet and triplet states was located with the code developed by Harvey and coworkers at the PCM(DCE)/B3LYP/SDD(Co)-6-311+G(d,p)//PCM(DCE)/B3LYP/Lanl2dz(Co)-6-31G(d) level of theory.[239-243]

5.3. Results and Discussion

5.3.1. C–H Activation

Co(II) species are known to easily oxidized in the presence of Ag_2CO_3, thus we used the Co(III) species in the catalytic cycle.[244] Initially, the singlet complex **Int1_S_5** is converted to the σ-complex **Int2_S_5** by κ^2-κ^1-displacement of the acetate ligand by the *ortho*-C–H bond. This leads to increase the acidity of the *ortho*-C–H bond because of the coordination of the C–H σ orbital to the cobalt atom (Figure 5.1). The C–H bond is then activated to give the five-membered cobaltacycle **Int3_S_5** through the

concerted-metalation deprotonation (CMD) transition state **TS1_S_5**. This mechanism involves an agostic interaction and is known as "ambiphilic metal–ligand activation (AMLA)", and can facilitate the CMD process (AMLA/CMD).[23] The triplet complex **Int1_T_5** was energetically unfavorable relative to **Int1_S_5** by 6.3 kcal mol^{-1}, and the triplet transition state **TS1_T_5** was also higher in energy than **TS1_S_5** by 1.6 kcal mol^{-1}. Interestingly, the σ-complex **Int2_T_5** could not be located, and the five-membered cobaltacycle **Int3_T_5** was highly stabilized compared to the singlet form. These data suggest that the C–H activation occurs on the singlet surface, and after the Co–C bond formation, spin crossover occurs to give the triplet cobaltacycle. The minimum energy crossing point (MECP) was energetically similar to **Int3_S_5**. During the C–H activation process on the triplet surface, the spin densities of the cobalt atom increased (1.12 for **Int1_T_5**, 1.21 for **TS1_T_5**, and 1.50 for **Int3_T_5**). A strong correlation between the spin density of the cobalt atom and the singlet-triplet energy gap was observed, indicating that the spin localization on the cobalt atom stabilizes the complexes (Scheme 5.3).

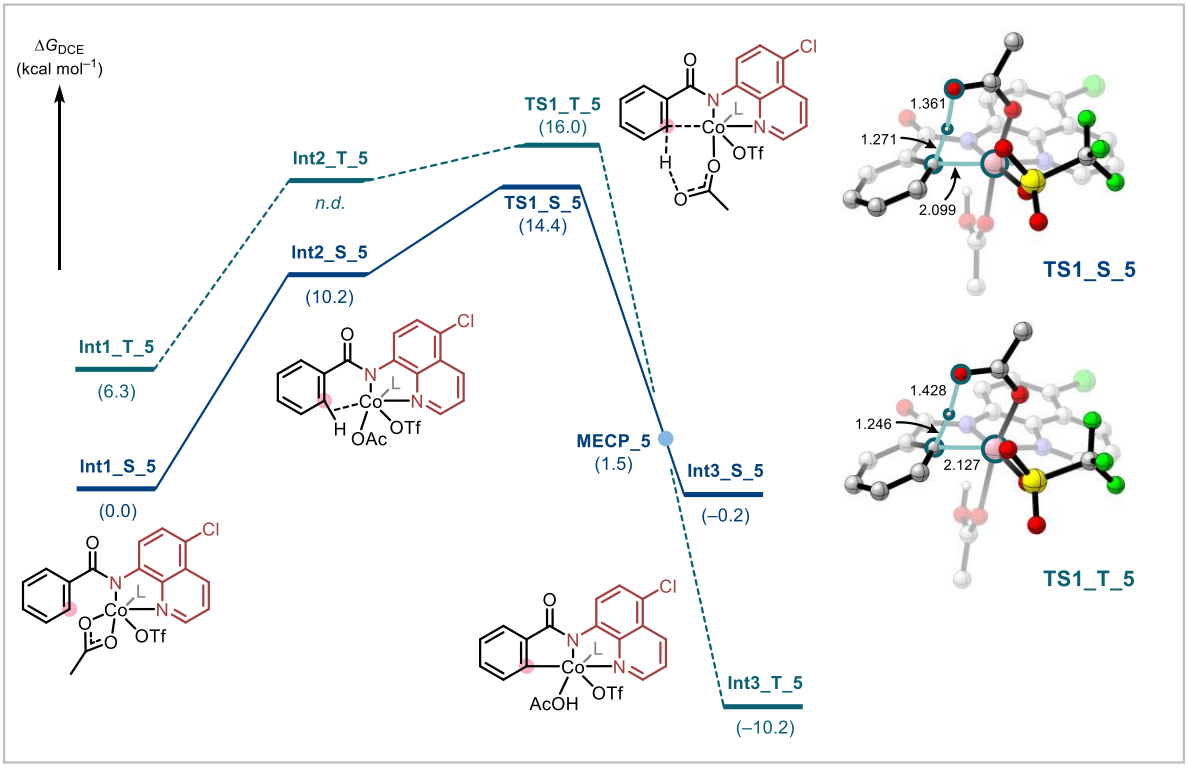
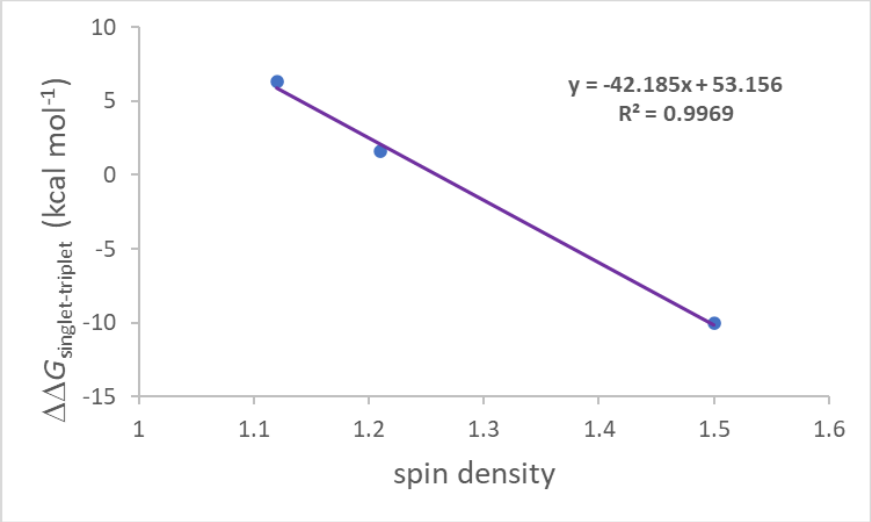


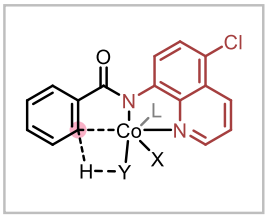
Figure 5.1. Computed reaction energy profile (Δ*G* [kcal mol^{-1}]) for the C–H activation step of cobalt-catalyzed C–H iodination with molecular iodine. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert. L = AcOH.



Scheme 5.3. Correlation between the singlet-triplet energy gaps (ΔΔ*G* [kcal mol^{-1}]) and the spin densities of the cobalt atom.

To investigate the nature of the AMLA/CMD process, the effect of coordinating deprotonating ligands (Y) and non-deprotonating ligands (X and L) were studied (Table 5.1). Both anionic and neutral non-deprotonating ligands had a minor effect on the C–H activation process (entries 1–4), and the deprotonating ligands had a huge impact with large energy barrier differences (entry 5). Thus, the choice of deprotonating ligands is crucial for the AMLA/CMD process.

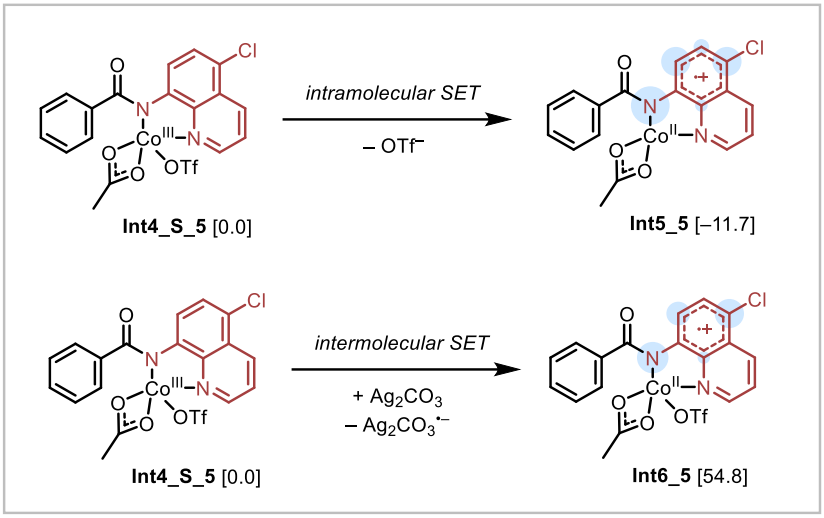
Table 5.1. Effects of deprotonating and non-deprotonating ligands for the AMLA/CMD process.



entry	X	Y	L	$\Delta G^{\ddagger}_{singlet}$
1	OTf	OAc	AcOH	4.2
2	I	OAc	AcOH	3.8
3	HCO_3	OAc	AcOH	5.3
4	OTf	OAc	TfOH	3.8
5	OTf	OTf	AcOH	15.2
6	OTf	HCO_3	AcOH	6.1

An alternative C–H activation pathway is the single electron transfer (SET) process, and this mechanism involves either intra- or intermolecular transfer of a single electron from the Ph ring to the cobalt atom.[245-247] Interestingly, both intra- and intermolecular SET process leads to the formation of Co(II) complex, however the spin was only localized on the amide nitrogen and the quinoline ring, but not on the Ph ring (Scheme 5.4). Experimental mechanistic studies showed that the deuterium KIE value was 1.1 and

the reaction was inhibited by radical scavengers.[238] Even though the experiments support the SET process rather than the CMD process, the absence of a radical on the *ortho* carbon atom of the Ph ring suggests that the Co–C bond cannot be formed by the SET process.



Scheme 5.4. Spin densities of the possible intermediates of intra- and intermolecular SET processes. Energies (kcal mol^{-1}) are provided in the insert. Blue dots represent the localized spin densities.

5.3.2. Mechanism of Iodination Process

After the acid ligand dissociation and iodine coordination, the cobaltacycles **Int7_T_5** and **Int8_T_5** are generated (Figure 5.2). As expected, the singlet states of the cobaltacycles **Int7_S_5** and **Int8_S_5** are less stable than their triplet forms. Three possible iodination pathways are the oxidative addition, the homolytic dissociation, and the electrophilic cleavage, and the reaction energy profile is shown. The oxidative addition pathway is initiated by the oxidative addition of molecular iodine to Co(III) through the transition state **TS2_T_5** to give the Co(V) intermediate **Int9_T_5**. The following reductive elimination has a higher energy barrier to furnish the iodinated complex **Int10_T_5**. The homolytic dissociation pathway is initiated by the I–I bond cleavage to obtain the Co(IV) species **Int11_D_5** and the iodine radical (ΔG = 6.0 kcal mol^{-1}). The following reductive elimination occurs through **TS4_D_5**, and this energy barrier is similar to the one for the previous pathway. Finally, the electrophilic cleavage pathway is initiated by the electrophilic attack of molecular iodine on the Co–C bond, and this goes through the three-membered transition state **TS5_T_5** ($\Delta G^{\ddagger}$ = 4.8 kcal mol^{-1}). After the C–I bond is formed, the iodine anion interacting with another iodine atom in **Int13_T_5** is transferred to the cationic cobalt atom to furnish the thermodynamically more stable complex **Int10_T_5**. The overall energy barrier is the lowest for the electrophilic cleavage pathway, and the valence of cobalt atom remains unchanged throughout the step.

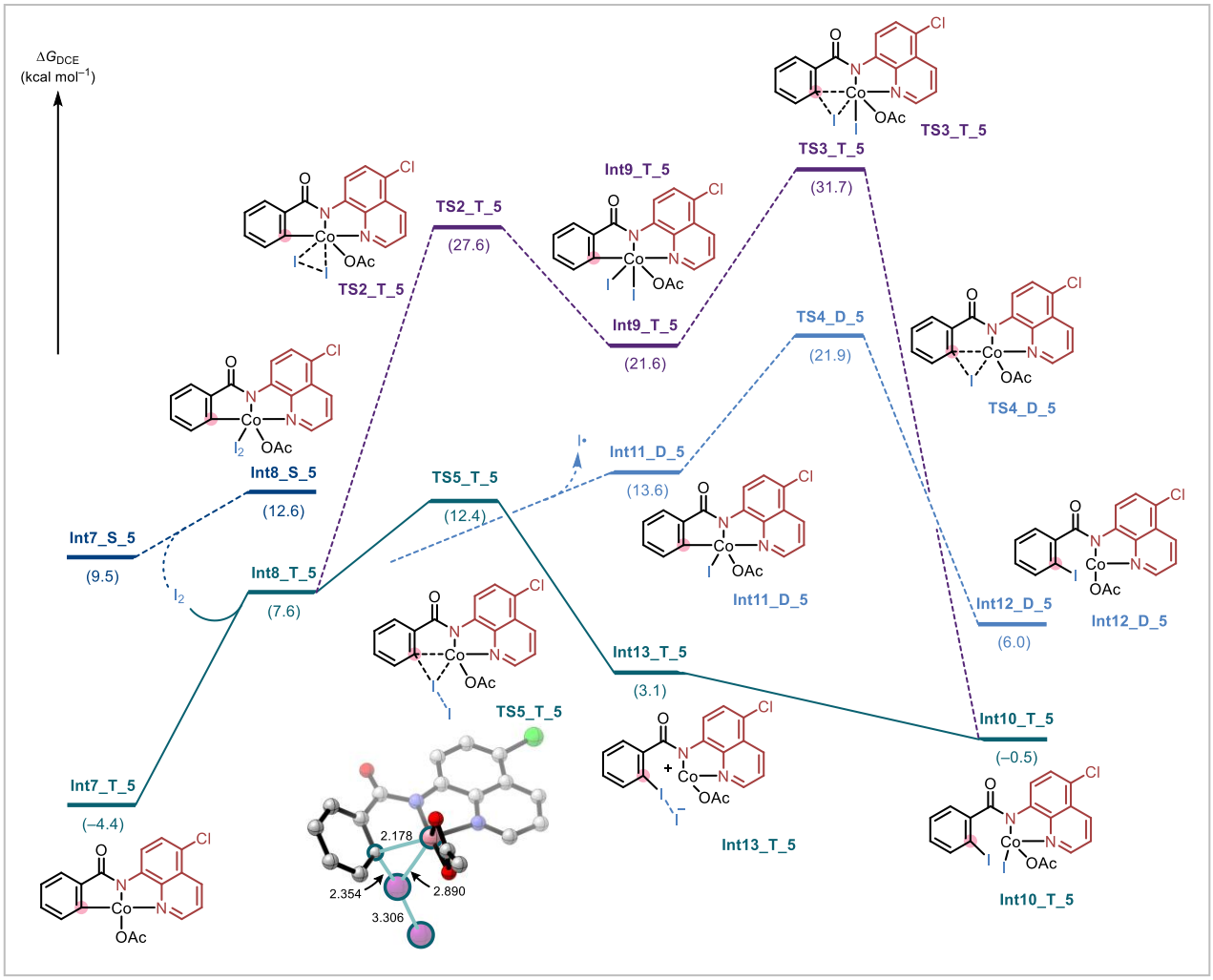


Figure 5.2. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the iodination step of the cobalt-catalyzed C–H iodination with molecular iodine. Energies (kcal mol^{-1}) and bond lengths (Å) are provided in the insert.

To further investigate the electrophilic cleavage pathway, the transition of spin densities of cobalt and iodine atoms throughout the pathway was studied (Figure 5.3). The molecular iodine coordination to **Int7_T_5** leads to the spin transfer from cobalt to iodine atoms, which results in the cobalt center being spin neutral. The cobalt atom regains the spin at the transition state **TS5_T_5**, and both the proximal and terminal iodine atoms are now spin neutral. Therefore, the facile spin transfer between cobalt and iodine atoms enables the lower energy barrier for the electrophilic cleavage pathway.

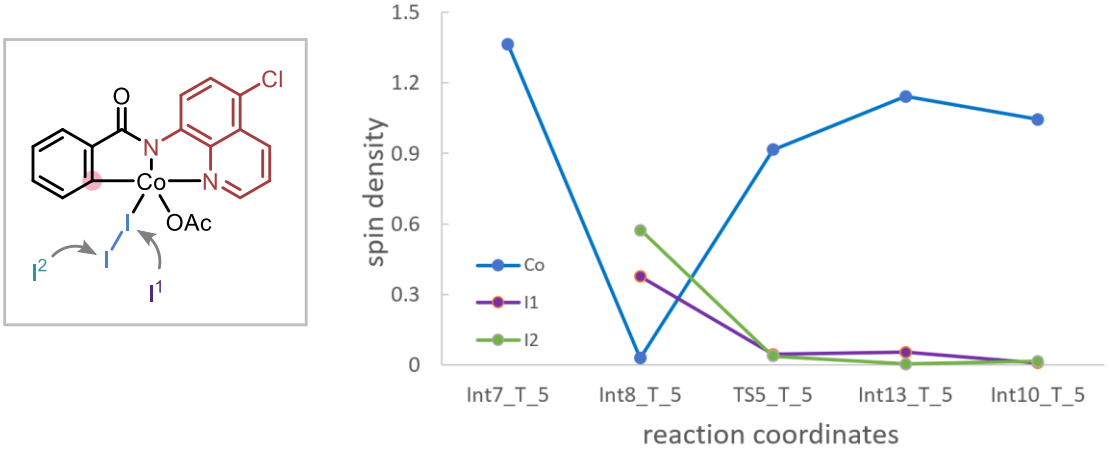


Figure 5.3. Transition of spin densities of cobalt and iodine atoms (I^1: proximal iodine, I^2: terminal iodine).

5.4. Conclusion

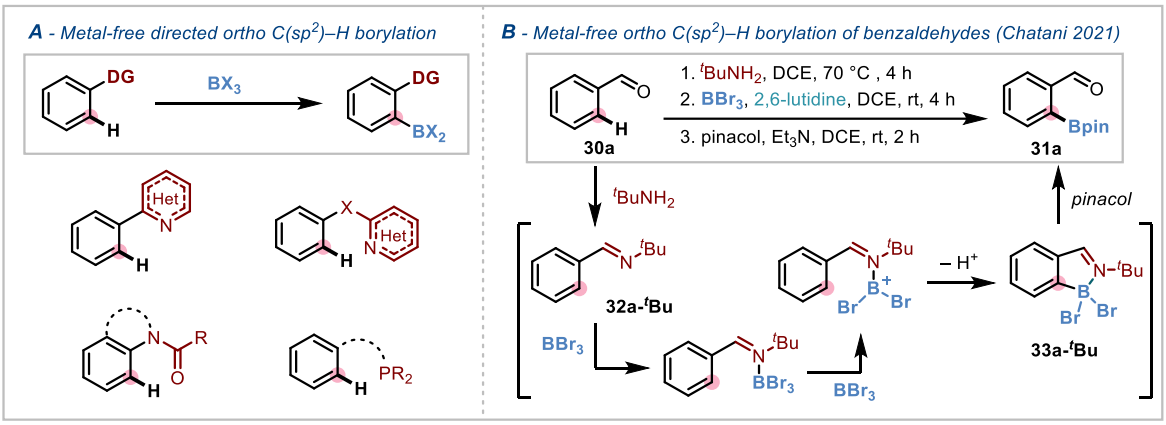
In conclusion, a mechanistic study of the cobalt-catalyzed C–H iodination with molecular iodine using the 8-aminoquinoline directing group was performed in this study. The reaction proceeds through C–H activation iodination steps, and the unique nature of the cobalt atom leads to the spin crossover between these two steps. The C–H activation is promoted by an agostic interaction and goes through the singlet surface. The singlet-triplet spin crossover takes place after the cobaltacycle formation due to the spin localization on the cobalt atom. The following iodination step proceeds through the electrophilic cleavage mechanism on a triplet surface, and the valency of the cobalt atom remains unchanged throughout the step. The current study will prove the unique nature of cobalt atoms and that both singlet and triplet states should be considered, and that mechanistic studies such as KIE or radical scavenger inhibition experiments may be misleading when considering mechanisms without computational analysis.

Chapter 6

Metal-Free *ortho* C–H Borylation of Benzaldehydes

6.1. Introduction

A borylation reaction is an exceptionally useful strategy for the synthesis of highly functionalized compounds.[248-254] Organoboron reagents can be used in a wide variety of applications such as natural product synthesis and drug discovery.[255,256] The most general C–H borylation of aromatic compounds is to use transition metal catalysis, which has been extensively studied over two decades.[250,257-261] Transition metal catalysts in this field often provide high selectivity, however the cost and toxicity of these precious transition metals limit their application. To avoid these limitations, a transition-metal-free borylation of C(sp^2)–H bonds has been achieved using boron trihalides (BX_3, X = Cl, Br) and various directing groups, such as *N*-heterocycles, amides, and phosphines (Scheme 6.1A).[262-285] Usually harsh reaction conditions are required, and the use of a directing group may cause decomposition of product during the directing group removal.



Scheme 6.1. Metal-free directed *ortho* C(sp^2)–H borylation of benzaldehydes.

In order to avoid these drawbacks, the metal-free *ortho* C–H borylation of benzaldehydes using a transient imine directing group was discovered and reported from the Chatani group (Scheme 6.1B).[286] The main advantages of this are that the reaction is step economical because the installation and removal of the directing group is not needed, and electron-deficient benzaldehydes can be used as a starting material under mild reaction conditions. Several experimental mechanistic studies were performed, and the proposed reaction mechanism is as follows: (i) complexation between the imine **32a-^{t}Bu** and BBr_3 provides a Lewis acid/base adduct, (ii) formation of borenium intermediate by disproportionation, (iii) electrophilic aromatic

substitution (S_EAr), and (iv) rearomatization to give the cyclic borylated compound **33a-^{t}Bu**. Finally, addition of pinacol and an aqueous work-up furnish the borylated aldehyde **31a**. To elucidate the detailed mechanism and the observed reactivity enhancement with a particular functional group, a detailed computational approach was used in this study.

6.2. Computational Details

Calculations were performed with the Gaussian 09 (G09) program.[85] Geometry optimizations and frequency calculations for all reported structures were performed using the B3LYP functional with the 6-31G(d) basis set.[86,87] Dispersion interactions were included using Grimme's DFT-D3 correction with Becke-Johnson damping.[287,288] Single point energy calculations were performed using the M06-2X functional with the 6-311+G(d,p) basis set.[133] The solvation model based on density (SMD) solvent effects were incorporated into all calculations with dichloroethane (DCE) as the solvent.[134] Each reported minimum has zero imaginary frequency and each transition state (TS) has only one imaginary frequency. Energy changes were shown by the use of Gibbs free energies (T = 298.15 K and P = 1 atm). Optimized structures were illustrated using CYLview20.[101]

Quantitative analyses of the activation barriers associated with the Lewis acid-base complexation were performed using the activation strain model (ASM). ASM involves the decomposition of the electronic energy (ΔE) of the structure into the strain energy (ΔE_{strain}) associated with the structural deformation of the Lewis acid and BBr_3 and the interaction energy (ΔE_{int}) between the deformed reactants [Eq. 1] (see Chapter 2).[135-141] The ΔE_{strain} value is the penalty required to deform the fragments from the complex. Since ΔE_{int} is related to the electronic structure of the deformed reactants, it accounts for the mutual interaction between these fragments.

6.3. Results and Discussion

6.3.1. Reaction Energy Profile

A full reaction energy profile was initially computed (Figure 6.1). The complexation of BBr_3 with the *tert*-butyl substituted imine **32a-^{t}Bu** is slightly exergonic by 1.1 kcal mol^{-1}, and **Int1-^{t}Bu_6** is generated. Then, another molecule of BBr_3 abstracts the bromine atom from the **Int1-^{t}Bu_6** adduct through **TS1-^{t}Bu_6**, and the borenium species **Int2-^{t}Bu_6** is obtained with an activation energy barrier of 20.8 kcal mol^{-1}. Since the boron atom in **Int2-^{t}Bu_6** is electropositive, the intramolecular electrophilic aromatic substitution (S_EAr) proceeds through **TS2-^{t}Bu_6** with a small energy barrier. Finally, the adjacent BBr_4^- anion deprotonates the Wheland intermediate **Int3-^{t}Bu_6** through **TS3-^{t}Bu_6** and the borylated product **33a-^{t}Bu** is generated.

The optimal reaction conditions require the addition of 2,6-lutidine, and the involvement of the base was computed. The boron-lutidine complex **Int4-L3_6** is relatively more stable (ΔG = 3.4 kcal mol^{-1}),

and the disproportionation transition state **TS4-L3_6** has a lower energy barrier, indicating that the borenium species **Int5-L3_6** is easily formed in the presence of 2,6-lutidine. In order to transfer the "BBr_2^+" species from **Int5-L3_6** to the imine substrate, the tetrahedral intermediate **Int6-L3_6** is generated after the interaction with **32a-^{t}Bu**, and the subsequent elimination of 2,6-lutidine gives thermodynamically stable **Int2-^{t}Bu_6**. Alternatively, the tetrahedral intermediate **Int7-L3_6** with two molecules of 2,6-lutidine can be formed, which was observed by an NMR experiment in the previous report.[286] Overall, the reaction rate is accelerated with 2,6-lutidine by rapid borenium intermediate formation.

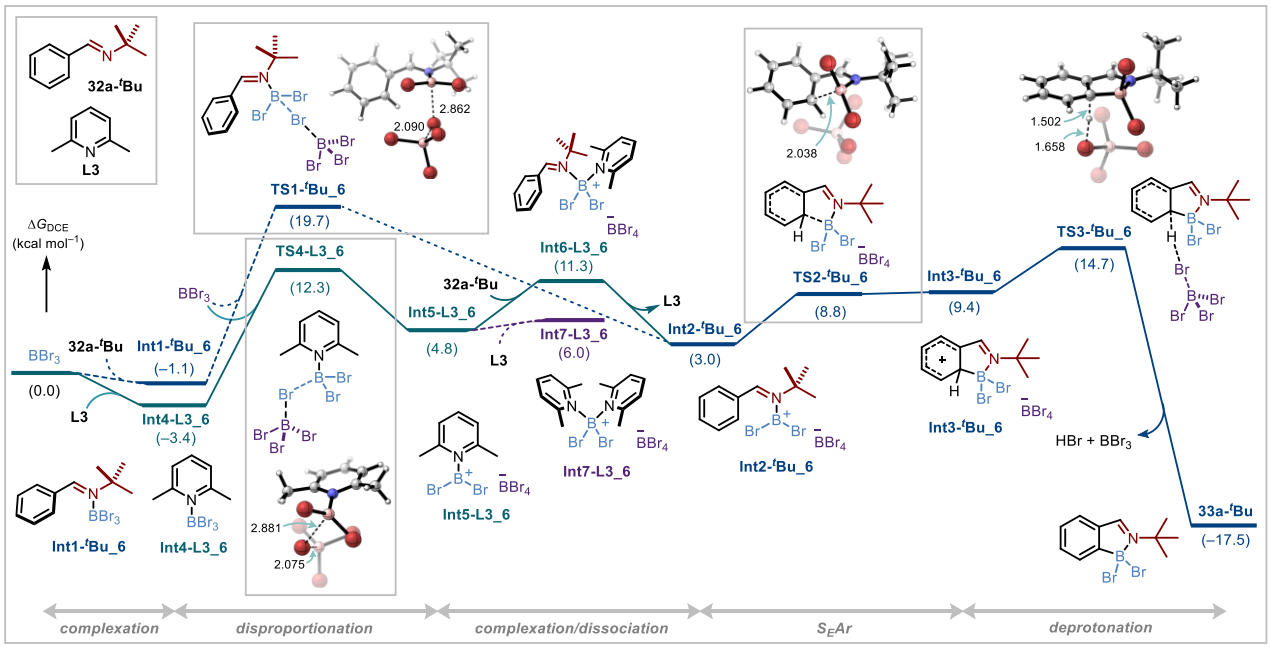


Figure 6.1. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the metal-free *ortho* C–H borylation. Energies (kcal mol^{-1}) and bond lengths (Å) of computed geometries are provided in the insert.

6.3.2. Reactivity Difference of Imines

The choice of substituent for the transient imine directing group was extremely important for achieving high reactivity (Figure 6.2). Especially, a bulkier substituent such as ^{t}Bu group improved the yield dramatically. To interpret this reactivity difference, we performed calculations with several different imines.

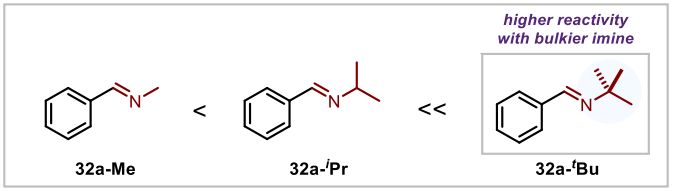


Figure 6.2. Reactivity enhancement with various imines.

Reaction energy profiles with various imines are shown in Figure 6.3. In comparison to the ^{t}Bu group, the complexation between BBr_3 and the ^{i}Pr-substituted imine **32a-^{i}Pr** furnished highly stabilized complex **Int1-^{i}Pr_6** (ΔG = –12.2 kcal mol^{-1}). The borenium species **Int2-^{i}Pr_6** is similar to **Int2-^{t}Bu_6** in terms of the stability (ΔG = 2.7 kcal mol^{-1}). In addition, the following S_EAr step through **TS2-^{i}Pr_6** and the deprotonation step through **TS3-^{i}Pr_6** have slightly smaller energy barriers, but the overall trend does not change dramatically. The Me-substituted imine **321-Me** is less hindered, and as expected, the imine-BBr_3 complex **Int1-Me_6** was even more stable with a strong B–N bond (ΔG = –14.8 kcal mol^{-1}). Furthermore, the S_EAr-deprotonation sequence also follows the similar trend. The potential energy surface with various imines revealed that the reaction rate is determined by the stability of the imime-BBr_3 complex **Int1_6** and the deprotonation transition state **TS3_6**. Since the trend of stability of **Int1_6** follows the experimentally observed reactivity difference, the complexation process is the key step to control the reaction.

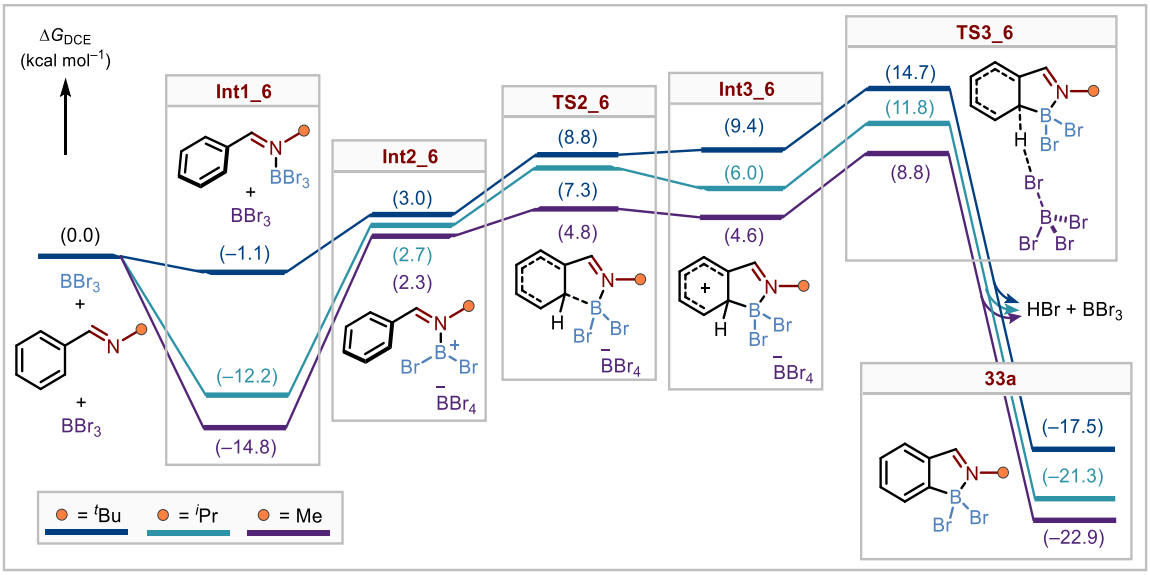
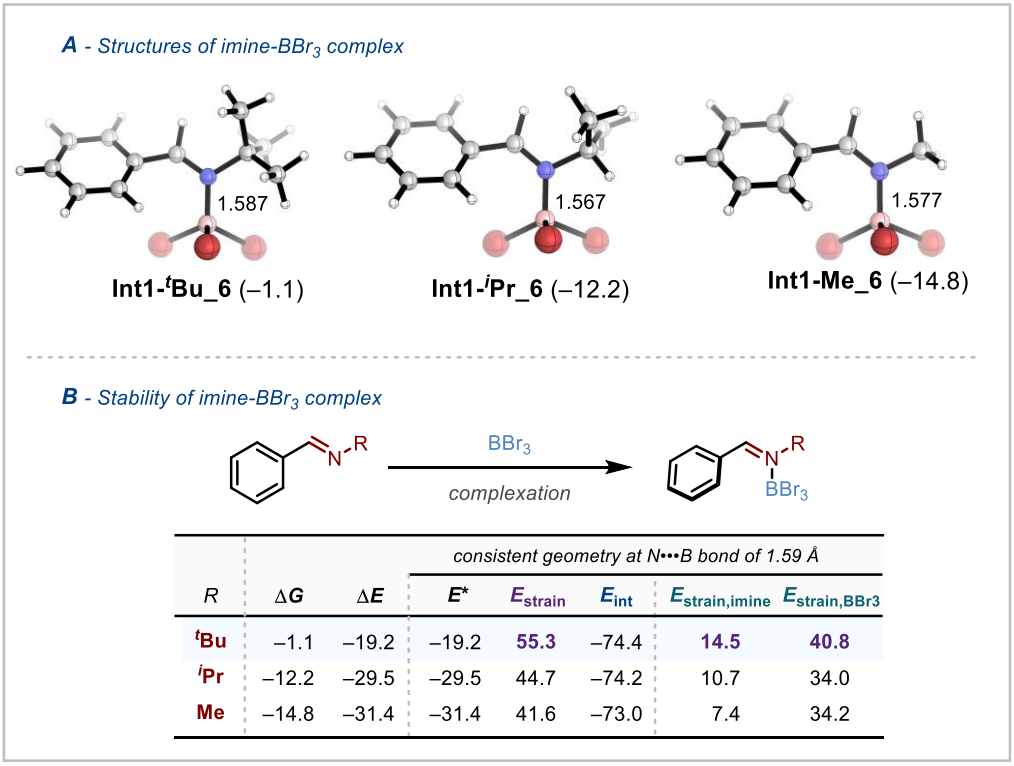


Figure 6.3. Computed reaction energy profile (ΔG [kcal mol^{-1}]) for the metal-free *ortho* C–H borylation from imines. Energies (kcal mol^{-1}) of computed geometries are provided in the insert.

The origin of the stability of imine-BBr_3 complexes was analyzed using the activation strain model (ASM).[135-141] The ASM involves the decomposition of the electronic energy into strain energy that is associated with the rigidity of the reactants and interaction energy between the deformed imine and BBr_3 fragments at consistent geometry with a B–N bond distance (1.59 Å) in order to ensure that the results are not skewed by the fact that the complexes have different equilibrium bond lengths (Figure 6.4).[289] The ASM revealed that the relative stability trend is controlled by the strain energy, and the interaction energies are identical in all cases. The E_{strain} can be further decomposed into the strain energies of the imine fragment ($E_{strain,imine}$) and boron tribromide fragment ($E_{strain,BBr3}$). Both fragments are responsible for the destabilized strain energies, but the majority of E_{strain} originates from the distortion of planar BBr_3 into a tetrahedral

geometry, which causes a steric repulsion with the imine substituent. Therefore, less hindered substituents such as ^{i}Pr or Me groups can avoid substantial steric clash with BBr_3, which results in the irreversible complexation process.



			consistent geometry at N•••B bond of 1.59 Å				
R	Δ*G*	Δ*E*	*E*‡	E_{strain}	E_{int}	$E_{strain,imine}$	$E_{strain,BBr3}$
^{t}Bu	–1.1	–19.2	–19.2	**55.3**	–74.4	**14.5**	**40.8**
^{i}Pr	–12.2	–29.5	–29.5	44.7	–74.2	10.7	34.0
Me	–14.8	–31.4	–31.4	41.6	–73.0	7.4	34.2

Figure 6.4. Structures (A) and relative stabilities (B) of imine-BBr_3 complexes. The activation strain analysis was performed at consistent geometry with a B–N bond distance of 1.59 Å. Energies (kcal mol^{-1}) and bond lengths (Å) of computed geometries are provided in the insert.

6.3.3. Reactivity Difference of Bases

The reactivity can also be tuned by the choice of a base (Figure 6.5). Unsubstituted pyridine or 4-dimethylaminopyridine (DMAP) inhibited the product formation, while 2,6-lutidine improved the yield dramatically and gave the borylated product in an excellent yield.

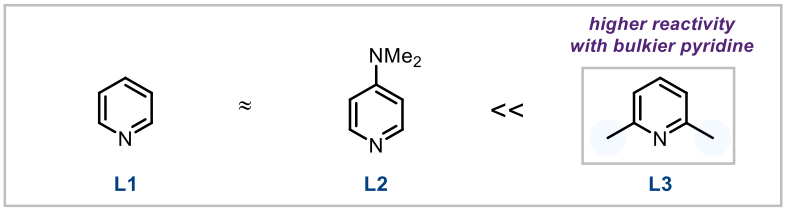
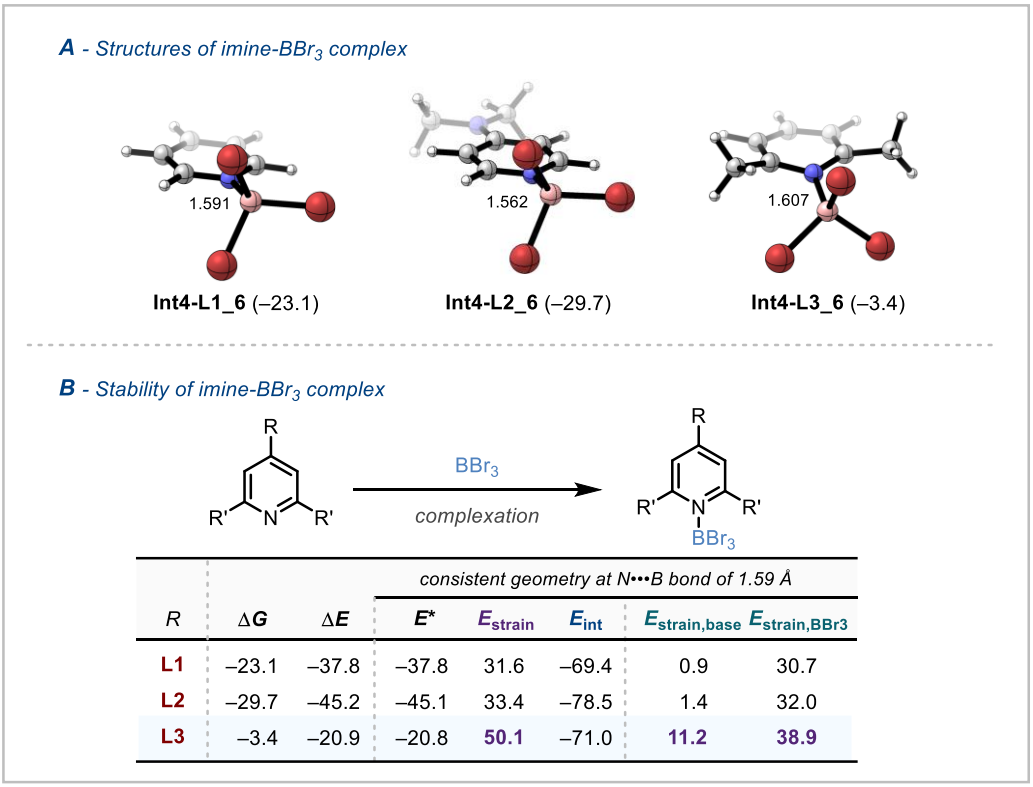


Figure 6.5. Reactivity enhancement with various imines.

Surprisingly, the base-BBr_3 complexes with pyridine (**L1**) or 4-dimethylaminopyridine (**L2**) are extremely stable (ΔG = –23.1 and –29.7 kcal mol^{-1}, respectively), considering the fact that the 2,6-lutidine-BBr_3 complex **Int4-L3_6** is more labile (ΔG = –3.4 kcal mol^{-1}) (Figure 6.6). The longest B–N bond length with **L3** (1.607 Å) also agrees that the complexation is reversible. In order to pinpoint the reason behind this stability difference, the activation strain analysis at a consistent geometry with a B–N bond distance was performed (1.59 Å), and a significant amount of strain energy was observed in **Int4-L3_6**.[289] When **Int4-L3_6** is compared to **Int4-L1_6**, two adjacent methyl groups increased the strain energy to destabilize the complex. Further decomposition of E_{strain} into strain energies of both fragments revealed that both fragments are responsible for this phenomenon. As described above, the complexation process causes the planar BBr_3 to distort into a tetrahedral geometry, and the two adjacent methyl groups of 2,6-lutidine are forced to bend, which causes the pyridine ring to be slightly twisted from the planar structure. As a result, the complexation between BBr_3 and **L3** becomes a reversible process, and the borenium species "BBr_2^+" can be transferred smoothly to the imine substrate.



			consistent geometry at N•••B bond of 1.59 Å				
R	Δ*G*	Δ*E*	*E**	E_{strain}	E_{int}	$E_{strain,base}$	$E_{strain,BBr3}$
L1	–23.1	–37.8	–37.8	31.6	–69.4	0.9	30.7
L2	–29.7	–45.2	–45.1	33.4	–78.5	1.4	32.0
L3	–3.4	–20.9	–20.8	**50.1**	–71.0	**11.2**	**38.9**

Figure 6.6. Structures (A) and relative stabilities (B) of pyridine-BBr_3 complexes. The activation strain analysis was performed at consistent geometry with a B–N bond distance of 1.59 Å. Energies (kcal mol^{-1}) and bond lengths (Å) of computed geometries are provided in the insert.

6.4. **Conclusion**

In conclusion, mechanistic details of the metal-free *ortho* C–H borylation of benzaldehydes using an imine transient directing group were thoroughly studied with a computational approach. The reaction is initiated by the complexation between BBr_3 and 2,6-lutidine, and "BBr_2^+" is smoothly transferred to the imine substrate after disproportionation. Then, the electrophilic aromatic substitution and deprotonation gives the final C–H borylated product. The origin of the reactivity enhancement was studied using activation strain analysis, and the increased destabilizing strain energies with a bulky transient directing group and base leads to a reversible complexation process with BBr_3. The detailed computational analysis revealed the tunability of such reactions, and the findings may be applied for further reaction development.

Conclusion

In this thesis, detailed computational studies of various C–H bond activation reactions have been discussed using the state-of-the-art density functional theory. In Chapter 1, the nickel-catalyzed oxidative C−H/N−H annulation of benzamides with alkynes was described. The first catalytic cycle is initiated from a Ni(II) species and undergoes the CMD-migratory insertion-reductive elimination sequence to furnish the cyclized product. The valency of the metal remains unchanged until the product release, where the formed Ni(0) triggers the main catalytic cycle as a form of nickelate complex. Our computational analysis revealed that the C−H activation step in the main catalytic cycle is through the LLHT mechanism, and the originally proposed oxidative addition does not occur under the reaction conditions. Experimentally observed regioselectivities with asymmetrical alkynes and *meta*-substituted aromatic amides were successfully explained using the current model. Furthermore, the computational results can be extended to an *N*-heterocyclic compounds. In Chapter 2, the rhodium-catalyzed oxidative C–H alkenylation and coupling sequence of unprotected 1-naphthylamines with *α,β*-unsaturated esters was described. Detailed calculations revealed that there are several steps in the catalytic cycle that determines the regioselectivities of the product, including the C–H activation, migratory insertion, and *β*-hydride elimination processes, and all the results agree with the experimentally observed selectivity. The quantitative analysis of the key C–C bond forming migratory insertion using the activation strain analysis revealed that the steric repulsion between the aromatic ring and the ester group is decisive for the selectivity. In Chapter 3, the iridium-catalyzed C–H alkynylation of 2-acylimidazoles with alkynyl bromides was described. The state-of-the-art DFT calculations revealed that the previously proposed oxidative addition pathway is energetically unfavored, and instead, the unexpected mechanism that involves sequential double 1,2-migration of bromine and silicon atoms is the favorable pathway. The experimentally observed reactivity difference with various alkynyl bromides originated from the second 1,2-migration step, and the transition state with the most reactive silyl group is stabilized by the *β*-silicon effect. In Chapter 4, the dimeric rhodium-catalyzed branch-selective C–H alkylation of aryl sulfonamides with vinylsilanes was described. The CMD process from the catalytically active twisted paddlewheel dirhodium complex leads to the formation of a rare perpendicular metallacycle, and this intermediate controls the regioselectivity during the migratory insertion process with the steric repulsion between the metallacycle and the vinylsilane. The computations with a model planar metallacycle also proved that the perpendicular metallacycle is the key for the reaction. In Chapter 5, the cobalt-catalyzed C–H iodination with molecular iodine using the 8-aminoquinoline directing group was described. The initial C–H activation proceeds through the singlet surface, and the unique character of cobalt leads to the spin crossover after the CMD step. The most favorable iodination step was the electrophilic cleavage mechanism on a triplet surface, and the valency of the cobalt atom remained unchanged throughout the catalytic cycle. In Chapter 6, the metal-free directed *ortho* C–H borylation of benzaldehydes using an imine transient directing group was described. The experimentally observed reactivity enhancement with a bulky imine and base was

thoroughly studied, and the reversibility during the complexation process between the imine or base and BBr_3 due to steric repulsion leads to a lower activation energy barrier. These results showcase the detailed mechanistic insights into the C–H activation reactions, and we believe that these studies will allow us to unveil broader reaction mechanisms and to further develop the field of organic and organometallic chemistry.

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Computational Details

Table 7.1. Energies (in Hartrees) and imaginary frequencies (in *i* cm^{-1}) of all stationary points in Chapter 1 are provided.

structure	*E*	*ZPE corr.*	*H corr.*	*G corr.*	Imag. Freq.
1a	-746.5589655	0.241498	0.257026	0.198220	-
^{t}Bu^{-}	-233.1362105	0.121180	0.128439	0.092531	-
^{t}BuOH	-233.6864178	0.135623	0.143314	0.106597	-
2a	-746.0423433	0.227312	0.242442	0.185036	-
Ni(OAc)$_2$	-626.3663171	0.103704	0.115232	0.065672	-
PPh$_3$	-1036.327968	0.273803	0.290666	0.227637	-
OAc^{-}	-228.5986816	0.048238	0.052749	0.022342	-
Int1_1	-2180.149231	0.557851	0.597682	0.480899	-
TS1_1	-2180.100224	0.552817	0.591860	0.478101	1375.41i
Int2_1	-2180.112107	0.557245	0.597022	0.480353	-
PhCCPh	-539.4839997	0.191624	0.203658	0.150820	-
AcOH	-229.0999814	0.061617	0.067160	0.034208	-
Int3_1	-2490.483905	0.686424	0.733066	0.600993	-
TS2_1	-2490.473533	0.686572	0.732158	0.603331	252.56i
TS3_1	-2490.445995	0.685943	0.731637	0.603187	273.20i
Int4_1	-2490.524998	0.688649	0.734451	0.604139	-
TS4_1	-2490.502897	0.687668	0.732794	0.604732	300.82i
Int5_1	-1951.704692	0.503310	0.538070	0.432551	-
3a	-1284.889558	0.414400	0.440218	0.357493	-
TS5_1	-1951.670764	0.497903	0.532174	0.429323	845.55i
Int6_1	-1951.697237	0.500563	0.534540	0.433597	-
Int7_1	-1454.842486	0.417084	0.446669	0.352926	-
TS6_1	-1454.837641	0.417040	0.445446	0.357216	62.01i
TS7_1	-1454.813580	0.416814	0.445023	0.356012	219.33i
Int8_1	-1454.868958	0.420665	0.449553	0.358563	-
Int9_1	-1454.882292	0.421042	0.450339	0.357645	-
TS8_1	-1454.836222	0.416180	0.445022	0.355194	351.36i
Int10_1	-1994.356106	0.613871	0.655378	0.535182	-
TS9_1	-1994.343369	0.613771	0.654312	0.536535	182.75i
Int11_1	-1994.403636	0.615772	0.656458	0.537829	-
TS10_1	-1994.368891	0.614786	0.654651	0.539422	312.52i
***cis*-stilbene**	-540.724310	0.215114	0.227151	0.176472	-
Int12_1	-1952.198364	0.516494	0.551692	0.443422	-
TS11_1	-1952.168653	0.511269	0.546084	0.439592	709.96i
TS12_1	-1952.173760	0.510573	0.545558	0.437771	1065.34i
Int13_1	-1952.186766	0.514147	0.548618	0.445228	-
Int14_1	-1952.198281	0.511685	0.547097	0.438416	-
Int15_1	-2491.220645	0.696390	0.742409	0.612693	-
TS13_1	-2491.140131	0.693799	0.740457	0.607900	313.78i
Int16_1	-2491.179990	0.697390	0.744033	0.609886	-
TS14_1	-2491.126227	0.691680	0.737478	0.608876	448.07i
Int17_1	-1454.801257	0.417821	0.446313	0.358091	–

Table 7.2. Energies (in Hartrees) and imaginary frequencies (in *i* cm^{-1}) of all stationary points in Chapter 1 are provided.

structure	*E*	*ZPE corr.*	*H corr.*	*G corr.*	Imag. Freq.
PhCCMe	-347.736414	0.138004	0.147301	0.103446	-
Int18_1	-1263.129016	0.367536	0.393903	0.308711	-
Int19_1	-1263.128318	0.367819	0.394070	0.310156	-
TS15_1	-1263.08699	0.362506	0.388560	0.304934	316.57i
TS16_1	-1263.085461	0.362584	0.388569	0.305552	300.55i
Int20_1	-1263.118779	0.367604	0.393388	0.310377	-
Int21_1	-1263.119277	0.367462	0.393287	0.310830	-
Int22_1	-1610.860665	0.507534	0.542869	0.436397	-
Int23_1	-1610.861955	0.507712	0.542922	0.438166	-
Int24_1	-1610.858292	0.507503	0.543185	0.435185	-
Int25_1	-1610.857492	0.507566	0.542832	0.440009	-
TS17_1	-1610.842144	0.507181	0.541506	0.439110	205.11i
TS18_1	-1610.844397	0.507310	0.541628	0.439412	142.63i
TS19_1	-1610.843444	0.506409	0.541135	0.437442	210.71i
TS20_1	-1610.845808	0.506994	0.541522	0.438906	144.98i
Int26_1	-1610.906159	0.509874	0.544112	0.440894	-
Int27_1	-1610.906129	0.509817	0.544105	0.441674	-
Int28_1	-1610.906959	0.509973	0.544229	0.442497	-
Int29_1	-1610.908689	0.509153	0.543905	0.439575	-
TS20_CF3_1	-1791.903902	0.420047	0.452754	0.352428	310.84i
TS21_CF3_1	-1791.897169	0.420117	0.452682	0.353767	413.37i
TS20_Me_1	-1494.153478	0.443110	0.474027	0.378564	392.15i
TS21_Me_1	-1494.150421	0.443753	0.474246	0.380862	280.12i
TS20_OMe_1	-1569.361692	0.448011	0.479833	0.381598	366.33i
TS21_OMe_1	-1569.361311	0.448307	0.479944	0.383677	532.52i
Int30_1	-1319.784167	0.393029	0.419206	0.331712	-
TS22_1	-1319.739035	0.387709	0.413361	0.329652	355.56i
Int31_1	-1319.769552	0.392925	0.418292	0.335016	-
Int32_1	-1859.256662	0.585769	0.623985	0.510726	-
TS23_1	-1859.239062	0.585791	0.622978	0.512065	201.94i
Int33_1	-1859.303632	0.587933	0.625071	0.514791	-
TS24_1	-1859.254661	0.586704	0.623231	0.515122	283.44i
Int34_1	-1859.259184	0.587932	0.624983	0.516133	-
8a	-610.9578451	0.199299	0.211013	0.161744	-
9a	-1149.293955	0.373014	0.395000	0.321484	-
Int35_1	-1319.757825	0.392566	0.418765	0.331364	-
TS25_1	-1319.726556	0.386119	0.412222	0.326188	989.12i
Int36_1	-1319.747455	0.387976	0.414341	0.327871	-
TS26_1	-1319.738276	0.387175	0.412750	0.329358	452.59i
Int37_1	-1319.765305	0.391632	0.417377	0.332398	-
TS27_1	-1319.725302	0.387851	0.412922	0.330977	1316.21i
Int38_1	-1319.788472	0.393917	0.418918	0.337973	-

Table 7.3. Energies (in Hartrees) and imaginary frequencies (in *i* cm^{-1}) of all stationary points in Chapter 2 are provided.

structure	*E*	*H*	*G*	E^{high}	Imag. Freq.
13a	-956.66431815	-956.311850	-956.389618	-957.39041224	-
10a	-441.25737314	-441.083457	-441.125402	-441.03598919	-
Int1_2	-1397.93164335	-1397.402062	-1397.499840	-1398.44597888	-
AcOH	-229.08771031	-229.020189	-229.053272	-229.04074492	-
Int2_2	-1168.80944806	-1168.351489	-1168.438774	-1169.36989731	-
TS1_2	-1168.77133319	-1168.319658	-1168.404666	-1169.33760176	1158.84i
Int3_2	-1168.79250537	-1168.334867	-1168.421936	-1169.36053829	-
TS2_2	-1168.76324312	-1168.310598	-1168.394932	-1169.32940634	756.98i
Int4_2	-1168.76516868	-1168.308411	-1168.395302	-1169.33108816	-
TS3_2	-1397.87461216	-1397.352139	-1397.450760	-1398.39902871	1314.56i
Int5_2	-1397.90379977	-1397.375711	-1397.474673	-1398.42660123	-
TS4_2	-1246.14924492	-1245.656436	-1245.743770	-1246.68137666	295.88i
TS5_2	-1246.15194909	-1245.658881	-1245.745769	-1246.68763921	290.41i
TS6_2	-1246.13652488	-1245.644150	-1245.730732	-1246.67083556	298.71i
TS7_2	-1246.14018981	-1245.647527	-1245.734576	-1246.67411546	311.50i
11a	-306.47278325	-306.369255	-306.406857	-306.37435639	-
Int6_2	-1246.17997720	-1245.685776	-1245.773362	-1246.70960766	-
Int7_2	-1246.17801954	-1245.682250	-1245.771201	-1246.70476257	-
TS8_2	-1246.13736680	-1245.647453	-1245.732576	-1246.66218394	1461.88i
Int8_2	-1475.29046338	-1474.723842	-1474.825318	-1475.77173257	-
TS9_2	-1475.26814167	-1474.706425	-1474.807864	-1475.75049701	680.59i
Int9_2	-1475.27471693	-1474.710931	-1474.812432	-1475.75340406	-
Int10_2	-1246.16610265	-1245.670477	-1245.758084	-1246.68898684	-
$Cu_2(OAc)_4$	-1306.36546006	-1306.133382	-1306.210605	-1308.59619996	-
$Cu_2(OAc)_2$	-849.43509184	-849.316570	-849.371167	-851.77791107	-
Int11_2	-1703.19986972	-1702.586908	-1702.701890	-1703.62860886	-
Int12_2	-1474.07333576	-1473.531901	-1473.632785	-1474.54640480	-
TS10_2	-1474.06012426	-1473.519678	-1473.619236	-1474.53592277	231.23i
TS11_2	-1474.04217014	-1473.502028	-1473.600230	-1474.52334306	132.51i
Int13_2	-1474.06580024	-1473.523756	-1473.621619	-1474.54274782	-
Int14_2	-1474.10534952	-1473.562721	-1473.662151	-1474.58067461	-
TS12_2	-1474.05423337	-1473.517348	-1473.615457	-1474.53236572	729.78i
TS13_2	-1474.07342713	-1473.536195	-1473.634461	-1474.55402718	704.32i
Int15_2	-728.74931764	-728.446639	-728.513424	-729.51892424	-
12a	-745.35454524	-745.120101	-745.173803	-745.03754204	-

Table 7.4. Energies (in Hartrees) and imaginary frequencies (in *i* cm^{-1}) of all stationary points in Chapter 3 are provided.

structure	*E*	*H*	*G*	E^{high}	Imag. Freq.
Int1_3	-1333.17268440	-1332.671117	-1332.765968	-1332.30414997	-
TS1_3	-1333.13804943	-1332.642067	-1332.731758	-1332.27622919	1165.02*i*
Int2_3	-1333.16191702	-1332.660721	-1332.753606	-1332.30055211	-
Int3_3	-1104.06661287	-1103.634055	-1103.713259	-1103.24635666	-
AcOH	-229.08941518	-229.023009	-229.053717	-229.04324993	-
TMSCCBr	-3057.12929895	-3056.995325	-3057.043956	-3059.33085420	-
TS2_3	-4161.15935623	-4160.592830	-4160.698875	-4162.54495966	168.22*i*
Int4_3	-4161.19637760	-4160.627016	-4160.732495	-4162.57494932	-
TS3_3	-4161.18346491	-4160.615901	-4160.720406	-4162.56846562	324.47*i*
TS4_3	-4161.13828373	-4160.572453	-4160.678463	-4162.52797908	531.51*i*
TS5_3	-4161.17889978	-4160.612569	-4160.716494	-4162.57587163	231.82*i*
TS6_3	-4161.16963716	-4160.603191	-4160.707152	-4162.57229940	314.40*i*
Int5_3	-4161.24648069	-4160.677257	-4160.781490	-4162.63335825	-
Int6_3	-4161.23299536	-4160.664141	-4160.768337	-4162.63143189	-
TS7_3	-4161.24009443	-4160.672554	-4160.777623	-4162.62322788	64.6*i*
Int7_3	-4161.25409516	-4160.685310	-4160.793198	-4162.63555408	-
TS8_3	-4161.21937498	-4160.651545	-4160.757388	-4162.61183411	263.48*i*
Int8_3	-4161.27443070	-4160.705075	-4160.815626	-4162.64879393	-
17a	-609.93876591	-609.735254	-609.785840	-609.67047116	-
NaOAc	-390.85746945	-390.799925	-390.837264	-390.79781959	-
NaBr	-2734.10182267	-2734.097448	-2734.124924	-2736.40018586	-
18a	-1094.77989453	-1094.454905	-1094.530197	-1094.39992781	-
PhCCBr	-2879.50368220	-2879.393456	-2879.435756	-2881.65582911	-
TS5_3_Ph	-3983.55723377	-3983.015233	-3983.115811	-3984.89370967	305.20*i*
TS6_3_Ph	-3983.54914894	-3983.006167	-3983.103120	-3984.89629763	323.24*i*
Int5_3_Ph	-3983.62383970	-3983.078710	-3983.177886	-3984.95929520	-
Int6_3_Ph	-3983.61946966	-3983.074810	-3983.174804	-3984.96393032	-
TS7_3_Ph	-3983.61721254	-3983.073827	-3983.173967	-3984.94613315	94.17*i*
Int7_3_Ph	-3983.62794242	-3983.083463	-3983.185836	-3984.95540353	-
TS8_3_Ph	-3983.57620847	-3983.033494	-3983.133216	-3984.91237515	212.09*i*
Int8_3_Ph	-3983.65044121	-3983.105038	-3983.210439	-3984.97419828	-
18a_Ph	-917.15577697	-916.854757	-916.923237	-916.72670971	-
tBuCCBr	-2805.70072358	-2805.558134	-2805.601442	-2807.89352792	-
TS5_3_tBu	-3909.77374636	-3909.198794	-3909.297935	-3911.14673942	82.39*i*
TS6_3_tBu	-3909.74077727	-3909.165396	-3909.263248	-3911.13180898	295.25*i*
Int5_3_tBu	-3909.81802238	-3909.240422	-3909.339466	-3911.19439415	-
Int6_3_tBu	-3909.80303352	-3909.225025	-3909.322555	-3911.19106669	-
TS7_3_tBu	-3909.80983062	-3909.233722	-3909.331609	-3911.18154413	89.40*i*
Int7_3_tBu	-3909.82436757	-3909.247002	-3909.347897	-3911.19553568	-
TS8_3_tBu	-3909.75730436	-3909.182382	-3909.283596	-3911.13315902	271.72*i*
Int8_3_tBu	-3909.84570264	-3909.267769	-3909.371941	-3911.21063037	-
18a_tBu	-843.35110161	-843.017633	-843.086520	-842.96294356	-

Table 7.5. Energies (in Hartrees), imaginary frequencies (in *i* cm^{-1}), and spin contaminations ($<S^2>$) of all stationary points in Chapter 4 are provided.

structure	*E*	*H*	*G*	E^{high}	Imag. Freq.	$<S^2>$
22a	-1236.92635646	-1236.665195	-1236.727680	-1236.56347120	-	-
25a	-801.7132832	-801.453227	-801.511377	-801.3429458	-	-
26a	-3148.83878085	-3148.217016	-3148.341333	-3150.07637196	-	-
26b	-3148.82582193	-3148.205468	-3148.329956	-3150.05770160	-	-
26c	-3148.83078383	-3148.210596	-3148.336147	-3150.06181329	-	-
27a	-2278.37497383	-2277.757080	-2277.873866	-2279.59088679	-	-
27b	-2278.38857787	-2277.771065	-2277.888191	-2279.59448985	-	-
27c	-2278.38877196	-2277.771535	-2277.889232	-2279.59490071	-	-
$Rh_2(OAc)_4$	-1133.15154110	-1132.917558	-1132.989040	-1134.96929918	-	-
AcOH	-229.08771031	-229.020189	-229.053272	-229.04074492	-	-
Int1_4	-3607.030943	-3606.270392	-3606.420501	-3608.195058	-	-
TS1_4	-3148.77162258	-3148.156888	-3148.281529	-3150.01551944	1386.52*i*	-
Int2_4	-3148.79109408	-3148.170370	-3148.296225	-3150.03976747	-	-
Int3_4	-1803.48895217	-1803.110615	-1803.199354	-1804.04899651	-	0.7563
Int4_4	-1574.38559438	-1574.076502	-1574.154229	-1574.99126618	-	0.7641
TS2_4	-1574.34644195	-1574.043412	-1574.116997	-1574.96084120	1360.39*i*	0.7672
Int5_4	-1574.36794299	-1574.059417	-1574.135686	-1574.98497687	-	0.7578
Int6_4	-3636.05454790	-3635.265971	-3635.414349	-3637.21251407	-	-
TS3_4	-3636.03302822	-3635.245855	-3635.390022	-3637.19463539	327.25*i*	-
TS4_4	-3636.03305794	-3635.245681	-3635.391038	-3637.19484615	336.61*i*	-
TS5_4	-3636.02552262	-3635.237946	-3635.380468	-3637.19257515	322.67*i*	-
TS6_4	-3636.01679244	-3635.229292	-3635.372779	-3637.18371709	286.11*i*	-
TS7_4	-1832.50472396	-1832.098868	-1832.183109	-1833.06832188	295.03*i*	0.7588
TS8_4	-1832.50543240	-1832.099783	-1832.183400	-1833.07038595	281.89*i*	0.7589
TS9_4	-1832.49935613	-1832.094186	-1832.177850	-1833.06614582	312.05*i*	0.7587
TS10_4	-1832.49519424	-1832.089670	-1832.172690	-1833.06051219	312.44*i*	0.7576
23a	-487.268658	-487.103567	-487.148789	-487.1475347	-	-
Int7_4	-3636.07309502	-3635.283010	-3635.427730	-3637.22238240	-	-
Int8_4	-3636.06554565	-3635.275823	-3635.421310	-3637.21670232	-	-
Int9_4	-3636.04669903	-3635.256866	-3635.399654	-3637.21031172	-	-
Int10_4	-3636.04503708	-3635.254582	-3635.397943	-3637.20361041	-	-
TS11_4	-3636.02662260	-3635.243061	-3635.388107	-3637.18129781	1219.04*i*	-
TS12_4	-3636.03655534	-3635.253060	-3635.397808	-3637.18849046	1413.55*i*	-
TS13_4	-3636.00265537	-3635.218614	-3635.360933	-3637.16510930	1471.45*i*	-
TS14_4	-3636.03237561	-3635.248834	-3635.392805	-3637.19112144	1451.96*i*	-
Int11_4	-3636.13280678	-3635.342176	-3635.490624	-3637.26293434	-	-
Int12_4	-3636.13358625	-3635.342943	-3635.489630	-3637.26567465	-	-
Int13_4	-3636.13574168	-3635.345393	-3635.495775	-3637.26217481	-	-
24a	-1724.22495013	-1723.794376	-1723.878288	-1723.75584712	-	-

Table 7.6. Energies (in Hartrees), imaginary frequencies (in *i* cm^{-1}), and spin contaminations ($<S^2>$) of all stationary points in Chapter 5 are provided.

structure	*E*	*ZPE corr.*	*H corr.*	*G corr.*	Imag. Freq.	$<S^2>$
Int1_S_5	-2824.857145	0.370233	0.406354	0.300645	-	-
Int1_T_5	-2824.835513	0.367819	0.405530	0.292560	-	2.059
Int2_S_5	-2824.836116	0.369715	0.406491	0.299209	-	-
TS1_S_5	-2824.827536	0.365512	0.401470	0.297462	884.60i	-
TS1_T_5	-2824.812367	0.363047	0.400446	0.289704	621.64i	2.117
Int3_S_5	-2824.852674	0.370536	0.407025	0.300963	-	-
Int3_T_5	-2824.854827	0.367968	0.405969	0.292342	-	2.164
MECP_5	-2824.845962	0.369420	0.406661	0.298092	-	-
Int2_S_ent2_5	-1874.807996	0.341190	0.371466	0.278572	-	-
TS1_S_ent2_5	-1874.800488	0.337108	0.366607	0.276339	939.52i	-
Int2_S_ent3_5	-2127.809378	0.369712	0.402333	0.304819	-	-
TS1_S_ent3_5	-2127.798474	0.365529	0.397320	0.303155	981.18i	-
Int2_S_ent4_5	-3557.741451	0.344510	0.384828	0.269021	-	-
TS1_S_ent4_5	-3557.732193	0.340385	0.379977	0.266605	853.58i	-
Int2_S_ent5_5	-3557.772134	0.346939	0.387217	0.271094	-	-
TS1_S_ent5_5	-3557.741215	0.341264	0.380715	0.267326	1221.15i	-
Int2_S_ent6_5	-2860.752032	0.347126	0.383077	0.277600	-	-
TS1_S_ent6_5	-2860.740028	0.342595	0.377753	0.275346	1009.16i	-
Int4_S_5	-2595.741949	0.306495	0.337554	0.241444	-	-
Int5_5	-1634.146914	0.276838	0.299563	0.222748	-	2.036
Int6_5	-2595.531003	0.306463	0.337580	0.241465	-	1.042
OTf-	-961.5779531	0.027166	0.035277	-0.005342	-	-
Ag_2CO_3	-555.3696793	0.015545	0.022932	-0.019463	-	-
Ag_2CO_3-	-555.4876126	0.015470	0.023689	-0.021395	-	0.7554
Int7_S_5	-1633.697005	0.265823	0.287578	0.215680	-	-
Int7_T_5	-1633.709846	0.264573	0.287017	0.211796	-	2.095
AcOH	-229.0875805	0.061820	0.067349	0.034489	-	-
TfOH	-962.0067425	0.038298	0.047099	0.004964	-	-
I_2	-22.77106236	0.000412	0.004308	-0.025550	-	-
Int8_S_5	-1656.479679	0.266842	0.293266	0.206516	-	-
Int8_T_5	-1656.488023	0.266441	0.293083	0.203765	-	2.037
TS2_T_5	-1656.453577	0.265357	0.291722	0.204262	69.07i	2.03
Int9_T_5	-1656.463579	0.265782	0.292580	0.204748	-	2.034
TS3_T_5	-1656.443767	0.264595	0.290996	0.204543	194.86i	2.138
Int10_T_5	-1656.497589	0.265632	0.292582	0.203531	-	2.059
I ▪	-11.36411078	0.000000	0.002360	-0.017503	-	0.7502
Int11_D_5	-1645.104607	0.266096	0.290123	0.211275	-	0.782
TS4_D_5	-1645.085419	0.264593	0.288429	0.209795	205.24i	0.858
Int12_D_5	-1645.108451	0.265381	0.290070	0.207051	-	0.966
TS5_T_5	-1656.476683	0.264761	0.291289	0.202866	79.36i	2.042
Int13_T_5	-1656.491354	0.265769	0.292875	0.201204	-	2.039

Table 7.7. Energies (in Hartrees) and imaginary frequencies (in *i* cm^{-1}) of all stationary points in Chapter 6 are provided.

structure	*E*	*H*	*G*	E^{high}	Imag. Freq.
BBr_3	-7740.09554461	-7740.083730	-7740.122238	-7747.48003855	-
32a-^{t}Bu	-483.01479842	-482.766532	-482.817627	-482.87139410	-
32a-^{i}Pr	-443.69555230	-443.476521	-443.525168	-443.56566985	-
32a-Me	-365.05027322	-364.890608	-364.932432	-364.94980225	-
L1	-248.31154371	-248.217138	-248.249746	-248.25054306	-
L2	-382.30375118	-382.131351	-382.174783	-382.20510626	-
L3	-326.96385231	-326.811036	-326.852566	-326.87214800	-
Int1-^{t}Bu_6	-8223.15694599	-8222.892486	-8222.957707	-8230.38195173	-
TS1-^{t}Bu_6	-15963.27042180	-15962.993161	-15963.074874	-15977.85180730	36.10*i*
Int2-^{t}Bu_6	-15963.27923770	-15963.001350	-15963.088552	-15977.87364120	-
TS2-^{t}Bu_6	-15963.27378630	-15962.997210	-15963.080050	-15977.86735370	132.12*i*
Int3-^{t}Bu_6	-15963.27556360	-15962.998529	-15963.081385	-15977.86682480	-
TS3-^{t}Bu_6	-15963.26365410	-15962.992778	-15963.074360	-15977.85362980	845.28*i*
33a-^{t}Bu	-5650.83803811	-5650.588257	-5650.647803	-5655.61094680	-
HBr	-2572.30601041	-2572.296844	-2572.319394	-2574.77478861	-
Int4-L3_6	-8067.10140710	-8066.933121	-8066.988928	-8074.38547425	-
TS4-L3_6	-15807.21690190	-15807.036070	-15807.109342	-15821.86233090	60.13*i*
Int5-L3_6	-15807.22274650	-15807.040867	-15807.118454	-15821.87099050	-
Int6-L3_6	-16290.27517060	-16289.839655	-16289.939871	-16304.76589370	-
Int7-L3_6	-16134.22363320	-16133.884107	-16133.975954	-16148.77326210	-
Int1-^{i}Pr_6	-8183.84950972	-8183.614436	-8183.678258	-8191.09269765	-
Int2-^{i}Pr_6	-15923.95970580	-15923.710878	-15923.795510	-15938.56869860	-
TS2-^{i}Pr_6	-15923.95106410	-15923.703833	-15923.785877	-15938.56236150	203.78*i*
Int3-^{i}Pr_6	-15923.95340700	-15923.705797	-15923.788286	-15938.56437880	-
TS3-^{i}Pr_6	-15923.94272480	-15923.701232	-15923.781717	-15938.55102980	868.80*i*
33a-^{i}Pr	-5611.52063668	-5611.300036	-5611.358163	-5616.31031533	-
Int1-Me_6	-8105.20350024	-8105.027744	-8105.085884	-8112.47990375	-
Int2-Me_6	-15845.31306670	-15845.123525	-15845.201536	-15859.95325750	-
TS2-Me_6	-15845.30387020	-15845.116313	-15845.191941	-15859.94962440	133.18*i*
Int3-Me_6	-15845.30492950	-15845.116670	-15845.193137	-15859.94987590	-
TS3-Me_6	-15845.29232130	-15845.110657	-15845.186626	-15859.93709020	886.86*i*
33a-Me	-5532.87441411	-5532.713547	-5532.765505	-5537.69586502	-

1a

C	-5.49877500	0.46816600	0.00571000
C	-4.55455000	1.38312500	0.47977500
C	-3.19857000	1.04672000	0.49474600
C	-2.77431300	-0.21216300	0.03939300
C	-3.73116800	-1.13234800	-0.41568000
C	-5.08339000	-0.79122700	-0.44066000
H	-6.55317900	0.73142000	-0.00771400
H	-4.87221200	2.35501100	0.84796100
H	-2.48484000	1.75888600	0.90161700
H	-3.39889700	-2.11111000	-0.74694700
H	-5.81412000	-1.50842500	-0.80509700
C	-1.33508600	-0.65016800	0.04936100
O	-1.02645000	-1.83822300	0.17082900
N	-0.41691100	0.35891900	-0.09642000
H	-0.79232100	1.27506400	-0.30441700
C	0.99680700	0.28948700	-0.08532100
C	1.72149900	-0.87312300	0.20313000
C	1.70208500	1.47426400	-0.36894500
C	3.12200100	-0.84845700	0.21109800
H	1.19668000	-1.79390700	0.41644400
C	3.08991700	1.49879200	-0.36219300
H	1.15655200	2.38813300	-0.59653900
C	3.81540200	0.33304900	-0.07058100
H	3.65139100	-1.76679700	0.43882100
H	3.62946400	2.41533400	-0.58149200
O	5.17871100	0.45589400	-0.08744100
C	5.96592500	-0.69635000	0.19938900
H	5.78483200	-1.49357500	-0.53268300
H	7.00473300	-0.36955400	0.13202700
H	5.76550800	-1.07288800	1.21051300

tBu-

C	-0.00012500	-0.00000900	0.14013500
C	0.49018600	-1.36958000	-0.43432100
H	1.50549500	-1.57415600	-0.06753500
H	-0.16405100	-2.17262600	-0.06803600
H	0.50428400	-1.40788700	-1.53722200
C	-1.43001300	0.26111200	-0.43718900
H	-2.11618800	-0.51571100	-0.07234400
H	-1.79826100	1.22967800	-0.07130000
H	-1.46768400	0.26840000	-1.54015700
C	0.94233000	1.10855700	-0.43345300
H	0.61245800	2.09079800	-0.06842500
H	1.96452900	0.94305600	-0.06568600
H	0.97017100	1.13877600	-1.53623800
O	-0.00312800	-0.00010100	1.50198900

tBuOH

C	0.00631300	-0.00000100	0.01115600
C	1.49687400	-0.00008000	-0.33611000
H	1.98676000	0.88785200	0.07878500
H	1.98666900	-0.88806700	0.07877300
H	1.63980500	-0.00008100	-1.42242100
C	-0.68270300	-1.26513100	-0.52142700
H	-0.20430900	-2.16183100	-0.11212000
H	-1.74353800	-1.28155700	-0.23789500
H	-0.63016300	-1.31212300	-1.61586200
C	-0.68256400	1.26520400	-0.52142800
H	-1.74339800	1.28174700	-0.23790100
H	-0.20407200	2.16185100	-0.11212100
H	-0.63001300	1.31218900	-1.61586300
O	-0.03942500	-0.00000100	1.45823100
H	-0.96986600	0.00007800	1.73762300

2a

C	-5.50503800	0.44436300	0.01473000
C	-4.54132000	1.46063500	0.03224700
C	-3.18068100	1.14291800	0.02257600
C	-2.75132900	-0.19484200	-0.00425600
C	-3.72710500	-1.20391000	-0.02163600
C	-5.09002600	-0.89127600	-0.01254900
H	-6.56493400	0.69142100	0.02238700
H	-4.85219900	2.50383300	0.05383900
H	-2.42553600	1.92150700	0.03563800
H	-3.38994500	-2.23559400	-0.04277100
H	-5.82896700	-1.69068100	-0.02680600
C	-1.27699300	-0.58434400	-0.01480800
O	-1.01219400	-1.82491600	-0.04298800
N	-0.44760400	0.46042200	0.00399000
C	0.93395100	0.31846100	0.00356500
C	1.69025300	-0.88033900	0.04184000
C	1.68725400	1.52392900	-0.03291400
C	3.09388000	-0.86861300	0.04118300
H	1.15901500	-1.82224200	0.07305900
C	3.07638900	1.54117200	-0.03597600
H	1.13402900	2.45991000	-0.05956600
C	3.79656800	0.33781900	-0.00018500
H	3.61946000	-1.81873200	0.07185000
H	3.62289700	2.48144100	-0.06613300
O	5.17898100	0.45168600	-0.00865900
C	5.93824400	-0.74431700	0.01181800
H	5.72755200	-1.37077300	-0.86645200
H	6.98694900	-0.43788700	-0.00604200
H	5.74631900	-1.32925200	0.92243800

$Ni(OAc)_2$

O	-1.59029500	1.07965900	-0.01599200
O	-1.58991800	-1.07946600	-0.01602600
O	1.59019900	-1.07963400	0.01598700
O	1.59004900	1.07951500	0.01595800
Ni	-0.00000900	0.00005300	-0.00007300
C	-2.28038900	-0.00001600	-0.01663500
C	2.28038300	-0.00000800	0.01669200
C	-3.77370900	-0.00027200	0.01087900
H	-4.10782400	0.00396000	1.05570100
H	-4.16172900	0.89685700	-0.47731700
H	-4.16139300	-0.90126100	-0.47034900
C	3.77370900	0.00006800	-0.01064200
H	4.16155900	-0.89716600	0.47749500
H	4.10794700	-0.00405800	-1.05542300
H	4.16144200	0.90095100	0.47075000

PPh_3

P	-0.00014900	-0.00013700	-1.20150500
C	0.32651500	1.64144800	-0.40095100
C	-0.34007800	2.11807400	0.73934500
C	1.28416500	2.46970600	-1.01380800
C	-0.04871700	3.38391100	1.25871700
H	-1.09225300	1.50311300	1.22515000
C	1.58566600	3.72839700	-0.48840400
H	1.79687200	2.12741800	-1.91056300
C	0.91697200	4.19047200	0.65004800
H	-0.57691800	3.73724500	2.14115900
H	2.33271100	4.35141600	-0.97408900
H	1.14218100	5.17388800	1.05497500
C	1.25808800	-1.10357400	-0.40028500
C	2.00416600	-0.76474900	0.74004200
C	1.49681300	-2.34682000	-1.01359000
C	2.95536500	-1.64976400	1.25869400
H	1.84729200	0.19378400	1.22635200
C	2.43663600	-3.23707100	-0.48880000
H	0.94382300	-2.61950500	-1.91028400
C	3.17147100	-2.88896500	0.64938800
H	3.52570700	-1.36915300	2.14101800
H	2.60295800	-4.19524700	-0.97495100
H	3.91120600	-3.57539000	1.05364100
C	-1.58502300	-0.53725900	-0.40029100
C	-2.78116200	-0.12171100	-1.01297400
C	-1.66448800	-1.35379900	0.73917700
C	-4.02197600	-0.49052200	-0.48797400
H	-2.74107100	0.49397800	-1.90937900
C	-2.90645800	-1.73530100	1.25794500
H	-0.75566300	-1.69768900	1.22452200
C	-4.08780300	-1.30200100	0.64953000
H	-4.93506300	-0.15487000	-0.97348300
H	-2.94837500	-2.37028000	2.13975300
H	-5.05207600	-1.59948600	1.05387700

OAc-

C	0.19737800	0.00013500	-0.00116300
O	0.81754700	-1.10138300	0.00027300
O	0.70102600	1.16111700	0.00015800
C	-1.35318100	-0.05584100	-0.00040300
H	-1.73800800	0.43434700	0.90355900
H	-1.74508000	0.50535300	-0.85860900
H	-1.73068400	-1.08333300	-0.03899700

Int1_1

N	-0.62429500	-1.74585300	0.34888800
C	-2.02478100	-1.49540500	0.31630900
C	-0.09912300	-2.77420700	-0.36918200
C	1.38532900	-3.01620000	-0.22841400
C	2.05442800	-2.91647200	1.00114000
C	3.41903000	-3.21197600	1.09101100
C	4.13144300	-3.60366800	-0.04523300
C	2.10152300	-3.44757100	-1.35645900
C	3.46684700	-3.72340400	-1.27129100
O	-0.75882200	-3.53379100	-1.10236500
C	-2.74741200	-1.34742400	-0.87636600
C	-4.11716600	-1.06654300	-0.86356600
C	-4.79037900	-0.91819900	0.35635800
C	-4.08039300	-1.06300600	1.55723000
H	3.92092700	-3.14758900	2.05360000
H	5.19261900	-3.82964700	0.02540700
H	1.57140300	-3.57498400	-2.29596300
H	4.01071900	-4.04281800	-2.15702300
H	-2.23990300	-1.46706600	-1.82601200
H	-4.64134200	-0.96898000	-1.80793500
H	-4.61286200	-0.96215700	2.49897800
H	1.50213100	-2.65094800	1.89743400
O	-6.12712500	-0.63835600	0.47820300
C	-6.90746200	-0.52832800	-0.70739300
H	-7.92688300	-0.32642900	-0.37413600
H	-6.55949000	0.29937400	-1.33903800
H	-6.88928000	-1.46192400	-1.28397700
C	-2.71964000	-1.35394900	1.53404200
H	-2.17948100	-1.49186600	2.46610800
Ni	0.32119100	-0.43775100	1.31968800
P	0.63515300	1.06128800	-0.34294800
C	-0.12787400	2.63379200	0.23619400
C	-0.06743000	0.76425900	-2.01494700
C	2.41120700	1.44213400	-0.64879800
C	0.51474300	3.87268000	0.09675600
C	-1.39602400	2.58033600	0.83990000
C	-1.06204400	1.58948500	-2.56026500
C	0.40864700	-0.32321300	-2.76718500
C	3.33343300	1.30861600	0.40299900
C	2.86096000	1.88849500	-1.90285200
C	-0.10655000	5.04193300	0.54547700
H	1.49989900	3.93065900	-0.35548600
C	-2.01627700	3.75111200	1.27980500
H	-1.90313400	1.62696400	0.96725800
C	-1.56841200	1.33299000	-3.83836900
H	-1.44525000	2.43333900	-1.99623000
C	-0.09808700	-0.57551000	-4.04203300
H	1.17839200	-0.97342100	-2.36284400
C	4.67999900	1.61967900	0.20073600
H	2.99736700	0.97271100	1.37830700
C	4.20965300	2.19561500	-2.10000400
H	2.16469000	1.99439700	-2.72880200
C	-1.37209600	4.98412000	1.13486800
H	0.40249200	5.99596700	0.43578300
H	-2.99835300	3.69685700	1.74198800
C	-1.08962600	0.25160000	-4.58083300
H	-2.33851800	1.98089200	-4.24883200
H	0.27598000	-1.42303200	-4.60979100
C	5.12176000	2.06131100	-1.04968000
H	5.38397800	1.51058400	1.02157100
H	4.54455100	2.53757500	-3.07584500
H	-1.85263700	5.89409600	1.48465900
H	-1.48631400	0.05129900	-5.57265300
H	6.17125100	2.29710200	-1.20570700
O	1.11101300	0.70558100	2.68753900
C	0.78446800	-0.12661900	3.61412500
O	0.20464900	-1.19552200	3.25475100
C	1.06157100	0.19180300	5.05496300
H	1.98153800	0.77481000	5.14962700
H	0.23555500	0.79699700	5.44858000
H	1.12606000	-0.72701000	5.64244200

TS1_1

N	-0.27596300	-1.99445400	-0.04950700
C	-1.65467100	-1.80640100	0.22107200
C	0.16300200	-3.18292400	-0.55993100
C	1.65584900	-3.26206500	-0.51917200
C	2.32840900	-2.34583900	0.31390600
C	3.73550000	-2.31232600	0.24836100
C	4.44192100	-3.20206600	-0.56617900
C	2.35496300	-4.15856300	-1.33240500
C	3.75075800	-4.13291600	-1.35162600
O	-0.54526700	-4.10502600	-0.99367700
C	-2.65583200	-2.01494300	-0.73753900
C	-4.00704600	-1.83952200	-0.42626100
C	-4.38336400	-1.44067200	0.86289500
C	-3.39464700	-1.23468900	1.83555200
H	4.29352300	-1.61428900	0.86925700
H	5.52909600	-3.17495400	-0.58385600
H	1.79475500	-4.85030200	-1.95577900
H	4.30017100	-4.82618300	-1.98384700
H	-2.37730700	-2.33006100	-1.73580000
H	-4.74942200	-2.01502000	-1.19694800
H	-3.69554800	-0.94945500	2.83998600
H	2.07229000	-2.05234600	1.71961100
O	-5.67727800	-1.23512000	1.26806600
C	-6.72589100	-1.49028200	0.33940900
H	-7.65396000	-1.28687700	0.87646100
H	-6.65643300	-0.82800400	-0.53314900
H	-6.71684200	-2.53623200	0.00736100
C	-2.05348900	-1.42492900	1.51580500
H	-1.29380600	-1.30441400	2.28465900
Ni	1.05395100	-0.77541600	0.52883800
P	0.22398500	1.25823000	-0.28204600
C	-0.21623800	2.51508600	0.99370200
C	-1.18149500	1.23274500	-1.47131100
C	1.56704600	2.04965700	-1.28084900
C	0.36145100	3.79354100	1.02400800
C	-1.13880800	2.16093400	1.99346600
C	-2.34579100	1.99341400	-1.29888600
C	-1.05112700	0.43059500	-2.61843600
C	2.91318900	1.75984000	-1.00416800
C	1.26575100	2.95216400	-2.31635200
C	0.01592000	4.70161900	2.02992000
H	1.08301100	4.08627700	0.26823500
C	-1.48865700	3.07262000	2.99127300
H	-1.59185900	1.17381500	1.98932300
C	-3.35984100	1.95860500	-2.26220800
H	-2.46757200	2.61911000	-0.42039500
C	-2.05810800	0.40730100	-3.58274700
H	-0.16077500	-0.17636500	-2.76125100
C	3.93398100	2.36285900	-1.74490900
H	3.16725900	1.07095000	-0.20679400
C	2.28805100	3.55288500	-3.05422900
H	0.23237400	3.18518400	-2.55445500
C	-0.91011200	4.34579900	3.01345600
H	0.47340600	5.68762400	2.04125500
H	-2.20951000	2.78524000	3.75233700
C	-3.21696400	1.17170100	-3.40670800
H	-4.25770500	2.55359200	-2.11562400
H	-1.94123200	-0.21430800	-4.46665000
C	3.62542300	3.25901900	-2.77106400
H	4.97061700	2.12474100	-1.52084200
H	2.03707200	4.24690900	-3.85227300
H	-1.17776300	5.05377500	3.79353400
H	-4.00341500	1.15037600	-4.15677400
H	4.42037500	3.72268900	-3.34944400

O	2.23288600	0.23678800	1.72998000
C	2.51615700	-0.41954100	2.78046400
O	2.30779300	-1.68213800	2.87766000
C	3.13118900	0.28792500	3.95767900
H	3.20324400	1.36005900	3.77018400
H	2.52573800	0.10383300	4.85106800
H	4.12762100	-0.12579800	4.14821500

Int2_1

N	-0.06538200	-2.12530700	-0.12335900
C	-1.43941800	-2.01395300	0.20684400
C	0.43609600	-3.33330500	-0.53397200
C	1.92821100	-3.31038000	-0.51606300
C	2.49946400	-2.14827300	0.02412200
C	3.89692500	-2.04351300	0.05163400
C	4.69456400	-3.09671100	-0.42518100
C	2.71240000	-4.35960500	-0.99878000
C	4.10611000	-4.25323400	-0.94740700
O	-0.22490600	-4.33521700	-0.84778300
C	-2.46701900	-2.41693300	-0.65918300
C	-3.81184300	-2.31598700	-0.29103500
C	-4.15899900	-1.79404500	0.96156700
C	-3.14537600	-1.38734900	1.83947100
H	4.38854500	-1.15154800	0.43505700
H	5.77865200	-3.00822700	-0.39006300
H	2.22583300	-5.24036100	-1.41058400
H	4.73045500	-5.06355200	-1.31589300
H	-2.21319700	-2.82754600	-1.62907000
H	-4.57234700	-2.64461300	-0.99098800
H	-3.41869200	-1.00005900	2.81730100
H	2.27534600	-1.64955900	2.24138000
O	-5.44574400	-1.64561300	1.41651500
C	-6.51166100	-2.08296100	0.58081300
H	-7.42782500	-1.88814900	1.14118300
H	-6.53479200	-1.52260800	-0.36283300
H	-6.43505100	-3.15683500	0.36739500
C	-1.80940100	-1.50403000	1.46516000
H	-1.03059400	-1.21270700	2.16582200
Ni	1.19545500	-0.77260300	0.30587000
P	0.01789400	1.28417400	-0.30022700
C	-0.51333400	2.35939600	1.10320000
C	-1.39800600	1.24642200	-1.48454000
C	1.22443100	2.32502500	-1.24924200
C	0.34615900	3.33347600	1.63912000
C	-1.74227400	2.11962700	1.74431000
C	-2.42547200	2.20250600	-1.50414600
C	-1.36817500	0.25749600	-2.48100000
C	2.43554200	1.76087100	-1.67551400
C	0.92154300	3.64495400	-1.62575900
C	-0.02231000	4.06197100	2.77410400
H	1.30475400	3.53107800	1.16991000
C	-2.10991000	2.85215100	2.87539900
H	-2.41653700	1.35815000	1.36458200
C	-3.40150300	2.17023000	-2.50413700
H	-2.47119400	2.97630500	-0.74380600
C	-2.33664000	0.23518000	-3.48660100
H	-0.58979000	-0.50067300	-2.46638500
C	3.33042800	2.50183800	-2.45497100
H	2.68444700	0.73870100	-1.40527700
C	1.81672300	4.38657300	-2.39766700
H	-0.01743800	4.09772800	-1.31938800
C	-1.25212700	3.82685300	3.39428500
H	0.65348100	4.81660400	3.16903400
H	-3.06839100	2.65813900	3.35004700
C	-3.35684600	1.19041000	-3.50007500
H	-4.19344900	2.91508600	-2.50494700
H	-2.29873200	-0.53601300	-4.25164100
C	3.02493500	3.81583100	-2.81453200
H	4.26299200	2.04766900	-2.77985900
H	1.56846500	5.40683300	-2.67914200
H	-1.53986500	4.39697000	4.27380200
H	-4.11438400	1.16968300	-4.27943900
H	3.71966100	4.39221800	-3.42009900
O	2.44159100	0.44778800	1.28834000
C	2.83174500	0.14469200	2.42687100
O	2.65459200	-1.05977700	2.94576800
C	3.54629900	1.10653400	3.32403000
H	3.62415600	2.08112000	2.84265900
H	3.00508600	1.19664300	4.27174700
H	4.54509600	0.71896400	3.55257700

PhCCPh

C	-0.60881100	-0.00022200	-0.00022700
C	0.60881100	0.00018000	-0.00001800
C	2.04027000	0.00008900	0.00000900
C	2.75682300	-0.85873700	-0.85837300
C	2.75689500	0.85884300	0.85840400
C	4.15174400	-0.85572900	-0.85528500
H	2.21091800	-1.52283400	-1.52219900
C	4.15181600	0.85569000	0.85533600
H	2.21104600	1.52300300	1.52221200
C	4.85404800	-0.00005700	0.00003300
H	4.69136400	-1.52308300	-1.52229900
H	4.69149300	1.52299300	1.52235500
H	5.94085900	-0.00011200	0.00004100
C	-2.04027000	-0.00010000	-0.00009100
C	-2.75685100	-0.85879900	0.85839500
C	-2.75686700	0.85869800	-0.85846500
C	-4.15177200	-0.85563700	0.85541200
H	-2.21096800	-1.52293100	1.52220300
C	-4.15178800	0.85569900	-0.85529300
H	-2.21099700	1.52275200	-1.52236100
C	-4.85404800	0.00007500	0.00011000
H	-4.69141400	-1.52290100	1.52249700
H	-4.69144300	1.52302100	-1.52231000
H	-5.94085900	0.00014000	0.00018500

AcOH

C	-0.08818700	0.12346000	-0.00026300
O	-0.63503800	1.20894600	0.00003300
O	-0.78980700	-1.03836800	-0.00006000
H	-1.73961600	-0.81095500	0.00073200
C	1.39701800	-0.12004800	-0.00008800
H	1.67995500	-0.69608300	0.88757900
H	1.67884200	-0.71120100	-0.87797800
H	1.92659900	0.83314700	-0.00801700

Int3_1

C	2.75850300	0.71893000	3.74232600
C	2.43926500	0.50796000	2.39042100
C	1.20042700	0.93958700	1.92660600
C	0.28629600	1.57278500	2.77235300
C	0.61000500	1.77197700	4.11801000
C	1.85096900	1.34824800	4.60175300
H	3.72691200	0.39350100	4.11604700
H	3.15549500	0.02157000	1.73567100
H	-0.12219700	2.24836100	4.76569100
H	2.11222900	1.50655000	5.64497300
C	-1.02603000	1.95510600	2.16707700
O	-1.93542600	2.51493600	2.80320400
N	-1.02934300	1.60648100	0.85299600
C	-2.14303700	1.75343600	0.01015000
C	-3.45993200	1.45760000	0.40670200
C	-1.93701900	2.16658900	-1.32372200
C	-4.52798600	1.57359500	-0.48543900
H	-3.64797200	1.14383300	1.42656200
C	-2.99395600	2.26885300	-2.22358400
H	-0.93359400	2.43070500	-1.64755300
C	-4.30044300	1.97475700	-1.81008700
H	-5.52871200	1.34448800	-0.13545100
H	-2.82498800	2.59384700	-3.24659800
O	-5.27874000	2.11133700	-2.76153200
C	-6.62978300	1.86657500	-2.38490900
H	-6.94939000	2.54643800	-1.58487300
H	-7.22561900	2.05289600	-3.28007600
H	-6.77221600	0.82731300	-2.06167400
C	1.85445100	1.87989200	-0.60294600
C	3.04753900	-0.14930600	-1.77153800

C	4.44070600	-0.03457300	-1.57522400
C	2.57282300	-1.08626400	-2.70948400
C	5.32726800	-0.83641900	-2.29463600
H	4.81864200	0.68201800	-0.85111900
C	3.46518600	-1.87419900	-3.43703800
H	1.50400100	-1.18729400	-2.86799500
C	4.84386000	-1.75687800	-3.23100500
H	6.39694200	-0.73755200	-2.12781800
H	3.08097300	-2.58494600	-4.16397600
H	5.53574400	-2.37681100	-3.79500700
C	2.08761300	3.30918000	-0.56806200
C	3.24660800	3.82241900	-1.18891600
C	1.19044200	4.20218600	0.04458200
C	3.49660600	5.19361600	-1.19348600
H	3.94311700	3.13966600	-1.66706700
C	1.44828600	5.57337200	0.03948600
H	0.29589400	3.81221800	0.51763200
C	2.59879100	6.07381500	-0.57808800
H	4.39250700	5.57562800	-1.67624600
H	0.74682100	6.25126200	0.51836200
H	2.79627400	7.14264700	-0.58005300
C	2.14863700	0.70851400	-1.02383900
Ni	0.56188800	0.68696200	0.16283400
P	-0.29847500	-1.66026400	0.22911000
C	0.83329200	-2.92887100	0.96152500
C	-0.74845100	-2.36557100	-1.42191500
C	-1.84191900	-1.86994100	1.22375300
C	0.37047200	-3.96205900	1.79304700
C	2.20494900	-2.86497300	0.66552100
C	-0.44538100	-3.68262200	-1.80061700
C	-1.41356100	-1.53130600	-2.33770000
C	-1.84537400	-1.39187900	2.54564200
C	-3.00143200	-2.47883500	0.72111000
C	1.25870600	-4.90776600	2.31361600
H	-0.68386100	-4.03192700	2.04081400
C	3.09044300	-3.81579200	1.17849800
H	2.58648500	-2.07519300	0.02700600
C	-0.80108900	-4.15507100	-3.06799100
H	0.07055400	-4.34365100	-1.11115700
C	-1.77716300	-2.00809500	-3.59922400
H	-1.65629600	-0.50615700	-2.06779200
C	-2.97936800	-1.52740700	3.34782300
H	-0.96020400	-0.91403400	2.95449800
C	-4.13836800	-2.61085600	1.52515900
H	-3.02617800	-2.85307600	-0.29733000
C	2.62027800	-4.83879100	2.00697700
H	0.88277300	-5.69835900	2.95819100
H	4.14771300	-3.75103700	0.93435800
C	-1.46835800	-3.32113600	-3.96937900
H	-0.55653000	-5.17685200	-3.34759200
H	-2.29583400	-1.35055200	-4.29208200
C	-4.13098500	-2.13683700	2.83913000
H	-2.96437000	-1.14644900	4.36545900
H	-5.02875900	-3.08530000	1.11990500
H	3.31009100	-5.57411200	2.41324000
H	-1.74393000	-3.69036000	-4.95390400
H	-5.01622500	-2.23709700	3.46196900

TS2_1

C	-3.07825700	-0.98246200	3.53005500
C	-2.77642700	-0.69304000	2.19338400
C	-1.59709700	-1.18579400	1.62292400
C	-0.70078600	-1.94521100	2.40150300
C	-1.02036700	-2.23139100	3.73198300
C	-2.20918400	-1.76296300	4.29681600
H	-4.00320200	-0.60641800	3.96071600
H	-3.47388900	-0.10890700	1.60315800
H	-0.30375800	-2.80707100	4.31220700
H	-2.45121200	-1.99649000	5.33036800
C	0.63420400	-2.34188000	1.83524700
O	1.36379400	-3.17285400	2.40965700
N	0.86974400	-1.68708300	0.67603900
C	2.01348700	-1.93260600	-0.10916500
C	3.30810900	-2.07246200	0.41737300
C	1.86285900	-2.01908600	-1.50837200
C	4.41058800	-2.28789100	-0.41553700
H	3.45275800	-2.01911000	1.48940000
C	2.95477900	-2.22551000	-2.34619500
H	0.86517900	-1.94503500	-1.93534000
C	4.24047800	-2.36182400	-1.80422800
H	5.39212700	-2.39406700	0.03367600
H	2.82573900	-2.30066900	-3.42261200
O	5.25597000	-2.56635600	-2.70596700
C	6.57648500	-2.74433100	-2.20664200
H	6.63933300	-3.62061500	-1.54856900
H	7.20710800	-2.90248100	-3.08340300
H	6.92208200	-1.85438400	-1.66459300
C	-2.12667000	-1.44210900	-0.34568800
C	-2.99168600	0.66417000	-1.64415000
C	-4.39893800	0.68444600	-1.51397600
C	-2.39412000	1.53906900	-2.57572700
C	-5.17529700	1.54516800	-2.28991400
H	-4.87668900	0.03085700	-0.78930800
C	-3.17541600	2.38436500	-3.36187800
H	-1.31394800	1.54163000	-2.68110100
C	-4.56793600	2.39451800	-3.22109700
H	-6.25581500	1.54929400	-2.17058200
H	-2.69591400	3.04129500	-4.08282200
H	-5.17415400	3.06001700	-3.82996400
C	-2.61111700	-2.80144600	-0.58112200
C	-3.81989200	-2.98759000	-1.28194300
C	-1.88643500	-3.93653300	-0.17584500
C	-4.28835400	-4.27097600	-1.56385300
H	-4.38804800	-2.12352800	-1.61042400
C	-2.35882900	-5.21815300	-0.45964900
H	-0.94685300	-3.81419000	0.34950100
C	-3.56118700	-5.39249900	-1.15202000
H	-5.22305700	-4.39363700	-2.10531100
H	-1.78193600	-6.08183100	-0.13971400
H	-3.92795200	-6.39231400	-1.36936800
C	-2.18837400	-0.22451000	-0.83262100
Ni	-0.55618700	-0.44551600	0.12957800
P	0.56021000	1.61192800	0.29843700
C	-0.40361000	2.89972900	1.21502100
C	1.04028200	2.44180400	-1.28224200
C	2.13318000	1.53263400	1.26373200
C	0.22954700	3.87000200	2.01051700
C	-1.80246300	2.92585500	1.10274300
C	0.81679100	3.80494700	-1.52822500
C	1.64346900	1.65907200	-2.28212900
C	2.09535000	0.92256000	2.52947000
C	3.34641300	2.05880300	0.79867800
C	-0.52056400	4.84503000	2.67301800
H	1.30967300	3.86526100	2.11912500
C	-2.55119300	3.90543000	1.76028600
H	-2.31055000	2.18050500	0.50123400
C	1.19316300	4.37433800	-2.74924000
H	0.34598000	4.42689300	-0.77343400
C	2.02856900	2.23205400	-3.49589600
H	1.82000000	0.60007700	-2.11192600
C	3.24519700	0.85124900	3.31623600
H	1.16733100	0.50059800	2.90469800
C	4.50004600	1.98115600	1.58668600
H	3.40055900	2.53066300	-0.17735500
C	-1.91285500	4.86644800	2.54872900
H	-0.01478800	5.58577600	3.28714300
H	-3.63360300	3.91071500	1.66055600
C	1.80155800	3.59176600	-3.73399600
H	1.01007500	5.43113900	-2.92677200
H	2.50090300	1.61398200	-4.25504100
C	4.45234100	1.37995800	2.84603500
H	3.19932200	0.37372800	4.29144200
H	5.43376500	2.39242100	1.21132200
H	-2.49585800	5.62372900	3.06658500
H	2.09462600	4.03661300	-4.68148700
H	5.34936900	1.31851700	3.45695300

TS3_1

C	1.52352800	-3.26612800	-0.58799000
C	0.35877500	-2.48281700	-0.62515100
C	-0.86499500	-3.18030200	-0.70877000
C	-0.93423400	-4.57932100	-0.74813400
C	0.23763600	-5.32809500	-0.71123500
C	1.46632000	-4.66393700	-0.63447600
C	-2.10730400	-2.37723900	-0.81152000
O	-3.21427200	-2.84816500	-1.05540300
N	-1.84044500	-1.00321000	-0.65379600
C	-2.67916200	-0.05603500	-1.30492300
C	-4.08149700	-0.09886700	-1.25308400
C	-4.85486700	0.86905000	-1.89927900
C	-4.23881000	1.91246100	-2.59958100
H	2.50379400	-2.80339100	-0.52642000
H	-1.91062000	-5.05248200	-0.81322200
H	0.20023400	-6.41386600	-0.74560800
H	2.39042200	-5.23837400	-0.61363600
H	-4.56947700	-0.90304000	-0.72066000
H	-5.93530600	0.79612800	-1.84515900
O	-4.90273200	2.91082200	-3.25867700
C	-6.32284700	2.88963600	-3.24847400
H	-6.72091900	2.97328500	-2.22871300
H	-6.64007300	3.75667800	-3.83085600
H	-6.71593500	1.97654700	-3.71394600
C	-2.07752000	0.98915000	-2.02995300
H	-0.99448100	1.01554700	-2.10338700
C	-2.83912400	1.96482500	-2.65950300
H	-2.36952400	2.76741100	-3.22042700
P	2.15643300	0.12590200	-0.33749800
C	2.41502500	1.93720500	-0.06563700
C	3.16937500	2.44856900	0.99759800
C	1.84116600	2.83236600	-0.98426200
C	3.35481400	3.82699800	1.13309700
H	3.62024100	1.77718200	1.72075300
C	2.03176900	4.20602400	-0.84979600
H	1.25598400	2.45648400	-1.81933800
C	2.79205900	4.70758200	0.21006900
H	3.94505900	4.20809200	1.96199800
H	1.58848300	4.88427500	-1.57396800
H	2.94347100	5.77857400	0.31406500
C	3.32974300	-0.67577200	0.84059500
C	4.64744500	-1.02391800	0.50957400
C	2.85842800	-0.95025800	2.13481200
C	5.47673400	-1.62770500	1.45710400
H	5.02825100	-0.83694500	-0.48890900
C	3.69273200	-1.54239100	3.08296200
H	1.83499700	-0.70054200	2.39887700
C	5.00383000	-1.88477800	2.74481300
H	6.49325500	-1.89861500	1.18499000
H	3.31453500	-1.74560300	4.08103100
H	5.65117400	-2.35548900	3.47959500
C	2.89139700	-0.06762500	-2.02566700
C	4.05261100	0.63707100	-2.39358600
C	2.26963000	-0.88995200	-2.97629000
C	4.58951600	0.49942400	-3.67288100
H	4.53110300	1.30630600	-1.68480600
C	2.80634100	-1.02000200	-4.25973300
H	1.36759300	-1.42867700	-2.70782600
C	3.96727600	-0.33081500	-4.60919200
H	5.48867600	1.04765400	-3.94075100
H	2.31029400	-1.65927400	-4.98480300
H	4.38276000	-0.43168100	-5.60821800
Ni	0.02029700	-0.61380200	-0.22272100
C	-1.75457100	-0.23135600	1.27141500
C	-0.82504900	0.64449200	1.15788600
C	-2.84156500	-0.87601500	1.96080100
C	-0.43164700	1.71761200	2.08265500
C	-2.70616600	-2.17363200	2.49337000
C	-4.04665500	-0.17303100	2.15828200
C	-0.50678100	3.06089900	1.67918100
C	-0.01922800	1.43245700	3.39706000
C	-3.75225200	-2.74901100	3.20762600
H	-1.78197000	-2.72136200	2.33581500
C	-5.08443600	-0.75403200	2.88550700
H	-4.15158600	0.82549100	1.74772400
C	-0.19466000	4.08756400	2.56939600
H	-0.81888800	3.29134500	0.66571000
C	0.31043700	2.46213800	4.27844100
H	0.02774300	0.39839300	3.72773100
C	-4.94190000	-2.04112000	3.40759800
H	-3.64001400	-3.75083400	3.61237200
H	-6.00697500	-0.20142400	3.04024000
C	0.22013200	3.79465000	3.87057500
H	-0.26826200	5.12081800	2.24060700
H	0.62611800	2.22104000	5.29045300
H	-5.75488900	-2.49328000	3.96892400
H	0.47039000	4.59665100	4.55983400

Int4_1

C	-2.39526500	2.89323900	-3.11626400
C	-1.84442700	2.90988200	-1.83628300
C	-0.59762500	2.31721700	-1.55846300
C	0.11409500	1.72222200	-2.62730300
C	-0.43318800	1.74587500	-3.92098300
C	-1.68490800	2.30649200	-4.16894100
H	-3.36862700	3.34448600	-3.29282100
H	-2.38691900	3.38951200	-1.02596900
H	0.14791600	1.32229500	-4.73524500
H	-2.09524700	2.30034000	-5.17570500
C	1.50331700	1.12892600	-2.50682600
O	2.38702700	1.51524200	-3.28836400
N	1.64994300	0.13277200	-1.58637500
C	2.92781300	-0.42230500	-1.32088100
C	3.04844800	-1.81114100	-1.17713200
C	4.08548800	0.36198200	-1.14083000
C	4.26713600	-2.41519400	-0.84504600
H	2.17532500	-2.43768100	-1.34691700
C	5.30143100	-0.22663900	-0.81938800
H	4.02550200	1.43769500	-1.25876000
C	5.40313200	-1.61881400	-0.66432200
H	4.31389800	-3.49442800	-0.74921800
H	6.19171300	0.38029800	-0.67982900
O	6.64751400	-2.09637500	-0.34371800
C	6.81048300	-3.49964200	-0.17488300
H	6.57619800	-4.04242700	-1.09979600
H	7.86183100	-3.64894000	0.07693400
H	6.18192800	-3.87821100	0.64180200
C	-0.05937000	2.37968200	-0.15956900
C	1.14605900	1.16384900	1.70850900
C	2.37893100	1.84076200	1.82193000
C	0.71758200	0.39001100	2.80517000
C	3.13939600	1.76121900	2.98837200
H	2.73164700	2.43478100	0.98453800
C	1.47358500	0.31822400	3.97633400
H	-0.22030300	-0.15265600	2.74651900
C	2.68972300	1.00194800	4.07383900
H	4.08556700	2.29340800	3.04935700
H	1.11281500	-0.27672600	4.81201100
H	3.28216500	0.94027600	4.98319900
C	-0.06394000	3.73022900	0.48901400
C	-0.44966500	3.91615000	1.82885600
C	0.31754100	4.86739900	-0.24919600
C	-0.44326800	5.18484900	2.41272100
H	-0.75616700	3.05924600	2.42078500
C	0.33031400	6.13583600	0.33415000
H	0.61482000	4.75346300	-1.28817800
C	-0.05131500	6.30218000	1.66935500
H	-0.74867600	5.29929600	3.45019800
H	0.63923200	6.99478700	-0.25678300
H	-0.04657100	7.28996200	2.12330600
C	0.37524100	1.25520300	0.45464300
Ni	0.21186400	-0.35264700	-0.51276100
P	-1.67693400	-1.40124500	0.24649800
C	-3.22666800	-0.46019400	0.56920600
C	-1.48155600	-2.51719500	1.70045800
C	-2.10553000	-2.53156400	-1.15161700
C	-4.48295500	-0.92511700	0.14748500
C	-3.14844900	0.75132100	1.27497200

C	-2.54106000	-2.83458600	2.56456300
C	-0.21501300	-3.07786400	1.93730700
C	-2.17817400	-1.97496200	-2.44226900
C	-2.32036400	-3.90904700	-0.98984600
C	-5.63898200	-0.19427500	0.43442100
H	-4.56328500	-1.85341200	-0.41016900
C	-4.30619200	1.47607200	1.56683900
H	-2.18188700	1.13915700	1.57977800
C	-2.33832000	-3.70528700	3.63941100
H	-3.52419800	-2.40210000	2.40482800
C	-0.01673200	-3.95509900	3.00539400
H	0.62223300	-2.81977000	1.29288000
C	-2.47364700	-2.77937600	-3.54402800
H	-2.00614800	-0.91129800	-2.58949000
C	-2.60998700	-4.71286600	-2.09713000
H	-2.26296400	-4.35925900	-0.00365000
C	-5.55360600	1.00564700	1.14650500
H	-6.60469000	-0.56357900	0.09898400
H	-4.22980800	2.41350200	2.11138700
C	-1.07874900	-4.27017300	3.85905700
H	-3.16588800	-3.94037000	4.30372500
H	0.96869100	-4.37996800	3.17700400
C	-2.68837900	-4.15111700	-3.37412400
H	-2.52723400	-2.33503600	-4.53426000
H	-2.77415100	-5.77834300	-1.95797600
H	-6.45330800	1.57437300	1.36652200
H	-0.92295900	-4.94552700	4.69628300
H	-2.91083500	-4.77843600	-4.23330300

TS4_1

C	1.82488900	3.41683800	3.20828700
C	1.27487300	3.28874100	1.94050300
C	0.22734300	2.37205500	1.66860500
C	-0.25421800	1.58719400	2.75812500
C	0.29162200	1.75780700	4.04527300
C	1.33108300	2.64839900	4.27632000
H	2.64132900	4.11671400	3.37038400
H	1.66511300	3.89296100	1.12809000
H	-0.12741500	1.16977600	4.85573000
H	1.75217200	2.75349200	5.27277000
C	-1.42105600	0.67478300	2.64485700
O	-2.13791700	0.41033900	3.61811400
N	-1.64892900	0.12576000	1.38051100
C	-2.89083000	-0.56033400	1.17249200
C	-2.91729200	-1.91575300	0.84736100
C	-4.10992500	0.12996100	1.28168400
C	-4.12606300	-2.58700900	0.62537800
H	-1.98126100	-2.46138800	0.76978400
C	-5.31569700	-0.52322800	1.07069500
H	-4.10553000	1.18463600	1.53876200
C	-5.33289900	-1.88843900	0.73842600
H	-4.10675000	-3.64121700	0.37303600
H	-6.25973900	0.00719000	1.15503600
O	-6.57079700	-2.43939100	0.54669600
C	-6.65441600	-3.82123400	0.21404300
H	-6.22754700	-4.44734600	1.00787000
H	-7.71902400	-4.03809800	0.11277900
H	-6.14609400	-4.03303600	-0.73543600
C	-0.34886600	2.26919200	0.32880300
C	-1.83838300	0.94232400	-1.25608000
C	-2.80320000	1.92174100	-1.56491800
C	-1.77543500	-0.19906800	-2.07463100
C	-3.64181600	1.78181000	-2.67007600
H	-2.89226600	2.79925000	-0.93249700
C	-2.61185600	-0.34190000	-3.18343700
H	-1.06642900	-0.98390300	-1.82564300
C	-3.54580200	0.65185500	-3.48957000
H	-4.37575500	2.55356400	-2.88873200
H	-2.53883100	-1.23322300	-3.80199800
H	-4.20098200	0.54204500	-4.35013600
C	-0.23221800	3.44917300	-0.58309700
C	0.33086400	3.33952100	-1.86587800
C	-0.68641200	4.71587300	-0.16664000
C	0.42048400	4.44933400	-2.71003300
H	0.70868700	2.37795600	-2.19935600
C	-0.59973000	5.82575100	-1.00911800
H	-1.12056100	4.82594300	0.82403200
C	-0.04669300	5.69735900	-2.28803500
H	0.86154200	4.33772700	-3.69781900
H	-0.96734100	6.79054700	-0.66739000
H	0.02289400	6.56090400	-2.94483200
C	-0.95385700	1.09014300	-0.07548300
Ni	-0.02978300	-0.44570000	0.60803700
P	1.91003300	-1.22593300	-0.21114100
C	2.75551800	-0.27353000	-1.55226200
C	1.77593500	-2.93502700	-0.91207400
C	3.19985400	-1.40232800	1.10393900
C	4.03019200	0.28793300	-1.38906400
C	2.08016700	-0.07742700	-2.76994900
C	2.53164900	-3.38623200	-2.00535600
C	0.88358600	-3.82664600	-0.29264500
C	3.20848800	-0.47498400	2.15950800
C	4.16395300	-2.42362900	1.08771100
C	4.61982200	1.02368600	-2.42305500
H	4.57105500	0.15448600	-0.45759500
C	2.67503700	0.64508900	-3.80529400
H	1.08633200	-0.49171800	-2.91647300
C	2.39558000	-4.69888300	-2.46849700
H	3.22648200	-2.71568400	-2.50199100
C	0.75617200	-5.14069900	-0.74739400
H	0.28682500	-3.49132700	0.55290900
C	4.17096200	-0.55957000	3.16942500
H	2.46159700	0.31354900	2.19796700
C	5.11976500	-2.51152600	2.10305700
H	4.16901000	-3.15767600	0.28757300
C	3.94771200	1.20077700	-3.63394100
H	5.60737200	1.45409500	-2.27767100
H	2.14047500	0.77943300	-4.74224300
C	1.51016600	-5.57902600	-1.84076100
H	2.98534700	-5.03162500	-3.31895300
H	0.06394700	-5.81768400	-0.25344300
C	5.12722900	-1.57851500	3.14459800
H	4.16335200	0.16578600	3.97851800
H	5.85638200	-3.31069200	2.08018200
H	4.40818700	1.76971200	-4.43742900
H	1.40581200	-6.59882000	-2.20203000
H	5.86956600	-1.64976500	3.93544700

Int5_1

N	2.05650000	1.38349800	0.14449900
C	3.24174400	0.62152500	0.12346500
C	2.04680900	2.70293100	-0.15186200
C	0.72218900	3.39514300	0.10351900
C	-0.12716000	3.03024900	1.16463800
C	-1.31735000	3.72938400	1.39820600
C	-1.68829500	4.78874400	0.56366000
C	0.35391200	4.48041700	-0.70657300
C	-0.84751100	5.16227400	-0.49203700
O	2.98900900	3.40633400	-0.59738700
C	4.50967200	1.03894900	-0.33572200
C	5.62305900	0.18373800	-0.29242300
C	5.50549400	-1.11285800	0.21069200
C	4.25507300	-1.54958900	0.67294800
H	-1.95625700	3.43853200	2.22917000
H	-2.61974400	5.32347500	0.73852500
H	1.02311500	4.77619200	-1.50920600
H	-1.12504100	5.98868800	-1.14353100
H	4.62000500	2.03943100	-0.72927600
H	6.57360300	0.55633800	-0.66188100
H	4.15975400	-2.55900200	1.06596300
O	6.54047700	-2.02728000	0.29470200
C	7.82483300	-1.61508200	-0.14248700
H	8.48616600	-2.47034700	0.01490100
H	7.82181800	-1.34977500	-1.20886600
H	8.19246900	-0.75869300	0.43991800
C	3.15775300	-0.70005200	0.62802300
H	2.18722600	-1.04137500	0.98325500
P	-1.39685300	-0.67857200	-0.04285200

C	-1.11615700	-2.51005700	-0.31098500
C	-2.56826400	-0.28333000	-1.44861000
C	-2.57317100	-0.71361900	1.41582500
C	-1.89825100	-3.52631300	0.26135200
C	-0.03161000	-2.88296000	-1.12461300
C	-3.30017700	-1.24224400	-2.16735200
C	-2.69700900	1.06721000	-1.81728500
C	-2.00146400	-0.81975600	2.69708600
C	-3.96807000	-0.59045400	1.32196300
C	-1.60689400	-4.87539000	0.02635400
H	-2.73754800	-3.26906000	0.90158900
C	0.25180900	-4.22754000	-1.37433300
H	0.60022700	-2.10587500	-1.54960800
C	-4.13958400	-0.86320600	-3.22131500
H	-3.21298000	-2.29435300	-1.91072000
C	-3.54473600	1.45028500	-2.85965800
H	-2.11715400	1.81884900	-1.28698200
C	-2.79718600	-0.82593600	3.84419200
H	-0.91934300	-0.88826300	2.78850600
C	-4.76838300	-0.57788400	2.47146700
H	-4.43982600	-0.49863400	0.34786100
C	-0.53364900	-5.23101800	-0.79504600
H	-2.22092400	-5.64667700	0.48705000
H	1.09629800	-4.49126600	-2.00710600
C	-4.26788700	0.48452900	-3.56868100
H	-4.69120600	-1.62355200	-3.77056100
H	-3.62841200	2.50140000	-3.12648500
C	-4.18764200	-0.69990200	3.73609500
H	-2.33140600	-0.91462400	4.82333800
H	-5.84715400	-0.47372800	2.37386600
H	-0.30533100	-6.27905700	-0.97566500
H	-4.91810100	0.77930700	-4.38939100
H	-4.80882000	-0.69057300	4.62889700
Ni	0.29298900	0.48732400	0.13174700
H	0.16488300	2.22010900	1.82727100

3a

C	-3.97799500	3.35101500	-0.10068500
C	-3.59719500	2.01709200	-0.08080300
C	-2.22944500	1.65284100	-0.03300700
C	-1.26636300	2.69113600	-0.02203500
C	-1.66635500	4.04066500	-0.03974700
C	-3.01191700	4.37372400	-0.07652200
H	-5.03443800	3.60519700	-0.13744000
H	-4.35465900	1.24119200	-0.10480300
H	-0.89612100	4.80485300	-0.02595000
H	-3.31822100	5.41609600	-0.09099500
C	0.16981300	2.39140600	0.01192900
O	1.04718500	3.25859700	0.05092200
N	0.51087200	1.02733500	0.00397400
C	1.92565000	0.73173100	0.10406300
C	2.74587200	0.85279300	-1.01361600
C	2.48170400	0.37244700	1.33594300
C	4.11745900	0.59884300	-0.92173700
H	2.31775400	1.15734500	-1.96425000
C	3.84336300	0.11153600	1.43955200
H	1.84704000	0.29779300	2.21412600
C	4.66976800	0.22182600	0.31013600
H	4.73493000	0.70246900	-1.80653900
H	4.28683800	-0.17354400	2.38878100
O	5.99196000	-0.05431900	0.51209100
C	6.88832500	0.05396800	-0.59104400
H	6.90993100	1.07749800	-0.98526400
H	7.87239200	-0.20590700	-0.19827900
H	6.61737900	-0.64532700	-1.39199100
C	-0.44245100	-0.00636800	-0.00876400
C	-1.78499000	0.26948500	-0.01779400
C	0.07655900	-1.40995300	-0.02020300
C	-0.04804600	-2.21994000	1.11739300
C	0.66459800	-1.94844600	-1.17483200
C	0.40848100	-3.54021400	1.10371800
H	-0.50637100	-1.81469500	2.01524700
C	1.11720300	-3.26895500	-1.19092500
H	0.76253000	-1.33345600	-2.06532100
C	0.99184900	-4.06886300	-0.05071600
H	0.30536500	-4.15445900	1.99455400
H	1.56628000	-3.67294600	-2.09470500
H	1.34532100	-5.09663700	-0.06317100
C	-2.80191200	-0.83012300	-0.04248800
C	-3.04814500	-1.56296500	-1.21359100
C	-3.55664200	-1.12748600	1.10424800
C	-4.01278500	-2.57447500	-1.23607900
H	-2.47796800	-1.33971900	-2.11158400
C	-4.52192800	-2.13752800	1.08512000
H	-3.38170500	-0.56438300	2.01818400
C	-4.75222300	-2.86589100	-0.08629600
H	-4.18556000	-3.13357700	-2.15235700
H	-5.09154100	-2.35628400	1.98504500
H	-5.50193300	-3.65288000	-0.10252900

TS5_1

N	1.75788200	1.56610700	0.14316500
C	2.83353600	0.65575600	0.15468600
C	2.01284500	2.89199600	0.24774100
C	0.76294300	3.74386900	0.21443400
C	-0.52792100	3.15148700	0.27900700
C	-1.63182900	4.01556500	0.11696600
C	-1.48272900	5.39267100	-0.08867200
C	0.90922700	5.12355100	0.02350600
C	-0.20467900	5.95555100	-0.12406300
O	3.13477600	3.44568900	0.35465000
C	4.04708200	0.85714300	-0.53151800
C	5.06676400	-0.10366800	-0.52649100
C	4.90289400	-1.29882300	0.18164300
C	3.70669500	-1.51981200	0.87489200
H	-2.64007500	3.60555500	0.17338200
H	-2.36428700	6.02145500	-0.20510000
H	1.91779400	5.52608400	-0.02702500
H	-0.07474500	7.02596400	-0.27149700
H	4.19988800	1.78423300	-1.07064000
H	5.98043100	0.10247200	-1.07531100
H	3.57646700	-2.45083900	1.42107100
O	5.84819200	-2.30816900	0.25391000
C	7.08375000	-2.10659800	-0.41105100
H	7.68064300	-3.00086300	-0.21721300
H	6.94493400	-1.99135200	-1.49530500
H	7.61188500	-1.22534600	-0.02118100
C	2.69702700	-0.56160000	0.85504700
H	1.76844100	-0.74730700	1.38718600
P	-1.34227400	-0.64649300	0.03130700
C	-0.57345200	-2.32845500	-0.25770400
C	-2.50117100	-0.57648400	-1.43435000
C	-2.49453100	-1.01394100	1.44954600
C	-0.89612000	-3.49155300	0.45837300
C	0.43194400	-2.40735800	-1.23775500
C	-2.96656500	-1.71381300	-2.11570000
C	-2.91726100	0.68737100	-1.88471700
C	-2.02606500	-0.73934400	2.74616900
C	-3.79547300	-1.52039400	1.30473900
C	-0.24197600	-4.70164400	0.19443500
H	-1.66174600	-3.46188600	1.22822600
C	1.07349800	-3.61503300	-1.51460200
H	0.72566000	-1.50871600	-1.77616500
C	-3.83261600	-1.59149200	-3.20719500
H	-2.64671400	-2.70314200	-1.80102800
C	-3.78649900	0.81213100	-2.97223700
H	-2.54011600	1.57441000	-1.38346700
C	-2.82393400	-0.98483200	3.86607300
H	-1.03353100	-0.31388500	2.87463500
C	-4.60357900	-1.75171500	2.42388200
H	-4.19017300	-1.72927600	0.31460100
C	0.73921300	-4.76972200	-0.79738800
H	-0.50483200	-5.59005200	0.76505900
H	1.84888900	-3.65047200	-2.27613000
C	-4.24818100	-0.32768600	-3.63753800
H	-4.17862800	-2.48509300	-3.72231000
H	-4.09129200	1.80142100	-3.30593300
C	-4.11903400	-1.49047200	3.70835500

H	-2.43912100	-0.76701200	4.85966400
H	-5.61238600	-2.13596900	2.28846600
H	1.24891100	-5.70838500	-1.00199500
H	-4.91780600	-0.23231800	-4.48932100
H	-4.74673000	-1.67076100	4.57802100
Ni	-0.22158800	1.19637000	0.24492400
H	-1.25492100	2.03128600	0.90011600

Int6_1

N	0.91006100	2.02793400	0.06418200
C	2.13846300	1.33197600	0.12611700
C	0.96354300	3.38223800	-0.05698400
C	-0.40170800	4.00467600	-0.02097200
C	-1.49618300	3.12967900	0.14802000
C	-2.77354600	3.71781800	0.20918500
C	-2.94932200	5.10658000	0.10226500
C	-0.56333500	5.38990600	-0.13097000
C	-1.84436500	5.94873000	-0.07012300
O	1.99730200	4.08482300	-0.15314500
C	3.13348500	1.45102300	-0.85846700
C	4.34879400	0.76137600	-0.76703000
C	4.59665800	-0.07431800	0.32757500
C	3.61596300	-0.21517800	1.31654300
H	-3.65255300	3.08986700	0.34256500
H	-3.95178800	5.53152600	0.15503100
H	0.31948900	6.01239600	-0.25774200
H	-1.97973300	7.02584700	-0.15371200
H	2.96173800	2.10924700	-1.70409800
H	5.08765100	0.89324700	-1.55110500
H	3.81087200	-0.86942000	2.16266200
O	5.76205400	-0.79453600	0.51678700
C	6.79648600	-0.64707600	-0.44194300
H	7.61900500	-1.27812700	-0.09719700
H	6.47527400	-0.98256000	-1.43796100
H	7.13962900	0.39468000	-0.50692200
C	2.41127600	0.47667300	1.21078500
H	1.65905500	0.37044000	1.98810900
P	-1.01443300	-0.96081700	-0.00079300
C	0.41537200	-2.13127200	-0.23340600
C	-2.08310100	-1.48457900	-1.43779500
C	-1.86821700	-1.67538400	1.48489800
C	0.76712800	-3.13099400	0.68525900
C	1.20804700	-1.96982200	-1.38356300
C	-2.05653200	-2.79030800	-1.95999800
C	-2.93056900	-0.54165600	-2.04242000
C	-1.67620200	-1.01917500	2.71138100
C	-2.68443000	-2.81583300	1.45395200
C	1.87438500	-3.95631200	0.45484700
H	0.17867100	-3.27444500	1.58652200
C	2.30394600	-2.79921700	-1.62050700
H	0.96901800	-1.18645800	-2.09896200
C	-2.86583100	-3.14742400	-3.04197800
H	-1.39093300	-3.53449600	-1.53213900
C	-3.73799200	-0.89751600	-3.12732900
H	-2.94664100	0.47290400	-1.65709000
C	-2.26542600	-1.50341800	3.88232900
H	-1.07791200	-0.11188500	2.74198900
C	-3.28495600	-3.29579100	2.62234400
H	-2.86585800	-3.33085600	0.51543600
C	2.64247500	-3.79769900	-0.69999800
H	2.13284100	-4.72293000	1.18203100
H	2.90291600	-2.65573700	-2.51656000
C	-3.71167800	-2.20133300	-3.62910600
H	-2.82903500	-4.16363300	-3.42820900
H	-4.38207200	-0.14913300	-3.58306200
C	-3.07297900	-2.64414500	3.84093100
H	-2.10421400	-0.98033200	4.82181300
H	-3.92041600	-4.17744500	2.57747800
H	3.50395300	-4.43693500	-0.87774000
H	-4.33742400	-2.47669700	-4.47499700
H	-3.54111000	-3.01677900	4.74905000
Ni	-0.93992400	1.30642800	0.17999500
H	-2.38922500	0.98880000	0.34538700

Int7_1

N	-0.54498300	1.03129500	-0.78240400
C	0.80882800	0.96558700	-1.18100700
C	-1.30540700	2.05408500	-1.24906600
C	-2.71909100	1.97580900	-0.74227100
C	-3.02639400	0.92612800	0.15086900
C	-4.34980300	0.85464000	0.62162200
C	-5.32272500	1.78178400	0.21621100
C	-3.67989800	2.90740900	-1.14973900
C	-4.99059000	2.81228600	-0.67057200
O	-0.94150100	2.96683000	-2.02687600
C	1.71238100	2.02290400	-0.98592700
C	3.05929800	1.92126400	-1.35414800
C	3.53650300	0.73933900	-1.93181100
C	2.65383400	-0.32769000	-2.13733000
H	-4.63417000	0.06654000	1.31498200
H	-6.34104400	1.69932800	0.59556800
H	-3.38767100	3.69527200	-1.83996500
H	-5.74394100	3.53278400	-0.98477600
H	1.35440300	2.94576500	-0.54143200
H	3.71663600	2.76773600	-1.18288100
H	3.02854600	-1.24163400	-2.59179600
O	4.84492600	0.53177500	-2.32819500
C	5.77065600	1.59057600	-2.14452200
H	6.72729800	1.22313700	-2.52308400
H	5.47564900	2.48558100	-2.70941000
H	5.87664400	1.85321000	-1.08278600
C	1.31474200	-0.20941900	-1.77035500
H	0.63560800	-1.03878100	-1.94481300
Ni	-1.50345500	-0.14843700	0.53698700
H	-2.39996400	-0.88311800	1.47173200
C	0.29213600	-0.92206700	1.43389300
C	-0.20702400	-1.82934800	0.75169300
C	1.09638300	-0.11391400	2.30214000
C	-0.48130600	-3.08731300	0.11825200
C	0.66499200	1.15389200	2.74007900
C	2.34618900	-0.59945800	2.74533200
C	-1.61011300	-3.27027600	-0.70478100
C	0.39945000	-4.17365700	0.31693400
C	1.46077200	1.90918500	3.60089000
H	-0.29211000	1.53137500	2.39355400
C	3.13605500	0.16319700	3.60378400
H	2.68964500	-1.57179900	2.40369800
C	-1.85057700	-4.50550700	-1.30699900
H	-2.28784600	-2.43587800	-0.85617300
C	0.15250400	-5.40395100	-0.29002800
H	1.27318900	-4.04064000	0.94881600
C	2.69709900	1.42027800	4.03636300
H	1.11483300	2.88623800	3.92915300
H	4.09825500	-0.22226800	3.93279300
C	-0.97329200	-5.57606600	-1.10468800
H	-2.72611100	-4.62999700	-1.93945000
H	0.84043700	-6.23040700	-0.12798600
H	3.31545000	2.01396700	4.70526100
H	-1.16313600	-6.53625200	-1.57814200

TS6_1

N	0.31142000	1.62865200	-0.09223900
C	1.60132700	1.19648700	-0.47644600
C	0.07502600	2.96780300	-0.03394200
C	-1.37814000	3.27103400	0.17773900
C	-2.25739500	2.17093800	0.26387300
C	-3.62568300	2.46726900	0.41072000
C	-4.09220300	3.78959400	0.46712800
C	-1.82921700	4.59410100	0.24102500
C	-3.19413600	4.85971000	0.38685900
O	0.91485200	3.88397300	-0.18590700
C	2.78333500	1.66403000	0.11928500
C	4.04366300	1.20504300	-0.28396700
C	4.14681400	0.25639200	-1.30644800
C	2.98039800	-0.22079700	-1.91731200
H	-4.35263400	1.66012300	0.48398100
H	-5.15904000	3.98283600	0.57706000
H	-1.10124400	5.39898500	0.16704900

H	-3.55353500	5.88621700	0.43352200
H	2.71774800	2.40261000	0.91029900
H	4.92720700	1.59733800	0.20936300
H	3.06636700	-0.95462600	-2.71501700
O	5.33771500	-0.26273600	-1.77879200
C	6.54356200	0.20961500	-1.20030400
H	7.35088700	-0.31584900	-1.71556700
H	6.66276700	1.29211800	-1.34630400
H	6.59066800	-0.01639800	-0.12604800
C	1.73416400	0.24600800	-1.50779000
H	0.83395300	-0.12638800	-1.98891700
Ni	-1.28596400	0.50864100	0.26525600
H	-2.63772500	0.02366300	0.55806700
C	-0.39846800	-1.30080800	0.57990100
C	-1.55882200	-1.47834200	0.10345800
C	0.84964500	-1.79432900	1.11195700
C	-2.62410000	-2.35661100	-0.33922000
C	1.54143900	-1.08758000	2.11486500
C	1.37771800	-3.02990600	0.67847900
C	-3.83587300	-1.87609300	-0.86843000
C	-2.43940700	-3.75429500	-0.25302900
C	2.70798300	-1.60713500	2.67638900
H	1.15247300	-0.12827400	2.44142600
C	2.54920400	-3.54178500	1.23534800
H	0.86650800	-3.57711100	-0.10868700
C	-4.82998600	-2.75969500	-1.29222500
H	-3.98358700	-0.80362300	-0.94651700
C	-3.43611500	-4.63362500	-0.67345600
H	-1.51079100	-4.14142200	0.15624200
C	3.21737800	-2.83532200	2.24174800
H	3.22619300	-1.04630900	3.45064400
H	2.94251700	-4.49228300	0.88171900
C	-4.63813400	-4.14161300	-1.19684800
H	-5.75753400	-2.36535800	-1.70064300
H	-3.27521900	-5.70612500	-0.59077800
H	4.13036900	-3.23501700	2.67682300
H	-5.41370500	-4.82801900	-1.52775900

TS7_1

C	2.26023000	-3.11811800	-2.34478200
C	2.12208200	-1.85386900	-1.75870700
C	0.94314900	-1.48700700	-1.08879400
C	-0.13325800	-2.40655500	-1.07845000
C	0.01716100	-3.67208000	-1.65535400
C	1.21443100	-4.04153400	-2.27402800
H	3.19028900	-3.37834900	-2.84624400
H	2.95369300	-1.15743700	-1.80676800
H	-0.83822500	-4.34267100	-1.63337600
H	1.32074700	-5.02987700	-2.71584500
C	-1.49922400	-1.98181600	-0.60532600
O	-2.37551000	-2.84224900	-0.35773300
N	-1.60773600	-0.63544500	-0.54415200
C	-2.81680800	-0.02245000	-0.15292900
C	-4.09185300	-0.52858800	-0.46468100
C	-2.76770000	1.19138700	0.56549600
C	-5.26201600	0.14405900	-0.08726500
H	-4.17238700	-1.46354800	-1.00434900
C	-3.92393000	1.86280100	0.94963400
H	-1.79640600	1.60800100	0.81175700
C	-5.18454400	1.34430100	0.62495600
H	-6.22056400	-0.28789000	-0.35659000
H	-3.86470000	2.79558400	1.50505900
O	-6.27549500	2.08013800	1.04846600
C	-7.56863800	1.59208700	0.72941600
H	-7.74828500	0.60517700	1.17776700
H	-8.27462800	2.31313100	1.14768500
H	-7.71703700	1.52632700	-0.35731100
C	1.71296500	-0.14873300	0.20577200
C	2.63311300	2.18453200	-0.53898000
C	4.04055200	2.13052800	-0.41025600
C	2.04710400	3.43873000	-0.81412700
C	4.82009500	3.28189500	-0.52999000
H	4.52145400	1.17157200	-0.23633000
C	2.82581200	4.59116100	-0.90709300
H	0.97153700	3.47637600	-0.95947800
C	4.21795500	4.52241200	-0.76809000
H	5.90167800	3.20948200	-0.43618500
H	2.34618500	5.54701200	-1.10660000
H	4.82528400	5.41998800	-0.85749100
C	2.17039300	-0.83459300	1.41247000
C	3.22183000	-0.26531700	2.16643200
C	1.56839000	-2.00684600	1.90996300
C	3.65667400	-0.85119000	3.35425100
H	3.68882800	0.65062000	1.82071400
C	2.00574700	-2.59037600	3.10022400
H	0.74869200	-2.45751000	1.36304700
C	3.05469100	-2.02227100	3.82921000
H	4.46812800	-0.38846800	3.91187900
H	1.51769200	-3.49345900	3.45928200
H	3.39458700	-2.48008200	4.75503600
C	1.81593900	0.99579900	-0.42865100
Ni	0.11061500	0.29871700	-0.84649100
H	-0.45364300	1.64687100	-1.29262500

Int8_1

N	0.76901800	1.78608200	-0.10906300
C	2.01259600	1.10768400	-0.13449800
C	0.76012400	3.14753100	-0.01780500
C	-0.63591900	3.68899000	0.00226100
C	-1.66072600	2.72384300	-0.04044400
C	-2.98265500	3.20326400	-0.02106600
C	-3.26184100	4.57899900	0.03212400
C	-0.89382900	5.06130400	0.05702600
C	-2.21862200	5.51209700	0.07050400
O	1.76880400	3.88321400	0.02858600
C	2.92361300	1.19622700	0.92621800
C	4.14966100	0.52024600	0.89912000
C	4.48051700	-0.27118300	-0.20616200
C	3.57941000	-0.37470600	-1.27399100
H	-3.82369300	2.50890300	-0.04927300
H	-4.29597100	4.92299800	0.04270300
H	-0.05840300	5.75773600	0.08609900
H	-2.43663500	6.57780300	0.11103900
H	2.67361900	1.81298400	1.78413500
H	4.82684600	0.62259300	1.74082900
H	3.84206200	-0.99798900	-2.12475200
O	5.65682800	-0.98179100	-0.33540400
C	6.60778300	-0.89568800	0.71411100
H	7.44964900	-1.52094000	0.40830100
H	6.95472700	0.13661600	0.85864000
H	6.19819000	-1.27509000	1.66036100
C	2.36636400	0.30679000	-1.23408600
H	1.66825100	0.22045500	-2.06194000
Ni	-0.91746500	0.93911600	-0.10510200
H	-2.51136500	0.15346100	-0.22731500
C	-0.75004100	-0.98707900	-0.09714100
C	-2.08512800	-0.90583200	-0.10835700
C	0.15070700	-2.12942400	-0.06613200
C	-3.21516700	-1.83716900	0.04926000
C	0.99288400	-2.36115100	1.04121100
C	0.25474400	-3.00687300	-1.16752000
C	-4.53754500	-1.36780900	-0.07786200
C	-3.02580500	-3.20405500	0.34247500
C	1.87794400	-3.43995200	1.05706000
H	0.95000900	-1.67818400	1.88516000
C	1.15273400	-4.07534500	-1.15512300
H	-0.37490500	-2.83705800	-2.03767500
C	-5.62883400	-2.22503100	0.07373900
H	-4.70823100	-0.31576500	-0.29775000
C	-4.11714700	-4.05896000	0.49446000
H	-2.01868700	-3.59097800	0.45511300
C	1.96722400	-4.30357400	-0.04029900
H	2.51379200	-3.59714200	1.92574300
H	1.21538500	-4.73293600	-2.01990900
C	-5.42581000	-3.57836700	0.36056800
H	-6.63828000	-1.83352500	-0.03038500
H	-3.94440400	-5.10826600	0.72361700
H	2.66847700	-5.13455800	-0.03130600

H	-6.27302400	-4.24898600	0.48151600

Int9_1

C	-0.84137500	-1.31090500	-0.21117800
C	-1.94852200	-0.84080100	0.29366100
Ni	-0.61607300	0.47568800	0.25658300
H	-1.14309600	2.06767900	1.24873300
C	-1.48283500	2.64865700	0.37297600
C	-2.82888100	3.03160500	0.30529300
C	-0.54505100	3.14639400	-0.55012800
C	-3.25452700	3.90915600	-0.69334300
C	-0.98332400	4.04110700	-1.53703500
C	-2.32643600	4.41365700	-1.61438400
H	-3.53805800	2.64042200	1.02998200
H	-4.30015600	4.20212900	-0.75343900
H	-2.65375700	5.09823900	-2.39406000
H	-0.25408200	4.43001800	-2.24152200
C	0.91007900	2.73774500	-0.49649500
O	1.76912300	3.54322300	-0.93428700
N	1.09139600	1.51418100	0.04553000
C	2.37589400	1.00087800	0.31216300
C	3.59296000	1.49873100	-0.19913600
C	2.46053600	-0.12313600	1.16820400
C	4.82258500	0.90809500	0.13112100
H	3.57426200	2.35880100	-0.85367200
C	3.67471300	-0.70895400	1.50174100
H	1.53489100	-0.53366100	1.56280000
C	4.87309800	-0.19580700	0.98488600
H	5.72877500	1.33164700	-0.29072400
H	3.71034900	-1.57314100	2.16050900
O	6.03147200	-0.84266800	1.37286300
C	7.26620900	-0.34159200	0.88704000
H	7.43380100	0.69535700	1.20956100
H	8.04055500	-0.98305400	1.31389300
H	7.31828500	-0.39032200	-0.20949500
C	-0.15319100	-2.47124400	-0.74377600
C	-0.69732500	-3.77135200	-0.62461500
C	1.08718800	-2.33571300	-1.40170600
C	-0.03193800	-4.88076400	-1.14589700
H	-1.64538000	-3.90055100	-0.10914400
C	1.74835300	-3.44613500	-1.92881900
H	1.52279100	-1.34473800	-1.48532000
C	1.19402100	-4.72531100	-1.80621300
H	-0.47034700	-5.87106900	-1.03785500
H	2.70327600	-3.31253300	-2.43260300
H	1.71115000	-5.59065700	-2.21454800
C	-3.33943300	-1.12867400	0.58650300
C	-4.01040100	-0.47413400	1.64243900
C	-4.08048200	-2.06246200	-0.17504000
C	-5.34777900	-0.74761500	1.93386500
H	-3.45768200	0.24694400	2.23914900
C	-5.42105100	-2.32532600	0.10732200
H	-3.59243600	-2.56860500	-1.00377300
C	-6.06438900	-1.67380700	1.16739100
H	-5.83427500	-0.23355300	2.76049900
H	-5.96728700	-3.04345000	-0.50126100
H	-7.10824500	-1.88265900	1.38960000

TS8_1

C	-0.58069500	-1.28161600	-0.14500000
C	-1.82190500	-1.13423300	0.14897500
Ni	-1.00008000	0.61237500	0.24705300
H	-2.15790800	0.66875800	1.11318200
C	-1.88614300	2.30601600	0.03663000
C	-3.24927200	2.63254000	-0.05291500
C	-0.95056900	3.31446400	-0.27308500
C	-3.66640900	3.91759100	-0.43033600
C	-1.36160000	4.59703100	-0.65333900
C	-2.72258900	4.90627600	-0.72839800
H	-4.00687200	1.88367500	0.16854400
H	-4.73018900	4.14531400	-0.48623200
H	-3.04394000	5.90471200	-1.01878400
H	-0.60008100	5.33605000	-0.89182300
C	0.50714800	2.96382100	-0.21126100
O	1.38934100	3.83591000	-0.38550800
N	0.69422900	1.64871000	0.06933600
C	1.99994500	1.16323500	0.29248600
C	3.11055500	1.50642600	-0.49819900
C	2.22450600	0.26424100	1.35542800
C	4.38277800	0.97370300	-0.24963800
H	2.98234600	2.20614900	-1.31532900
C	3.48386500	-0.26760200	1.61469300
H	1.38259800	-0.01716600	1.98207700
C	4.57595200	0.08301800	0.81081900
H	5.20716900	1.26968300	-0.89081300
H	3.63538800	-0.96143700	2.43783700
O	5.78748500	-0.49457200	1.14210000
C	6.91811600	-0.16544000	0.35192500
H	7.13895600	0.91012900	0.39314500
H	7.75574700	-0.72281600	0.77748100
H	6.77770700	-0.46450000	-0.69613400
C	0.46183000	-2.21689300	-0.51845300
C	0.48501200	-3.52395900	0.01532000
C	1.46783000	-1.85569000	-1.43548600
C	1.47567300	-4.43293700	-0.35804300
H	-0.27755700	-3.81464000	0.73336300
C	2.44759300	-2.77211000	-1.81977100
H	1.47403000	-0.84594900	-1.83289400
C	2.45955800	-4.06371100	-1.28279100
H	1.47849900	-5.43251300	0.07169200
H	3.21367000	-2.47038800	-2.53025300
H	3.23150700	-4.77217000	-1.57409500
C	-3.13014600	-1.75748500	0.25856800
C	-4.18457500	-1.19190600	0.99812600
C	-3.36514700	-2.98795600	-0.39496400
C	-5.42385600	-1.82855200	1.08764400
H	-4.01856500	-0.24708800	1.50815600
C	-4.60601500	-3.61865500	-0.31201000
H	-2.56444700	-3.43701000	-0.97620800
C	-5.64382100	-3.04415500	0.43218800
H	-6.22062100	-1.37094600	1.66968900
H	-4.76427400	-4.56181300	-0.83045900
H	-6.61085900	-3.53697000	0.49759400

Int10_1

C	-4.50367700	-2.85496100	1.21905600
C	-3.71524700	-1.80488800	0.72147900
C	-2.31701400	-1.91029900	0.64952400
C	-1.74586200	-3.11662800	1.08968300
C	-2.51415800	-4.17134200	1.59391800
C	-3.90500700	-4.04009400	1.66205600
H	-5.58753900	-2.74772500	1.25715900
H	-4.21740700	-0.90045400	0.37959600
H	-2.01614600	-5.08095500	1.92263700
H	-4.51608100	-4.85306200	2.04989500
C	-0.26080300	-3.22525100	0.95001200
O	0.35049300	-4.28030900	1.21894500
N	0.29097700	-2.07471600	0.45893000
C	1.67166900	-2.10750500	0.13266900
C	2.65530100	-2.49585500	1.05281000
C	2.09695000	-1.76339900	-1.16323400
C	4.00914200	-2.55329400	0.70156500
H	2.35985200	-2.76157800	2.06155200
C	3.44121000	-1.80465600	-1.52494700
H	1.35384400	-1.45381400	-1.89185600
C	4.40778700	-2.20675200	-0.59371900
H	4.73248400	-2.86253000	1.44902700
H	3.75694500	-1.53234100	-2.52883500
O	5.71281500	-2.22947600	-1.04445800
C	6.72275300	-2.64798000	-0.13982000
H	6.55091800	-3.67635300	0.20629700
H	7.66148000	-2.60512000	-0.69667600
H	6.78600700	-1.97997700	0.73011600
C	-2.20663500	0.30724000	-1.15013500
C	-2.77236800	2.00004800	0.81486800
C	-3.23056200	1.64634700	2.10053800
C	-2.74942400	3.36269100	0.45018700
C	-3.66693800	2.63000000	2.98761400

H	-3.23897300	0.60002300	2.38915300
C	-3.18332900	4.34012900	1.34562400
H	-2.37863700	3.64237100	-0.53137800
C	-3.64556900	3.97903400	2.61588700
H	-4.01961600	2.34182700	3.97483600
H	-3.15415600	5.38666700	1.05231000
H	-3.98093300	4.74321500	3.31267100
C	-2.37168800	-0.18001400	-2.49435200
C	-2.91442400	0.68250600	-3.47164800
C	-2.00812600	-1.48820400	-2.86613400
C	-3.09448500	0.24032400	-4.78131300
H	-3.18860000	1.69601800	-3.19223400
C	-2.19424300	-1.92301200	-4.17878400
H	-1.58710300	-2.14871100	-2.11552300
C	-2.73589600	-1.06448900	-5.14102300
H	-3.51307100	0.91619100	-5.52323000
H	-1.91066500	-2.93687100	-4.44973300
H	-2.87453900	-1.40664200	-6.16363100
C	-2.35411100	1.00267800	-0.12906700
Ni	-0.93692700	-0.57472500	0.19808400
C	0.49308300	0.85240100	0.13470600
C	0.73425000	1.59036700	-0.97531300
H	0.20558800	1.29924700	-1.88685400
C	1.21563600	1.04358000	1.41171600
C	0.52874700	1.35573100	2.60486900
C	2.61335200	0.86343700	1.50172400
C	1.20564000	1.51893900	3.81587700
H	-0.54852300	1.48839800	2.57582400
C	3.28944900	1.01471800	2.71308300
H	3.16643900	0.60056700	0.60506600
C	2.59319100	1.35012600	3.88007100
H	0.64448100	1.77252200	4.71348100
H	4.36743600	0.86727900	2.74558900
H	3.12092400	1.46858700	4.82399700
C	1.60581700	2.76521800	-1.20585100
C	2.02494900	3.04198200	-2.52567600
C	1.99981900	3.67875200	-0.20412300
C	2.82128000	4.14765700	-2.82998000
H	1.72110300	2.36523900	-3.32269700
C	2.79171400	4.78787900	-0.50617100
H	1.67117300	3.52276500	0.81732200
C	3.21486500	5.03028600	-1.81863500
H	3.13286900	4.32080700	-3.85827300
H	3.07564500	5.47241900	0.29086500
H	3.83324700	5.89490500	-2.04890300

TS9_1

C	3.83322700	0.21516700	3.11890700
C	3.17867000	-0.20201900	1.95300700
C	2.20525800	0.60818900	1.35006800
C	1.86030900	1.82852100	1.97074100
C	2.52533700	2.24171500	3.12847700
C	3.52243800	1.44747100	3.70031200
H	4.59194400	-0.42536400	3.56427300
H	3.44570500	-1.15508500	1.50755400
H	2.21576600	3.18007600	3.58166000
H	4.03658600	1.77608400	4.60067600
C	0.68189500	2.60655600	1.45975600
O	0.47511600	3.78841800	1.81771500
N	-0.05626800	1.85498100	0.61618700
C	-1.18987800	2.40834000	-0.01607500
C	-2.24542900	2.99909100	0.69227700
C	-1.29715200	2.35189800	-1.41831100
C	-3.37068400	3.51245100	0.03644900
H	-2.18445200	3.06301800	1.77368300
C	-2.41011500	2.85866300	-2.08375500
H	-0.48520300	1.90298100	-1.98502800
C	-3.45767000	3.44119200	-1.35863800
H	-4.16431600	3.95967300	0.62590900
H	-2.48191400	2.81103200	-3.16746400
O	-4.52053200	3.91239200	-2.10207100
C	-5.61316000	4.49623000	-1.40847100
H	-5.30144900	5.38542600	-0.84377600
H	-6.33310300	4.78932000	-2.17577600
H	-6.08327100	3.77801500	-0.72325500
C	2.43843000	0.01095100	-0.62261700
C	1.92901900	-2.42228300	-1.40094400
C	3.15090300	-3.13364200	-1.39920200
C	0.82011700	-3.01895300	-2.03897900
C	3.26056500	-4.38001900	-2.01768200
H	4.01085300	-2.70754800	-0.88881500
C	0.93912100	-4.25637200	-2.67131800
H	-0.13202700	-2.49978300	-2.02142600
C	2.15718900	-4.94672600	-2.66498600
H	4.21116300	-4.90869900	-1.99436700
H	0.07102000	-4.68959200	-3.16311800
H	2.24275500	-5.91601100	-3.15027600
C	3.44574400	0.86010200	-1.25021800
C	4.42140400	0.28151400	-2.09007800
C	3.44324900	2.25996000	-1.10096600
C	5.36059700	1.07527600	-2.74876100
H	4.43449500	-0.79484700	-2.22798500
C	4.38454400	3.05074700	-1.76095500
H	2.69342100	2.72488900	-0.47089100
C	5.35048200	2.46513600	-2.58599600
H	6.10340300	0.60555100	-3.38980100
H	4.35944400	4.12989700	-1.63002700
H	6.08508200	3.08304400	-3.09676900
C	1.82391900	-1.13571600	-0.74394500
Ni	0.67893100	0.04707800	0.24950300
C	-0.99506100	-0.97924300	0.30824300
C	-1.95801400	-1.03796500	-0.63767700
H	-1.79661000	-0.45518400	-1.54620000
C	-1.08795100	-1.57429700	1.65827100
C	-0.28145700	-2.66340700	2.05376800
C	-1.94412500	-1.01121400	2.62995400
C	-0.35507100	-3.18639000	3.34594300
H	0.40269400	-3.09954000	1.33043600
C	-2.00789100	-1.52694600	3.92550100
H	-2.56077400	-0.16073300	2.35089800
C	-1.21836000	-2.62258200	4.29328100
H	0.27127300	-4.03430400	3.61720000
H	-2.67790800	-1.07060900	4.65181800
H	-1.26736000	-3.02412900	5.30288700
C	-3.25586900	-1.75051400	-0.65477200
C	-4.24706900	-1.30866200	-1.55851100
C	-3.56647300	-2.87523600	0.13947900
C	-5.49056800	-1.93584100	-1.65063500
H	-4.03283300	-0.44697200	-2.18792000
C	-4.80867000	-3.50602300	0.04666900
H	-2.82472800	-3.26356800	0.82827700
C	-5.78289200	-3.04149200	-0.84478200
H	-6.23210600	-1.56022600	-2.35309700
H	-5.01432300	-4.37215800	0.67280800
H	-6.74925100	-3.53593700	-0.91361100

Int11_1

C	-0.58217800	3.85698400	-3.12264200
C	-0.37944400	3.52305200	-1.78536700
C	0.41806000	2.42651500	-1.40092800
C	1.05842600	1.67943900	-2.41900700
C	0.86997800	2.04385200	-3.76337300
C	0.04389100	3.10682900	-4.12434900
H	-1.22191200	4.69824000	-3.38114800
H	-0.85719300	4.11337100	-1.00773600
H	1.40027500	1.48158500	-4.52734400
H	-0.09733200	3.35707200	-5.17354800
C	2.05931300	0.56344600	-2.17546200
O	3.19552200	0.69086900	-2.68429700
N	1.60310200	-0.50902200	-1.48983800
C	2.46942500	-1.58928400	-1.19425400
C	3.80222500	-1.43788200	-0.77806500
C	1.95724100	-2.90097000	-1.25704800
C	4.58992600	-2.54211300	-0.43270400
H	4.23122700	-0.44458900	-0.72528000
C	2.73007500	-4.00669400	-0.91356700
H	0.93330600	-3.04835300	-1.59319400
C	4.05643400	-3.83420400	-0.49782400

H	5.61318100	-2.37420900	-0.11315100
H	2.32046800	-5.01189600	-0.96924800
O	4.74832800	-4.98474200	-0.18214500
C	6.09822300	-4.85754100	0.23952600
H	6.17675400	-4.26475200	1.16086600
H	6.44911300	-5.87362400	0.43221300
H	6.72092800	-4.39909900	-0.54063500
C	0.58362800	2.13469900	0.06057500
C	0.70530300	0.44968100	1.92361800
C	-0.23930500	-0.15315000	2.77762800
C	2.02559100	0.58369800	2.40282800
C	0.10867300	-0.56580600	4.06456600
H	-1.25184800	-0.29870000	2.41675500
C	2.37908600	0.15645200	3.68440900
H	2.77681300	1.02830400	1.75630900
C	1.42124000	-0.41515100	4.52778300
H	-0.64640800	-1.01702900	4.70533200
H	3.40661300	0.27108100	4.02359300
H	1.69439400	-0.74739400	5.52682700
C	0.96675700	3.30659600	0.91157500
C	2.00310100	4.17264500	0.51009600
C	0.30174800	3.59831200	2.11694700
C	2.37526800	5.26865000	1.29139000
H	2.52626400	3.97610400	-0.42256600
C	0.66896300	4.69630500	2.89899300
H	-0.51496600	2.95793500	2.43638400
C	1.71030400	5.53726500	2.49304600
H	3.18651000	5.91380700	0.96034800
H	0.13466600	4.89797100	3.82511600
H	1.99598300	6.39284300	3.10087200
C	0.36859300	0.88760000	0.54968200
Ni	-0.13331200	-0.46488700	-0.63598500
C	-1.95425200	-0.73585900	-0.14736100
C	-2.19389900	-2.06019300	0.06797800
H	-1.31926600	-2.69868000	0.22879700
C	-3.00812600	0.29948800	-0.18011500
C	-3.81930800	0.55130600	0.94689900
C	-3.20546600	1.11173900	-1.31521300
C	-4.79041200	1.55463200	0.93517000
H	-3.68514300	-0.05601100	1.83893600
C	-4.19141900	2.10021300	-1.33707300
H	-2.57389200	0.96035700	-2.18689400
C	-4.99031000	2.33139900	-0.21139700
H	-5.39660100	1.72626900	1.82264500
H	-4.32497000	2.70295500	-2.23303500
H	-5.74878000	3.11083200	-0.22430900
C	-3.45338500	-2.83662200	0.12507200
C	-3.43018100	-4.10246800	0.74985600
C	-4.67454100	-2.42241800	-0.44886100
C	-4.57114200	-4.90265800	0.82971900
H	-2.49593100	-4.45541400	1.18298000
C	-5.81520400	-3.22303100	-0.37403400
H	-4.72568600	-1.47078800	-0.96587200
C	-5.77625200	-4.46561200	0.27000700
H	-4.51782400	-5.86990500	1.32519600
H	-6.74079100	-2.87603300	-0.82876100
H	-6.66762200	-5.08611700	0.32522800

TS10_1

C	-0.63781500	4.09192300	-3.06007700
C	-0.36561100	3.68629300	-1.76525900
C	0.31460400	2.46706200	-1.47870000
C	0.73682800	1.68732000	-2.60440200
C	0.46493400	2.13153200	-3.91657800
C	-0.22541500	3.30815000	-4.15802700
H	-1.18698600	5.01688100	-3.22685500
H	-0.71315900	4.29331600	-0.93542400
H	0.82048900	1.51734000	-4.73820600
H	-0.44391000	3.62208500	-5.17590200
C	1.61555000	0.50917400	-2.47507600
O	2.33947100	0.12207100	-3.41024100
N	1.60858400	-0.14762400	-1.23558700
C	2.68086800	-1.05779900	-0.96457200
C	2.42465300	-2.37501300	-0.58496600
C	4.01895600	-0.63047400	-1.03337100
C	3.46531600	-3.25904800	-0.26916600
H	1.39448300	-2.71620900	-0.52860600
C	5.06024900	-1.49812600	-0.73354800
H	4.23771900	0.38932500	-1.33431300
C	4.79003700	-2.82010800	-0.34431500
H	3.22237400	-4.27321700	0.02832000
H	6.09402400	-1.16840900	-0.78966800
O	5.88760900	-3.59742700	-0.06106600
C	5.67082700	-4.94274500	0.34372000
H	5.16125800	-5.51862900	-0.44002400
H	6.66225000	-5.36551500	0.51780100
H	5.08521300	-4.99105800	1.27120500
C	0.56960900	2.04034300	-0.12329000
C	1.37671800	0.22767600	1.44567000
C	2.60088600	0.75029200	1.90161400
C	0.72292600	-0.72047800	2.25007900
C	3.14858600	0.34624000	3.12026900
H	3.12244000	1.48213300	1.29155000
C	1.25894000	-1.11463000	3.47865500
H	-0.21697300	-1.13779600	1.89993700
C	2.47660500	-0.58570000	3.91828400
H	4.09935500	0.76078300	3.44832700
H	0.72581300	-1.83994300	4.08973200
H	2.89981100	-0.89843300	4.87036400
C	0.53510600	3.04386600	0.97823000
C	-0.26375000	2.86250200	2.12444600
C	1.30247600	4.22582500	0.90610600
C	-0.27841300	3.80280100	3.15756700
H	-0.89051400	1.97872600	2.19514500
C	1.28609100	5.17089800	1.93362600
H	1.92854900	4.39431500	0.03297400
C	0.49713400	4.96325900	3.07130900
H	-0.90871400	3.63139000	4.02776600
H	1.89793700	6.06711600	1.84992400
H	0.48421100	5.69681700	3.87434500
C	0.79459200	0.67350700	0.14011100
Ni	-0.22016700	-0.59545800	-0.80311900
C	-2.02656900	-1.01052200	-0.28140500
C	-2.38352900	-2.32823200	-0.28588200
H	-1.58303300	-3.05859000	-0.43755500
C	-3.69695500	-2.99444300	-0.12675600
C	-3.71852600	-4.35521700	0.25170300
C	-4.94321800	-2.38087700	-0.38085600
C	-4.91406900	-5.05933900	0.40505600
H	-2.77184700	-4.86174900	0.43386900
C	-6.13990700	-3.08365500	-0.23240500
H	-4.97151000	-1.34764300	-0.70794600
C	-6.13840600	-4.42543500	0.16760100
H	-4.88938900	-6.10471200	0.70690900
H	-7.08223700	-2.57991600	-0.43858100
H	-7.07365500	-4.96868700	0.28181100
C	-2.96785400	0.07583400	0.06964700
C	-3.25899300	1.11422000	-0.83920000
C	-3.54665500	0.16182500	1.35478300
C	-4.11969300	2.15922800	-0.49884000
H	-2.79351900	1.09440500	-1.82158900
C	-4.39212300	1.21732600	1.70427100
H	-3.32963200	-0.61819400	2.08119300
C	-4.69381800	2.22076000	0.77673600
H	-4.32885700	2.93900500	-1.22858200
H	-4.81993700	1.25402100	2.70476100
H	-5.35111700	3.04400500	1.04747000

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C	-0.67597400	1.83703500	0.00138400
H	-1.14459000	2.82092200	-0.03859200
C	0.67590400	1.83682600	-0.00115000
H	1.14478800	2.82057500	0.03900800
C	-1.64344800	0.72316700	0.07077100
C	-2.88650800	0.86205300	-0.57643000
C	-1.41530000	-0.44686500	0.82057700
C	-3.85120800	-0.14565000	-0.51313200
H	-3.09230300	1.76910500	-1.14107300

C	-2.38254500	-1.44954600	0.89391700
H	-0.48004500	-0.56389300	1.35896600
C	-3.60210900	-1.30870900	0.22141000
H	-4.79879500	-0.01860900	-1.03075600
H	-2.18688100	-2.34113200	1.48466500
H	-4.35353900	-2.09193800	0.27971800
C	1.64325900	0.72291900	-0.07088200
C	2.88662100	0.86227000	0.57574200
C	1.41504100	-0.44748800	-0.82004900
C	3.85146000	-0.14527400	0.51253300
H	3.09251100	1.76962100	1.13986700
C	2.38245400	-1.45003500	-0.89331900
H	0.47968400	-0.56499500	-1.35813200
C	3.60226100	-1.30871900	-0.22138800
H	4.79924300	-0.01780800	1.02969200
H	2.18667600	-2.34190500	-1.48359800
H	4.35380100	-2.09184400	-0.27967400

Int12_1

C	1.07148300	5.39636100	-0.20617500
C	0.63386900	4.66092500	-1.31280800
C	-0.12826500	3.50561200	-1.13494000
C	-0.48064700	3.06817400	0.15640100
C	-0.03470600	3.81619700	1.25999100
C	0.73544100	4.96578100	1.08086600
H	1.66967900	6.29290200	-0.34711300
H	0.89241500	4.98204500	-2.31882100
H	-0.41530300	2.94006300	-2.01784600
H	-0.31155000	3.48139300	2.25411100
H	1.06985100	5.52903100	1.94861000
C	-1.32054100	1.85621200	0.45205400
O	-1.65572500	1.55234800	1.61266500
C	-3.30684000	0.64122200	-0.54515300
C	-3.48333500	-0.43795400	0.32129500
C	-4.39698300	1.10050900	-1.29683200
C	-4.73372100	-1.05257700	0.44345300
H	-2.64595200	-0.79915700	0.90644100
C	-5.64042400	0.48475000	-1.19262200
H	-4.27590400	1.94777500	-1.96882100
C	-5.81832700	-0.59581300	-0.31649300
H	-4.84107500	-1.88527700	1.12904100
H	-6.48589500	0.83505100	-1.77712700
O	-7.07646000	-1.13343900	-0.27727800
C	-7.32178600	-2.22415600	0.60589000
H	-7.13809300	-1.93929700	1.64949800
H	-8.37537200	-2.47725700	0.47769100
H	-6.70305500	-3.09273700	0.34675100
H	-2.04053200	1.91422000	-1.50232200
N	-2.02939300	1.28751100	-0.70109100
Ni	-0.35731900	0.29063400	-0.59520500
P	1.46946900	-0.74655800	-0.10929100
C	1.88844400	-2.11936000	-1.28290300
C	1.42274200	-1.59041200	1.53930600
C	3.02438100	0.25837800	-0.05435300
C	3.19723200	-2.42421900	-1.68678700
C	0.82728400	-2.88712200	-1.79382000
C	2.09457600	-2.79484100	1.80447200
C	0.67203700	-0.98825500	2.56392400
C	3.23482200	1.19834000	-1.07746100
C	3.98825800	0.13373200	0.95720300
C	3.43975900	-3.47731600	-2.57544500
H	4.03227300	-1.83834800	-1.31395700
C	1.06996400	-3.94501000	-2.67225400
H	-0.19470500	-2.65226900	-1.50372500
C	2.02535700	-3.38110100	3.07184100
H	2.66808200	-3.28396900	1.02207300
C	0.61304100	-1.57147300	3.83283900
H	0.12029300	-0.07213800	2.36667600
C	4.39200400	1.97859500	-1.10169500
H	2.48443800	1.32428600	-1.85427700
C	5.14166800	0.92539200	0.94061800
H	3.84174900	-0.57663500	1.76515000
C	2.37884100	-4.24207800	-3.06726400
H	4.45964300	-3.69793000	-2.88104300
H	0.23736000	-4.52983100	-3.05519300
C	1.28824700	-2.76864800	4.08994500
H	2.54700900	-4.31614200	3.26137000
H	0.02830500	-1.09389400	4.61503500
C	5.34909200	1.84532800	-0.08994800
H	4.54004600	2.69878400	-1.90245500
H	5.87608400	0.82057700	1.73550400
H	2.56876700	-5.05995700	-3.75771700
H	1.23435000	-3.22589200	5.07487000
H	6.24542900	2.46033000	-0.10160300

TS11_1

C	2.62582100	0.89156700	-0.15116600
C	1.39243300	2.91108800	0.62357100
C	0.31136700	3.83586900	0.19578200
C	-0.84144600	3.26748300	-0.41311400
C	-1.75138100	4.17637300	-0.99807700
C	-1.53228500	5.55499400	-0.96218100
C	0.50625200	5.22166100	0.28934600
C	-0.41918700	6.08620200	-0.29419100
O	2.10720800	3.03196500	1.60463900
C	3.55087900	0.76335600	-1.18603300
C	4.62349700	-0.13122000	-1.08670700
C	4.77772800	-0.89534200	0.07528100
C	3.84978600	-0.76101300	1.12102500
H	-2.65788300	3.79573700	-1.46453800
H	-2.24653100	6.22516500	-1.43570000
H	1.39493200	5.60572400	0.78430400
H	-0.27224100	7.16171500	-0.24184100
H	3.44747300	1.36603200	-2.08627400
H	5.32320000	-0.20931000	-1.91101000
H	3.97820200	-1.36338400	2.01526500
O	5.78786200	-1.79333800	0.28588400
C	6.77415000	-1.95579300	-0.72854600
H	7.47242200	-2.70197600	-0.34635800
H	6.32763400	-2.31816800	-1.66340500
H	7.30924100	-1.01618700	-0.91615800
C	2.78124600	0.11789600	1.00656600
H	2.06507800	0.20563300	1.81608800
P	-1.31839400	-0.73581900	-0.03988900
C	-0.16349200	-2.15231300	-0.35786700
C	-2.77854200	-1.15807300	-1.10860200
C	-1.94781300	-1.06966700	1.67065800
C	-0.06865400	-3.28463900	0.46487300
C	0.66844600	-2.06885600	-1.48708900
C	-2.91530500	-2.38207600	-1.78123300
C	-3.79582800	-0.19721400	-1.24508600
C	-1.32083400	-0.41533900	2.74377300
C	-3.01576200	-1.93975800	1.94178200
C	0.83256700	-4.31101500	0.16183900
H	-0.69400900	-3.37011500	1.34830300
C	1.55768600	-3.09861100	-1.79868700
H	0.62254100	-1.18949700	-2.12588800
C	-4.04236600	-2.63996900	-2.56983000
H	-2.14323100	-3.14060200	-1.69633100
C	-4.92653600	-0.45957900	-2.02060100
H	-3.69547900	0.76144300	-0.74279600
C	-1.73611200	-0.63992000	4.05861700
H	-0.51153100	0.28380700	2.54864300
C	-3.43884200	-2.15748900	3.25654000
H	-3.52624500	-2.44546700	1.12705500
C	1.64342200	-4.22393700	-0.97231400
H	0.89780700	-5.17847600	0.81416100
H	2.19092900	-3.01668300	-2.67848700
C	-5.05197500	-1.68225700	-2.68940100
H	-4.12824800	-3.59234200	-3.08742500
H	-5.70495500	0.29422500	-2.10988500
C	-2.79792800	-1.51181700	4.31803300
H	-1.23868900	-0.12422500	4.87610900
H	-4.27052900	-2.83081700	3.44916900
H	2.34377900	-5.02169100	-1.20636700
H	-5.92757600	-1.88353100	-3.30146600
H	-3.12898300	-1.68051600	5.33964500
Ni	-0.60765700	1.33690900	-0.31763100

H	-1.73431600	2.23560800	0.07772800
N	1.51699400	1.79683200	-0.28935800
H	1.41206100	2.12133400	-1.25100500

TS12_1

C	-0.67781800	5.81051700	-0.12939600
C	-1.01874700	4.54651100	-0.61772100
C	-0.07190400	3.51836700	-0.62639100
C	1.22844300	3.74170200	-0.15050100
C	1.56560300	5.02093700	0.32372600
C	0.61868800	6.04461900	0.34338500
H	-1.41486900	6.60981300	-0.12198200
H	-2.02015600	4.35846900	-0.99627300
H	-0.34599400	2.53866300	-1.01400400
H	2.57742900	5.19515400	0.67574700
H	0.89193300	7.02581300	0.72329500
C	2.31422200	2.70148600	-0.14622600
O	3.50082200	3.04288200	-0.20501700
C	3.00002500	0.39868800	0.03711500
C	3.46314100	-0.24879600	-1.10994500
C	3.57202700	0.07222800	1.27649800
C	4.48034600	-1.20806000	-1.03742700
H	3.03412300	0.00730400	-2.07476300
C	4.57705600	-0.88388600	1.36320100
H	3.22212500	0.57314400	2.17506200
C	5.03937200	-1.53027300	0.20507200
H	4.81960100	-1.68794100	-1.94850600
H	5.02168600	-1.14151500	2.32016800
O	6.03028900	-2.45561800	0.39435900
C	6.55804100	-3.12738800	-0.74533600
H	7.00903600	-2.41809900	-1.45077200
H	7.32787400	-3.79954600	-0.36300000
H	5.78280500	-3.71244400	-1.25656100
H	0.94190100	1.17435500	0.93464500
N	1.93981300	1.36958800	-0.05789700
Ni	0.31191100	0.43801400	-0.23987400
P	-1.51232900	-0.72343400	-0.00120000
C	-1.42824700	-2.01750000	1.31560800
C	-1.97264600	-1.66006400	-1.52951800
C	-3.03895400	0.23417100	0.41459400
C	-2.54213500	-2.41248500	2.07258700
C	-0.18851700	-2.63271500	1.55669000
C	-2.45216100	-2.97852800	-1.52017400
C	-1.80645100	-1.00745700	-2.76370100
C	-2.92403400	1.28252000	1.34361500
C	-4.29438300	-0.03919400	-0.14980200
C	-2.41971400	-3.41007700	3.04476300
H	-3.50651500	-1.93929800	1.91204100
C	-0.06923500	-3.63609400	2.52100900
H	0.68743600	-2.31725000	0.99517300
C	-2.76696800	-3.62628700	-2.71934200
H	-2.57635500	-3.50633300	-0.57929300
C	-2.13024000	-1.65051300	-3.95998200
H	-1.42170200	0.01009000	-2.78860400
C	-4.04469100	2.02895000	1.71325800
H	-1.95302900	1.51885400	1.77147000
C	-5.41405400	0.71681000	0.21283400
H	-4.40309800	-0.83845700	-0.87715500
C	-1.18515800	-4.02625900	3.26825500
H	-3.28974300	-3.70256900	3.62733700
H	0.89694200	-4.10227700	2.69601300
C	-2.61053300	-2.96412800	-3.93995900
H	-3.13367500	-4.64944100	-2.69670900
H	-1.99884500	-1.13028000	-4.90529500
C	-5.29297500	1.74864200	1.14731000
H	-3.93994600	2.83573200	2.43414300
H	-6.37950500	0.49602200	-0.23560800
H	-1.09112400	-4.80014600	4.02581400
H	-2.85503000	-3.46978700	-4.87054200
H	-6.16386000	2.33522700	1.42857700

Int13_1

C	2.29350200	1.20862000	-0.18110000
C	1.03547500	3.27346700	0.33009800
C	-0.22042700	3.98473800	0.03728400
C	-1.32439000	3.18414600	-0.33669200
C	-2.52049200	3.87441600	-0.61931000
C	-2.59330500	5.26885000	-0.54655900
C	-0.28678900	5.38479300	0.15247000
C	-1.48083000	6.03021700	-0.15255100
O	1.94239600	3.64639700	1.04974700
C	3.16118300	1.03231600	-1.25618500
C	4.35929300	0.32279100	-1.10505200
C	4.69485500	-0.20149500	0.14781300
C	3.82077400	-0.02116700	1.23237800
H	-3.41212500	3.31750300	-0.89572500
H	-3.52848900	5.77236400	-0.78497400
H	0.58965200	5.94377200	0.47098200
H	-1.55299400	7.11278000	-0.08503800
H	2.91890600	1.45799500	-2.22808700
H	5.01228000	0.20178400	-1.96183300
H	4.09088200	-0.43849500	2.19754700
O	5.83989200	-0.90022500	0.41555900
C	6.79267900	-1.07011000	-0.62949900
H	7.62077500	-1.62664400	-0.18790400
H	6.37115200	-1.64458800	-1.46435900
H	7.15651400	-0.10180700	-0.99578500
C	2.62911200	0.67118300	1.06734100
H	1.95907100	0.80441200	1.91077400
P	-1.12053500	-0.95450900	-0.01657000
C	0.30057500	-2.10834100	0.27708700
C	-1.92946700	-1.70682900	-1.50641000
C	-2.26124400	-1.33183500	1.39113100
C	0.51392300	-2.74139000	1.51091900
C	1.23176500	-2.31471500	-0.75578000
C	-1.86763500	-3.08416500	-1.78296900
C	-2.63395600	-0.87383700	-2.39152300
C	-2.33806200	-0.40351000	2.44126400
C	-3.03338400	-2.50142000	1.46276200
C	1.62304700	-3.57264400	1.70264500
H	-0.18725300	-2.59712700	2.32698700
C	2.33251600	-3.15034400	-0.56678100
H	1.09486500	-1.82719600	-1.71793200
C	-2.50542300	-3.61456900	-2.90706100
H	-1.31070100	-3.74836400	-1.12861300
C	-3.27162500	-1.40549300	-3.51623600
H	-2.68025200	0.19290200	-2.19539400
C	-3.15466200	-0.64679300	3.54916000
H	-1.77018300	0.52153900	2.38268400
C	-3.85795200	-2.74062100	2.56526700
H	-3.00333100	-3.22788200	0.65643600
C	2.53200600	-3.78402200	0.66434700
H	1.76980500	-4.05686400	2.66496600
H	3.03767900	-3.30241300	-1.37987100
C	-3.21110300	-2.77686700	-3.77627400
H	-2.44775500	-4.68237700	-3.10317000
H	-3.81116900	-0.74454900	-4.18988600
C	-3.91747400	-1.81609800	3.61285400
H	-3.20243600	0.08295800	4.35331000
H	-4.45545600	-3.64808600	2.60300300
H	3.39238700	-4.43135300	0.81282700
H	-3.70497800	-3.19008100	-4.65208900
H	-4.56056000	-2.00270000	4.46918500
Ni	-0.94112500	1.31819700	-0.21691900
H	-2.39361200	1.16832100	-0.21346400
N	1.07724800	1.96947000	-0.34503300
H	0.89289400	2.13102100	-1.33852900

Int14_1

C	-1.80826900	5.38791700	-0.34090000
C	-1.59869400	4.29293800	-1.18435300
C	-0.44509200	3.51475300	-1.05070800
C	0.51848300	3.82706100	-0.07989600
C	0.31261200	4.94503800	0.74233200
C	-0.84815600	5.71151800	0.62449800
H	-2.70735500	5.99108600	-0.44182100
H	-2.33026200	4.04718500	-1.95040800
H	-0.27790400	2.67742100	-1.72212900

H	1.07355700	5.20390700	1.47249900
H	-1.00024300	6.56626100	1.27917100
C	1.80933000	3.05842500	0.06641200
O	2.85223900	3.68045800	0.32682800
C	2.93147800	0.93366600	-0.04132600
C	3.25475900	0.05491700	-1.08362100
C	3.77171500	0.95401800	1.09134400
C	4.36747300	-0.79504800	-1.01377200
H	2.63510300	0.04942400	-1.97756600
C	4.87898000	0.12059500	1.16992400
H	3.54521000	1.62974200	1.90872100
C	5.18630100	-0.76161400	0.11859600
H	4.58098200	-1.45661200	-1.84604300
H	5.52612200	0.13615800	2.04263800
O	6.29996100	-1.54018200	0.29881100
C	6.67524400	-2.43372900	-0.74341200
H	6.89409300	-1.89160600	-1.67232500
H	7.57896700	-2.93572900	-0.39385500
H	5.89182900	-3.17981300	-0.93016800
H	-0.11221200	1.00240000	1.33893800
N	1.73931500	1.70817300	-0.13869400
Ni	0.26058300	0.58130800	0.00359000
P	-1.36884500	-0.91416800	0.07935700
C	-1.26408800	-2.06083300	1.51359700
C	-1.31466700	-1.98657200	-1.42108000
C	-3.07980000	-0.23491200	0.11550200
C	-2.37120800	-2.79266600	1.97220500
C	-0.02668200	-2.21121100	2.15969900
C	-1.10493400	-3.37229100	-1.36299100
C	-1.41160700	-1.36340700	-2.67928500
C	-3.31245900	0.94989500	0.83381900
C	-4.15590400	-0.86841800	-0.52749000
C	-2.23842900	-3.66765900	3.05285300
H	-3.34012000	-2.67622400	1.49513500
C	0.10501500	-3.09159800	3.23701300
H	0.83011900	-1.63004500	1.82928200
C	-1.00687600	-4.12182300	-2.54024800
H	-1.01818300	-3.87169500	-0.40294100
C	-1.32025200	-2.11429900	-3.85177300
H	-1.56989800	-0.28911500	-2.74568000
C	-4.60158400	1.48012100	0.92175300
H	-2.48496100	1.46133100	1.31675200
C	-5.44310600	-0.33053900	-0.44396200
H	-3.99355100	-1.77608800	-1.10168500
C	-1.00003400	-3.82068000	3.68485100
H	-3.10313300	-4.22543700	3.40293400
H	1.06760800	-3.19760900	3.73006900
C	-1.11535400	-3.49704100	-3.78469800
H	-0.84591300	-5.19506000	-2.48010200
H	-1.40362100	-1.61968700	-4.81592700
C	-5.66906600	0.84163900	0.28352500
H	-4.76715500	2.39756200	1.48012800
H	-6.26722300	-0.82872600	-0.94815400
H	-0.89975500	-4.49917900	4.52803400
H	-1.03867800	-4.08132100	-4.69781100
H	-6.67065400	1.25897700	0.34675600

Int15_1

C	-2.77703700	0.00796800	3.63454900
C	-2.28313600	-1.87274500	2.16187400
C	-3.11844100	-2.67163700	2.96284000
C	-3.77505500	-2.14399900	4.07620100
C	-3.60679500	-0.79760100	4.41950000
C	-1.59740400	-2.54635800	0.98141500
O	-1.76218800	-3.79190600	0.87040400
N	-0.88132800	-1.77970100	0.13730900
C	-0.19272200	-2.46146400	-0.90289700
C	-0.33644900	-2.05435500	-2.23773200
C	0.37507800	-2.66318100	-3.28343900
C	1.25986300	-3.70680100	-3.00318500
H	-2.63607800	1.05716600	3.88600200
H	-3.23482300	-3.71492800	2.68844900
H	-4.41927200	-2.78347800	4.67663100
H	-4.11623400	-0.38224700	5.28674700
H	-1.01779900	-1.24096000	-2.46698800
H	0.22140000	-2.30942400	-4.29792300
O	2.01405600	-4.37543300	-3.94937100
C	1.86775000	-3.99042500	-5.30664100
H	2.15917100	-2.94222300	-5.46148100
H	2.53569600	-4.63923700	-5.87780800
H	0.83587200	-4.13216800	-5.65626000
C	0.70953500	-3.51740300	-0.64916100
H	0.84681200	-3.85639100	0.37102900
C	1.42231300	-4.12762300	-1.67535000
H	2.11705900	-4.93669100	-1.46276300
P	1.48386900	0.47570000	0.73073800
C	2.76880000	1.08397200	-0.46934600
C	3.79444500	1.98681200	-0.14862300
C	2.68453400	0.60270500	-1.78712000
C	4.71632800	2.39449500	-1.11873100
H	3.87652200	2.38407000	0.85867700
C	3.61268100	0.99885800	-2.75290500
H	1.88303400	-0.08052400	-2.05732500
C	4.63120600	1.89837300	-2.42257900
H	5.49993100	3.10051200	-0.85253000
H	3.53102600	0.61281300	-3.76608700
H	5.34734400	2.21606700	-3.17683000
C	1.59662200	1.69344000	2.13721800
C	2.62825400	1.66417900	3.09169000
C	0.59780900	2.67263500	2.26172400
C	2.66871100	2.59661200	4.13184400
H	3.39991300	0.90183200	3.03074600
C	0.63994700	3.61036400	3.29848200
H	-0.22006800	2.69075900	1.54686900
C	1.67544000	3.57583000	4.23631000
H	3.47373000	2.55406000	4.86210100
H	-0.14399500	4.36003800	3.37597600
H	1.70396200	4.29924200	5.04786500
C	2.32967100	-0.99369700	1.49594800
C	3.57424500	-1.48340700	1.07475900
C	1.65534300	-1.67071900	2.52783100
C	4.13711300	-2.61620500	1.67416900
H	4.11050600	-0.98745300	0.27163500
C	2.21986300	-2.79487300	3.13235300
H	0.67974000	-1.32399300	2.85698500
C	3.46424100	-3.27346200	2.70644400
H	5.10101800	-2.98285600	1.32811700
H	1.67875100	-3.30562600	3.92510300
H	3.89912500	-4.15589000	3.17004800
Ni	-0.59524200	0.22532000	-0.12231300
C	-2.15975800	0.92810000	-0.91143100
C	-1.21292700	1.82449000	-0.96310300
C	-3.54750600	0.61006700	-1.18674900
C	-0.90581300	3.13005300	-1.53069200
C	-4.54161200	1.61541800	-1.24486200
C	-3.96027600	-0.72693600	-1.37908000
C	-1.80003000	3.76678800	-2.42568700
C	0.29893300	3.80412800	-1.24058400
C	-5.87593300	1.29980000	-1.50264000
H	-4.25791900	2.64918700	-1.06730700
C	-5.29241200	-1.03861000	-1.65358100
H	-3.21959800	-1.51580400	-1.29779500
C	-1.50668100	5.00859900	-2.98765900
H	-2.72636100	3.26473400	-2.68809600
C	0.58968000	5.05265600	-1.79394600
H	1.01455900	3.32938900	-0.57888200
C	-6.26008400	-0.02937200	-1.71873600
H	-6.61939300	2.09418700	-1.53527200
H	-5.57789700	-2.07781700	-1.80209600
C	-0.31074100	5.66652500	-2.67094100
H	-2.21419100	5.46650000	-3.67646300
H	1.52863400	5.54296100	-1.54507800
H	-7.29975100	-0.27539500	-1.92278000
H	-0.08316100	6.63677500	-3.10652100
C	-2.12407400	-0.52563800	2.51919400
H	-1.49531900	0.11682800	1.90589900

TS13_1

C	0.31665800	4.30075200	-0.80634900
C	1.64074400	2.54509500	-1.85041300
C	2.31888800	3.53302300	-2.58568100
C	2.01454800	4.88449100	-2.42213700
C	1.00578200	5.27476200	-1.53335800
C	1.98880400	1.10293200	-2.14757600
O	2.47760300	0.85177100	-3.26839700
N	1.74924800	0.13753300	-1.20515400
C	1.92302400	-1.21427500	-1.63157600
C	2.93744400	-2.01986800	-1.11157900
C	3.08819500	-3.35563300	-1.51009500
C	2.20906200	-3.90072900	-2.44922600
H	-0.47297300	4.58752000	-0.11553100
H	3.08409400	3.22129500	-3.28941200
H	2.56036900	5.63366700	-2.99153400
H	0.76046900	6.32741200	-1.40953100
H	3.61857100	-1.60956000	-0.37329200
H	3.88534100	-3.94780800	-1.07352200
O	2.26231700	-5.19859600	-2.90989200
C	3.27663600	-6.04851600	-2.39487000
H	3.18029100	-6.17475500	-1.30815900
H	3.13671100	-7.01387300	-2.88601700
H	4.27853300	-5.66330800	-2.62781200
C	1.03803800	-1.78502900	-2.56334000
H	0.23198700	-1.17829900	-2.96529600
C	1.18055100	-3.10408200	-2.97584300
H	0.49520900	-3.53890600	-3.69869000
P	-2.21876300	0.01865600	0.05888500
C	-2.96900800	-1.48119900	0.87107100
C	-4.21713100	-1.48492400	1.51418500
C	-2.22235500	-2.67068700	0.84391400
C	-4.71263000	-2.65251700	2.10473400
H	-4.80618100	-0.57297700	1.56224600
C	-2.72222200	-3.84113000	1.42025600
H	-1.23434300	-2.66689800	0.38920900
C	-3.96937800	-3.83575200	2.05376300
H	-5.67869000	-2.63509000	2.60490300
H	-2.12725000	-4.75082100	1.39003300
H	-4.35336600	-4.74307500	2.51452200
C	-3.11930600	1.41442400	0.90375500
C	-4.29468200	2.00557800	0.41403200
C	-2.56272000	1.91587200	2.09425700
C	-4.90069500	3.06636100	1.09698600
H	-4.73909900	1.64454500	-0.50911500
C	-3.17321300	2.96568000	2.78374500
H	-1.63777700	1.48120500	2.46771600
C	-4.34511300	3.54740100	2.28555000
H	-5.80756500	3.51495500	0.69696100
H	-2.72739200	3.33705300	3.70370400
H	-4.81588600	4.37193100	2.81599200
C	-3.05073900	-0.00768500	-1.61774700
C	-4.09863800	-0.87092000	-1.97441100
C	-2.54719800	0.86751700	-2.59700600
C	-4.63358700	-0.85381000	-3.26819400
H	-4.50067000	-1.56792000	-1.24499700
C	-3.08742500	0.89622000	-3.88421700
H	-1.71764200	1.52689000	-2.35165700
C	-4.13376900	0.03199400	-4.22604800
H	-5.44064400	-1.53687900	-3.52466400
H	-2.68002300	1.58237300	-4.62301400
H	-4.54706300	0.04281700	-5.23192300
Ni	-0.09620500	0.13558300	0.17586600
C	1.86400800	0.35991900	0.61632200
C	1.28258800	-0.58182500	1.34653300
C	2.88150600	1.38248100	0.91220500
C	1.52678700	-1.11572200	2.65511700
C	2.68663000	2.22376600	2.02657100
C	4.10149400	1.48959000	0.21678500
C	2.83905100	-1.44776700	3.09584100
C	0.46817500	-1.38450700	3.56380000
C	3.66844900	3.12803600	2.43130100
H	1.75172100	2.15056500	2.57498400
C	5.08505100	2.39532200	0.62215600
H	4.28242600	0.85494300	-0.64564000
C	3.06933600	-1.99863900	4.35494400
H	3.67695100	-1.26336100	2.42754100
C	0.70813100	-1.91828100	4.82867600
H	-0.54865100	-1.16794200	3.24683600
C	4.87652400	3.22200700	1.73035900
H	3.48739700	3.76481600	3.29488100
H	6.01901500	2.45350200	0.06669800
C	2.00970100	-2.23767100	5.24247900
H	4.08985600	-2.23795600	4.65178400
H	-0.13301700	-2.10116700	5.49620800
H	5.64177300	3.92902700	2.04258300
H	2.19270300	-2.66585900	6.22538400
C	0.63906200	2.94933500	-0.95820600
H	0.09555000	2.19928900	-0.37628500

Int16_1

C	2.71424400	-2.75983800	2.89319500
C	3.21982600	-0.43314800	2.42786300
C	4.42200800	-0.56651000	3.13779500
C	4.78203000	-1.79399100	3.69682300
C	3.92637500	-2.89470900	3.57834300
C	2.82333800	0.93751400	1.94563300
O	3.00764600	1.90855800	2.69449500
N	2.24251400	1.05129800	0.70162100
C	1.59461500	2.27925100	0.34966800
C	1.81305500	2.87300100	-0.89488300
C	1.16294500	4.05841300	-1.26123100
C	0.28154000	4.67025100	-0.36593700
H	2.03988800	-3.60867900	2.80483900
H	5.06863700	0.29935600	3.24556600
H	5.72544400	-1.89028100	4.22935000
H	4.20148500	-3.85040400	4.01910000
H	2.48081400	2.39865200	-1.60623000
H	1.35446300	4.47970200	-2.24202700
O	-0.40950700	5.83363200	-0.62075100
C	-0.20796500	6.46969200	-1.87534100
H	-0.51080600	5.81987000	-2.70711000
H	-0.83821500	7.36139400	-1.86315000
H	0.84090000	6.76676700	-2.00913500
C	0.69657300	2.89905100	1.23527600
H	0.50064400	2.44823900	2.20110100
C	0.05344700	4.08024500	0.88628700
H	-0.64406600	4.55345300	1.57217500
P	-2.54893500	-0.50988400	0.15006100
C	-3.63260900	0.78237200	-0.65386600
C	-4.87423400	0.52197600	-1.25477000
C	-3.13859300	2.09927200	-0.68574100
C	-5.60640500	1.54914200	-1.86257700
H	-5.27575900	-0.48734800	-1.25664100
C	-3.87432800	3.12809900	-1.27758900
H	-2.16531300	2.31519200	-0.25127300
C	-5.11234300	2.85612200	-1.87172600
H	-6.56375700	1.32395600	-2.32819000
H	-3.47327200	4.13907100	-1.28386600
H	-5.68148500	3.65420200	-2.34328000
C	-3.40892500	-2.09415100	-0.34151800
C	-4.47801200	-2.67232900	0.36217000
C	-2.92892100	-2.75286400	-1.48677800
C	-5.05707200	-3.87047600	-0.07182800
H	-4.86060500	-2.19227700	1.25877600
C	-3.51388800	-3.94170100	-1.92995200
H	-2.07847100	-2.33212600	-2.01870200
C	-4.58031200	-4.50668400	-1.22174000
H	-5.88076200	-4.30518900	0.49081000
H	-3.12652200	-4.43245400	-2.81994100
H	-5.02997000	-5.43822200	-1.55835700
C	-3.06654900	-0.35833800	1.94101700
C	-4.18012100	0.36941400	2.38935400
C	-2.25694500	-0.99366600	2.89930300
C	-4.47901600	0.45563700	3.75444200
H	-4.81771600	0.87997000	1.67305900
C	-2.56047800	-0.92223000	4.26042800
H	-1.37371000	-1.53611800	2.56935300
C	-3.67361900	-0.19294000	4.69427200

H	-5.34265800	1.03175900	4.08029900
H	-1.91840800	-1.42098400	4.98293800
H	-3.90406800	-0.12351200	5.75494500
Ni	-0.49703700	-0.41377900	-0.32680000
C	2.44868900	0.03607700	-0.34460300
C	1.34691500	-0.57360500	-0.86645600
C	3.88096700	-0.12961300	-0.71637200
C	1.42896400	-1.45484200	-2.05006900
C	4.39374200	-1.35873400	-1.18659000
C	4.80158000	0.93607700	-0.58881800
C	1.70234300	-0.94199700	-3.33997900
C	1.15861400	-2.84129500	-1.95990800
C	5.73531000	-1.50320600	-1.54029700
H	3.73308100	-2.21404500	-1.26172400
C	6.14435300	0.79280000	-0.94431700
H	4.46180300	1.89335000	-0.20389500
C	1.71351300	-1.76583700	-4.46736900
H	1.90014200	0.12181600	-3.44907500
C	1.18885600	-3.66715600	-3.08342000
H	0.92056500	-3.26220200	-0.98587300
C	6.62412600	-0.42784200	-1.42930700
H	6.09038500	-2.46910500	-1.89428900
H	6.81791500	1.64094300	-0.83695100
C	1.46292500	-3.13836700	-4.35278600
H	1.92490100	-1.33190400	-5.44360200
H	0.98599500	-4.73110800	-2.96990600
H	7.67052800	-0.54297900	-1.70283800
H	1.47367000	-3.78004600	-5.23101100
C	2.36453900	-1.53885100	2.31070900
H	1.43207500	-1.43816900	1.76207200

TS14_1

C	-0.35050500	2.73642600	-2.93326700
C	1.07897600	0.78337800	-2.88187900
C	1.39261500	1.01527100	-4.23827300
C	0.86267200	2.09727800	-4.93332200
C	-0.03463900	2.95238000	-4.27241300
C	1.53472400	-0.54526400	-2.34258500
O	1.71384700	-1.48776900	-3.12496300
N	1.64811400	-0.75455700	-0.94990600
C	1.35723900	-2.05489900	-0.43436400
C	0.28879700	-2.80965600	-0.94198200
C	-0.04663200	-4.05592300	-0.40804700
C	0.68069300	-4.57644400	0.66927600
H	-1.03029100	3.42631100	-2.43538300
H	2.04840600	0.31078100	-4.74280900
H	1.13029300	2.26849200	-5.97371000
H	-0.47910100	3.79263400	-4.80540900
H	-0.29935400	-2.42173200	-1.76550700
H	-0.88695100	-4.59390100	-0.83313400
O	0.42869200	-5.79023100	1.27277400
C	-0.64446600	-6.57415300	0.77192200
H	-0.48573800	-6.84472300	-0.28072100
H	-0.66213700	-7.48095600	1.38036700
H	-1.60439800	-6.04985400	0.87118900
C	2.07518000	-2.59279100	0.64841200
H	2.90268300	-2.03684200	1.07237000
C	1.74115600	-3.83139400	1.19432600
H	2.30689500	-4.23358600	2.03065900
P	-2.01310000	0.43539300	0.20305900
C	-2.32759500	-0.32502400	1.87437300
C	-3.49261400	-0.09889400	2.62569300
C	-1.33074200	-1.15555600	2.41076900
C	-3.66112700	-0.69587300	3.87902600
H	-4.27158800	0.55100000	2.23637100
C	-1.50412500	-1.76430200	3.65702400
H	-0.40946700	-1.31329500	1.85633700
C	-2.66879300	-1.53471900	4.39598600
H	-4.56665600	-0.50335600	4.45052700
H	-0.72168400	-2.40701300	4.05319900
H	-2.79808400	-1.99770500	5.37166500
C	-3.11718500	1.93040200	0.26035700
C	-4.38943900	1.99257800	-0.32774500
C	-2.62513300	3.07328600	0.91786800
C	-5.15253900	3.16445900	-0.25970200
H	-4.79064500	1.12713300	-0.84682700
C	-3.39026300	4.23819300	0.99603600
H	-1.63288800	3.04855900	1.36205000
C	-4.65818700	4.28927400	0.40480000
H	-6.13453500	3.19317600	-0.72692500
H	-2.99141100	5.10958100	1.51017400
H	-5.25118100	5.19935800	0.45795500
C	-2.94222100	-0.71018900	-0.93134000
C	-3.77895000	-1.74718300	-0.48995700
C	-2.75654300	-0.53995200	-2.31519300
C	-4.42368200	-2.58455700	-1.40711600
H	-3.92820200	-1.90913900	0.57303400
C	-3.40690700	-1.36996700	-3.23121600
H	-2.08806800	0.23892600	-2.67166400
C	-4.24362900	-2.39668400	-2.78020600
H	-5.06559200	-3.38474300	-1.04469200
H	-3.24652500	-1.22206900	-4.29642500
H	-4.74266800	-3.04945200	-3.49275100
Ni	0.00585100	1.21394100	-0.32978100
C	2.39728200	0.16611000	-0.06101800
C	1.63749000	0.95138000	0.75713200
C	3.86680600	0.14205400	-0.26430200
C	2.13485400	1.72296000	1.89525500
C	4.70853600	1.17531200	0.21297100
C	4.49204400	-0.89411700	-0.99829800
C	2.70807000	1.07512100	3.01630200
C	1.97444000	3.12630600	1.98009100
C	6.08640400	1.15258500	0.00139000
H	4.27561400	2.01367800	0.74464000
C	5.87188400	-0.91260600	-1.21272400
H	3.88861000	-1.69325100	-1.41456300
C	3.11034900	1.78969100	4.14525400
H	2.83166000	-0.00503200	2.99028300
C	2.40132400	3.84181000	3.09869700
H	1.51161900	3.64600900	1.14508600
C	6.68610900	0.10575400	-0.70923900
H	6.69478100	1.96981900	0.38441200
H	6.30917800	-1.73073400	-1.78185900
C	2.96997800	3.18203400	4.19649100
H	3.54428500	1.25566000	4.98904800
H	2.27807200	4.92346900	3.11959100
H	7.76057900	0.09287500	-0.87761100
H	3.28736600	3.73955600	5.07472100
C	0.19561800	1.66655000	-2.17895200
H	0.82875600	2.35236200	-0.76672200

Int17_1

C	-1.00631800	3.74284100	0.08284200
C	-1.12030200	1.86684700	-1.39872600
C	-2.29465200	2.38637900	-1.96702800
C	-2.86062500	3.56131800	-1.47252900
C	-2.21781900	4.22681100	-0.42313400
C	-0.57038100	0.57360300	-1.92527400
O	-0.11390900	0.46016200	-3.05643300
N	-0.54375500	-0.53071100	-1.02146100
C	-1.63356600	-0.73791400	-0.13428600
C	-2.93981500	-0.75889000	-0.64363200
C	-4.04523900	-0.98606300	0.18230800
C	-3.85307400	-1.23653300	1.54549900
H	-0.49545800	4.31905000	0.84817800
H	-2.77365000	1.85173700	-2.78565600
H	-3.78426000	3.94966100	-1.89726200
H	-2.64399600	5.14411000	-0.01812300
H	-3.09903000	-0.60251700	-1.70705000
H	-5.03771900	-0.97959000	-0.25513200
O	-4.86493200	-1.49089800	2.44455100
C	-6.20469600	-1.43786800	1.97578500
H	-6.39298400	-2.20230900	1.20968300
H	-6.83424100	-1.63594700	2.84571500
H	-6.44635300	-0.44720700	1.56817500
C	-1.45876500	-0.99140700	1.23784500
H	-0.46040300	-0.97345200	1.65941300
C	-2.55096400	-1.24565100	2.06211600

H	-2.40881900	-1.43766600	3.12228600
Ni	1.35382700	2.06835300	0.18092000
C	0.80163700	-0.87784100	-0.57872300
C	1.48938100	0.15836300	-0.06316000
C	1.21043800	-2.28677400	-0.78988400
C	2.77543300	0.32049600	0.58654500
C	2.50600500	-2.74776300	-0.46995600
C	0.31151300	-3.22124400	-1.34415900
C	3.05690500	-0.18728700	1.89053400
C	3.68017400	1.27941700	0.05227600
C	2.87530600	-4.07592800	-0.68006200
H	3.23509300	-2.05671600	-0.06313400
C	0.68080600	-4.55234400	-1.55080600
H	-0.68292400	-2.89099800	-1.62352300
C	4.19794700	0.19428700	2.57679700
H	2.36007900	-0.89188600	2.33764300
C	4.83625400	1.65661400	0.76263600
H	3.52379400	1.65188000	-0.95755900
C	1.96469900	-4.99301600	-1.21832800
H	3.88431400	-4.39462900	-0.42625500
H	-0.03980200	-5.24566700	-1.97968300
C	5.10277400	1.11873800	2.01435800
H	4.39568800	-0.22233000	3.56243600
H	5.51991200	2.37576700	0.31759000
H	2.25449700	-6.02850000	-1.38135900
H	5.99358100	1.41324700	2.56370900
C	-0.40448800	2.54994200	-0.37915400
H	1.69113400	3.55613600	0.45521700

PhCCMe

C	1.39653200	-0.00019700	-0.00077600
C	2.61156500	0.00006300	-0.00115800
C	-0.03567000	-0.00010200	-0.00028000
C	-0.75392500	1.21328500	-0.00017100
C	-0.75410800	-1.21338100	-0.00015600
C	-2.14895100	1.20951700	0.00021300
H	-0.20830800	2.15255400	-0.00019200
C	-2.14913800	-1.20939100	0.00020500
H	-0.20862700	-2.15273000	-0.00018600
C	-2.85216800	0.00011600	0.00036400
H	-2.68832400	2.15331400	0.00039400
H	-2.68866300	-2.15310200	0.00036100
H	-3.93902400	0.00019900	0.00072000
C	4.07344700	0.00004600	0.00074900
H	4.46927600	0.90626400	-0.47326900
H	4.46855000	-0.04157700	1.02347500
H	4.46961900	-0.86464700	-0.54525400

Int18_1

C	-0.79020800	-1.66285900	-0.71797500
C	-1.91412400	-1.28480200	-0.18747400
Ni	-0.53755800	-0.02808900	0.10895300
H	-0.94315600	1.30138200	1.44951100
C	-1.24093400	2.11409000	0.76212600
C	-2.55183000	2.60176400	0.83880400
C	-0.27737600	2.75958500	-0.03430200
C	-2.91824400	3.73661300	0.11262300
C	-0.65487400	3.90821900	-0.74499700
C	-1.96411400	4.38880600	-0.67966800
H	-3.28039800	2.09316900	1.46497700
H	-3.93706800	4.11357400	0.16494300
H	-2.24388300	5.27404100	-1.24700500
H	0.09394200	4.40794800	-1.35207600
C	1.14102600	2.24301000	-0.14102300
O	2.05326000	3.06360200	-0.41415400
N	1.23419600	0.91634600	0.08724700
C	2.47575500	0.25563400	0.14119700
C	3.70023800	0.74544400	-0.35948300
C	2.50530900	-1.02484300	0.74381400
C	4.88396900	-0.00227200	-0.26376100
H	3.72496900	1.72361400	-0.81913200
C	3.67532000	-1.76663700	0.84826100
H	1.57241900	-1.42456200	1.13210600
C	4.88121300	-1.26065700	0.34183800
H	5.79739500	0.42262400	-0.66835300
H	3.67097000	-2.74580900	1.32138800
O	5.99249900	-2.06995000	0.49002700
C	7.23172400	-1.59312600	-0.00860000
H	7.53341500	-0.66073500	0.48832400
H	7.96479000	-2.37303500	0.20987300
H	7.19159500	-1.42596700	-1.09388800
C	-3.30771600	-1.65875400	-0.03745700
C	-4.09125800	-1.17682900	1.03385500
C	-3.93954200	-2.52533300	-0.96151000
C	-5.42941900	-1.54609000	1.18185500
H	-3.62655100	-0.51056900	1.75623500
C	-5.27813300	-2.89040300	-0.81741800
H	-3.36356300	-2.90008700	-1.80404800
C	-6.03484400	-2.40528400	0.25719100
H	-6.00398300	-1.16055500	2.02202400
H	-5.73541300	-3.55547400	-1.54786000
H	-7.07877800	-2.68919200	0.36879100
C	-0.05636000	-2.70874600	-1.48029500
H	0.11859200	-2.38210900	-2.51531300
H	0.93162300	-2.90710500	-1.04637700
H	-0.61419800	-3.65748400	-1.51810500

Int19_1

C	-0.66451100	2.14477800	-0.20440500
C	-1.86509200	2.14412600	-0.69620000
Ni	-1.27592100	0.38993400	-0.48669400
H	-2.36769600	-0.84655200	-1.55643700
C	-3.05591600	-1.10567200	-0.73473500
C	-4.41538600	-0.79164800	-0.86892700
C	-2.59958000	-1.88435900	0.34422200
C	-5.33261000	-1.24209900	0.08173500
C	-3.53460200	-2.34171100	1.28556400
C	-4.88606800	-2.01699400	1.16183800
H	-4.74905500	-0.20003100	-1.71807300
H	-6.38797700	-0.99788200	-0.01688800
H	-5.59700500	-2.36949700	1.90623000
H	-3.17993500	-2.94987400	2.11255400
C	-1.13767800	-2.24768200	0.49190900
O	-0.85300700	-3.31693100	1.08897600
N	-0.31288300	-1.33724700	-0.06711700
C	1.07474200	-1.54720700	-0.16902500
C	1.80300300	-2.61251900	0.40417600
C	1.81749200	-0.60872700	-0.92602700
C	3.19043300	-2.73036400	0.22840500
H	1.27397500	-3.35337100	0.98649400
C	3.19002000	-0.72288200	-1.10504300
H	1.28031400	0.22471800	-1.37029400
C	3.89344100	-1.78850400	-0.52545300
H	3.69995000	-3.56851200	0.69360500
H	3.73512400	0.01499800	-1.68854400
O	5.25749500	-1.81597300	-0.75222700
C	6.00514500	-2.86715900	-0.16304100
H	5.67982500	-3.84961800	-0.53257700
H	7.04455200	-2.69788400	-0.45348600
H	5.92627200	-2.85129000	0.93287500
C	0.43360900	2.96764800	0.26437100
C	0.51795000	4.33690300	-0.08429600
C	1.45382600	2.44002900	1.08427400
C	1.56348400	5.13803900	0.37476100
H	-0.24861800	4.76243200	-0.72750000
C	2.49986100	3.24271800	1.54273600
H	1.41193700	1.38872300	1.35275100
C	2.56331300	4.59686100	1.19381600
H	1.60239400	6.18799300	0.08980200
H	3.27237800	2.80721100	2.17332400
H	3.38098400	5.22004200	1.54898900
C	-3.02595500	2.98894800	-1.09590500
H	-3.14680500	2.99675700	-2.18903400
H	-3.96501700	2.59805200	-0.68175100
H	-2.91907500	4.03426400	-0.76730600

TS15_1

C	-0.59537300	-1.58602000	-0.55707900

C	-1.79538800	-1.35668800	-0.19246400
Ni	-0.75124600	0.24703500	0.15155300
H	-1.82592900	0.49061300	1.09667100
C	-1.30739100	2.08406700	0.17529600
C	-2.58882800	2.66089700	0.15357700
C	-0.20373300	2.93688100	-0.04456000
C	-2.76695800	4.03361400	-0.07110000
C	-0.37783700	4.30738400	-0.26851200
C	-1.65992300	4.86396200	-0.27770000
H	-3.46774700	2.03984500	0.31434200
H	-3.77197900	4.45383800	-0.07682500
H	-1.79497200	5.93049100	-0.44731200
H	0.50456200	4.91875700	-0.44265700
C	1.16765100	2.32612800	-0.07665500
O	2.19434700	3.03968200	-0.16990300
N	1.11216200	0.97530300	0.02539500
C	2.30786900	0.23645900	0.12419700
C	3.41632100	0.42520000	-0.71935700
C	2.41477100	-0.77009000	1.10604100
C	4.57398100	-0.35503500	-0.59977600
H	3.37579600	1.19831100	-1.47789700
C	3.56094800	-1.55013500	1.23772300
H	1.57154000	-0.93018600	1.77293200
C	4.65238000	-1.34767000	0.38288400
H	5.40153200	-0.17074900	-1.27732600
H	3.62731500	-2.31857600	2.00425500
O	5.74637700	-2.16800800	0.58651200
C	6.88235600	-1.97950300	-0.24234900
H	7.29688700	-0.96799800	-0.13297900
H	7.62195900	-2.71152500	0.08986500
H	6.64386900	-2.15868300	-1.29994000
C	-3.15995400	-1.83545200	-0.06069000
C	-4.09363100	-1.24492000	0.81036800
C	-3.58067500	-2.94821300	-0.82312200
C	-5.39289700	-1.74436200	0.92023100
H	-3.78221600	-0.38916700	1.40258200
C	-4.88035500	-3.44313000	-0.71739800
H	-2.87541500	-3.41600200	-1.50502000
C	-5.79595000	-2.84514900	0.15706600
H	-6.09344700	-1.27027300	1.60420400
H	-5.17995200	-4.29861700	-1.31914300
H	-6.80908600	-3.23124200	0.24015800
C	0.41948100	-2.48881500	-1.14690200
H	0.88001400	-2.03016700	-2.03088000
H	1.23542200	-2.67900200	-0.44088900
H	-0.01537700	-3.45361600	-1.44658100

TS16_1

C	-0.15494400	2.15456300	-0.06138700
C	-1.27763900	2.66891900	-0.38491400
Ni	-1.52805300	0.75690300	-0.42301100
H	-2.48589600	1.21006600	-1.40998100
C	-3.21316300	-0.13081100	-0.20640300
C	-4.52595200	0.36998900	-0.20277700
C	-3.01810800	-1.46104800	0.21990900
C	-5.60616300	-0.42207800	0.21325500
C	-4.09304100	-2.25385300	0.63826500
C	-5.39278600	-1.73940100	0.63375400
H	-4.72066600	1.38969900	-0.52974200
H	-6.61460600	-0.01024100	0.20128800
H	-6.22929000	-2.35728500	0.95469200
H	-3.88791700	-3.26908300	0.97024700
C	-1.61677300	-2.00092200	0.24172000
O	-1.39923900	-3.20518800	0.51499300
N	-0.70612300	-1.04906900	-0.08318900
C	0.65202700	-1.39523100	-0.22760700
C	1.33042200	-2.31339500	0.59563000
C	1.40629100	-0.77710700	-1.24792800
C	2.69003400	-2.60159500	0.41209500
H	0.78622800	-2.81931100	1.38290900
C	2.75457900	-1.05938300	-1.44196500
H	0.90894500	-0.05797300	-1.89266900
C	3.40924500	-1.97817700	-0.61176700
H	3.16472900	-3.31848000	1.07475900
H	3.31642000	-0.57067500	-2.23412000
O	4.74781600	-2.19937200	-0.88121600
C	5.43982800	-3.13901100	-0.07579900
H	4.99388700	-4.14041700	-0.15247800
H	6.46281800	-3.16841300	-0.45812200
H	5.45560800	-2.83215300	0.97933600
C	1.21662700	2.40535700	0.33808500
C	1.95507000	3.45914800	-0.24275800
C	1.84544900	1.62207600	1.32578200
C	3.26715500	3.72199400	0.15492000
H	1.48934500	4.06480900	-1.01620800
C	3.15250700	1.89487400	1.73128500
H	1.29795800	0.79136500	1.76001900
C	3.87214600	2.94387600	1.14837400
H	3.81808100	4.53626400	-0.31154100
H	3.61594200	1.27621000	2.49643400
H	4.89502600	3.14665600	1.45723200
C	-2.13314400	3.86168800	-0.60316100
H	-2.36646400	3.98757500	-1.66828200
H	-3.08875800	3.77065800	-0.07270000
H	-1.62966300	4.77455300	-0.25431000

Int20_1

C	-0.83068800	-1.31902800	-0.01857400
C	-2.13231900	-1.01184700	0.05128900
Ni	-0.63289900	0.57642300	0.08397900
H	-2.35534100	0.10852600	0.18589700
C	-0.96627500	2.49221800	0.06021900
C	-2.14177000	3.26573700	0.06845800
C	0.24987400	3.20010300	-0.03811600
C	-2.10407300	4.66703400	-0.01778200
C	0.30828800	4.59414200	-0.13213600
C	-0.87837500	5.33588700	-0.12152000
H	-3.11749600	2.78278700	0.14362600
H	-3.03254300	5.23809400	-0.00547700
H	-0.84891100	6.42184500	-0.19209300
H	1.27600700	5.08538700	-0.21154500
C	1.49027700	2.35781900	-0.02743300
O	2.64034500	2.84427100	-0.08330900
N	1.19651000	1.02995900	0.07453900
C	2.26012300	0.09633500	0.12620000
C	3.13512200	-0.09070200	-0.95171700
C	2.46545900	-0.68838100	1.27491300
C	4.18120700	-1.02072100	-0.89768300
H	2.99991900	0.50691700	-1.84825800
C	3.49862600	-1.61996000	1.34355900
H	1.79204000	-0.56180300	2.11846500
C	4.36622300	-1.79069900	0.25611400
H	4.83619100	-1.12780200	-1.75610500
H	3.64868600	-2.22260000	2.23591700
O	5.35930900	-2.73571800	0.41601800
C	6.26444300	-2.94107000	-0.65801500
H	6.82466200	-2.02570600	-0.89177500
H	6.95863300	-3.71430100	-0.32185900
H	5.74394500	-3.28724500	-1.56142300
C	-3.41195600	-1.72855800	-0.01839400
C	-4.63102400	-1.02089300	0.05281300
C	-3.47936700	-3.13318500	-0.15195600
C	-5.85875600	-1.67966100	-0.01072300
H	-4.60846300	0.06216100	0.15766800
C	-4.70882700	-3.79042900	-0.21531100
H	-2.56402900	-3.71174300	-0.20534400
C	-5.90768300	-3.07170600	-0.14560300
H	-6.78025300	-1.10426400	0.04568000
H	-4.72972900	-4.87335400	-0.31846200
H	-6.86333000	-3.58785100	-0.19503500
C	-0.15271900	-2.63832500	-0.19387000
H	-0.48677500	-3.13942900	-1.11593700
H	0.93475700	-2.53081500	-0.24828500
H	-0.37446700	-3.32144500	0.64110300

Int21_1

C	0.02473400	2.04265400	-0.09430300
C	-0.97263300	2.91761100	-0.24035300

Ni	-1.44903900	0.78986300	-0.13937000
H	-1.99442500	2.47524700	-0.50186700
C	-3.24836100	0.09252600	-0.04718800
C	-4.50901300	0.71654500	-0.05158000
C	-3.23500600	-1.30833800	0.09745900
C	-5.69432400	-0.02539200	0.07970000
C	-4.40397000	-2.06320600	0.23400200
C	-5.64548900	-1.41758200	0.22381300
H	-4.58871000	1.79963700	-0.15782200
H	-6.65806300	0.48380200	0.06947200
H	-6.56469800	-1.99161100	0.32653700
H	-4.33148300	-3.14331500	0.34348000
C	-1.87996900	-1.94584800	0.08408500
O	-1.72141400	-3.18133100	0.18492800
N	-0.88778800	-1.02008100	-0.07797300
C	0.45496900	-1.45481100	-0.18160500
C	1.03804800	-2.33328300	0.74443600
C	1.26197700	-1.00649200	-1.24405800
C	2.36639700	-2.76012700	0.61700800
H	0.44115500	-2.70087200	1.57163400
C	2.58292600	-1.42197100	-1.38238500
H	0.83431100	-0.31522600	-1.96426900
C	3.14457100	-2.30733300	-0.45332300
H	2.77071200	-3.44369800	1.35667900
H	3.19514800	-1.06622900	-2.20700700
O	4.45941200	-2.66792500	-0.67533400
C	5.05939400	-3.58287900	0.22759800
H	4.52486800	-4.54271000	0.24143400
H	6.07738700	-3.74055500	-0.13585700
H	5.09717800	-3.17633200	1.24768400
C	1.43576700	2.31516500	0.15222300
C	2.17744600	3.20258500	-0.65834300
C	2.11552900	1.67205600	1.20810500
C	3.53176100	3.44486700	-0.41608700
H	1.68203600	3.68977700	-1.49491200
C	3.46334700	1.92765200	1.46122400
H	1.56914700	0.96159100	1.82197000
C	4.18182700	2.81457800	0.65039600
H	4.08038200	4.12845700	-1.06123000
H	3.96051600	1.41982600	2.28500400
H	5.23647100	3.00128000	0.83943900
C	-1.09408100	4.41063700	-0.04764400
H	-1.40141100	4.91700800	-0.97363200
H	-1.84705500	4.65162400	0.71525100
H	-0.13493500	4.83304500	0.27036000

Int22_1

C	5.12463200	1.77459200	0.91007500
C	4.07281200	0.84580200	0.95865700
C	2.75879100	1.19984100	0.60917400
C	2.55181200	2.53284300	0.20998200
C	3.58537100	3.47470500	0.15452400
C	4.88403200	3.09407800	0.50814900
H	6.13412100	1.46733900	1.18378700
H	4.30015100	-0.17378000	1.27077600
H	3.36204400	4.49181800	-0.16145100
H	5.69885800	3.81502400	0.46986900
C	1.14832100	2.89090900	-0.16455200
O	0.84900500	4.02256700	-0.60204600
N	0.28688600	1.84469700	0.00775600
C	-1.06557500	2.06232200	-0.36897100
C	-1.85024200	3.06347400	0.21950300
C	-1.66834400	1.26526500	-1.35789600
C	-3.18613000	3.26602800	-0.14861100
H	-1.40833900	3.70327700	0.97696300
C	-2.99602300	1.45173300	-1.73463500
H	-1.08046400	0.48174500	-1.82547700
C	-3.76503100	2.45462200	-1.13049500
H	-3.75277400	4.05445200	0.33588000
H	-3.45359000	0.82287000	-2.49398100
O	-5.07041900	2.56478000	-1.56718100
C	-5.88847600	3.56247100	-0.97753800
H	-5.48618600	4.56938700	-1.15450900
H	-6.86515700	3.47348300	-1.45851700
H	-6.00016200	3.40334900	0.10384100
C	2.11500100	-1.61520900	0.54810100
C	2.55865700	-2.15403000	-0.70980600
C	2.83214400	-3.53608800	-0.80457600
C	2.73186800	-1.34770300	-1.85124600
C	3.27197600	-4.08946100	-2.00643800
H	2.69026400	-4.16608900	0.06928800
C	3.17342000	-1.91008800	-3.04952500
H	2.52390900	-0.28530700	-1.77997000
C	3.44476500	-3.27956700	-3.13517600
H	3.47608600	-5.15615700	-2.06308500
H	3.30337700	-1.27290200	-3.92077900
H	3.78421300	-3.71325000	-4.07263300
C	1.84932000	-1.45504600	1.74702300
Ni	1.05442900	0.19260600	0.71325400
C	-0.71472300	-0.63984400	1.09121800
C	-1.13907300	-1.75661300	0.44869900
H	-0.47300200	-2.15805100	-0.32062600
C	-2.39201000	-2.53213300	0.53395300
C	-2.72596400	-3.37652700	-0.55229100
C	-3.28432100	-2.53511000	1.63126000
C	-3.88375100	-4.15267300	-0.56108000
H	-2.05439700	-3.40908700	-1.40850200
C	-4.44486200	-3.31393600	1.62552200
H	-3.05993800	-1.94389600	2.51036100
C	-4.76017500	-4.12465200	0.53063800
H	-4.10427000	-4.78126100	-1.42186300
H	-5.10499700	-3.29026400	2.49072800
H	-5.66553500	-4.72721400	0.53022500
C	1.75790800	-1.55317900	3.20761600
H	2.35658300	-2.39810600	3.57294400
H	2.12449500	-0.63722000	3.68536100
H	0.71912000	-1.70365800	3.52185400
C	-1.51988200	0.06257100	2.16695200
H	-2.59488100	0.12092600	1.93924800
H	-1.42399900	-0.45487800	3.13588400
H	-1.16392900	1.08644200	2.32352700

Int23_1

C	-4.81085300	-1.94149700	-1.72908300
C	-3.89222800	-0.92471200	-1.42096000
C	-2.59468700	-1.21366800	-0.96611000
C	-2.26565000	-2.57617400	-0.83678900
C	-3.16294400	-3.60551200	-1.13914700
C	-4.44878200	-3.28681800	-1.59007900
H	-5.81150500	-1.68335600	-2.07656900
H	-4.21184900	0.11142300	-1.53941300
H	-2.84754600	-4.64047300	-1.02116300
H	-5.15972600	-4.07579800	-1.82945900
C	-0.87848400	-2.86131800	-0.35081900
O	-0.45864900	-4.02321100	-0.15991800
N	-0.16433700	-1.71860600	-0.14232400
C	1.16846200	-1.89011200	0.32444800
C	1.49430600	-1.69677700	1.66925300
C	2.20314500	-2.26721900	-0.54987900
C	2.80586000	-1.85102000	2.14050000
H	0.70701800	-1.41671700	2.36428000
C	3.50931100	-2.42935700	-0.10011100
H	1.96636800	-2.43265100	-1.59744900
C	3.81954200	-2.21761600	1.25090700
H	3.01299600	-1.68507300	3.19262400
H	4.30548400	-2.71864800	-0.78167700
O	5.14219700	-2.39761200	1.60238000
C	5.50446000	-2.19253300	2.95864200
H	4.97560200	-2.88768100	3.62511500
H	6.57833200	-2.38415000	3.01526700
H	5.30157900	-1.16090100	3.27696600
C	-1.85939600	1.67559900	-1.45692200
C	-3.00753600	1.96444200	0.91488000
C	-3.28745400	0.97512300	1.87690300
C	-3.42708600	3.28998800	1.15870200
C	-3.97477000	1.30447500	3.04569900
H	-2.96744100	-0.04440100	1.68798500
C	-4.11215100	3.61067500	2.33020000

H	-3.20826300	4.05994400	0.42373100
C	-4.38903200	2.61982900	3.27947500
H	-4.18596200	0.52833400	3.77712900
H	-4.42805400	4.63672300	2.50366000
H	-4.92107800	2.87219900	4.19342900
C	-2.31514600	1.65604200	-0.30720200
Ni	-1.04815900	-0.04397700	-0.52613100
C	0.56707000	1.05331800	-0.19279000
C	1.51186200	1.18145300	-1.15488500
H	1.40895500	0.54814600	-2.04222100
C	-1.53528100	1.92228800	-2.86445500
H	-1.85988000	1.08199400	-3.48979200
H	-2.03461400	2.83380600	-3.21912300
H	-0.45372100	2.04321800	-2.99020000
C	2.75578400	1.98316600	-1.18337900
C	3.87213400	1.48777500	-1.89413600
C	2.89484700	3.25414000	-0.58445400
C	5.06917900	2.19920600	-1.97463600
H	3.79173800	0.51500300	-2.37558900
C	4.09280800	3.97005200	-0.66247200
H	2.04512000	3.69789000	-0.07549000
C	5.19178800	3.44780200	-1.35260400
H	5.91070100	1.77742700	-2.52105200
H	4.16316700	4.94815900	-0.18984000
H	6.12325900	4.00617400	-1.41237300
C	0.64777200	1.74500500	1.15072800
H	1.66700300	2.04256100	1.43758800
H	0.02017300	2.64891100	1.17334200
H	0.26146500	1.08985900	1.94197500

Int24_1

C	-3.93103600	-2.51040700	-2.06040500
C	-3.34858500	-1.82383500	-0.98533600
C	-2.05275600	-1.29343600	-1.07201700
C	-1.36788000	-1.48815200	-2.28303200
C	-1.93081200	-2.17148400	-3.36363400
C	-3.22394800	-2.68702300	-3.25360200
H	-4.94240800	-2.90611700	-1.96805700
H	-3.92903600	-1.70278700	-0.07092600
H	-1.34689100	-2.28621700	-4.27413100
H	-3.67765500	-3.21985200	-4.08726100
C	0.00384800	-0.89915100	-2.36840400
O	0.66517000	-0.92971700	-3.42111600
N	0.37484700	-0.31169500	-1.18663400
C	1.57139800	0.44235400	-1.17408600
C	2.78279200	-0.02496100	-1.70926300
C	1.57253800	1.73649900	-0.62011500
C	3.94191400	0.75745600	-1.69803500
H	2.81677600	-1.01321100	-2.15052400
C	2.72063000	2.52077600	-0.59368300
H	0.64856200	2.11989200	-0.20067500
C	3.91744000	2.03688300	-1.13647000
H	4.85322100	0.35139200	-2.12457400
H	2.70587800	3.51866500	-0.16315900
O	5.00030800	2.89003400	-1.07301200
C	6.22089700	2.44019100	-1.62858300
H	6.12528800	2.22302500	-2.70166700
H	6.93752800	3.25356100	-1.48974600
H	6.59501400	1.54046300	-1.11988500
C	-2.53824100	0.28363200	1.23881200
C	-3.19019100	1.49180300	0.80253900
C	-4.09547000	2.13154900	1.67516700
C	-2.95152300	2.05993700	-0.46210800
C	-4.74442400	3.30074900	1.28748000
H	-4.28009900	1.70143200	2.65551700
C	-3.60727600	3.23001000	-0.84203300
H	-2.25569100	1.56872000	-1.13329700
C	-4.50389600	3.85567300	0.02698800
H	-5.43920200	3.78094700	1.97216900
H	-3.41313300	3.65457900	-1.82348200
H	-5.01022600	4.76947100	-0.27304600
C	-2.24411700	-0.72067700	1.90446000
Ni	-0.87794500	-0.51433800	0.29775500
C	0.48951100	-0.17887600	1.73411900
C	0.41499300	0.82732800	2.62847400
H	-0.41106000	1.53777100	2.52847000
C	1.57445100	-1.18734000	1.78237900
C	1.27545100	-2.56688000	1.78414800
C	2.94139300	-0.83560400	1.78532400
C	2.27636200	-3.53694700	1.82405800
H	0.23432600	-2.87707700	1.74921400
C	3.94605000	-1.80375900	1.81712800
H	3.21020200	0.21550500	1.73944700
C	3.62248300	-3.16219900	1.84440500
H	2.00391800	-4.59061100	1.83181700
H	4.98924100	-1.49320100	1.81387300
H	4.40548300	-3.91668600	1.86856400
C	-2.22250500	-1.80476800	2.89188300
H	-3.06135300	-1.70566500	3.59311500
H	-2.29816000	-2.78472900	2.40587800
H	-1.28672000	-1.78167800	3.45987700
C	1.31568900	1.12760200	3.80800400
H	0.72425000	1.29895200	4.72032900
H	2.02259900	0.31711600	4.00939900
H	1.90298700	2.04546000	3.64769800

Int25_1

C	-3.40500900	3.90704500	-0.58282800
C	-2.98830000	2.71060800	0.02355700
C	-1.65071700	2.28240300	-0.02812900
C	-0.75212700	3.11494000	-0.71890800
C	-1.14682900	4.30761200	-1.33456200
C	-2.48503100	4.70902600	-1.26840100
H	-4.44959300	4.21262400	-0.51961700
H	-3.73476300	2.11458200	0.54938300
H	-0.40150200	4.90728200	-1.85275400
H	-2.80671400	5.63535000	-1.74112100
C	0.67430700	2.66628400	-0.73251500
O	1.57911600	3.36209900	-1.24206600
N	0.83994800	1.46843600	-0.09781400
C	2.17528500	1.02394300	0.08630300
C	3.05155500	0.81476600	-0.98631100
C	2.67347100	0.80316800	1.38224300
C	4.37710700	0.41057000	-0.78587400
H	2.69421000	0.97524800	-1.99791400
C	3.98599200	0.39024000	1.59907400
H	2.01039000	0.95927400	2.22774400
C	4.84882300	0.19435000	0.51285800
H	5.01865800	0.26397100	-1.64857800
H	4.35937900	0.22240100	2.60635300
O	6.13379700	-0.20928900	0.82366200
C	7.04273800	-0.41557300	-0.24606000
H	7.19895500	0.50530100	-0.82414300
H	7.98598300	-0.71779900	0.21479200
H	6.69633200	-1.21051800	-0.92077200
C	-2.19163900	0.45055600	2.09132000
C	-3.38637200	-1.27496800	0.46251400
C	-4.02326400	-0.89105500	-0.73488200
C	-3.50589100	-2.60870500	0.90150300
C	-4.76750300	-1.81788700	-1.46507500
H	-3.92065900	0.13205400	-1.08360600
C	-4.25050000	-3.52981300	0.16416000
H	-3.00111600	-2.91093300	1.81374700
C	-4.88470500	-3.13949100	-1.02021300
H	-5.25226600	-1.50810000	-2.38773700
H	-4.33032600	-4.55685100	0.51224300
H	-5.46055800	-3.86065900	-1.59505800
C	-2.64388300	-0.32025700	1.23920800
Ni	-0.78196200	0.60443400	0.56146900
C	0.07801000	-1.20030100	0.82399000
C	0.17360100	-1.79584400	2.03099900
H	-0.18121300	-1.23919200	2.90465400
C	0.54650800	-1.87450100	-0.41148400
C	-0.29133600	-1.97372500	-1.54388400
C	1.84814900	-2.40761000	-0.53575800
C	0.13016100	-2.60301400	-2.71712000
H	-1.29207000	-1.55451500	-1.49615000
C	2.27768800	-3.03021600	-1.71033300

H	2.53585600	-2.30643300	0.29902900
C	1.41957500	-3.13962400	-2.80965700
H	-0.54898300	-2.66648200	-3.56546000
H	3.29148400	-3.42288400	-1.76955300
H	1.75313300	-3.62205600	-3.72607500
C	-2.00391300	1.30182500	3.27342100
H	-2.02221900	2.35857400	2.98610700
H	-2.80334500	1.11909600	4.00442800
H	-1.04145400	1.10328100	3.75836300
C	0.67410300	-3.18259300	2.38643700
H	1.62771200	-3.14390800	2.93723900
H	-0.04262100	-3.69491700	3.04711700
H	0.82899000	-3.81241600	1.50458800

TS17_1

C	-4.23206900	-0.59387900	-2.79816400
C	-3.33835000	-1.06422300	-1.82769100
C	-2.42065500	-0.19914900	-1.20966800
C	-2.38197300	1.14867600	-1.63226700
C	-3.28814800	1.61565900	-2.58980300
C	-4.22553900	0.75456000	-3.16674800
H	-4.94069000	-1.28332900	-3.25356800
H	-3.37647800	-2.10969900	-1.53551800
H	-3.21538700	2.65758300	-2.89265100
H	-4.92820700	1.12626800	-3.90936800
C	-1.26070900	2.03632900	-1.16958600
O	-1.31930200	3.28013400	-1.31256000
N	-0.25530400	1.30663800	-0.64010700
C	0.89132200	1.95838100	-0.13434200
C	1.63333200	2.88579400	-0.87983900
C	1.34782100	1.65551100	1.16246700
C	2.78346700	3.49343100	-0.35995500
H	1.30536600	3.14267700	-1.88158900
C	2.48758100	2.25306800	1.69252500
H	0.79021800	0.93536900	1.75415700
C	3.21469300	3.17882600	0.93298400
H	3.32495400	4.20512300	-0.97455400
H	2.82885100	2.01087500	2.69605400
O	4.33064700	3.72047500	1.54051500
C	5.10147500	4.65603400	0.80330800
H	4.51213500	5.54545700	0.54105400
H	5.92554100	4.94865300	1.45781000
H	5.50729700	4.20844700	-0.11423200
C	-2.27108800	-1.14648400	0.63153200
C	-3.40054300	-0.69279400	1.43331700
C	-4.21456100	-1.64522100	2.08215800
C	-3.68054200	0.67193200	1.63614200
C	-5.26423300	-1.24488000	2.91070900
H	-4.02029800	-2.70284600	1.92525200
C	-4.73201400	1.06864300	2.46299000
H	-3.06510300	1.41779000	1.14360900
C	-5.52944900	0.11495300	3.10599600
H	-5.88010500	-1.99716000	3.39895000
H	-4.92810000	2.12878400	2.60543200
H	-6.34997400	0.42752600	3.74744700
C	-1.40529300	-2.10901500	0.51117100
Ni	-0.66407200	-0.63632400	-0.42764700
C	1.11044600	-1.37946700	-0.72979500
C	1.98321100	-1.79205300	0.22058500
H	1.68990300	-1.65583600	1.26509500
C	3.34792800	-2.34894100	0.08631900
C	4.29951500	-2.08588900	1.09747600
C	3.76042600	-3.18788700	-0.97235700
C	5.59598000	-2.59791900	1.04084500
H	4.00902200	-1.45354100	1.93423200
C	5.05850000	-3.70242400	-1.03271700
H	3.04650800	-3.46530900	-1.74078800
C	5.98955200	-3.40777400	-0.03150100
H	6.30287700	-2.36260200	1.83425400
H	5.33944900	-4.34741200	-1.86335300
H	6.99942100	-3.80868600	-0.08027100
C	-1.06742100	-3.44162900	1.07212700
H	-1.53460200	-3.61320200	2.05359600
H	-1.41538700	-4.23699700	0.39650200
H	0.01656100	-3.56118300	1.16953500
C	1.42194400	-1.39884600	-2.21430700
H	2.49883700	-1.39366100	-2.44037800
H	0.98594300	-2.28752000	-2.69720800
H	0.97418000	-0.52977100	-2.71173500

TS18_1

C	-4.43065400	-2.57019700	1.76442000
C	-3.74058200	-1.52716000	1.13130400
C	-2.48766600	-1.75205400	0.54119100
C	-1.91552900	-3.03589200	0.64413900
C	-2.61264000	-4.07832500	1.26203200
C	-3.87847700	-3.85446400	1.81276300
H	-5.40454400	-2.37707900	2.21112000
H	-4.19271900	-0.53969000	1.08468500
H	-2.13047400	-5.05058700	1.33189400
H	-4.41888200	-4.66724700	2.29327900
C	-0.48586300	-3.20626000	0.21942000
O	0.03378800	-4.33844900	0.09186600
N	0.10655900	-2.00532900	0.04268700
C	1.45746300	-1.97366400	-0.38058400
C	2.50817200	-2.34380400	0.46747900
C	1.78613700	-1.53649500	-1.67568100
C	3.84297100	-2.28831100	0.04954600
H	2.27695100	-2.68435800	1.47281400
C	3.10962000	-1.47380900	-2.10669400
H	0.98352700	-1.24284500	-2.34763100
C	4.14731100	-1.85018900	-1.24437400
H	4.62537600	-2.58475100	0.74033300
H	3.35575900	-1.13543800	-3.11012100
O	5.42526600	-1.75311400	-1.75703200
C	6.51021600	-2.12498000	-0.92049600
H	6.44410700	-3.18031800	-0.62299800
H	7.41340300	-1.97292100	-1.51563600
H	6.55757500	-1.49712400	-0.02049400
C	-2.63597700	-0.39076900	-1.10308300
C	-2.77742600	2.17334300	-0.89552700
C	-4.08675500	2.46619500	-1.34230000
C	-1.89557500	3.25354200	-0.68763900
C	-4.49078800	3.78041300	-1.57997000
H	-4.78794900	1.64869100	-1.49141400
C	-2.29988700	4.56624000	-0.93586500
H	-0.89045700	3.03914500	-0.33976100
C	-3.59833400	4.84040400	-1.38072500
H	-5.50514300	3.97790100	-1.92075900
H	-1.59647900	5.38068300	-0.77612800
H	-3.91219200	5.86508300	-1.56585600
C	-2.37973800	0.79680800	-0.66087600
Ni	-1.10130800	-0.43264600	0.13387800
C	0.15244800	0.88103100	0.86624100
C	1.19893500	1.47125600	0.24288500
H	1.40419800	1.16642000	-0.78551500
C	2.18899700	2.44848700	0.74738100
C	3.48982400	2.44517800	0.19406400
C	1.91105000	3.44024600	1.71382000
C	4.46648500	3.35277600	0.60376200
H	3.72959600	1.70141500	-0.56316700
C	2.88753000	4.35153800	2.12626500
H	0.91079000	3.51812100	2.12679100
C	4.17460000	4.31313400	1.58046700
H	5.45935700	3.31170900	0.15960700
H	2.63521600	5.10404200	2.87124400
H	4.93291500	5.02350800	1.90190700
C	-3.28349600	-1.21405600	-2.15769600
H	-4.19711800	-1.69973000	-1.79337100
H	-3.54861800	-0.57117800	-3.00831200
H	-2.61349200	-2.00357600	-2.51687200
C	-0.19677900	1.11340100	2.32432400
H	0.66010200	1.43490900	2.93556200
H	-0.98407800	1.87741800	2.42320500
H	-0.60198800	0.20030000	2.77954900

TS19_1

C	-3.49365200	1.69717800	2.39100300

C	-2.94080900	1.47058900	1.12456600
C	-1.91087300	0.53386700	0.94382300
C	-1.40597900	-0.13802200	2.07868300
C	-1.97252300	0.08203400	3.33823400
C	-3.02517200	0.98698000	3.50004800
H	-4.29749500	2.42228300	2.50393900
H	-3.33281500	2.01408000	0.26986600
H	-1.54429700	-0.44510900	4.18729900
H	-3.46088800	1.15129700	4.48319600
C	-0.15762300	-0.96524400	1.95527900
O	0.18040700	-1.76042500	2.86334000
N	0.48773500	-0.70184200	0.79835000
C	1.69774700	-1.36441100	0.50419300
C	2.75961200	-1.46089000	1.41766200
C	1.88953700	-1.93056900	-0.77123200
C	3.96571300	-2.08841200	1.08026500
H	2.63863100	-1.04460800	2.41160100
C	3.08192000	-2.55941900	-1.11812500
H	1.08290400	-1.86496700	-1.49499900
C	4.13135100	-2.64178000	-0.19377400
H	4.75700300	-2.13677400	1.82144000
H	3.21700900	-2.99135700	-2.10658100
O	5.27583600	-3.28208900	-0.62903300
C	6.36916900	-3.37418400	0.27032300
H	6.10139600	-3.94063800	1.17290500
H	7.15794700	-3.90410200	-0.26839800
H	6.73374100	-2.37990500	0.56323900
C	-2.33733900	-0.06227400	-0.98983300
C	-3.35874900	-1.09868800	-0.90192900
C	-4.52719400	-0.98733700	-1.68459000
C	-3.19859100	-2.24692400	-0.10321400
C	-5.49379100	-1.99455100	-1.67577800
H	-4.67352900	-0.10048800	-2.29537100
C	-4.16765400	-3.25052900	-0.09492400
H	-2.30768400	-2.34698100	0.50811900
C	-5.31984700	-3.13255300	-0.88061400
H	-6.38773200	-1.88644100	-2.28632600
H	-4.02075900	-4.12875800	0.52937200
H	-6.07452300	-3.91536200	-0.86971200
C	-1.81541500	0.81301000	-1.79576900
Ni	-0.51346000	0.51675600	-0.44498700
C	0.97304800	1.43602700	-1.33664100
C	1.55840600	1.12062800	-2.50449000
H	1.17600500	0.26173600	-3.06362400
C	1.41524800	2.58334000	-0.50894900
C	0.79310700	3.84516600	-0.61986100
C	2.44671600	2.45190100	0.44569700
C	1.19057300	4.92610400	0.17026300
H	-0.01377400	3.96800500	-1.33919300
C	2.84311900	3.53147800	1.23864000
H	2.93093100	1.48557600	0.56093100
C	2.21997400	4.77804300	1.10723600
H	0.69336400	5.88790800	0.05544100
H	3.64305900	3.39776300	1.96482100
H	2.52680100	5.61735000	1.72749600
C	-1.99626800	1.40280300	-3.14562700
H	-2.65889000	0.79665000	-3.78159500
H	-2.43950900	2.40649300	-3.06750600
H	-1.03113100	1.52183200	-3.64901100
C	2.74100100	1.80412200	-3.15983900
H	2.49509100	2.14298300	-4.17862000
H	3.07897600	2.67525400	-2.58845600
H	3.59438200	1.11522000	-3.25790800

TS20_1

C	2.54387300	4.00678000	0.17690600
C	2.38471900	2.64004800	-0.08911600
C	1.13273300	2.12789900	-0.45794600
C	0.03014500	3.00181000	-0.51295400
C	0.19617100	4.36741800	-0.26239000
C	1.45426900	4.87785100	0.07125900
H	3.52360200	4.38845600	0.45882700
H	3.24332600	1.97756200	-0.02283400
H	-0.68291400	5.00633200	-0.30276600
H	1.58027200	5.94060600	0.26669300
C	-1.33619200	2.41246200	-0.70098800
O	-2.32930700	3.13292000	-0.95236300
N	-1.30585600	1.06898000	-0.54650700
C	-2.49597900	0.32701400	-0.70131900
C	-3.67975700	0.63242200	-0.01282100
C	-2.51657200	-0.78551600	-1.56322500
C	-4.84076300	-0.13412300	-0.17382800
H	-3.69847600	1.48881400	0.65277300
C	-3.66332500	-1.55614500	-1.73304800
H	-1.60966300	-1.03957100	-2.10494200
C	-4.83631800	-1.23436500	-1.03827000
H	-5.73365100	0.14278000	0.37737100
H	-3.66612900	-2.41280900	-2.40245000
O	-5.92370400	-2.05391800	-1.27048400
C	-7.13625300	-1.75987900	-0.59476900
H	-7.51432400	-0.76360600	-0.86202600
H	-7.85263900	-2.51773700	-0.91969500
H	-7.01393500	-1.81917900	0.49543200
C	1.74355100	0.60395900	-1.81623300
C	3.18391100	-1.42499200	-1.13924500
C	4.36801900	-1.22920600	-1.88771500
C	3.04366000	-2.63869800	-0.43566100
C	5.36036100	-2.20846200	-1.93791800
H	4.50491200	-0.29248800	-2.42238500
C	4.03456900	-3.62000000	-0.49476700
H	2.14285200	-2.79228200	0.14947400
C	5.19893500	-3.41342000	-1.24344200
H	6.26271600	-2.03037800	-2.51931400
H	3.89913300	-4.55029400	0.05300300
H	5.97213100	-4.17725300	-1.28140900
C	2.16543900	-0.39150900	-1.10468900
Ni	0.52170900	0.28434200	-0.31711000
C	0.06688700	-1.17460700	0.93700400
C	-0.45133000	-2.39092900	0.70038800
H	-0.62486300	-2.69155100	-0.33572000
C	0.32411400	-0.66256300	2.30368200
C	1.62355200	-0.65792900	2.85645900
C	-0.71373700	-0.11397500	3.08889900
C	1.86900000	-0.15335600	4.13508700
H	2.44556400	-1.05517600	2.26587900
C	-0.46805300	0.39658000	4.36576900
H	-1.71996500	-0.08870600	2.67834500
C	0.82488900	0.37901300	4.90102900
H	2.88172000	-0.17122900	4.53428700
H	-1.29099100	0.81167800	4.94506700
H	1.01689500	0.77857600	5.89437500
C	1.77251100	1.30520800	-3.12609300
H	2.36417900	2.22801600	-3.08090700
H	2.21648500	0.64566200	-3.88423900
H	0.76255900	1.57779400	-3.45255000
C	-0.84692000	-3.44141300	1.71804200
H	-1.91785000	-3.68458000	1.64268100
H	-0.30206200	-4.38423700	1.55106800
H	-0.64830600	-3.11592100	2.74483000

Int26_1

C	2.47672000	3.02569300	-2.97321100
C	2.27391500	2.79840000	-1.61301400
C	1.98724900	1.51642000	-1.10053600
C	1.95493500	0.43040000	-2.01009200
C	2.18872700	0.66778300	-3.37560000
C	2.42638400	1.95058800	-3.86679000
H	2.67355200	4.03378000	-3.33235300
H	2.32528000	3.63354700	-0.91817100
H	2.19102100	-0.18186300	-4.05327600
H	2.58469800	2.10748000	-4.93154300
C	1.80806400	-1.02876200	-1.61047200
O	2.72730800	-1.80827900	-1.95074200
N	0.65795800	-1.36207100	-0.98300600
C	0.43370000	-2.68231600	-0.53164700
C	1.43022200	-3.54089300	-0.03355700
C	-0.89379500	-3.16175200	-0.51267800
C	1.11783500	-4.81090300	0.46790300

H	2.46228400	-3.21437300	-0.03904500
C	-1.21495600	-4.42137200	-0.01576300
H	-1.68507200	-2.52554900	-0.90327000
C	-0.20729400	-5.25902100	0.47944000
H	1.92229200	-5.43411000	0.84494300
H	-2.24371300	-4.77222500	-0.00987100
O	-0.61624200	-6.49179500	0.94623600
C	0.37185600	-7.36982900	1.46407300
H	0.88117200	-6.93311200	2.33390000
H	-0.16051400	-8.27233700	1.77208400
H	1.11796200	-7.62992400	0.70095600
C	1.75688800	1.37094300	0.37494800
C	2.80736200	1.97280800	1.25608000
C	2.48672600	2.84521400	2.31365200
C	4.17153000	1.69422100	1.03490500
C	3.47991600	3.39777000	3.12849100
H	1.44530600	3.10355200	2.48686700
C	5.16629100	2.24428200	1.84519300
H	4.44769500	1.03101200	0.21886300
C	4.82652900	3.09914400	2.90070200
H	3.19947200	4.07021100	3.93684700
H	6.20984300	2.00287400	1.65372500
H	5.60080600	3.52984300	3.53154800
C	0.64776900	0.74443000	0.83950000
Ni	-0.54985200	0.04517900	-0.39197600
C	-1.92492900	1.30434500	-0.07013800
C	-3.14882600	0.73255800	0.11417000
H	-3.18151600	-0.36111000	0.17024800
C	-4.50279600	1.32207700	0.19796700
C	-5.61138400	0.52123600	-0.16127600
C	-4.78395100	2.62756600	0.65923500
C	-6.91942200	1.00034700	-0.09911300
H	-5.42972700	-0.49636500	-0.50282300
C	-6.09421100	3.10944100	0.72439800
H	-3.97415700	3.26262900	0.99917500
C	-7.17206300	2.30551400	0.34024900
H	-7.74444300	0.35411400	-0.39238100
H	-6.27294100	4.11933100	1.08861600
H	-8.19013800	2.68421300	0.39212500
C	0.34482700	0.44805300	2.28607700
H	1.20000600	0.62377900	2.95277400
H	-0.50124700	1.05177100	2.64214000
H	0.03807400	-0.60005600	2.39792200
C	-1.70398400	2.79521000	-0.19969300
H	-2.54304300	3.32161600	-0.67832700
H	-1.55222500	3.25886000	0.78817200
H	-0.79811000	3.00489900	-0.77785100

Int27_1

C	-1.44417000	4.73572600	-1.87945300
C	-1.09275400	4.22195600	-0.63133400
C	-0.14713600	3.18737900	-0.48628100
C	0.48361200	2.69462100	-1.65499600
C	0.14558800	3.24333300	-2.90354000
C	-0.82115100	4.24028300	-3.02884200
H	-2.19707400	5.51781900	-1.95316500
H	-1.57772000	4.61556800	0.25926100
H	0.66532100	2.87703500	-3.78507300
H	-1.07758300	4.63272200	-4.01042300
C	1.61102100	1.67446500	-1.66597000
O	2.68274800	2.02287000	-2.21275900
N	1.32338200	0.45962000	-1.14494500
C	2.29793200	-0.56059100	-1.08027100
C	3.69020800	-0.35869700	-1.01053600
C	1.84646700	-1.89860100	-1.02131400
C	4.58072300	-1.43258200	-0.87737600
H	4.08047300	0.64847600	-1.06420600
C	2.72284600	-2.97066500	-0.89048800
H	0.77832500	-2.09479300	-1.07828700
C	4.10363000	-2.74545500	-0.81709800
H	5.64372200	-1.22067000	-0.82276100
H	2.35021900	-3.99070600	-0.84540300
O	4.89743300	-3.86782700	-0.69173800
C	6.30152800	-3.68290600	-0.59674100
H	6.56901400	-3.08554100	0.28559300
H	6.73023500	-4.68284100	-0.50031400
H	6.70518500	-3.19897700	-1.49655400
C	0.17075100	2.69312000	0.89273700
C	0.29003300	0.78693900	2.52243700
C	-0.42263300	1.20068200	3.66661700
C	1.23253600	-0.25044200	2.68397600
C	-0.19914500	0.61313000	4.91568800
H	-1.16703600	1.98673900	3.56819300
C	1.46383800	-0.83147200	3.93128700
H	1.78420800	-0.59700300	1.81467600
C	0.74816600	-0.40527700	5.05715300
H	-0.76902100	0.95180800	5.77898300
H	2.20275800	-1.62477100	4.02394600
H	0.92308600	-0.86454300	6.02750900
C	0.04325100	1.38240400	1.19067200
Ni	-0.38610500	0.21945300	-0.21354700
C	-2.13983200	-0.23553500	0.29920700
C	-2.47605700	-1.31030000	-0.46301000
H	-1.70116700	-1.69828400	-1.14199900
C	-3.74453200	-2.05212100	-0.61843200
C	-3.99920400	-2.72412300	-1.83545000
C	-4.71932500	-2.17285500	0.39630900
C	-5.17335000	-3.44734200	-2.04377900
H	-3.25830500	-2.66402500	-2.63071900
C	-5.89629400	-2.89706200	0.18906000
H	-4.54055900	-1.72316400	1.36660800
C	-6.13766200	-3.53424100	-1.03245700
H	-5.33691700	-3.94481900	-2.99771800
H	-6.62429900	-2.97324000	0.99442800
H	-7.05412900	-4.09799700	-1.19008500
C	0.65461200	3.76339200	1.86228500
H	-0.12915000	4.49789300	2.09923900
H	0.99734600	3.32853500	2.80502300
H	1.48888900	4.32719100	1.42150200
C	-3.07878400	0.48084900	1.23279000
H	-4.13308000	0.41352000	0.92753000
H	-3.00379200	0.07283100	2.25207100
H	-2.81138400	1.54079000	1.30493200

Int28_1

C	2.81841400	1.82867400	3.05724000
C	2.59985400	1.61705100	1.69722700
C	1.30922300	1.41364500	1.16665200
C	0.21126500	1.46930100	2.05952800
C	0.44081400	1.71297300	3.42445700
C	1.72863700	1.87162700	3.93364600
H	3.83214100	1.96123100	3.43004000
H	3.44773500	1.59548400	1.01708500
H	-0.41844900	1.78733800	4.08576600
H	1.87925000	2.04090700	4.99765900
C	-1.24413800	1.40151500	1.63581700
O	-1.98422300	2.35996400	1.95555000
N	-1.62828100	0.26929500	1.00659500
C	-2.95151100	0.14190500	0.52163100
C	-3.65344200	1.17126200	-0.12812800
C	-3.59212100	-1.10960400	0.62472700
C	-4.93023000	0.96213900	-0.66286300
H	-3.19596700	2.14936200	-0.21701400
C	-4.86115200	-1.33022800	0.09536300
H	-3.07885300	-1.91966700	1.13793500
C	-5.54101500	-0.29267600	-0.55471300
H	-5.42964700	1.78753500	-1.15977900
H	-5.34063600	-2.30170900	0.18331300
O	-6.79290800	-0.60113700	-1.04638100
C	-7.51163700	0.41608200	-1.72776700
H	-6.96949200	0.76306000	-2.61791200
H	-8.45659600	-0.03806000	-2.03379700
H	-7.71554900	1.27281500	-1.07135400
C	1.17293800	1.18603800	-0.30988900
C	1.88304000	2.17822900	-1.17927300
C	2.76198000	1.77688000	-2.20291100
C	1.70678000	3.56210100	-0.97814900
C	3.41948600	2.71460700	-3.00532000

H	2.94223100	0.71626700	-2.35562700
C	2.36217300	4.50171300	-1.77614500
H	1.04122800	3.89858600	-0.18688100
C	3.22235300	4.08323400	-2.79853300
H	4.09542100	2.37291700	-3.78674100
H	2.19963500	5.56325000	-1.60072000
H	3.73606300	4.81391000	-3.41933300
C	0.47377700	0.13041100	-0.79383900
Ni	-0.33391000	-1.04029800	0.39486800
C	0.70565800	-2.59769400	0.02733400
C	-0.06343000	-3.71181000	0.08483600
H	-1.15025200	-3.58615400	0.15560800
C	2.17141100	-2.66712100	-0.16182800
C	2.73950700	-3.21510500	-1.33096500
C	3.05844300	-2.14950700	0.80464900
C	4.12436500	-3.25524600	-1.52150100
H	2.07802800	-3.60812100	-2.10010300
C	4.44175700	-2.20294300	0.62551100
H	2.64571200	-1.69452600	1.70153100
C	4.98655100	-2.75466200	-0.54075600
H	4.52976800	-3.68140400	-2.43760800
H	5.09834000	-1.80162000	1.39516500
H	6.06423300	-2.78537400	-0.68521900
C	0.19896400	-0.14874700	-2.24913300
H	0.46337300	0.68913500	-2.90838200
H	0.74848900	-1.03859600	-2.58525100
H	-0.86631800	-0.37093400	-2.39459200
C	0.37167500	-5.16357900	0.11435000
H	-0.00842100	-5.71570000	-0.75919400
H	1.46127800	-5.26650200	0.12950200
H	-0.03061500	-5.67355900	1.00253200

Int29_1

C	4.11575100	0.01702300	-3.21979600
C	3.52663100	-0.91854100	-2.36938800
C	2.15339400	-0.88507500	-2.05466500
C	1.35803500	0.11719000	-2.66203000
C	1.95626800	1.03516000	-3.54125200
C	3.32420500	1.00715000	-3.81046800
H	5.18430400	-0.02845600	-3.42065400
H	4.14805500	-1.68730200	-1.91571800
H	1.32052800	1.77349100	-4.02322100
H	3.76476200	1.74127300	-4.48169800
C	-0.15097700	0.22393000	-2.52432500
O	-0.82226500	0.21304100	-3.58272300
N	-0.62102100	0.39738200	-1.26996800
C	-2.00909300	0.48485300	-1.02372900
C	-2.99324200	-0.23252100	-1.72845700
C	-2.44842300	1.29319400	0.04751600
C	-4.34739600	-0.15603800	-1.37813000
H	-2.69730200	-0.85726200	-2.56170800
C	-3.79156900	1.37555800	0.40287500
H	-1.71457500	1.86880200	0.60674300
C	-4.75466000	0.64911000	-0.30916500
H	-5.06655700	-0.73274700	-1.95088100
H	-4.10912100	2.00319500	1.23168400
O	-6.06150700	0.79264100	0.11378300
C	-7.06707000	0.06648000	-0.57632300
H	-6.89842200	-1.01688400	-0.50741600
H	-8.00976900	0.31815700	-0.08550000
H	-7.11857400	0.35732900	-1.63442200
C	1.59815700	-1.93541300	-1.14031100
C	0.38135900	-2.54023000	0.96624600
C	1.19916100	-3.47357000	1.63634900
C	-0.99078200	-2.52671100	1.29490600
C	0.67193300	-4.35832600	2.58235500
H	2.26277700	-3.49698600	1.41257400
C	-1.52088700	-3.41604300	2.23025300
H	-1.64036100	-1.80789600	0.80351300
C	-0.69287200	-4.33766400	2.88372900
H	1.33113400	-5.06330900	3.08561000
H	-2.58513000	-3.38511900	2.45526100
H	-1.10555700	-5.02401500	3.61981300
C	0.93256500	-1.58448500	-0.01856700
Ni	0.60226000	0.24597000	0.25317500
C	1.72696100	0.57885500	1.73495300
C	2.53646400	-0.10242500	2.56265100
H	2.62081100	-1.18137400	2.42088800
C	1.47422600	2.03965100	1.82282900
C	1.94647900	2.91288400	0.81599100
C	0.65420300	2.59610500	2.83249300
C	1.64244600	4.27752500	0.83671300
H	2.56721000	2.50748500	0.02059300
C	0.35310800	3.95836700	2.85403000
H	0.25615700	1.93844700	3.60173900
C	0.84652900	4.80883800	1.85579300
H	2.02469900	4.92477600	0.05021800
H	-0.27391500	4.35925500	3.64811000
H	0.60441900	5.86899300	1.86879000
C	1.83886100	-3.36880200	-1.59793100
H	2.90016100	-3.65353100	-1.54140400
H	1.27321200	-4.08470800	-0.99533300
H	1.53723700	-3.49076400	-2.64771600
C	3.38493700	0.45395200	3.68445000
H	3.10522300	0.01851800	4.65634800
H	4.44855300	0.21364800	3.53255000
H	3.29585200	1.54281800	3.76604000

TS20_CF_3_1

C	1.31090100	1.58226200	0.21701900
C	0.39250900	2.38709200	-0.17297500
Ni	-0.28206600	0.58443800	-0.39992000
H	-1.06287700	1.37175700	-1.33243700
C	-2.10856000	0.02222100	-0.33959600
C	-3.30108200	0.76395200	-0.29989700
C	-2.19073100	-1.36089100	-0.07556700
C	-4.52888800	0.15670800	-0.01715500
C	-3.40795500	-1.97796200	0.21459800
C	-4.58408300	-1.21904600	0.24136300
H	-3.28659800	1.83497000	-0.48594000
H	-5.43752100	0.75217300	0.00366300
H	-3.41291300	-3.04317900	0.42785200
C	-0.91853900	-2.15909600	-0.08428400
O	-0.94434200	-3.40350000	0.04878000
N	0.16299300	-1.36344700	-0.27269700
C	1.43905200	-1.93701800	-0.45538900
C	1.91073700	-3.05983700	0.24814000
C	2.32030700	-1.34847400	-1.38646500
C	3.20131800	-3.56629500	0.04176600
H	1.25840900	-3.55079900	0.95918700
C	3.60213300	-1.84399600	-1.60050200
H	1.98024700	-0.48104300	-1.94552000
C	4.05503800	-2.95984100	-0.88443700
H	3.51767400	-4.43418800	0.61153600
H	4.26740000	-1.37322300	-2.31991200
O	5.34163800	-3.37957700	-1.16133700
C	5.84482200	-4.49830200	-0.44855200
H	5.25130100	-5.40172700	-0.64511300
H	6.86461600	-4.65081200	-0.80910800
H	5.86640100	-4.30914400	0.63357800
C	2.64444100	1.43216600	0.76418700
C	3.66985600	2.34153200	0.42652600
C	2.94522900	0.39169300	1.66400100
C	4.94723600	2.21421100	0.97334200
H	3.45551300	3.14288400	-0.27589700
C	4.21899000	0.27652900	2.22180700
H	2.16900200	-0.32498100	1.91183100
C	5.22676800	1.18400700	1.87890700
H	5.72529200	2.92154300	0.69435000
H	4.42824700	-0.53302400	2.91697200
H	6.22200600	1.08553000	2.30592600
C	-0.05318200	3.76234500	-0.31674200
C	-1.11167900	4.13720800	-1.16370200
C	0.60308700	4.77794600	0.41392500
C	-1.49959000	5.47308600	-1.28209100
H	-1.62367000	3.36753600	-1.73428100
C	0.20919900	6.11069500	0.30117100
H	1.41992300	4.50639000	1.07696000

C	-0.84376300	6.46772700	-0.54996000
H	-2.31833700	5.73654900	-1.94774600
H	0.72615700	6.87371800	0.87882000
H	-1.14899700	7.50739500	-0.63958100
C	-5.89660700	-1.88946800	0.49543300
F	-6.43773500	-2.44795000	-0.63511500
F	-5.80973400	-2.90721700	1.39584300
F	-6.84859200	-1.03602900	0.96957500

TS21_CF_3_1

C	-0.12336500	1.36559400	-0.37597700
C	1.04691400	1.53330600	0.11161200
Ni	0.62258700	-0.37211400	0.13995400
H	1.79094500	-0.40516300	1.01101300
C	1.70300500	-1.96221300	-0.05167300
C	3.07196700	-2.18077500	-0.32936700
C	0.86339600	-3.09772700	-0.10770800
C	3.56989300	-3.46473900	-0.61404100
C	1.35792200	-4.37487200	-0.38547000
C	2.71696000	-4.56644800	-0.63142500
H	4.62694000	-3.60027300	-0.81692300
H	3.11010500	-5.55733700	-0.84525100
H	0.65252200	-5.20145500	-0.41329700
C	-0.61477900	-2.91447600	0.08398200
O	-1.37395300	-3.90724700	0.16963500
N	-0.95457100	-1.60708200	0.15190500
C	-2.29533000	-1.25962000	0.43416200
C	-3.39774200	-1.84039100	-0.21440000
C	-2.56578200	-0.26367800	1.39368000
C	-4.71130900	-1.44754400	0.07267700
H	-3.22915100	-2.61608200	-0.95212600
C	-3.86586500	0.13567400	1.68780300
H	-1.73174200	0.20184300	1.91131400
C	-4.95130500	-0.45514400	1.02835000
H	-5.52870900	-1.92728400	-0.45611300
H	-4.05659200	0.90792600	2.42887200
O	-6.20377600	0.00307700	1.38792700
C	-7.33289500	-0.57757200	0.75520800
H	-7.39338300	-1.65699300	0.95118200
H	-8.20636600	-0.08258500	1.18567700
H	-7.31799700	-0.40805100	-0.33031000
C	-1.31672100	1.98275300	-0.92333100
C	-1.64540100	3.31610200	-0.59797300
C	-2.15158400	1.28946100	-1.81892300
C	-2.76878500	3.93084400	-1.15169800
H	-1.01317900	3.86143800	0.09783100
C	-3.26871600	1.90955200	-2.37995100
H	-1.91221700	0.25969300	-2.06334500
C	-3.58405100	3.23156000	-2.04936500
H	-3.00847500	4.95746300	-0.88307400
H	-3.90018500	1.35465000	-3.06987600
H	-4.45934700	3.71095900	-2.48156100
C	2.10578900	2.46112300	0.46422000
C	2.93232600	2.26507400	1.58477700
C	2.29491200	3.62694300	-0.30884400
C	3.90501600	3.20438100	1.92975300
H	2.80239100	1.36654400	2.17974800
C	3.27736600	4.55794600	0.02951100
H	1.66766300	3.78901400	-1.18141100
C	4.08597900	4.35411600	1.15381900
H	4.52966400	3.03275600	2.80342000
H	3.41139500	5.44504700	-0.58571300
H	4.85014700	5.08087800	1.41902500
C	4.06890200	-1.05168400	-0.31342100
F	4.31879900	-0.57969600	0.94590700
F	3.69280200	0.01828200	-1.05634700
F	5.29358300	-1.42260100	-0.80151000

TS20_Me_1

C	-0.11227000	1.55905100	0.13331000
C	-1.35956700	1.71741800	-0.13032500
Ni	-0.97756400	-0.17073600	-0.27188700
H	-2.14297800	0.07851100	-1.09054900
C	-2.24449400	-1.61736100	-0.13390800
C	-3.64115200	-1.62593400	-0.01204000
C	-1.57538900	-2.84420100	0.05830100
C	-4.34185200	-2.80660000	0.28157700
C	-2.27378900	-4.01847300	0.35052700
C	-3.67221900	-4.02345000	0.46215600
H	-4.20915700	-0.70648300	-0.14086300
H	-5.42851500	-2.77630200	0.36513400
H	-1.70239100	-4.93311100	0.50062700
C	-0.07623300	-2.84135600	-0.01548900
O	0.58070100	-3.90620800	0.04451000
N	0.41473400	-1.58434200	-0.16445200
C	1.80685000	-1.40968100	-0.32275900
C	2.75720800	-2.01532300	0.51585000
C	2.29337800	-0.57471100	-1.34779700
C	4.13112600	-1.80083500	0.34638500
H	2.41858500	-2.67091500	1.31018000
C	3.65625800	-0.35593500	-1.52937300
H	1.57673200	-0.09037700	-2.00580600
C	4.58726600	-0.96962700	-0.68214000
H	4.82555500	-2.29228900	1.02047000
H	4.01473400	0.29339500	-2.32422000
O	5.91787900	-0.69578300	-0.93833700
C	6.89348900	-1.31070400	-0.11308900
H	6.84550000	-2.40639500	-0.18091100
H	7.86184800	-0.96731300	-0.48433000
H	6.78022800	-1.00985000	0.93769400
C	1.12957300	2.22391500	0.47572000
C	1.47540200	3.45547000	-0.12189100
C	2.01803700	1.67031300	1.41823800
C	2.66295800	4.10700900	0.21352600
H	0.80622600	3.88966800	-0.86041000
C	3.19619100	2.33291100	1.76462100
H	1.77605000	0.71187800	1.86631300
C	3.52761000	3.55231400	1.16419600
H	2.91266600	5.05092400	-0.26657800
H	3.86614600	1.88686600	2.49609400
H	4.45328700	4.05957300	1.42571600
C	-2.47403200	2.64751800	-0.20205300
C	-3.65477500	2.37020100	-0.91446300
C	-2.37671600	3.89194500	0.45981000
C	-4.69696600	3.29773900	-0.96997400
H	-3.74460200	1.41768100	-1.42930600
C	-3.42134000	4.81423300	0.41043800
H	-1.47388000	4.12123200	1.01915000
C	-4.58844700	4.52436400	-0.30716100
H	-5.59746400	3.05919600	-1.53144500
H	-3.32461900	5.76307200	0.93362500
H	-5.40222300	5.24444100	-0.34642200
C	-4.42207600	-5.30176400	0.77126700
H	-4.28020300	-6.05395600	-0.01657200
H	-4.07677100	-5.75423200	1.71048400
H	-5.49891000	-5.11896300	0.86578600

TS21_Me_1

C	0.43046000	-1.27580600	0.31549000
C	1.63867300	-1.26328500	-0.10690800
Ni	0.94617700	0.56761400	-0.16398700
H	2.16086200	0.55074800	-0.96359300
C	1.83832500	2.26484700	0.06638100
C	3.20329400	2.57896700	0.26182900
C	0.88576600	3.28392800	0.26782900
C	3.56269300	3.88881700	0.62776900
C	1.25729000	4.58466700	0.62948200
C	2.60499600	4.89252100	0.80562400
H	4.61648000	4.12598300	0.77336400
H	2.91234300	5.89850900	1.08551400
H	0.47670800	5.32760600	0.77354100
C	-0.56531600	2.93684400	0.11998600
O	-1.44930900	3.82363500	0.16651300
N	-0.74919800	1.60598300	-0.07793200
C	-2.04154900	1.12195700	-0.37418600
C	-3.20764400	1.54844900	0.28600400
C	-2.19724800	0.14260900	-1.37673500
C	-4.46766700	1.02483700	-0.03287400

H	-3.13052900	2.30705800	1.05522600
C	-3.44294100	-0.38611300	-1.70074900
H	-1.31315900	-0.20411800	-1.90409800
C	-4.59190000	0.05389300	-1.03145100
H	-5.33612600	1.38893200	0.50694500
H	-3.54141900	-1.14125000	-2.47675000
O	-5.78562500	-0.52182200	-1.42526500
C	-6.97593700	-0.07943300	-0.79378500
H	-7.14023000	0.99521100	-0.95331700
H	-7.78969700	-0.64255000	-1.25648200
H	-6.96028900	-0.28487900	0.28552700
C	-0.65950900	-2.08944300	0.81934200
C	-0.78229100	-3.44338300	0.44011500
C	-1.60170200	-1.56124600	1.72142000
C	-1.81162000	-4.23758600	0.94648800
H	-0.06506300	-3.86226200	-0.26105000
C	-2.62185700	-2.36127400	2.23789900
H	-1.52358400	-0.51669900	2.00468400
C	-2.73447100	-3.70114900	1.85222600
H	-1.89313500	-5.27693600	0.63542700
H	-3.33911700	-1.93291100	2.93417000
H	-3.53682000	-4.31993700	2.24736400
C	2.84865900	-2.02332200	-0.36922900
C	3.69102900	-1.74424200	-1.46096800
C	3.18435800	-3.10839400	0.46945900
C	4.82133100	-2.52328500	-1.71308300
H	3.44475100	-0.91007900	-2.11162400
C	4.32178800	-3.87808400	0.22321300
H	2.54703700	-3.33386500	1.32032400
C	5.14602000	-3.59261600	-0.87175000
H	5.45295400	-2.29101500	-2.56761400
H	4.56509900	-4.70371100	0.88842600
H	6.03104100	-4.19427400	-1.06428600
C	4.30304600	1.55217800	0.09422400
H	4.37613600	1.20752900	-0.94524700
H	4.12206500	0.66090700	0.70496300
H	5.27813900	1.96731200	0.37739100

TS20_OMe_1

C	0.49877000	1.62956200	0.15460000
C	-0.65291800	2.10935000	-0.14990800
Ni	-0.76694100	0.18835800	-0.32821200
H	-1.79331600	0.73404700	-1.18831000
C	-2.36168800	-0.88524600	-0.23475900
C	-3.71692500	-0.54200100	-0.18001500
C	-2.03299400	-2.23537800	0.01837400
C	-4.71729300	-1.48886900	0.10887100
C	-3.00912200	-3.18842900	0.30571200
C	-4.35893800	-2.81932500	0.34720100
H	-4.03155100	0.48436900	-0.35792900
H	-5.75518800	-1.17143900	0.13682800
H	-2.71584600	-4.21574900	0.50368400
C	-0.58081900	-2.61970900	0.00291400
O	-0.22557100	-3.81307200	0.13697500
N	0.21716200	-1.53858500	-0.19003200
C	1.60682100	-1.71858000	-0.35370400
C	2.38297700	-2.58661100	0.43369900
C	2.28189500	-0.97727700	-1.34504500
C	3.76741900	-2.70579600	0.25009500
H	1.89760800	-3.18325000	1.19627000
C	3.65479100	-1.08940300	-1.53904400
H	1.70464700	-0.29766500	-1.96572500
C	4.41061300	-1.95693100	-0.74022200
H	4.32175000	-3.38913800	0.88572100
H	4.15766600	-0.50585500	-2.30616900
O	5.76672900	-2.00342900	-1.00488500
C	6.56967300	-2.86041600	-0.20990000
H	6.26112800	-3.91014200	-0.31033600
H	7.59066400	-2.74689300	-0.58155100
H	6.53524300	-2.57494200	0.85078500
C	1.85475100	1.93609300	0.56588400
C	2.51878800	3.07735100	0.06559700
C	2.54221700	1.11522100	1.48106700
C	3.82022400	3.38261400	0.46605100
H	2.00559800	3.71529300	-0.64945500
C	3.83751200	1.43197300	1.89239000
H	2.05097100	0.22256600	1.85419500
C	4.48496500	2.56437900	1.38679000
H	4.31560000	4.26234000	0.06042800
H	4.34851900	0.78325100	2.60004700
H	5.49927600	2.80212500	1.69882200
C	-1.49171400	3.29254900	-0.23899900
C	-2.67377700	3.33357700	-1.00046400
C	-1.11102700	4.46234000	0.45616100
C	-3.44355400	4.49612800	-1.07275800
H	-2.97908500	2.44247800	-1.54177100
C	-1.88511000	5.62026300	0.39014200
H	-0.20398700	4.44710800	1.05428100
C	-3.05601800	5.64598100	-0.37756800
H	-4.35022900	4.50227400	-1.67361600
H	-1.57373300	6.50610100	0.93939600
H	-3.65847900	6.54959700	-0.43053000
O	-5.25561300	-3.83052300	0.63284500
C	-6.63388700	-3.50223000	0.69597600
H	-7.15397700	-4.43263400	0.93475300
H	-6.83610000	-2.76110400	1.48169000
H	-7.00111900	-3.11753600	-0.26565000

TS21_OMe_1

C	-0.13798400	1.37437700	0.25300100
C	-1.37844100	1.41815100	-0.07597100
Ni	-0.79226300	-0.42214100	-0.14140600
H	-2.05291100	-0.45005100	-0.85763400
C	-1.85557600	-2.04153400	0.01320500
C	-3.24151200	-2.26348700	0.14571400
C	-1.00746500	-3.14235300	0.23215800
C	-3.75254200	-3.52685900	0.47959300
C	-1.50439500	-4.41183400	0.56419900
C	-2.87704400	-4.60101500	0.68673800
H	-4.82131300	-3.68889100	0.57474700
H	-3.28100300	-5.57812000	0.94419900
H	-0.79833100	-5.22145900	0.72626100
C	0.47697200	-2.92866500	0.12893900
O	1.26987000	-3.89665400	0.19803300
N	0.78910800	-1.62386000	-0.06085600
C	2.13311800	-1.26840500	-0.30882600
C	3.21658300	-1.74794700	0.44617800
C	2.42858900	-0.37480500	-1.35806900
C	4.53439300	-1.35731000	0.17282600
H	3.02947500	-2.44536500	1.25443500
C	3.73293500	0.01974700	-1.64084500
H	1.60780900	0.01033200	-1.95670500
C	4.79879800	-0.47120900	-0.87620400
H	5.33633400	-1.75771700	0.78498300
H	3.94181600	0.71054200	-2.45395000
O	6.05875800	-0.02707500	-1.23165700
C	7.16769300	-0.51435600	-0.49430400
H	7.25196900	-1.60740600	-0.56869300
H	8.05191700	-0.05253800	-0.93967400
H	7.10416600	-0.22929100	0.56507200
C	1.03079300	2.14486700	0.63139500
C	1.27647700	3.41021100	0.05601200
C	1.93765800	1.66508600	1.59561300
C	2.38773700	4.16523500	0.43317300
H	0.58998700	3.78905900	-0.69694000
C	3.03932300	2.42903600	1.98296800
H	1.76850600	0.68398800	2.02772600
C	3.27294800	3.68066500	1.40322600
H	2.56268300	5.13407900	-0.03010000
H	3.72643000	2.03876300	2.73027200
H	4.13959200	4.26849100	1.69682500
C	-2.54233800	2.26887400	-0.25664900
C	-3.59368300	1.93854600	-1.13117700
C	-2.61906100	3.49483200	0.44066200
C	-4.67368900	2.80458700	-1.31297700
H	-3.55335800	0.99163200	-1.65970300
C	-3.70457300	4.35335500	0.26681500
H	-1.81753300	3.76238800	1.12399500

C	-4.73799000	4.01567900	-0.61551400
H	-5.47037300	2.53094400	-2.00162100
H	-3.74304100	5.28941100	0.81991700
H	-5.58231300	4.68668400	-0.75516600
O	-4.06557600	-1.17912100	-0.08194800
C	-5.46417300	-1.33348600	0.07756900
H	-5.87643900	-2.06582000	-0.63146600
H	-5.72272200	-1.63843300	1.10127700
H	-5.89747000	-0.35135100	-0.12481600

Int30_1

C	-1.98827500	0.64647800	0.16250800
C	-1.77621200	-0.38568300	-0.58243000
Ni	-0.15540600	0.39570400	-0.10276500
H	0.67263000	-1.89456800	0.82146600
C	1.39672400	-1.95201600	1.62846700
C	1.20813400	-2.84742700	2.68091000
C	2.52275200	-1.11102200	1.60940900
C	2.13769000	-2.91917600	3.72334800
C	3.45281300	-1.18588200	2.66281700
C	3.25987100	-2.08490600	3.71218100
H	0.33341300	-3.49180300	2.68338600
H	1.98671700	-3.61766700	4.54206400
H	3.97935600	-2.12424300	4.52548300
H	4.30986800	-0.51727300	2.68781200
C	-2.90045900	1.57885100	0.79079500
C	-4.28487300	1.55359600	0.50837300
C	-2.42990300	2.54752400	1.70190800
C	-5.15694000	2.45785600	1.11401200
H	-4.66707000	0.82327300	-0.19935000
C	-3.30429400	3.44854200	2.30979600
H	-1.36711600	2.57961500	1.92712500
C	-4.67287700	3.40954800	2.01983800
H	-6.21817000	2.42102900	0.87854700
H	-2.91763400	4.18419400	3.01133400
H	-5.35422500	4.11241400	2.49262800
C	-2.23198300	-1.55059500	-1.31023600
C	-1.37511400	-2.23496800	-2.19762800
C	-3.54762000	-2.04105800	-1.14853800
C	-1.81537800	-3.35742500	-2.89944100
H	-0.36126700	-1.86718800	-2.33205600
C	-3.98368300	-3.16581000	-1.84842100
H	-4.21982100	-1.53615600	-0.46036200
C	-3.12161100	-3.83014000	-2.72934600
H	-1.13785100	-3.86498700	-3.58223200
H	-4.99994000	-3.52625900	-1.70603200
H	-3.46424600	-4.70515800	-3.27584300
C	2.73869400	-0.17880500	0.49601800
C	3.88238800	1.05356600	-0.98135800
C	2.49418300	1.19312200	-1.18791300
C	4.83018700	1.70856300	-1.77174700
C	2.01313400	2.01956100	-2.21161900
C	4.33761700	2.52355500	-2.78968900
H	5.89697700	1.59136200	-1.60398100
C	2.95049800	2.67682300	-3.00472300
H	0.94538400	2.13322000	-2.37151500
H	5.03688600	3.05337000	-3.43052200
H	2.60842600	3.32281200	-3.80842300
N	3.99575900	0.18669600	0.09333000
N	1.80733100	0.41584400	-0.25274400
H	4.85465100	-0.20950500	0.45005000

TS22_1

C	-1.01225800	1.18426800	0.08083300
C	-1.96695200	0.37368100	-0.15397500
Ni	-0.31017000	-0.65336000	-0.18041800
H	-1.25534500	-1.44199500	-0.93178300
C	-0.05861400	-2.55079000	0.10645400
C	-0.98517000	-3.56826600	0.37783200
C	1.31498100	-2.88822200	0.23781700
C	-0.57340000	-4.85656900	0.74567700
C	1.73558500	-4.17568500	0.60442400
C	0.78655400	-5.16724000	0.85239200
H	-2.05023900	-3.36448100	0.30194700
H	-1.31908400	-5.62348700	0.94374700
H	1.10341300	-6.16762500	1.13455000
H	2.79378200	-4.40495800	0.71924100
C	-0.56087600	2.53549800	0.34768200
C	-0.85826700	3.58037100	-0.55167800
C	0.16450200	2.83953700	1.51622200
C	-0.44245100	4.88619400	-0.28575000
H	-1.41273000	3.35718100	-1.45910100
C	0.56418600	4.14933600	1.78457800
H	0.40919400	2.04006000	2.20981800
C	0.26684200	5.17829100	0.88442100
H	-0.67824500	5.67814300	-0.99255100
H	1.11689800	4.36516100	2.69561700
H	0.58636300	6.19642400	1.09120500
C	-3.39816500	0.14589600	-0.26543800
C	-3.94823500	-0.97005400	-0.91823300
C	-4.27768100	1.09739700	0.29426500
C	-5.33161000	-1.13313500	-1.01200900
H	-3.28306700	-1.70689500	-1.35981900
C	-5.65886300	0.92917100	0.20471100
H	-3.86546300	1.96416600	0.80319900
C	-6.19336200	-0.18672000	-0.44974100
H	-5.73590900	-2.00188900	-1.52551800
H	-6.31957500	1.67089700	0.64668800
H	-7.27022200	-0.31651000	-0.51975600
C	2.21300600	-1.76947500	0.02108100
C	3.98264900	-0.46105300	-0.31490300
C	2.78772200	0.29779500	-0.37296200
C	5.24381500	0.10460900	-0.50724700
C	2.84759500	1.67063800	-0.64492200
C	5.28501800	1.47419300	-0.76974600
H	6.15116600	-0.49086100	-0.46083300
C	4.10405100	2.24184700	-0.83957300
H	1.94335100	2.26485200	-0.70094700
H	6.24566200	1.95661900	-0.92752400
H	4.17550700	3.30507600	-1.05170300
N	3.57581000	-1.76352100	-0.05694300
N	1.70859700	-0.54790600	-0.14391600
H	4.17484900	-2.57490800	0.00795100

Int31_1

C	-1.21021700	0.47878800	-0.03632000
C	-1.90523100	-0.65154200	-0.12308300
Ni	0.22702000	-0.79265000	-0.04312700
H	-1.27464700	-1.61738800	-0.23717600
C	1.24244900	-2.47483300	0.02205900
C	0.85426200	-3.82353000	0.05516200
C	2.63982000	-2.23318100	0.06717700
C	1.79537100	-4.86219200	0.12454000
C	3.59694800	-3.25580400	0.13816700
C	3.16686800	-4.58307700	0.16610000
H	-0.20122700	-4.09045200	0.02745600
H	1.45794600	-5.89668300	0.14644900
H	3.89156700	-5.39116500	0.22008800
H	4.66295900	-3.03451100	0.17234600
C	-1.60783200	1.87847000	0.05478200
C	-2.01689900	2.59240600	-1.09063400
C	-1.55994500	2.56368400	1.28604300
C	-2.37388100	3.93948000	-1.00310600
H	-2.04899900	2.08257400	-2.05003100
C	-1.92841000	3.90765600	1.37055400
H	-1.23149000	2.03248600	2.17556400
C	-2.33533400	4.60442200	0.22740000
H	-2.68629500	4.46978900	-1.89965400
H	-1.89201300	4.41315100	2.33267000
H	-2.61585300	5.65241100	0.29401700
C	-3.32133100	-1.05553200	-0.08523600
C	-3.67477000	-2.40937800	-0.23393700
C	-4.35047800	-0.11099200	0.09950000
C	-5.01104800	-2.81109700	-0.20124700
H	-2.89408600	-3.15355100	-0.37729800
C	-5.68476300	-0.51507600	0.13138200
H	-4.10195700	0.93799000	0.21994300
C	-6.02369200	-1.86499700	-0.01877400

H	-5.25994100	-3.86282500	-0.31850900
H	-6.46455700	0.22864900	0.27599000
H	-7.06519700	-2.17462100	0.00741900
C	2.94147900	-0.81483300	0.02558300
C	3.90858500	1.19248600	-0.04725500
C	2.50001700	1.33122300	-0.09011800
C	4.77329500	2.28637600	-0.08752000
C	1.92712300	2.60486700	-0.18324200
C	4.18670600	3.54920100	-0.17606600
H	5.85221900	2.16276800	-0.05549000
C	2.78612400	3.70221100	-0.22430900
H	0.85208300	2.72830500	-0.22206200
H	4.82227400	4.42963000	-0.21095700
H	2.36441100	4.70091400	-0.29655600
N	4.14306600	-0.17522800	0.02748300
N	1.93377100	0.06246000	-0.03728800
H	5.04709100	-0.62512300	0.06637700

Int32_1

C	-4.45531300	2.25744900	1.47300700
C	-3.18152000	2.11261700	0.90104500
C	-2.62391900	0.85266700	0.64301400
C	-3.43207300	-0.26256100	0.98330800
C	-4.70194900	-0.14166700	1.56685500
C	-5.21475900	1.13272900	1.81563500
H	-4.85928100	3.25258600	1.65022500
H	-2.62679700	3.01345800	0.64274100
H	-5.29067500	-1.01924100	1.83121000
H	-6.19716400	1.24763900	2.26614300
C	-0.50674500	2.03953400	-1.02383400
C	0.76138200	2.92743400	1.13718700
C	0.12217000	3.25411100	2.35001600
C	2.13004600	3.22581000	0.97833300
C	0.83641200	3.87806400	3.37219700
H	-0.92821300	3.01411900	2.48097200
C	2.83581200	3.84882600	2.00726000
H	2.62825000	2.95760900	0.05199100
C	2.19299500	4.17772000	3.20530900
H	0.33308300	4.12888900	4.30228400
H	3.89073600	4.07357400	1.87411500
H	2.74648200	4.66167000	4.00569400
C	-0.96904400	2.12600500	-2.38525500
C	-0.24831400	2.93676000	-3.28838900
C	-2.11129000	1.44178200	-2.84103100
C	-0.67139300	3.06365600	-4.61064100
H	0.63853900	3.46030600	-2.94341900
C	-2.52705400	1.57607600	-4.16570000
H	-2.66330300	0.81592800	-2.14831800
C	-1.81137300	2.38434500	-5.05479900
H	-0.10812100	3.69191600	-5.29574100
H	-3.41223100	1.04430200	-4.50483100
H	-2.13717900	2.48252800	-6.08697400
C	0.04076200	2.32283500	0.05146100
Ni	-0.77778500	0.29619100	0.08722700
C	1.09561200	-0.36336400	0.01239400
C	1.90312400	-0.20759800	-1.06157900
H	1.44741800	0.20216500	-1.96652000
C	1.47003000	-1.03301400	1.28088900
C	1.18870100	-0.43380700	2.52816700
C	2.03534300	-2.32793100	1.30623400
C	1.47610800	-1.08048600	3.73302200
H	0.75702400	0.56160100	2.55395400
C	2.31319400	-2.98012000	2.50737200
H	2.26413400	-2.82439900	0.36881300
C	2.03809000	-2.36017000	3.73193500
H	1.25626600	-0.58123000	4.67424700
H	2.74707500	-3.97761300	2.48712000
H	2.25619500	-2.86823300	4.66816400
C	3.34921700	-0.48126800	-1.24098900
C	3.83059400	-0.74223400	-2.54085600
C	4.29486400	-0.43275900	-0.19616400
C	5.18457100	-0.98175400	-2.78502700
H	3.12439200	-0.76079600	-3.36927400
C	5.64941200	-0.66596900	-0.43846800
H	3.96521700	-0.20004400	0.81091700
C	6.10407100	-0.94894600	-1.73196200
H	5.52163200	-1.18915600	-3.79826700
H	6.35582300	-0.61914600	0.38747000
H	7.16001500	-1.13022400	-1.91676500
C	-2.81296900	-1.51935300	0.60298500
C	-2.41447000	-3.62915500	0.00976400
C	-1.31673200	-2.80766500	-0.34187300
C	-2.45807000	-4.99363700	-0.27769600
C	-0.23495900	-3.35644800	-1.04102700
C	-1.36367000	-5.52790400	-0.95809800
H	-3.30823900	-5.60881000	0.00339900
C	-0.27496600	-4.71722100	-1.33983400
H	0.59452500	-2.72889000	-1.34413000
H	-1.35602100	-6.58541900	-1.20712600
H	0.55287600	-5.16484000	-1.88320100
N	-3.33215100	-2.77832100	0.61415500
N	-1.58972100	-1.50615600	0.06777500
H	-4.25293200	-3.03259500	0.94424600

TS23_1

C	-3.64661700	0.12200800	3.06681700
C	-2.72339200	0.60405000	2.13053000
C	-2.14289500	-0.24335600	1.17781700
C	-2.47536600	-1.62432100	1.24165300
C	-3.41365200	-2.10235200	2.16662300
C	-4.01755000	-1.22482500	3.06824200
H	-4.08467900	0.80745200	3.78799600
H	-2.47706300	1.66098100	2.12780100
H	-3.63604000	-3.16601900	2.22220000
H	-4.74570800	-1.59574700	3.78398300
C	-1.93979000	1.05181600	-0.38078500
C	-0.41648900	3.15095200	-0.33424700
C	-1.21791000	4.21755000	0.13216500
C	0.82252400	3.46565100	-0.92902100
C	-0.80260700	5.54267000	-0.00280300
H	-2.16202400	3.99824500	0.62342400
C	1.22660700	4.79265800	-1.07499300
H	1.46253000	2.66102400	-1.26976300
C	0.42010200	5.83894900	-0.61345100
H	-1.43611600	6.34389800	0.37029600
H	2.18225100	5.00937400	-1.54614000
H	0.74356200	6.87094800	-0.72214900
C	-3.18274400	0.98698200	-1.14639000
C	-3.92211800	2.16303500	-1.38289600
C	-3.63573700	-0.21471900	-1.72166600
C	-5.07559600	2.13323900	-2.16812600
H	-3.58731800	3.10078500	-0.95275600
C	-4.78934700	-0.24107400	-2.50514000
H	-3.06861900	-1.12666300	-1.56521200
C	-5.51735300	0.93194300	-2.73088100
H	-5.63097600	3.05234300	-2.33757700
H	-5.11772200	-1.17944600	-2.94532600
H	-6.41725600	0.91001200	-3.33992700
C	-0.88497000	1.78670200	-0.17153900
Ni	-0.38281200	-0.02028300	0.25187000
C	1.55331400	0.18369400	0.19482700
C	2.30414000	0.26324800	-0.92345700
H	1.76341600	0.27393500	-1.87331100
C	2.02747600	0.11322100	1.59242100
C	2.03908000	1.25825200	2.41764200
C	2.41396900	-1.11594700	2.16844600
C	2.44755900	1.18160300	3.74996500
H	1.73108600	2.21237200	1.99781400
C	2.81828000	-1.19092000	3.50298100
H	2.40520200	-2.01299100	1.55447800
C	2.84051600	-0.04311200	4.30277000
H	2.45826800	2.08240600	4.35990700
H	3.12002700	-2.15003100	3.91871200
H	3.15646400	-0.10195800	5.34135100
C	3.76897200	0.33567300	-1.12447100
C	4.24964500	0.27881300	-2.45094800
C	4.72757100	0.47111700	-0.09690600
C	5.61315900	0.34077700	-2.74320500

H	3.53300200	0.18398500	-3.26510900
C	6.09113300	0.53522700	-0.38827500
H	4.40644300	0.53205400	0.93587000
C	6.54630600	0.46823600	-1.71004300
H	5.94549000	0.29213900	-3.77783000
H	6.80417600	0.64123200	0.42638700
H	7.60985300	0.51853400	-1.92984200
C	-1.63698000	-2.49773400	0.44073900
C	-0.72008500	-4.22104900	-0.62423700
C	0.11494500	-3.08012400	-0.71848800
C	-0.38646200	-5.44687800	-1.20329500
C	1.33412200	-3.16041000	-1.40608400
C	0.82681100	-5.50755100	-1.88774700
H	-1.03759700	-6.31283600	-1.12407600
C	1.67197100	-4.38164600	-1.98474600
H	1.98506600	-2.29686300	-1.47432900
H	1.12793400	-6.44191000	-2.35319200
H	2.61163500	-4.47086200	-2.52283100
N	-1.81928100	-3.81172900	0.11941800
N	-0.48969600	-2.02936300	-0.03861900
H	-2.62699600	-4.37312300	0.35240900

Int33_1

C	-2.08093800	-1.23153600	-4.11545000
C	-2.01966100	-1.50155100	-2.75012100
C	-1.84006200	-0.48927700	-1.78628900
C	-1.74745800	0.84565100	-2.26460000
C	-1.82705500	1.11306100	-3.64596600
C	-1.98592700	0.08670300	-4.57226500
H	-2.20236500	-2.04882300	-4.82183600
H	-2.11268500	-2.52746500	-2.40573000
H	-1.73253600	2.13899900	-3.99381800
H	-2.02748300	0.31155100	-5.63431500
C	-1.83627000	-0.87290800	-0.33907200
C	-0.94193200	-0.67629200	1.99688100
C	-2.00180100	-0.11414700	2.73738600
C	0.05064700	-1.38190100	2.70437000
C	-2.07446800	-0.26293700	4.12438700
H	-2.77440900	0.44235400	2.21361400
C	-0.03041200	-1.54549300	4.08765500
H	0.88476600	-1.81031600	2.15863300
C	-1.09139100	-0.98413300	4.80815200
H	-2.90353400	0.18267800	4.66962700
H	0.74195000	-2.10895300	4.60651500
H	-1.14796300	-1.10478700	5.88719700
C	-2.95471400	-1.79309700	0.06251400
C	-2.70591300	-3.00034400	0.73848300
C	-4.29009600	-1.47690900	-0.24991100
C	-3.75273000	-3.84936800	1.10677500
H	-1.68157000	-3.27485000	0.97196200
C	-5.33936300	-2.32144400	0.11913500
H	-4.50860300	-0.55408900	-0.78267900
C	-5.07530000	-3.51326500	0.80228600
H	-3.53235400	-4.77748100	1.62894600
H	-6.36324500	-2.04813000	-0.12590100
H	-5.88998500	-4.17356100	1.08912600
C	-0.87518600	-0.46365100	0.52959000
Ni	0.51589300	0.67008900	0.00530800
C	2.01713600	-0.43177200	0.04267900
C	2.93208100	0.54275900	0.29118900
H	2.54101300	1.47760400	0.72809000
C	4.38922700	0.62734900	0.04591400
C	5.14301700	1.58454800	0.75468900
C	5.06544900	-0.17414000	-0.89593500
C	6.51835200	1.71915500	0.55618400
H	4.63963500	2.22551000	1.47620400
C	6.43920800	-0.03767000	-1.09758400
H	4.50910600	-0.90041900	-1.47901300
C	7.17615800	0.90499900	-0.37076300
H	7.07484400	2.46173800	1.12328600
H	6.93633800	-0.66657200	-1.83253600
H	8.24625400	1.00830200	-0.53177700
C	2.27748800	-1.83662200	-0.29629400
C	1.60244500	-2.46410500	-1.36217500
C	3.16549700	-2.61886800	0.47264900
C	1.83116000	-3.80670900	-1.66880100
H	0.89594800	-1.88556000	-1.95032900
C	3.37772100	-3.96689300	0.18025400
H	3.68798900	-2.15711700	1.30652100
C	2.71703800	-4.56722200	-0.89755700
H	1.30702600	-4.26427300	-2.50490500
H	4.06311200	-4.54894600	0.79222000
H	2.88454800	-5.61633300	-1.12847600
C	-1.60538300	2.00380500	-1.36961800
C	-0.92670000	3.39956600	0.17035700
C	-1.96033300	4.04998700	-0.53892800
C	-0.28419400	4.04235600	1.23572700
C	-2.38868700	5.34031400	-0.21755100
C	-0.70548400	5.32937500	1.56063400
H	0.50738900	3.54701300	1.79003300
C	-1.74150600	5.96858400	0.84546600
H	-3.18575100	5.83240300	-0.76740800
H	-0.22936100	5.85424900	2.38399600
H	-2.04188000	6.97305900	1.12999800
N	-0.73036600	2.13699600	-0.37920000
N	-2.35785500	3.14116700	-1.50696100
H	-3.13159900	3.24685700	-2.14960900

TS24_1

C	-2.54116300	-2.47582900	-3.66220100
C	-2.18324200	-2.42055600	-2.33440900
C	-1.98696800	-1.17948800	-1.64710000
C	-2.19078900	0.01815000	-2.43124500
C	-2.57997400	-0.06764200	-3.79841500
C	-2.74942500	-1.28698800	-4.41117100
H	-2.64930900	-3.44228400	-4.14795800
H	-2.01252900	-3.34260500	-1.78992500
H	-2.70395100	0.84610500	-4.37557300
H	-3.01955600	-1.34121200	-5.46183400
C	-1.68482700	-1.13238000	-0.25502100
C	-1.33298700	0.24658100	1.85015600
C	-2.62742000	0.31309600	2.39504000
C	-0.23340700	0.41234900	2.70722200
C	-2.81856800	0.54140900	3.75897600
H	-3.48725400	0.18571200	1.74216600
C	-0.42259500	0.62494200	4.07502800
H	0.76777800	0.37213800	2.28780200
C	-1.71520100	0.69563900	4.60458500
H	-3.82711600	0.59476600	4.16153000
H	0.44076600	0.73914200	4.72590100
H	-1.86204800	0.86918600	5.66772000
C	-1.89814600	-2.35572500	0.58106800
C	-0.83438100	-2.94827600	1.28268100
C	-3.17284800	-2.94306100	0.68567000
C	-1.04028900	-4.08419400	2.07037400
H	0.16276000	-2.52725300	1.19385900
C	-3.38080900	-4.07686700	1.47353800
H	-4.00854800	-2.49892500	0.15008400
C	-2.31335200	-4.65192000	2.17168300
H	-0.20055600	-4.52787900	2.59963100
H	-4.37645400	-4.50851100	1.54530700
H	-2.47287800	-5.53498400	2.78550500
C	-1.14844300	0.02618100	0.37919900
Ni	0.30820800	0.87552000	-0.43313000
C	2.10124000	0.24750400	-0.22993300
C	3.02287800	1.24251600	-0.09075700
H	2.64039200	2.25030700	0.09682300
C	4.50312700	1.22900100	-0.16189000
C	5.20946400	2.30570000	0.41508400
C	5.25971300	0.23465200	-0.81675500
C	6.60305700	2.37454100	0.37357200
H	4.64859300	3.09762000	0.90873900
C	6.65281000	0.30413900	-0.86408900
H	4.75209800	-0.59281500	-1.29956900
C	7.33578300	1.36922300	-0.26525400
H	7.11613200	3.21498400	0.83590500
H	7.20890300	-0.47656200	-1.37842200
H	8.42116900	1.41886900	-0.30468200

C	2.43766500	-1.18956600	-0.31418800
C	2.03771400	-1.97252100	-1.41674200
C	3.09637700	-1.84952100	0.74570700
C	2.31787200	-3.33921600	-1.47717900
H	1.50374800	-1.49345100	-2.23404600
C	3.36029300	-3.21998700	0.69550300
H	3.40763400	-1.27158600	1.61272400
C	2.97952000	-3.97434100	-0.42007800
H	2.00739500	-3.91272200	-2.34806900
H	3.87041100	-3.69943900	1.52859300
H	3.18702600	-5.04083200	-0.46112300
C	-2.12802100	1.26407100	-1.77614000
C	-1.84289900	2.75853300	-0.11213400
C	-2.58002500	3.37943400	-1.13813800
C	-1.49925500	3.45640200	1.04631600
C	-3.01578400	4.70122400	-1.03729700
C	-1.93591000	4.77920400	1.15325500
H	-0.92459600	2.98928700	1.83678000
C	-2.68387400	5.38985700	0.13084700
H	-3.58719700	5.17302300	-1.83113000
H	-1.68848400	5.34655100	2.04556500
H	-3.00735100	6.42017900	0.24843300
N	-1.54216200	1.44037600	-0.54456800
N	-2.72108200	2.44181000	-2.15383500
H	-3.35554900	2.52571000	-2.93646700

Int34_1

C	-3.41541400	-2.59065100	-3.13286200
C	-2.86380500	-2.46579800	-1.88396600
C	-2.44091700	-1.19269800	-1.36378100
C	-2.61265800	-0.05068300	-2.24457200
C	-3.19899400	-0.21454300	-3.53833400
C	-3.59472200	-1.45113200	-3.97634200
H	-3.70943300	-3.57265000	-3.49437200
H	-2.72077100	-3.34754600	-1.26933700
H	-3.31441200	0.64731200	-4.19171400
H	-4.02923700	-1.56973900	-4.96474900
C	-1.90931100	-1.04116200	-0.07148400
C	-1.43951100	0.52198700	1.87333000
C	-2.67816900	0.88541600	2.42579700
C	-0.32249900	0.43632800	2.71395200
C	-2.79551200	1.17195500	3.78765600
H	-3.55514400	0.94399000	1.78467100
C	-0.44135600	0.70685000	4.08031400
H	0.63761700	0.16485100	2.28518700
C	-1.67541900	1.08157700	4.62029200
H	-3.76062200	1.45868300	4.19805300
H	0.43346400	0.62925000	4.72106500
H	-1.76472800	1.29961700	5.68155100
C	-1.89978200	-2.19634700	0.87861700
C	-0.69644300	-2.80107000	1.27570000
C	-3.10574100	-2.70072000	1.39644700
C	-0.69956200	-3.87816900	2.16653600
H	0.24293300	-2.43554100	0.87285100
C	-3.10988200	-3.77473900	2.28939100
H	-4.04568500	-2.24169400	1.09959200
C	-1.90439400	-4.36754000	2.67864800
H	0.24330200	-4.33603700	2.45529000
H	-4.05354900	-4.14576700	2.68230800
H	-1.90533100	-5.20445700	3.37265700
C	-1.34883900	0.21190400	0.39672400
Ni	0.25543900	0.72181400	-0.52306400
C	2.04147500	0.07640300	-0.34712200
C	2.97670500	1.02216600	-0.04295800
H	2.60890200	1.99724600	0.28577200
C	4.45789700	0.98311100	-0.08579400
C	5.17493200	1.90427700	0.70677800
C	5.20586600	0.12359800	-0.91707000
C	6.57032100	1.94430700	0.70222900
H	4.62117200	2.59499600	1.34054500
C	6.60077500	0.16681400	-0.92914200
H	4.68981500	-0.57469700	-1.56681100
C	7.29402900	1.07099500	-0.11596200
H	7.09199000	2.66066000	1.33314800
H	7.15022500	-0.50627000	-1.58362300
H	8.38078600	1.10073900	-0.12813600
C	2.37432900	-1.33692300	-0.63358400
C	1.96491600	-1.95862800	-1.83177500
C	3.04219200	-2.13954700	0.31668600
C	2.24134200	-3.30362800	-2.08517400
H	1.42433200	-1.36959500	-2.56961000
C	3.30320600	-3.48970600	0.07323500
H	3.36037200	-1.68943300	1.25411000
C	2.91047700	-4.08100700	-1.13264500
H	1.92249400	-3.74976100	-3.02489200
H	3.81979900	-4.08110900	0.82661200
H	3.11482400	-5.13169300	-1.32359300
C	-2.24556300	1.19801500	-1.75292000
C	-1.55609700	2.77118800	-0.24156400
C	-2.08126700	3.42445400	-1.37125900
C	-1.05142900	3.49877200	0.83613300
C	-2.13107300	4.81535400	-1.45939300
C	-1.10262700	4.89412300	0.75171100
H	-0.63886100	3.00956400	1.70831300
C	-1.63426100	5.54145500	-0.37485200
H	-2.54186700	5.30983100	-2.33423500
H	-0.71800700	5.48430200	1.57795700
H	-1.65895900	6.62689200	-0.40727100
N	-1.62606300	1.36829200	-0.51031600
N	-2.47693600	2.44630700	-2.27099000
H	-2.97600900	2.61691700	-3.13213300

8a

C	4.53469900	-0.02816800	0.00529200
C	3.84308600	1.18536700	-0.04210800
C	2.44703500	1.19893300	-0.04719800
C	1.71952400	-0.00335700	-0.00366400
C	2.42494100	-1.22011700	0.04264100
C	3.81838000	-1.23007000	0.04690100
H	5.62141100	-0.03770800	0.00895500
H	4.38881400	2.12451200	-0.07749200
H	1.93749700	2.15797700	-0.09219100
H	1.86297600	-2.14755100	0.07572900
H	4.34803800	-2.17846000	0.08372100
C	0.25098000	-0.03216600	-0.00516700
C	-1.79759500	-0.70715200	-0.02044900
C	-1.85410700	0.70873800	0.01702000
C	-2.98633600	-1.45249100	-0.03863700
C	-3.06068700	1.41359500	0.03927600
C	-4.19371600	-0.75789400	-0.01699100
H	-2.95468700	-2.53795300	-0.06812300
C	-4.23060600	0.65384000	0.02174100
H	-3.09235900	2.49944300	0.06847900
H	-5.12960800	-1.31020000	-0.02996700
H	-5.19204600	1.16019300	0.03805600
N	-0.48095900	-1.13221100	-0.03323400
N	-0.53069900	1.10839400	0.02365000
H	-0.20200700	2.06211200	0.06797700

9a

C	3.47579200	0.91560200	0.01268300
C	2.59679600	-0.20004700	0.02859300
C	3.08664600	-1.51299700	0.07543800
C	4.47046500	-1.67988600	0.09757800
C	5.35159400	-0.57780500	0.07507100
C	4.86688600	0.72406000	0.03357500
C	1.50422100	1.75452800	-0.01867200
H	2.43499400	-2.37572400	0.09615500
H	4.87590600	-2.68745800	0.13403200
H	6.42409700	-0.75339100	0.09289900
H	5.53235700	1.58255300	0.02006000
C	0.35594800	2.62241100	-0.02915900
C	-0.93837900	2.03953600	-0.01147000
C	0.51141600	4.02258700	-0.05340600
C	-2.05723200	2.90481800	-0.02439500
C	-0.60295600	4.84725500	-0.06236200
H	1.51554600	4.43407400	-0.06513900
C	-1.89209600	4.28253300	-0.04862400

H	-3.05616600	2.48200900	-0.01690300
H	-0.48087800	5.92681400	-0.08104300
H	-2.76651900	4.92804300	-0.05825800
C	-1.07317300	0.58800400	0.00476900
C	0.03359000	-0.21783800	0.00231500
C	-0.04825900	-1.70870400	-0.01359800
C	-0.19673700	-2.42851400	1.18029000
C	0.02191600	-2.40538200	-1.22923100
C	-0.26893000	-3.82394800	1.15958900
H	-0.25252200	-1.89545500	2.12561700
C	-0.05107000	-3.79990800	-1.24987000
H	0.13876800	-1.85358200	-2.15843300
C	-0.19432800	-4.51235800	-0.05489300
H	-0.38397300	-4.37120700	2.09150300
H	0.00373700	-4.32868800	-2.19785000
H	-0.24994000	-5.59769000	-0.07077000
C	-2.44539800	-0.01526900	0.01307400
C	-3.14802700	-0.16899700	1.21843000
C	-3.06798200	-0.40230100	-1.18309900
C	-4.43677200	-0.70935100	1.22985600
H	-2.67982700	0.13566800	2.15141900
C	-4.35702200	-0.94285500	-1.17441900
H	-2.53892500	-0.27989100	-2.12485700
C	-5.04461400	-1.09923500	0.03256300
H	-4.96422800	-0.82579200	2.17334900
H	-4.82227500	-1.24162400	-2.11044700
H	-6.04693200	-1.51982000	0.04019400
N	2.77657900	2.10284500	-0.01590300
N	1.30956500	0.36365900	0.00086400

Int35_1

C	-1.81835700	-0.83137900	-0.11771200
C	-0.79382100	-1.60442700	-0.02560300
Ni	-0.25092300	0.15599300	-0.35969000
H	1.19344500	1.59567500	-1.86187100
C	4.43545100	1.03547800	0.60104900
C	5.57658100	0.26411000	0.39022400
C	3.28231600	0.82577700	-0.17800300
C	5.59075400	-0.71962900	-0.60546100
C	3.30081900	-0.17048500	-1.17061200
C	4.44970400	-0.93309000	-1.38451700
H	6.45954100	0.43439500	1.00038800
H	6.48315800	-1.31747300	-0.77023200
H	4.44732700	-1.70176000	-2.15251200
H	2.41170100	-0.37726200	-1.76076200
C	-3.24384000	-0.58258400	-0.12956100
C	-4.15210800	-1.60806300	-0.47363000
C	-3.76526400	0.68552600	0.20022100
C	-5.52680300	-1.37237300	-0.48007600
H	-3.76879700	-2.58728700	-0.74583800
C	-5.14106300	0.91543700	0.19866600
H	-3.07769700	1.48369900	0.46536900
C	-6.02957100	-0.11077800	-0.14161300
H	-6.20799900	-2.17597500	-0.74972400
H	-5.52183000	1.89857600	0.46505900
H	-7.10135600	0.07025000	-0.14415000
C	-0.21625300	-2.90313100	0.25310300
C	1.17692400	-3.07467000	0.37798000
C	-1.04384300	-4.03598100	0.41874000
C	1.72271900	-4.32828000	0.65496800
H	1.82616600	-2.21212100	0.26130600
C	-0.49549000	-5.28785900	0.69529400
H	-2.12073300	-3.92313000	0.33502600
C	0.89089600	-5.44203400	0.81352500
H	2.80061900	-4.43562200	0.74998200
H	-1.15193600	-6.14565900	0.82106100
H	1.31679300	-6.41858400	1.02923900
C	2.11246600	1.68196800	0.04267200
C	0.79460300	3.23686500	0.76672300
C	0.18796500	2.76961200	-0.41824000
C	0.20930100	4.28631900	1.48480400
C	-0.96482300	3.34126400	-0.95332700
C	-0.95317100	4.85842600	0.96763800
H	0.66048900	4.64440600	2.40522300
C	-1.52570200	4.40187700	-0.23660000
H	-1.41304200	2.98061900	-1.87428300
H	-1.42542100	5.68037000	1.49870100
H	-2.42465600	4.88004400	-0.61525700
N	1.97488700	2.54684600	1.01472400
N	1.00454200	1.69082300	-0.86502300
H	4.42174300	1.80796500	1.36278000

TS25_1

C	0.59323700	2.09314100	0.10743000
C	-0.65118200	2.00241500	-0.07322500
Ni	0.11515900	0.20372100	0.03209700
H	0.28114100	-0.71620500	-1.14338400
C	-2.43855500	-3.88201100	-0.14666600
C	-3.82654400	-3.87977700	-0.02054700
C	-1.68574500	-2.74495100	0.20362300
C	-4.49136600	-2.74498900	0.45996100
C	-2.36249300	-1.61576600	0.69278600
C	-3.75349200	-1.61359000	0.81740000
H	-4.39250000	-4.76481700	-0.29992000
H	-5.57380300	-2.74535000	0.55900800
H	-4.25615000	-0.73054800	1.20261600
H	-1.79993600	-0.73856000	1.01005400
C	1.92483600	2.64924400	0.15479200
C	2.28735300	3.67212800	-0.74603000
C	2.86894900	2.19990200	1.09820500
C	3.56382800	4.23095000	-0.69602000
H	1.56385300	4.01722700	-1.47886400
C	4.14359300	2.76508100	1.14237400
H	2.59367100	1.41528300	1.79708600
C	4.49503500	3.78005300	0.24653900
H	3.83271700	5.01872500	-1.39476000
H	4.86244600	2.41262600	1.87714900
H	5.48912300	4.21761900	0.28195600
C	-2.01505300	2.47407500	-0.17038100
C	-2.96524500	1.80381700	-0.96254400
C	-2.39953100	3.64156800	0.52129400
C	-4.26728100	2.29449300	-1.06682700
H	-2.67372700	0.90447000	-1.49623100
C	-3.70371900	4.12333600	0.41615000
H	-1.67062800	4.15978400	1.13782100
C	-4.64111900	3.45289800	-0.37823700
H	-4.99030500	1.77063700	-1.68637400
H	-3.98888500	5.02350700	0.95439600
H	-5.65650200	3.83175300	-0.45925800
C	-0.22214200	-2.78861100	0.06903600
C	1.78938800	-3.53989600	-0.09040100
C	1.87926300	-2.13094200	-0.18396600
C	2.94492800	-4.33074300	-0.16261400
C	3.10135000	-1.48068900	-0.37803700
C	4.16633100	-3.68592200	-0.34995900
H	2.87921900	-5.41207800	-0.07868500
C	4.24232900	-2.28075900	-0.46139100
H	3.16714400	-0.39942800	-0.46006000
H	5.07904600	-4.27281900	-0.41407900
H	5.21032500	-1.81012900	-0.61309900
N	0.46701100	-3.91636700	0.06495600
N	0.57238600	-1.64275400	-0.05529200
H	-1.91821500	-4.75874900	-0.51820900

Int36_1

C	-1.96890800	0.56044500	-0.60601500
C	-1.80074000	-0.67313000	-0.72773600
Ni	0.01452500	0.16224700	-0.44135700
H	0.25678700	0.14487200	-1.85111900
C	1.89082800	-1.01609400	3.29010600
C	1.02108800	-1.27766800	4.34800600
C	1.49573600	-0.17269800	2.23721600
C	-0.25993500	-0.70962800	4.37489300
C	0.21934000	0.41821600	2.28994800
C	-0.65828200	0.14233300	3.34304900
H	1.33837700	-1.93557600	5.15310900
H	-0.93483100	-0.92173200	5.19979300
H	-1.63735900	0.61349000	3.36675900

H	-0.05862700	1.18142800	1.55825600
C	-2.54202800	1.87419800	-0.48470300
C	-1.80274900	3.03791900	-0.77407400
C	-3.88631700	1.99591100	-0.07134600
C	-2.39891400	4.29295400	-0.65673100
H	-0.76924700	2.95241900	-1.09609800
C	-4.47219500	3.25526500	0.04161500
H	-4.45883300	1.10195900	0.15840900
C	-3.73188400	4.40681000	-0.24901600
H	-1.82013500	5.18360400	-0.88511000
H	-5.50813500	3.33783700	0.35917800
H	-4.19199300	5.38692000	-0.15826400
C	-2.04959500	-2.07227600	-0.95842200
C	-1.00586000	-2.98837900	-1.18642300
C	-3.38423600	-2.53081400	-0.96379000
C	-1.29286000	-4.33363800	-1.41505500
H	0.02273900	-2.64144200	-1.18589400
C	-3.66020800	-3.87785500	-1.18989300
H	-4.19329800	-1.82713500	-0.79102800
C	-2.61718200	-4.78307000	-1.41655900
H	-0.47925300	-5.03167200	-1.59160400
H	-4.69125100	-4.22113900	-1.19127900
H	-2.83618700	-5.83264700	-1.59291800
C	2.37670500	0.05980600	1.08435500
C	4.08892000	0.29028300	-0.17439800
C	2.93784500	0.46937600	-0.99102000
C	5.37616900	0.39427900	-0.72489200
C	3.05446800	0.74044600	-2.36097600
C	5.48671100	0.66931700	-2.08571100
H	6.25503500	0.26071600	-0.09927700
C	4.33891400	0.83930200	-2.89358100
H	2.17590100	0.87088600	-2.98780200
H	6.47126600	0.75391300	-2.53927200
H	4.46137300	1.05041000	-3.95315200
N	3.70191700	0.02577600	1.12678200
N	1.83870300	0.32102200	-0.16173600
H	2.87762700	-1.46726200	3.25691700

TS26_1

C	1.83835100	0.43754400	-0.47633700
C	1.24132200	1.47121600	-0.05387600
Ni	-0.09142100	-0.01950900	-0.37887100
H	-0.38172800	1.38550300	-0.60499700
C	-1.40630800	-3.23384800	2.00436300
C	-0.33221000	-3.94800700	2.53338600
C	-1.22829400	-2.43232700	0.86520800
C	0.93900500	-3.87284100	1.94513400
C	0.04601700	-2.39039500	0.25952900
C	1.12705600	-3.09450900	0.80281600
H	-0.48094300	-4.56105000	3.41867600
H	1.77051900	-4.42944900	2.36847500
H	2.09706000	-3.05569700	0.31643700
H	0.15234800	-1.97076500	-0.75529600
C	2.96795500	-0.39410300	-0.81862400
C	2.95218900	-1.20312700	-1.97164000
C	4.11346800	-0.39619100	0.00424600
C	4.05927300	-1.98669600	-2.29749600
H	2.07534600	-1.20440800	-2.61305900
C	5.21384600	-1.18671600	-0.32600900
H	4.12833900	0.21544700	0.90158000
C	5.19166600	-1.98314900	-1.47634400
H	4.03660300	-2.60145700	-3.19320000
H	6.08991600	-1.18132700	0.31705500
H	6.05127900	-2.59716700	-1.73071000
C	1.22710800	2.83171600	0.45025900
C	0.04929400	3.47337500	0.86833700
C	2.45422800	3.52168500	0.53618400
C	0.09541400	4.77953100	1.35706300
H	-0.89849000	2.94513200	0.81648800
C	2.49198100	4.82614200	1.02441600
H	3.36825500	3.03319800	0.21118100
C	1.31387300	5.45982900	1.43711800
H	-0.82285700	5.26365400	1.67780700
H	3.44245800	5.34994000	1.08100300
H	1.34697400	6.47685700	1.81817600
C	-2.29132000	-1.58128400	0.33107500
C	-4.15015000	-0.68630400	-0.19943700
C	-3.11090500	0.13763100	-0.72460800
C	-5.49718400	-0.34481700	-0.40519800
C	-3.40038300	1.30522000	-1.44539900
C	-5.77776900	0.81474300	-1.12318100
H	-6.29142600	-0.97327000	-0.01033300
C	-4.74165400	1.63062000	-1.63618600
H	-2.60706100	1.93132800	-1.84697100
H	-6.81205700	1.10307900	-1.29483100
H	-4.99925500	2.52853900	-2.19274900
N	-3.60043400	-1.76370100	0.46928600
N	-1.91896900	-0.46085600	-0.37469800
H	-2.38486300	-3.26955400	2.47275200

Int37_1

C	-1.75517600	0.23287700	0.69660900
C	-1.04878200	1.38970300	1.05859700
Ni	-0.08325700	-0.33561900	0.73359200
H	-0.82162500	1.50458600	2.12517300
C	1.46985200	-3.85106400	-1.03687200
C	0.54780700	-4.89544900	-1.07603300
C	1.35284500	-2.83368600	-0.07303600
C	-0.51157900	-4.94907000	-0.15795100
C	0.30129100	-2.91065100	0.86423600
C	-0.63012000	-3.95579000	0.81497800
H	0.64904100	-5.67246400	-1.82962900
H	-1.22454900	-5.76859400	-0.19333300
H	-1.42267000	-4.00599200	1.55731200
H	0.28279100	-2.22898800	1.72076700
C	-3.07876900	-0.07195000	0.25471600
C	-4.11550000	0.89214700	0.34872300
C	-3.38619300	-1.35507700	-0.26230300
C	-5.40704200	0.58046200	-0.06099300
H	-3.88540800	1.87682300	0.74413300
C	-4.67830200	-1.65799200	-0.67656800
H	-2.59555400	-2.09612300	-0.33066300
C	-5.68951400	-0.69259900	-0.57523500
H	-6.19571100	1.32368300	0.01545000
H	-4.90441300	-2.64249300	-1.07627000
H	-6.69956300	-0.93270000	-0.89667800
C	-0.89660500	2.62834600	0.26590000
C	-0.58713000	3.83208300	0.92607000
C	-1.06314300	2.65232400	-1.13217900
C	-0.46417000	5.02706500	0.21486800
H	-0.44654300	3.82878500	2.00496300
C	-0.94186200	3.84619200	-1.84085700
H	-1.26870700	1.72746300	-1.66460800
C	-0.64305500	5.03931200	-1.17142800
H	-0.22508800	5.94642300	0.74323600
H	-1.06718400	3.84491400	-2.92051900
H	-0.54063600	5.96701700	-1.72802500
C	2.26525600	-1.68415600	-0.05863600
C	3.93815500	-0.38949000	-0.31317100
C	2.88246400	0.37144700	0.27121500
C	5.17770900	0.20898000	-0.58905500
C	3.04678500	1.73222400	0.56939700
C	5.33507400	1.56017000	-0.28590400
H	5.98579200	-0.37063900	-1.02835900
C	4.28183100	2.31235400	0.28405500
H	2.23925400	2.31685600	1.00190800
H	6.28414400	2.04954200	-0.49182800
H	4.43990200	3.36577700	0.50299400
N	3.51295800	-1.68893600	-0.51851000
N	1.80894300	-0.48106400	0.43334700
H	2.28186000	-3.79882000	-1.75531300

TS27_1

C	-1.40954900	-0.13602200	0.02948100
C	-1.67630600	0.97485300	0.76783500
Ni	0.48191900	-0.04222600	-0.33067800
H	-0.87070500	1.32487500	1.41872100
C	2.86145400	-2.82444700	1.53559200

C	2.13515200	-3.99372200	1.77065500
C	2.24550100	-1.70170500	0.96805000
C	0.78836500	-4.06857600	1.40838900
C	0.85764300	-1.75642600	0.66114800
C	0.15331500	-2.95371200	0.84656900
H	2.62937300	-4.85525800	2.21196400
H	0.22421300	-4.98388000	1.56569800
H	-0.89932000	-3.01779800	0.58680300
H	-0.27956200	-0.91157100	0.73172500
C	-2.33431600	-1.01926200	-0.70304800
C	-3.45491300	-1.57807300	-0.05468800
C	-2.08805100	-1.37561300	-2.04297400
C	-4.30676100	-2.45165700	-0.73069700
H	-3.64959000	-1.32371400	0.98373500
C	-2.94541000	-2.24354500	-2.72072700
H	-1.22336700	-0.96047100	-2.55483500
C	-4.05686000	-2.78541100	-2.06671800
H	-5.16475500	-2.87412200	-0.21414800
H	-2.74368800	-2.49943600	-3.75750400
H	-4.72149200	-3.46561300	-2.59263500
C	-2.87188200	1.83102700	0.82243500
C	-2.97332400	2.74927900	1.88728400
C	-3.89534900	1.81514100	-0.14696000
C	-4.07294300	3.59987900	2.00138200
H	-2.18218900	2.78849400	2.63270900
C	-4.98783800	2.67351500	-0.03758100
H	-3.82972900	1.13976700	-0.99264700
C	-5.08581800	3.56381600	1.03865600
H	-4.13475800	4.29384800	2.83534700
H	-5.76449900	2.65185300	-0.79755500
H	-5.94085700	4.22968400	1.11969700
C	3.00497600	-0.53878700	0.51643200
C	4.48869400	0.90497500	0.02747600
C	3.28561300	1.27083000	-0.65420400
C	5.64514400	1.69066300	-0.10981300
C	3.22916900	2.40977900	-1.47186700
C	5.58118300	2.81949500	-0.92290100
H	6.56088100	1.41708600	0.40831100
C	4.38792300	3.17396600	-1.59576800
H	2.31618700	2.68893900	-1.99327300
H	6.46309500	3.44345900	-1.04608400
H	4.37644700	4.06255900	-2.22249000
N	4.28020900	-0.24714300	0.75978100
N	2.34639400	0.31975400	-0.32456200
H	3.92551000	-2.77618800	1.74828200

Int38_1

C	-1.72698800	-1.63885000	-0.32256300
C	-1.68951100	-1.35545200	1.04044700
Ni	0.03857300	-0.57599700	0.15692900
H	-1.36278800	-2.17336200	1.67865600
C	3.65458900	-2.52386200	0.10963700
C	3.37463700	-3.87348600	0.34383200
C	2.60794000	-1.59665300	0.06404300
C	2.05628200	-4.29283600	0.53612500
C	1.27394100	-2.02283600	0.24808800
C	0.99919600	-3.36579000	0.48883100
H	4.18553900	-4.59632000	0.38011500
H	1.83696800	-5.34143100	0.72304900
H	-0.01264900	-3.72949100	0.64574100
H	-1.37338200	-2.62944700	-0.59882800
C	-2.41606400	-0.92835200	-1.43270700
C	-3.73650400	-0.46060100	-1.30263200
C	-1.78167600	-0.81942000	-2.68479800
C	-4.39389000	0.11987600	-2.38833400
H	-4.25385000	-0.56774200	-0.35362100
C	-2.43513700	-0.22467000	-3.76518300
H	-0.76837300	-1.19428300	-2.80473600
C	-3.74275900	0.24867100	-3.61981600
H	-5.41711200	0.46773400	-2.27319800
H	-1.92412700	-0.13576300	-4.71994200
H	-4.25449100	0.70621200	-4.46224500
C	-2.10688300	-0.16023600	1.80190900
C	-2.11155100	-0.26673300	3.21019500
C	-2.42179700	1.09327400	1.23104900
C	-2.43605400	0.82205200	4.01495800
H	-1.85489000	-1.21790500	3.67020100
C	-2.72807400	2.18725200	2.04198600
H	-2.44103200	1.21949400	0.15451200
C	-2.74354000	2.05697400	3.43301200
H	-2.43993400	0.71118400	5.09578700
H	-2.96079800	3.14344400	1.58139700
H	-2.98885500	2.91044800	4.05895600
C	2.74301100	-0.16072200	-0.14419400
C	3.30019100	1.86978900	-0.44935600
C	1.87742600	1.83558800	-0.31072100
C	3.95798100	3.09030300	-0.66119900
C	1.11012200	3.00565000	-0.38355600
C	3.18940900	4.25174500	-0.73163100
H	5.03970600	3.11999100	-0.76566200
C	1.78426400	4.20915600	-0.59437100
H	0.02815500	2.98389400	-0.27732000
H	3.67751200	5.20957800	-0.89448600
H	1.21617100	5.13450500	-0.65400300
N	3.81836300	0.58902500	-0.33871000
N	1.54757200	0.50918600	-0.11605500
H	4.67527300	-2.17929100	-0.03332900

13a

Rh	0.01266200	0.21776000	-0.09141600
C	1.30883800	-1.08907700	1.09896900
C	0.94357200	-1.77559000	2.37661400
C	1.19252100	-1.64935100	-0.21789100
C	0.66063700	-3.00970200	-0.54005800
C	1.68072300	-0.67838000	-1.16123100
C	1.79005700	-0.85331900	-2.64420300
C	2.18798400	0.46292900	-0.40447800
C	2.83054500	1.67252100	-1.00797700
C	1.95704400	0.21294500	0.97744100
C	2.31412200	1.09863000	2.13036900
C	-1.38153000	2.35264700	0.07293300
O	-0.75385000	2.07435100	-0.99876100
O	-1.20328500	1.62222700	1.09937200
C	-2.35547700	3.50009400	0.10869400
H	-0.01672100	-2.28538800	2.27295700
H	0.85973900	-1.06289000	3.20164000
H	1.71217400	-2.51294100	2.64763500
H	-0.16361500	-3.27397100	0.12491400
H	1.45965100	-3.75499800	-0.42249400
H	0.30091500	-3.06859900	-1.57056900
H	1.70410900	0.10305900	-3.16796800
H	1.00984400	-1.51512800	-3.02974200
H	2.76253100	-1.29143100	-2.90883900
H	2.34113000	1.96152500	-1.94237900
H	3.88556000	1.46730800	-1.23497900
H	2.79363300	2.53037800	-0.33183700
H	3.22630400	0.73260200	2.62047700
H	1.51943000	1.11376600	2.88194000
H	2.49597100	2.12812900	1.81184500
H	-3.33993600	3.13632400	-0.21059100
H	-2.44944600	3.89744300	1.12249400
H	-2.04593900	4.29026800	-0.58043200
O	-2.05000200	-1.95882300	1.01838200
O	-1.83358600	-0.50817900	-0.71002800
C	-2.46878400	-1.39369500	0.00459400
C	-3.86803300	-1.68464100	-0.53386100
H	-3.84196500	-1.86188200	-1.61412200
H	-4.29770700	-2.55082200	-0.02506100
H	-4.51296900	-0.81462600	-0.36238400

10a

C	1.38917500	0.74837200	-0.00009100
C	2.31456400	-0.28480500	-0.01980000
C	1.90314400	-1.63465800	-0.02660400
C	0.56828800	-1.96771200	0.00461300
C	-2.75572500	-0.25113600	0.01889600
C	-2.35906100	1.10526800	-0.03225600
C	-1.02091400	1.43661300	-0.04640500

C	-0.01460600	0.43433900	-0.00634400
C	-0.41628200	-0.94308200	0.01599200
C	-1.80503900	-1.24686000	0.03743500
H	3.37619500	-0.04701500	-0.02027300
H	2.66076200	-2.41433500	-0.03970900
H	0.25078300	-3.00709900	0.01532600
H	-3.81258700	-0.50468000	0.03341300
H	-3.11237500	1.88776800	-0.06873900
H	-0.73658000	2.48253400	-0.11672400
H	-2.10526500	-2.29196000	0.06259900
N	1.80310500	2.08469300	-0.03469300
H	2.78824600	2.20617300	0.17445500
H	1.24781900	2.71773000	0.52988500

Int1_2

Rh	-1.05718600	-0.03385900	-0.04752000
C	-2.58921000	-1.05317700	-1.32400200
C	-2.46885400	-1.34538100	-2.78928000
C	-2.17839200	-1.94669100	-0.24570300
C	-1.65441200	-3.34118900	-0.41205800
C	-2.55947600	-1.33494400	0.99462100
C	-2.40574900	-1.93311600	2.35674800
C	-3.12982200	-0.04606900	0.70872100
C	-3.71897400	0.89756100	1.70923500
C	-3.17304800	0.10485900	-0.73904700
C	-3.75163200	1.28513000	-1.45505700
C	-0.32923000	2.77997700	-1.05143300
O	-0.81181600	2.08851900	-0.08148200
O	0.19712700	2.33205500	-2.09395100
C	-0.38447800	4.28824600	-0.83465500
H	-1.61635000	-1.99657600	-3.00856100
H	-2.35815900	-0.43155900	-3.38005300
H	-3.36591600	-1.86667800	-3.15019200
H	-1.15323500	-3.47500600	-1.37497600
H	-2.47880900	-4.06717400	-0.37419300
H	-0.94499000	-3.60539900	0.37720100
H	-2.14125100	-1.16689000	3.08781100
H	-1.63286600	-2.70636200	2.37246500
H	-3.35212700	-2.40030800	2.66397100
H	-3.07175300	0.97293400	2.58551600
H	-4.71372200	0.55176900	2.02498400
H	-3.83372700	1.89996700	1.28794800
H	-4.84878200	1.25191500	-1.41777600
H	-3.45263600	1.31184800	-2.50606900
H	-3.43052500	2.22017400	-0.98748700
H	0.44539000	4.58235400	-0.17995000
H	-0.27765300	4.81483000	-1.78635800
H	-1.31299700	4.58487800	-0.33884400
O	-0.78911000	0.80025100	3.09784700
O	0.44119200	-0.04919400	1.39055800
C	0.27132100	0.42434000	2.59230100
C	1.57969000	0.49170900	3.37830900
H	2.13894000	-0.44507100	3.28764800
H	2.21164200	1.28629100	2.96490500
H	1.37833100	0.70565300	4.43098000
C	1.90309900	-0.93345200	-1.04922800
C	1.98549800	-2.31245000	-1.09749200
C	3.15416600	-2.99263300	-0.69557100
C	4.24409000	-2.28719200	-0.24242800
C	5.30849600	1.25032900	0.29203600
C	4.15135300	1.94474200	-0.13218200
C	3.03895500	1.25776800	-0.56744900
C	3.02547400	-0.16338300	-0.60328500
C	4.20735400	-0.86884400	-0.18902400
C	5.33271400	-0.12439200	0.25900000
H	1.12941400	-2.88402700	-1.44610700
H	3.18226700	-4.07772300	-0.74718500
H	5.14769400	-2.80183000	0.07409200
H	6.17715100	1.80548400	0.63622900
H	4.13947400	3.03128500	-0.11723200
H	2.17349000	1.81686500	-0.90251300
H	6.22002900	-0.66864700	0.57394500
N	0.67863300	-0.31083400	-1.45626300
H	0.74445300	0.67290400	-1.77717600
H	0.26740400	-0.83992900	-2.22303200

AcOH

O	0.64390200	1.20230300	0.00001200
C	0.09134900	0.12338200	0.00002000
C	-1.39576500	-0.11104800	0.00002200
H	-1.91892400	0.84584600	-0.00051600
H	-1.68510700	-0.69205100	-0.88241800
H	-1.68545300	-0.69152400	0.88264000
O	0.77974000	-1.04386900	0.00001400
H	1.72684400	-0.80375000	-0.00016700

Int2_2

Rh	1.02657600	0.22257600	-0.00226100
C	2.28675700	-1.13785300	-1.26117400
C	1.82132100	-1.69232500	-2.57195700
C	2.94321200	0.11947700	-1.04789100
C	3.39581300	1.08040900	-2.10526600
C	3.25881600	0.23464700	0.38014900
C	4.03428600	1.36181400	0.98900300
C	2.71545900	-0.89406900	1.03382700
C	2.77175600	-1.22146800	2.49387100
C	2.05030100	-1.72338400	0.02919800
C	1.44036800	-3.06672200	0.28947300
H	-5.67409900	1.28624900	-0.43371200
H	-4.97672300	-3.02721800	1.48206300
H	-2.59003200	-3.57923500	1.00429300
H	-1.16073200	-1.95121500	-0.19094200
H	2.37592700	-1.25636800	-3.40798100
H	0.75290500	-1.47722700	-2.71682200
H	1.96026400	-2.77800800	-2.60771500
H	2.80293900	0.98184100	-3.01878500
H	4.44784000	0.90136500	-2.36813600
H	3.31577000	2.11742700	-1.76400500
H	3.90994600	1.40057600	2.07439800
H	3.71897800	2.32802700	0.58270000
H	5.10692600	1.25101300	0.77832300
H	3.04785200	-0.35281800	3.09728200
H	3.51343900	-2.00986700	2.68225100
H	1.80622800	-1.58794000	2.85730800
H	2.22326100	-3.83572500	0.35909800
H	0.75897300	-3.36008400	-0.51338200
H	0.88260700	-3.08142200	1.23078400
H	-5.91825100	-0.86797200	0.72796700
N	-0.54816800	0.18004700	-1.41663000
H	-0.21558300	0.91457100	-2.04579800
O	-0.37277600	0.67651700	1.64562300
O	0.44360700	2.30365200	0.42522100
C	-0.32485300	1.91582000	1.36512300
C	-1.18783900	2.89915000	2.10888600
H	-0.79963300	3.91514100	2.00370400
H	-2.20159500	2.86481300	1.69313000
H	-1.24977000	2.62707300	3.16649600
C	-1.86804300	0.49095700	-1.11078000
C	-2.46565500	1.68089700	-1.53823800
C	-3.82814000	1.95875900	-1.30929000
C	-4.62567800	1.06877900	-0.62259500
C	-4.35058100	-2.31205400	0.95405700
C	-2.99689300	-2.62205400	0.68672700
C	-2.19651300	-1.71688000	0.02142600
C	-2.69880000	-0.46404200	-0.40827300
C	-4.07769200	-0.15867400	-0.15975000
C	-4.87483500	-1.10929900	0.53589600
H	-1.85414100	2.41159000	-2.06419300
H	-4.24406600	2.89649100	-1.67146000

TS1_2

Rh	0.69583800	0.05479200	-0.15717100
C	1.55389700	-1.89022000	-0.86566200
C	1.20851600	-2.56264500	-2.15916300
C	2.62555800	-0.96864400	-0.65282700
C	3.62461600	-0.48929800	-1.66072900
C	2.66875300	-0.65367700	0.77246200
C	3.69134800	0.23987100	1.40549400

C	1.61439700	-1.34773800	1.41153200
C	1.34440400	-1.41062000	2.88436600
C	0.86916000	-2.07959800	0.39158900
C	-0.22748700	-3.06605500	0.65944800
H	-5.58873300	-0.67045300	-0.25169900
H	-3.03904700	0.26368200	3.74821800
H	-0.77136600	0.86206400	2.94677100
H	-0.62353900	1.70672700	0.58677300
H	1.53043600	-1.97359700	-3.02305900
H	0.13441800	-2.74444500	-2.25176100
H	1.71396300	-3.53649600	-2.22164000
H	3.24100300	-0.57128200	-2.68169300
H	4.55077600	-1.07863600	-1.60469800
H	3.88846900	0.55832000	-1.48773200
H	3.43259800	0.48418800	2.43942600
H	3.78718900	1.17955700	0.85143900
H	4.67818000	-0.24256900	1.41373700
H	1.66268800	-0.49936400	3.39861000
H	1.89416300	-2.25084100	3.33155300
H	0.28370100	-1.56473400	3.09467800
H	0.19204000	-4.04097400	0.94643900
H	-0.85433900	-3.22318300	-0.22264200
H	-0.87883900	-2.73446100	1.47257800
H	-4.83206700	-0.29213300	2.14800100
N	-0.60488600	0.38076800	-1.73558800
H	-0.31430500	0.04086900	-2.64967000
O	-0.32275600	2.99927800	0.42129600
O	1.46914300	2.05483000	-0.54002300
C	0.78616900	3.06228700	-0.19300400
C	1.31184800	4.43761500	-0.54820900
H	2.37484200	4.39952800	-0.79559300
H	0.75996100	4.80875400	-1.42024400
H	1.13833800	5.13517800	0.27593900
C	-1.91540200	0.10885000	-1.44565000
C	-2.91614900	-0.24170700	-2.35991700
C	-4.22974900	-0.49709600	-1.91433400
C	-4.57765800	-0.44015400	-0.57742600
C	-2.82373300	0.23955500	2.68220700
C	-1.52463800	0.55390300	2.22483100
C	-1.22521100	0.55629100	0.86180400
C	-2.26565600	0.20039200	-0.05531700
C	-3.58749300	-0.09816500	0.38531100
C	-3.83029200	-0.06878200	1.78621500
H	-2.67720900	-0.32092300	-3.41850400
H	-4.98412100	-0.76484800	-2.65174000

Int3_2

Rh	0.66489200	0.01404300	-0.12229900
C	2.35590900	-1.18098400	-1.13652900
C	2.40437700	-1.51504300	-2.59736200
C	2.99941800	-0.11995000	-0.47908600
C	3.86164200	0.94724700	-1.08287200
C	2.70078400	-0.21534400	0.95475400
C	3.28390500	0.69433000	1.99464300
C	1.90727500	-1.36741000	1.16925100
C	1.53620700	-1.97811500	2.48628800
C	1.58035500	-1.92417200	-0.13719800
C	0.88815000	-3.23267300	-0.38033100
H	-5.60609900	-1.01651700	-0.20777700
H	-2.89129500	-0.44528100	3.78113200
H	-0.59722900	-0.06088700	2.95197200
H	-1.44035400	1.86304000	0.58555900
H	2.67674000	-0.64753000	-3.20603000
H	1.43950000	-1.88692000	-2.95604000
H	3.14534100	-2.30289200	-2.79251000
H	3.84752800	0.91042100	-2.17577000
H	4.90647000	0.83817700	-0.76112000
H	3.52957200	1.94577100	-0.77790300
H	2.74025800	0.63096500	2.94174100
H	3.26467800	1.73909600	1.66805600
H	4.33314400	0.43616900	2.19841700
H	1.54520000	-1.24360700	3.29638400
H	2.25803500	-2.76449600	2.74926900
H	0.54419200	-2.43559300	2.45895400
H	1.60862700	-4.06356500	-0.37153300
H	0.38094900	-3.24389800	-1.34955300
H	0.13614500	-3.43538300	0.38711200
H	-4.76831100	-0.82876300	2.22732200
N	-0.65511400	0.12973000	-1.68937600
H	-0.33828300	-0.07241900	-2.63500100
O	-1.42476200	2.83957300	0.42636400
O	0.70925900	2.38341500	-0.13511500
C	-0.21656100	3.18108600	0.00189100
C	-0.08922400	4.64865700	-0.29837100
H	0.94393800	4.89379100	-0.54700700
H	-0.73910900	4.90183500	-1.14394300
H	-0.42155900	5.24147600	0.55982300
C	-1.94084600	-0.25446700	-1.42505500
C	-2.96777800	-0.49398200	-2.34450600
C	-4.27314700	-0.76615400	-1.88089000
C	-4.58879700	-0.81446800	-0.53397700
C	-2.71453300	-0.43095000	2.70722400
C	-1.39662100	-0.20505000	2.22868700
C	-1.13738300	-0.18076000	0.86321400
C	-2.23955400	-0.35725800	-0.02585800
C	-3.56528300	-0.60897300	0.43349300
C	-3.76850100	-0.64248100	1.84043600
H	-2.76955900	-0.44010800	-3.41315800
H	-5.05759900	-0.93535200	-2.61637600

TS2_2

Rh	0.91312700	0.02673100	-0.17462000
C	1.72220600	-1.99362400	-0.89204400
C	1.43741200	-2.63224100	-2.21816500
C	2.83385600	-1.19044200	-0.55521700
C	3.96382000	-0.77248100	-1.44574100
C	2.73060300	-0.83858200	0.86549400
C	3.76150700	-0.05288400	1.61852700
C	1.56963900	-1.46179500	1.39281300
C	1.14365700	-1.50518000	2.82929000
C	0.87270600	-2.10203400	0.28970200
C	-0.33466300	-2.98356700	0.41735000
H	-3.48506700	0.48030100	2.94110500
H	-6.80238700	-0.63641300	-0.30601800
H	-5.61503200	-0.65607900	-2.49808500
H	-0.20770400	2.14649200	0.60823800
H	1.94948800	-2.11720400	-3.03588800
H	0.36639900	-2.63758300	-2.44453800
H	1.77427900	-3.67858400	-2.22164700
H	3.71955200	-0.90957700	-2.50294200
H	4.86939100	-1.35831500	-1.23405500
H	4.21513300	0.28288700	-1.29742400
H	3.37060400	0.31583200	2.57114400
H	4.10104900	0.81297200	1.04094500
H	4.64552300	-0.66868600	1.83677600
H	1.53647200	-0.65656900	3.39675200
H	1.51651100	-2.42275100	3.30617200
H	0.05527200	-1.50206700	2.92862500
H	-0.04530600	-4.00736700	0.69570600
H	-0.89058400	-3.04656400	-0.52288800
H	-1.02291700	-2.61418200	1.18274300
H	-5.57993600	-0.09519600	1.76896700
N	-0.69754600	0.44262900	-1.50106600
H	-0.97671300	-0.18554100	-2.25513100
O	0.25215200	3.18255100	0.45152800
O	1.77083100	1.98243200	-0.69492900
C	1.29610000	3.07002100	-0.29876300
C	1.95227700	4.36849600	-0.70234200
H	2.88554300	4.18232000	-1.23621000
H	1.26948700	4.93137100	-1.34875700
H	2.14268900	4.98177300	0.18429600
C	-1.58804100	0.50841900	-0.46849400
C	-0.89795400	0.83512700	0.72171700
C	-1.59087300	0.73920000	1.95902000
C	-2.94294400	0.47242700	1.99769100
C	-5.73978500	-0.40957100	-0.34594300
C	-5.06773700	-0.42546600	-1.58791300
C	-3.71815600	-0.13238900	-1.64193200

C	-2.99599600	0.18754300	-0.46911200
C	-3.66989200	0.19432800	0.79647700
C	-5.05674500	-0.10570300	0.81518000
H	-3.20676000	-0.11889200	-2.60165600
H	-1.06276500	0.93884700	2.89079500

Int4_2

Rh	0.91866200	0.04320700	-0.13577200
C	2.13197500	-1.70063200	-1.04607400
C	1.98484700	-2.22666200	-2.44247800
C	3.08099000	-0.77252700	-0.58029400
C	4.13975500	-0.06858900	-1.37404100
C	2.88263600	-0.59421400	0.86198100
C	3.75606900	0.24850000	1.74327900
C	1.83396200	-1.45396700	1.27540000
C	1.40209900	-1.73057700	2.68422100
C	1.27866200	-2.07582900	0.08321900
C	0.25850000	-3.17536300	0.06910400
H	-3.55025200	0.07280800	2.97559000
H	-6.89836900	-0.71791500	-0.33457600
H	-5.70176400	-0.67369900	-2.52218100
H	-0.58670700	2.14494600	0.68662400
H	2.39555400	-1.53568100	-3.18421400
H	0.93560800	-2.40437300	-2.69799600
H	2.51054100	-3.18570300	-2.55368400
H	4.01770000	-0.23256000	-2.44823300
H	5.14149400	-0.42330700	-1.09484900
H	4.11736000	1.01270900	-1.19732200
H	3.23995200	0.53740400	2.66379700
H	4.07171400	1.16595700	1.23640100
H	4.66787300	-0.29417400	2.03149700
H	1.60665500	-0.88421600	3.34645800
H	1.94642900	-2.59862500	3.08288400
H	0.33463900	-1.95675500	2.74515400
H	0.73653100	-4.15285400	0.22869000
H	-0.27072600	-3.22315900	-0.88735700
H	-0.49098200	-3.03952000	0.85394700
H	-5.66623500	-0.34430000	1.76984400
N	-0.72743700	0.27307700	-1.45157400
H	-0.89188400	-0.39087000	-2.20981400
O	-0.36536100	3.12053800	0.51660100
O	1.42063100	2.19547500	-0.49409800
C	0.74776700	3.18415100	-0.17915600
C	1.14735000	4.57871700	-0.57217600
H	2.14831700	4.57883100	-1.00531300
H	0.43274000	4.96165500	-1.31006600
H	1.11039000	5.24313400	0.29677900
C	-1.64534100	0.18518000	-0.41549900
C	-0.94885500	0.35328200	0.78585400
C	-1.63095400	0.27303300	2.01644700
C	-3.00756800	0.09071100	2.03258600
C	-5.82650600	-0.53641700	-0.35759200
C	-5.14727200	-0.51513000	-1.60069200
C	-3.78906900	-0.28071600	-1.63826700
C	-3.05478400	-0.06124000	-0.44508700
C	-3.73550000	-0.09137400	0.82318400
C	-5.13911800	-0.32632200	0.81799800
H	-3.26890100	-0.24064400	-2.59269400
H	-1.09542200	0.37285900	2.95986400

TS3_2

Rh	0.82934200	-0.26813000	0.01456500
C	1.03037900	-2.48401000	0.12224600
C	0.75828900	-3.38741400	1.28726200
C	0.12831000	-2.17555500	-0.95197600
C	-1.27668500	-2.67333400	-1.08601000
C	0.83126400	-1.35591500	-1.90195500
C	0.30309000	-0.84390700	-3.20733900
C	2.22185000	-1.26345700	-1.46670900
C	3.32850300	-0.58547500	-2.21564500
C	2.33717200	-1.94573300	-0.22975200
C	3.56997400	-2.09017800	0.60619900
C	1.20026200	1.43184900	2.44732800
O	1.57226700	0.33451900	1.94468600
O	0.17674200	2.08582900	2.04887800
C	2.01878200	2.01935800	3.57105300
H	-0.29943300	-3.38368700	1.56425300
H	1.33848500	-3.09250500	2.16730200
H	1.03347600	-4.42417300	1.04571500
H	-1.76089800	-2.79182400	-0.11391600
H	-1.27208900	-3.65547400	-1.57961300
H	-1.89260200	-2.00316200	-1.69000700
H	0.68905500	0.15632900	-3.42381500
H	-0.78801600	-0.78304200	-3.20505200
H	0.60140000	-1.50353800	-4.03434600
H	2.93638800	0.12837200	-2.94444800
H	3.92618200	-1.32518400	-2.76662400
H	3.98826600	-0.03630300	-1.54091000
H	3.93148200	-3.12724900	0.58175700
H	3.36959600	-1.83152700	1.65098300
H	4.37406900	-1.44177000	0.25041400
H	2.83993000	2.59479300	3.12758000
H	1.41434300	2.68746700	4.18855700
H	2.45620100	1.22493100	4.18106400
O	3.21926500	1.96220000	-0.04834500
O	1.07744500	1.70432900	-0.74575900
C	2.18633800	2.36841900	-0.58535800
C	2.09990200	3.79133100	-1.14099000
H	1.77720700	3.77865700	-2.18815600
H	1.35130300	4.36149100	-0.57857400
H	3.06846700	4.29150100	-1.06313500
C	-3.93762100	-0.54628900	1.15185600
C	-2.92263700	-0.93568000	2.02387400
C	-1.60094100	-0.52602000	1.81116400
C	-1.20239900	0.28402500	0.74010700
C	-2.96666900	2.01296200	-2.10619500
C	-4.30741100	1.62523200	-1.89473900
C	-4.62268100	0.80072700	-0.83643400
C	-3.61738500	0.31818600	0.04466800
C	-2.25078200	0.71612900	-0.15994100
C	-1.97034100	1.57651600	-1.25758500
H	-3.17053300	-1.56227100	2.87902500
H	-0.84978600	-0.84645300	2.53051300
H	-0.43961700	1.30871500	1.29479400
H	-2.72102200	2.67280300	-2.93487600
H	-5.09179800	1.98900900	-2.55330500
H	-5.66514400	0.54861900	-0.66291800
H	-0.94149700	1.89182900	-1.39616200
N	-5.24416100	-0.93229800	1.38985600
H	-5.85261700	-1.03241500	0.58838600
H	-5.35921300	-1.68759900	2.05462500

Int5_2

Rh	-0.88275100	0.12950100	-0.10968800
C	-1.91448900	0.97369700	-1.84246800
C	-1.84126200	2.40998700	-2.26284100
C	-1.08151900	-0.09709000	-2.29789500
C	0.03327400	-0.00279900	-3.29418400
C	-1.54763200	-1.29667100	-1.65041800
C	-1.06193100	-2.68952900	-1.90898000
C	-2.81491200	-0.98206400	-0.96655900
C	-3.67347600	-2.00301700	-0.28479700
C	-3.03353900	0.39125000	-1.07719700
C	-4.15626300	1.20122400	-0.50514200
C	-0.71111100	2.20204200	2.34033000
O	-1.10383800	1.98078500	1.18177800
O	-0.23371400	1.28878600	3.14348900
C	-0.73636900	3.59047700	2.91925800
H	-0.84472000	2.67109800	-2.62790100
H	-2.08466300	3.08078200	-1.43266800
H	-2.55534400	2.61393500	-3.07330800
H	0.53690400	0.96598100	-3.25123000
H	-0.36427800	-0.13131700	-4.31079200
H	0.78733300	-0.77679400	-3.13197700
H	-1.13191500	-3.29576700	-1.00359400
H	-0.02347200	-2.69901200	-2.24956500
H	-1.67347700	-3.16100200	-2.69253300
H	-3.06619600	-2.66928900	0.33346300

H	-4.19885300	-2.62001600	-1.02741900
H	-4.43081100	-1.53713100	0.35230000
H	-4.77967400	1.62506100	-1.30391800
H	-3.77528300	2.03954200	0.08895100
H	-4.80306100	0.60007700	0.13936800
H	-1.12573400	3.57204600	3.94132600
H	0.29127400	3.97137600	2.96354700
H	-1.33639700	4.25513900	2.29596400
O	-0.95499400	-2.99742100	1.40432400
O	-0.50800900	-0.82534700	1.79658700
C	-0.65014400	-2.07582600	2.15937900
C	-0.37120300	-2.31871000	3.63716700
H	0.68379600	-2.11107200	3.85251100
H	-0.97156400	-1.64772600	4.26197200
H	-0.59284700	-3.35544700	3.89846500
C	3.86959800	1.39895100	-0.54058000
C	2.82684500	2.30440800	-0.57408800
C	1.48414300	1.88578900	-0.41473300
C	1.13323800	0.55860300	-0.24582700
C	2.97333700	-2.72226000	0.01880200
C	4.31759100	-2.29714700	-0.06336800
C	4.60210200	-0.95958600	-0.23024200
C	3.56907100	0.01235100	-0.32955800
C	2.19319400	-0.40860800	-0.20623100
C	1.94896800	-1.80208800	-0.04376400
H	3.04026200	3.36106400	-0.73134100
H	0.71605300	2.65437600	-0.43728900
H	-0.27376000	0.36562000	2.67539500
H	2.74409500	-3.77724900	0.14843300
H	5.12495600	-3.02113300	0.01468000
H	5.63879200	-0.63631000	-0.25662000
H	0.92336200	-2.13527300	0.05028500
N	5.20964500	1.82058100	-0.65106500
H	5.77639800	1.22971600	-1.25155400
H	5.28445900	2.78240100	-0.96733500

TS4_2

Rh	-0.51641400	-0.26546200	-0.06027000
C	-2.10377100	-0.92245500	1.34244500
C	-2.84772400	-0.01089500	2.27264200
C	-2.52604100	-1.35134000	0.03693100
C	-3.77641100	-0.91052300	-0.66600200
C	-1.56904700	-2.30058000	-0.44603600
C	-1.65849100	-3.07956600	-1.72684700
C	-0.59930800	-2.53860400	0.61042100
C	0.51173500	-3.54188300	0.54143300
C	-0.92662000	-1.70406300	1.70612500
C	-0.22906100	-1.60840400	3.02759800
H	5.71221900	0.87365100	0.58588200
H	3.75891600	-2.25288900	-2.55501700
H	1.34411200	-1.70979600	-2.56939400
C	1.99426800	-1.21957400	-1.84809000
H	-3.46625800	0.70658000	1.72524800
H	-2.15779100	0.55544900	2.90633700
H	-3.51192100	-0.58145000	2.93797800
H	-3.98598400	0.14994500	-0.49842000
H	-4.64173800	-1.48119200	-0.30090500
H	-3.71648000	-1.07295300	-1.74645400
H	-0.67196100	-3.40275300	-2.07224800
H	-2.11935200	-2.49659700	-2.53062300
H	-2.26636600	-3.98611200	-1.59356600
H	1.00585300	-3.52984000	-0.43478200
H	0.12763600	-4.55875200	0.70320700
H	1.27760400	-3.35165500	1.29787700
H	-0.85629800	-2.01865900	3.83069300
H	-0.00466300	-0.56491500	3.27413200
H	0.71601000	-2.15813600	3.02840400
H	5.32887300	-0.97659600	-1.13941900
N	0.46237400	1.15073400	1.10457500
H	-0.00294600	2.01229300	1.37818100
C	1.48230100	-0.26694500	-0.97360500
H	0.98291800	1.70966700	-1.91125800
C	2.37514300	0.39227700	-0.07350000
C	3.78628800	0.19689300	-0.16216600
C	4.25892400	-0.79211700	-1.07129800
H	2.28141100	2.84026700	2.31499900
H	4.72680600	2.60149100	2.06156300
C	1.80849500	1.27344800	0.90425000
C	2.68191900	2.11677000	1.60848100
C	4.07377200	1.96143600	1.47123300
C	4.63445500	1.00251500	0.64250400
C	3.38046300	-1.50008100	-1.86704200
C	-1.05857000	1.20570500	-1.48646500
H	-1.89496900	0.77597300	-2.03313900
C	0.27788100	0.88417700	-1.95665700
H	0.31274300	0.33490500	-2.89187800
C	-1.34710600	2.55320300	-0.95154900
O	-0.54143300	3.42683000	-0.68221100
O	-2.69074600	2.73225200	-0.80315300
C	-3.09026000	4.02298900	-0.31914800
H	-2.68967600	4.20877600	0.68196200
H	-4.18116100	4.00196500	-0.28877600
H	-2.74752900	4.81501700	-0.99148800

TS5_2

Rh	-0.34051700	0.16223300	-0.18325100
C	-0.11176700	2.42829800	-0.09590400
C	1.01593100	3.20338000	-0.70868600
C	-1.34324500	2.05085000	-0.78287700
C	-1.70082100	2.42998500	-2.18980000
C	-2.21576000	1.45339300	0.18518500
C	-3.65348100	1.08851900	-0.02465800
C	-1.50547400	1.36008100	1.42891900
C	-2.07057800	0.83834900	2.71808000
C	-0.22610800	2.01833200	1.25865100
C	0.77868700	2.25806000	2.34308600
H	5.89718700	-0.84496100	-0.26559000
H	3.07490400	-1.40959500	3.61360400
H	0.75660500	-1.30157000	2.75392500
C	1.58517900	-1.14136800	2.06837200
H	1.17124600	2.92897700	-1.75614400
H	1.95873400	3.03478400	-0.18088100
H	0.80652100	4.28212400	-0.68026100
H	-0.82704600	2.40435400	-2.84896700
H	-2.10606600	3.45133300	-2.22980000
H	-2.45548000	1.75842700	-2.61012300
H	-3.96544200	0.29066000	0.65343700
H	-3.85511700	0.76892600	-1.05068000
H	-4.29077600	1.96059500	0.18021100
H	-2.63439400	-0.08569200	2.55779200
H	-2.74649700	1.57119700	3.18145900
H	-1.27950700	0.62410100	3.44295500
H	0.53226100	3.17707200	2.89344500
H	1.78956200	2.37109100	1.94288500
H	0.79955500	1.43844300	3.06606200
H	5.00274000	-1.23808800	2.07986600
N	0.87681700	-0.22646900	-1.83825900
H	0.69851100	0.24650100	-2.71958300
C	1.34841000	-0.92134200	0.71754600
H	0.69052900	-2.74588600	-0.33420800
C	2.46112500	-0.75780700	-0.16652400
C	3.80052000	-0.89125600	0.30753100
C	3.98947800	-1.13496100	1.69792400
H	3.10766800	0.00347400	-3.44793700
H	5.41952100	-0.33150800	-2.64077300
C	2.19379800	-0.39639000	-1.53266600
C	3.28257900	-0.26421500	-2.40797200
C	4.59661300	-0.44873200	-1.93797600
C	4.87276200	-0.74389700	-0.61428100
C	2.91122600	-1.23160700	2.55305400
C	-1.17519500	-1.74615900	-0.68417600
C	-2.53805400	-1.98085300	-0.16753100
C	-0.06119700	-2.13876300	0.16070600
H	-0.34624600	-2.50291100	1.14225300
H	-1.06831700	-1.88705600	-1.75351000
O	-2.86979500	-2.11058600	1.00281900
O	-3.42899600	-2.08129400	-1.18914400
C	-4.77105500	-2.42965900	-0.81865100

H	-5.32389300	-2.50468400	-1.75667000
H	-5.22037400	-1.66485900	-0.17934400
H	-4.79194400	-3.38882400	-0.29283100

TS6_2

Rh	0.97690000	0.18608100	-0.29514200
C	2.97209200	-0.61978800	-0.81268300
C	3.35081100	-1.11220700	-2.17827900
C	3.19826200	0.69086500	-0.27784900
C	3.81931100	1.84987000	-0.99998600
C	2.77171300	0.67984900	1.09041600
C	2.91344500	1.81237100	2.06712600
C	2.40672600	-0.68489800	1.43955200
C	2.00376800	-1.12925200	2.81342000
C	2.52259200	-1.48254700	0.28416200
C	2.26458500	-2.95194600	0.14604200
H	-4.58040300	-2.74710900	0.69247000
H	-2.40911900	0.23909200	3.81986400
H	-0.65998600	1.38378200	2.50087600
C	-1.21599100	0.56728200	2.04674000
H	3.35874800	-0.30282600	-2.91492800
H	2.65494800	-1.87988400	-2.53149200
H	4.35488000	-1.56038300	-2.16976400
H	3.64089200	1.80130600	-2.07825400
H	4.90781000	1.85991300	-0.84717300
H	3.43679800	2.81069500	-0.64059900
H	2.19491800	1.72929300	2.88841000
H	2.76373800	2.78635200	1.58942400
H	3.91736700	1.82346000	2.51625300
H	1.24758600	-0.46673800	3.24775500
H	2.86717300	-1.12936300	3.49311000
H	1.58856900	-2.14038200	2.80683800
H	3.20466000	-3.50891800	0.02851200
H	1.64387100	-3.16119800	-0.73176600
H	1.74508900	-3.35689900	1.01889600
H	-3.91102800	-1.40639700	2.75655900
N	-0.17665900	-0.95108300	-1.58938100
H	-0.00495800	-1.01721000	-2.58796600
C	-0.97498600	0.19315700	0.72683600
C	-2.15954700	1.93589500	-0.80645800
C	-1.77096300	-0.84283500	0.14306700
C	-2.88539700	-1.39416000	0.84537900
C	-3.08253900	-0.98135900	2.19381500
H	-2.09726900	-2.51339200	-2.83072300
H	-4.10638400	-3.34679300	-1.66565400
C	-1.40551100	-1.32578300	-1.16011600
C	-2.31305800	-2.17554200	-1.81950700
C	-3.44580800	-2.65780600	-1.14215900
C	-3.72694100	-2.31922300	0.17323700
C	-2.24532800	-0.05596000	2.78580300
C	0.30166700	1.87062400	-1.31513100
H	1.06058500	2.64634700	-1.22191200
C	-0.73277700	1.85380400	-0.29847400
H	-0.56785100	2.51323800	0.54805200
O	-2.50810300	1.69485400	-1.94240400
O	-2.98877000	2.38780700	0.15223200
C	-4.37182800	2.49765200	-0.22863000
H	-4.89112600	2.86106900	0.65912800
H	-4.76485300	1.52191700	-0.52611500
H	-4.49140100	3.20429400	-1.05480300
H	-0.01796700	1.67101500	-2.33449800

TS7_2

Rh	0.84941500	-0.08905100	-0.39105500
C	2.25162300	-1.54821300	0.75125700
C	2.07430600	-3.03660900	0.79530200
C	2.92090800	-0.82606300	-0.33904100
C	3.64216700	-1.47656200	-1.48321700
C	2.98486900	0.55944300	0.03401100
C	3.71835800	1.64486000	-0.69674900
C	2.25687500	0.71537900	1.25536600
C	2.11616900	1.98870300	2.03812200
C	1.85924000	-0.60680900	1.72241000
C	1.14929600	-0.87238700	3.01528500
H	-4.65095200	-2.99724100	0.72406900
H	-3.11297500	0.97509600	2.99316600
H	-1.20688900	1.79654300	1.64944200
C	-1.69464800	0.87033300	1.36390700
H	1.79642200	-3.43524500	-0.18563300
H	1.29242200	-3.33149800	1.50029800
H	3.00592700	-3.53434100	1.09896500
H	3.11292600	-2.36618900	-1.83964300
H	4.64996700	-1.79828300	-1.18234200
H	3.75397800	-0.79416300	-2.33112600
H	3.24689300	2.62164600	-0.55170300
H	3.77107900	1.45201400	-1.77257000
H	4.75094000	1.72408000	-0.32806900
H	1.91500300	2.84492200	1.38850300
H	3.03410500	2.20316300	2.60458500
H	1.29715500	1.92422600	2.76061800
H	1.81233100	-0.68964100	3.87191000
H	0.80121800	-1.90664500	3.08144000
H	0.27474700	-0.22308600	3.13321800
H	-4.39128700	-1.01645100	2.28532800
N	-0.17089900	-1.44340300	-1.62036400
H	0.31911200	-2.09473300	-2.22535400
C	-1.27757900	0.17095300	0.23601300
H	-1.70803000	0.94133500	-1.80501800
C	-1.94573200	-1.04644800	-0.11481100
C	-3.10529100	-1.47478500	0.59875100
C	-3.51382100	-0.70195000	1.72447600
H	-1.65687200	-3.66812600	-2.30955200
H	-3.75323400	-4.31194500	-1.17467600
C	-1.36437300	-1.87418800	-1.14010100
C	-2.06319400	-3.03218400	-1.52565900
C	-3.24777800	-3.39932000	-0.86409700
C	-3.76491000	-2.66427400	0.19029900
C	-2.80252800	0.41239500	2.11561100
C	0.41713300	1.24285500	-1.91864500
H	1.06775300	2.11296800	-1.85239100
C	-0.87512900	1.34036700	-1.23546300
C	-1.16927800	2.70968800	-0.68073100
O	-0.37812800	3.42407100	-0.09500000
O	-2.43142400	3.07444200	-0.96811500
C	-2.82702100	4.37973000	-0.50855800
H	-3.85175200	4.51391500	-0.85692800
H	-2.17780700	5.15186200	-0.92998300
H	-2.78958800	4.42897000	0.58338400
H	0.40848600	0.75035900	-2.88741900

11a

O	-0.05870500	1.33054100	0.00014300
C	0.04360300	0.11841700	0.00012000
H	3.43138900	-0.56442400	-0.00033700
H	-3.03243900	-0.90589200	-0.00002800
H	-2.43465600	0.52968300	-0.89156000
H	-2.43479200	0.53006900	0.89087800
O	-1.01544800	-0.72136200	0.00009500
C	-2.30682600	-0.09116500	-0.00019100
C	1.31629500	-0.64500300	0.00012600
H	1.23928200	-1.72836900	0.00023300
C	2.49362600	-0.01622500	-0.00016100
H	2.54425300	1.06935800	-0.00046100

Int6_2

Rh	-0.36939500	-0.25760200	-0.12310200
C	-1.64112400	-0.87554900	1.81028200
C	-1.63796700	-0.06649400	3.06707100
C	-2.59294500	-0.85200600	0.76501800
C	-3.87858200	-0.08268700	0.71307700
C	-2.16625800	-1.81001800	-0.23506800
C	-2.97326400	-2.19123300	-1.43969600
C	-0.97937200	-2.46265500	0.22817800
C	-0.35011300	-3.68245700	-0.37508400
C	-0.60552900	-1.83928300	1.46882900
C	0.50179800	-2.26343800	2.38606200
H	5.81732600	1.16811800	0.15010200
H	3.84524900	-2.43302900	-2.43392500

H	1.41909300	-2.25605200	-2.03641300
C	2.08233800	-1.57058300	-1.51572600
H	-2.45832100	0.65655700	3.09178700
H	-0.69335800	0.48533300	3.15329600
H	-1.73015300	-0.71241000	3.94997200
H	-3.99081400	0.56742500	1.58578100
H	-4.73843800	-0.76630000	0.70297600
H	-3.94510300	0.54554300	-0.18181400
H	-2.35586700	-2.64347400	-2.22133200
H	-3.49419600	-1.32952000	-1.86885000
H	-3.74220500	-2.92729200	-1.16404500
H	-0.46443200	-3.70809600	-1.46329700
H	-0.82901200	-4.58880100	0.02262200
H	0.71622000	-3.74661000	-0.14671600
H	0.13558100	-2.98028400	3.13505100
H	0.91929100	-1.40702300	2.92354400
H	1.31816300	-2.74293000	1.83928800
H	5.44020800	-0.88659800	-1.35571900
N	0.60460800	1.12238400	1.09257700
H	0.12366300	2.01545500	1.19662800
C	1.59088600	-0.61613400	-0.64301600
H	0.20837600	-0.10822900	-2.82142200
C	2.50910700	0.26641900	-0.01194500
C	3.91210200	0.20695500	-0.26723200
C	4.37512600	-0.80835000	-1.14827100
H	2.39323200	3.02685600	2.01209000
H	4.82826100	2.93791400	1.56277000
C	1.95496800	1.26422700	0.84527200
C	2.79763900	2.24052400	1.37864700
C	4.18522800	2.17787200	1.12333500
C	4.74645800	1.18781700	0.33721400
C	3.48049300	-1.66741500	-1.75163300
C	-0.56795600	1.43828400	-1.53545800
C	-1.77998700	2.23174700	-1.22895300
C	-0.64804300	0.24413200	-2.25902900
H	-1.62089700	-0.11329300	-2.58250800
H	0.37297000	1.97360300	-1.46685100
O	-2.91868500	1.97359700	-1.58525100
O	-1.46748600	3.33058000	-0.49913200
C	-2.56643400	4.19770700	-0.17255500
H	-2.12644000	5.03907900	0.36474300
H	-3.29357200	3.68371500	0.46272600
H	-3.06634500	4.54801900	-1.07977600

Int7_2

Rh	0.55316900	-0.39884100	-0.26030200
C	2.47869200	-1.28034600	-0.52015600
C	3.32350200	-1.19136800	-1.75423100
C	2.63150100	-0.44395000	0.66847800
C	3.63576500	0.65395100	0.83284700
C	1.74714300	-0.95069500	1.64404900
C	1.50995300	-0.40982900	3.02092900
C	1.16385700	-2.20662700	1.14697100
C	0.23993400	-3.07373800	1.94745300
C	1.64615300	-2.43183000	-0.14994700
C	1.37321400	-3.60396300	-1.04178100
H	-5.24202300	-1.28091400	1.17457000
H	-4.30882500	3.34812000	1.26362800
H	-2.35190000	3.65723700	-0.22159100
C	-2.73112400	2.65448200	-0.04627100
H	3.61260900	-0.15890600	-1.96958100
H	2.80100800	-1.58469700	-2.63165700
H	4.24723800	-1.77546600	-1.62843500
H	3.72649800	1.26650200	-0.06625300
H	4.62424200	0.22340500	1.04828300
H	3.37938200	1.31409100	1.66574200
H	0.45881200	-0.50704100	3.31188500
H	1.77783700	0.64708400	3.09494200
H	2.10491600	-0.96062200	3.76352000
H	-0.57115000	-2.49125700	2.39804500
H	0.78073700	-3.56480400	2.76843500
H	-0.21559700	-3.85649400	1.33564400
H	2.22370000	-4.29978000	-1.03725600
H	1.22109600	-3.29613000	-2.08223000
H	0.49026000	-4.16487100	-0.72283300
H	-5.22984100	1.07215400	1.63462600
N	-0.82806800	-0.84781500	-1.77450900
H	-0.60002800	-1.78827700	-2.10337400
C	-2.09445700	1.58758900	-0.66066200
H	-1.10449100	1.35465100	-2.54062900
C	-2.58518500	0.25526800	-0.43037100
C	-3.75744900	0.08761600	0.39497900
C	-4.35380200	1.22251400	1.00772600
H	-2.19688000	-3.05659400	-1.28439800
H	-4.26602600	-3.27469500	0.05678800
C	-1.99233100	-0.93966300	-1.02060200
C	-2.63296900	-2.17396500	-0.82012900
C	-3.80161800	-2.29743700	-0.05591200
C	-4.34633100	-1.19359300	0.56497300
C	-3.84692000	2.48159000	0.79679300
C	0.48556400	1.54385000	-1.12817000
C	1.00254500	2.56139600	-0.17120000
C	-0.94563800	1.89262700	-1.60466600
H	-0.98609800	2.96675000	-1.83707500
H	1.14354100	1.50307500	-1.99944200
O	0.46454300	2.95501700	0.85169700
O	2.19890300	3.08741200	-0.58601400
C	2.74739300	4.11107900	0.25434100
H	3.71917500	4.36101800	-0.17629600
H	2.86912300	3.76270500	1.28375900
H	2.10461800	4.99710200	0.25823000

TS8_2

Rh	0.92586700	-0.07377200	-0.10891900
C	3.00924400	0.13362200	-0.98767900
C	3.40145800	1.01785500	-2.13388600
C	3.10272200	0.46784500	0.40356600
C	3.66163700	1.75271700	0.94242600
C	2.77043700	-0.71066400	1.17992800
C	2.82761400	-0.81447500	2.67488200
C	2.42202100	-1.75507300	0.28361400
C	2.12449100	-3.18004100	0.64739200
C	2.51721300	-1.21467200	-1.07243500
C	2.36151900	-2.00893300	-2.33659800
H	-5.15671600	-2.15373000	1.64333100
H	-5.94000100	2.15322700	-0.23981000
H	-3.87092000	2.70583300	-1.49443400
C	-3.93310200	1.76427000	-0.95369700
H	3.26904600	2.07615800	-1.88825700
H	2.81086400	0.80778600	-3.03082900
H	4.45993100	0.87340500	-2.39678400
H	3.24543900	2.62687000	0.43155400
H	4.75256300	1.78396200	0.81074900
H	3.46298600	1.86656300	2.01139900
H	2.18529300	-1.61838700	3.04620400
H	2.50921600	0.11361000	3.16063100
H	3.85178500	-1.02465600	3.01504600
H	1.54536600	-3.25177700	1.57367000
H	3.05316300	-3.75057200	0.79548900
H	1.55927800	-3.69049600	-0.13829700
H	3.30972100	-2.49128600	-2.61266700
H	2.05638500	-1.37715600	-3.17666700
H	1.61876900	-2.80720300	-2.23188000
H	-6.11283600	0.01411400	1.00025400
N	-0.70880800	-1.00560600	-1.06725800
H	-0.37345400	-1.84420600	-1.54370900
C	-2.84328000	0.90814500	-0.96924700
H	-1.11186600	0.00602700	-1.83314400
C	-2.93480600	-0.34121800	-0.27264500
C	-4.13491400	-0.66741300	0.44251900
C	-5.20850300	0.26326400	0.44991100
H	-1.24610700	-3.28044300	0.24308800
H	-3.32023600	-3.81334100	1.50067100
C	-1.88181300	-1.31828000	-0.32295700
C	-2.04647000	-2.54606600	0.29859600
C	-3.22546600	-2.84590800	1.01354800
C	-4.24592200	-1.92584000	1.09483900
C	-5.11058900	1.44986100	-0.24017700

C	-0.48717600	1.89372300	-1.15382300
C	-0.17089200	1.91771100	0.24162400
C	-1.61390100	1.24754000	-1.77213800
H	-1.83973800	1.66576100	-2.75509400
H	0.13248100	2.53844500	-1.77183300
O	-0.56514000	1.05869800	1.09711500
O	0.53865400	3.02295800	0.64314700
C	0.70532700	3.16478800	2.05701000
H	-0.26076300	3.32683700	2.54758100
H	1.33670600	4.04532200	2.19311200
H	1.18208400	2.28854000	2.50325100

Int8_2

Rh	-0.79030100	0.27633800	0.28152600
C	-2.77056800	0.41868200	1.07788300
C	-3.97270500	0.89238100	0.32870600
C	-2.36815500	-0.96613100	1.26303100
C	-3.08560300	-2.18042400	0.76065800
C	-1.23533700	-0.95320300	2.11641000
C	-0.50504100	-2.15111600	2.63232000
C	-1.01551400	0.41960000	2.59577100
C	0.06023200	0.80811200	3.56178900
C	-1.97202700	1.24851000	1.99476600
C	-2.15995600	2.72083200	2.18466500
H	5.93376300	-1.01413500	1.43909600
H	2.23586100	-3.88030400	1.13547400
H	0.74033600	-2.85865800	-0.56595700
C	1.62628700	-2.32272200	-0.23961900
H	-4.20562300	0.23069700	-0.50914300
H	-3.80701400	1.89320000	-0.07287600
H	-4.84520400	0.91651800	0.99839300
H	-3.79925700	-1.92187200	-0.02344200
H	-3.64953300	-2.64388300	1.58174900
H	-2.39983500	-2.93160600	0.35916400
H	0.57034300	-1.97305100	2.71563000
H	-0.66112300	-3.02458700	1.99501700
H	-0.87646900	-2.39917200	3.63746100
H	1.01424000	0.33160700	3.31111900
H	-0.20209000	0.49361500	4.58154200
H	0.21923400	1.88951400	3.57713800
H	-3.03233100	2.91188800	2.82495100
H	-2.33152000	3.21830900	1.22700200
H	-1.29052500	3.18082800	2.66220900
H	4.36989800	-2.74783900	1.71916800
N	2.67102500	1.71022200	-1.74933400
H	3.06238800	2.63645600	-1.89227600
C	1.89474000	-1.09746500	-0.83982800
H	1.32815700	0.16475200	-2.50757000
C	3.10013900	-0.38564800	-0.46773400
C	4.01168000	-1.04072300	0.44751000
C	3.66584200	-2.28917500	1.02865900
H	5.05929200	2.38168600	-1.03574400
H	6.63759400	1.14367400	0.41304100
C	3.50722400	0.91975300	-0.95274700
C	4.77333500	1.40787400	-0.64261800
C	5.66328500	0.71398700	0.19393900
C	5.27772400	-0.47633800	0.75954200
C	2.48839400	-2.91496800	0.70343200
C	-0.56028000	-0.49636600	-1.69884400
C	-1.40841300	-1.67587300	-1.99561300
C	0.95187600	-0.71527900	-1.99508500
H	1.02661300	-1.53793800	-2.71907500
H	-0.93427900	0.34448100	-2.28437300
O	-1.09908800	-2.85655500	-1.89424600
O	-2.64125300	-1.31047100	-2.45525000
C	-3.48396700	-2.38211100	-2.89960200
H	-4.41485400	-1.91054000	-3.22034800
H	-3.68208700	-3.10117200	-2.10011800
H	-3.02611400	-2.91173900	-3.74110400
O	-1.96764400	2.96399800	-1.18305400
H	1.71552800	1.79715700	-1.39487200
O	-0.00116000	2.01497700	-0.60082600
C	-0.73778800	2.95612000	-1.13397400
C	0.07731900	4.09395300	-1.74259800
H	0.88284600	4.40724100	-1.07022000
H	0.53667800	3.75456100	-2.67946600
H	-0.57170400	4.94441100	-1.96280200

TS9_2

Rh	1.12151800	-0.32617000	0.07492700
C	3.29163600	-0.36632500	0.77273200
C	4.43058300	-0.83614100	-0.07935600
C	2.85984200	0.96587600	0.98137600
C	3.47772300	2.21627200	0.43718000
C	1.72070400	0.92906900	1.88180700
C	1.04918400	2.13285300	2.46963600
C	1.53476000	-0.43590300	2.31433200
C	0.55978300	-0.89908200	3.35615100
C	2.46145700	-1.24848900	1.59923300
C	2.67653300	-2.72335300	1.75768900
H	-6.53736800	0.81792600	1.07728500
H	-2.85140400	3.65424200	1.55263300
H	-0.98665200	2.54327300	0.37652100
C	-1.93708000	2.03450200	0.45217800
H	4.79647600	-0.04334900	-0.73759700
H	4.12850900	-1.67861100	-0.71045200
H	5.27267800	-1.17113100	0.54191100
H	4.09672000	2.01539900	-0.44191700
H	4.12157200	2.68246600	1.19652200
H	2.71516300	2.95029800	0.16174500
H	0.03758400	1.90336500	2.81620400
H	0.98180700	2.94781200	1.74473600
H	1.61698500	2.50137600	3.33633200
H	-0.35890700	-0.30550800	3.34345400
H	0.99892000	-0.80533900	4.35925900
H	0.28370400	-1.94713400	3.21144800
H	3.43589000	-2.92263400	2.52752400
H	3.02800800	-3.17601100	0.82624600
H	1.75780800	-3.23774800	2.04954500
H	-5.08079400	2.55737200	1.62214300
N	-2.66553900	-2.08757900	-1.12911500
H	-3.06388800	-2.98361800	-1.39433000
C	-2.06773700	0.78676700	-0.14203500
H	-0.38343100	-0.86115900	0.20596300
C	-3.33803400	0.08149100	-0.05278300
C	-4.43715900	0.78666300	0.57035900
C	-4.23307200	2.06774300	1.14879900
H	-5.12925900	-2.73048100	-0.87667600
H	-6.99556800	-1.42051100	0.07636900
C	-3.62937400	-1.25296800	-0.54167200
C	-4.93714500	-1.73091100	-0.49205400
C	-5.99569400	-0.99470600	0.06117000
C	-5.74575300	0.23807500	0.61062900
C	-3.00474200	2.67493100	1.10689300
C	0.21746500	0.82970200	-1.56174200
H	0.52845600	0.28428800	-2.44665400
C	-0.92075200	0.21513600	-0.91128600
H	-1.22041900	-0.64875900	-1.49102300
C	0.66013600	2.23690400	-1.63961500
O	0.53022400	3.15193500	-0.83660400
O	1.31755400	2.41966000	-2.81429600
C	1.82520600	3.74053000	-3.05244900
H	1.01915800	4.47946100	-3.02931200
H	2.27338100	3.70418900	-4.04669600
H	2.58171500	4.01122300	-2.31040200
H	-1.80850900	-2.27530000	-0.60548900
O	1.35241700	-1.81871300	-1.41315200
O	-0.10666900	-3.27736000	-0.47255200
C	0.74657300	-2.96159800	-1.31557200
C	1.14737600	-3.95246500	-2.40579300
H	0.86413800	-4.96854200	-2.12023700
H	0.62422400	-3.69332300	-3.33484100
H	2.22105300	-3.90442500	-2.61011100

Int9_2

Rh	0.97740200	-0.41326200	0.13904100
C	3.14314900	-0.39400500	1.08509600
C	4.34857400	-0.95471200	0.39532800

C	2.73069200	0.94751800	1.15110100
C	3.46200100	2.15090400	0.64110900
C	1.47409000	0.99567300	1.90037500
C	0.78757200	2.25506900	2.33263100
C	1.18210800	-0.32036300	2.37559300
C	0.10803700	-0.68695800	3.35803700
C	2.15938000	-1.21126600	1.79791000
C	2.33083900	-2.67059200	2.10005200
H	-6.44291800	0.84192400	1.00620000
H	-2.88674800	3.86376600	1.09802800
H	-1.00976000	2.74212300	-0.03949900
C	-1.93165900	2.19814000	0.10887200
H	4.87641700	-0.19204400	-0.18385100
H	4.06362400	-1.75912600	-0.29217500
H	5.05704500	-1.37507100	1.12160000
H	4.16929300	1.89087000	-0.15144300
H	4.03381100	2.62196600	1.45357800
H	2.77219500	2.90632000	0.25475400
H	-0.26623600	2.08246800	2.56699200
H	0.83946600	3.02818000	1.56233700
H	1.26753600	2.65406600	3.23841600
H	-0.79476100	-0.08703600	3.21335400
H	0.45910100	-0.51572400	4.38546100
H	-0.17404800	-1.73985100	3.27524600
H	2.99956200	-2.80888400	2.96189200
H	2.77242800	-3.20371000	1.25323800
H	1.37868800	-3.15253500	2.33381500
H	-5.05092500	2.66892200	1.36141200
N	-2.56276800	-2.04850300	-1.20561500
H	-2.95023200	-2.96340400	-1.41738000
C	-2.01323100	0.89346300	-0.36820900
H	-0.23220500	-1.34393700	0.42538400
C	-3.25773400	0.15032300	-0.19550000
C	-4.36309600	0.85336900	0.41971300
C	-4.19877200	2.18257500	0.89257500
H	-4.97918400	-2.76025300	-0.79976100
H	-6.85326600	-1.47006400	0.16340500
C	-3.52190000	-1.21680100	-0.60476700
C	-4.80879500	-1.73637500	-0.47331500
C	-5.87173400	-1.01020800	0.08296900
C	-5.64732200	0.26159300	0.54695300
C	-3.00609400	2.84250700	0.74553500
C	0.33202700	0.83094800	-1.64879200
H	0.74495100	0.21111800	-2.43715300
C	-0.86914000	0.31543200	-1.10838700
H	-1.12866800	-0.60397100	-1.61221700
C	0.91686900	2.19047700	-1.70236300
O	0.68489400	3.17934800	-1.02083600
O	1.82565100	2.22589300	-2.71001400
C	2.43964100	3.49886900	-2.96234100
H	1.68635300	4.24457700	-3.23292200
H	3.11953300	3.33154800	-3.79907000
H	2.99595500	3.85188000	-2.09015700
H	-1.68644400	-2.20101500	-0.70559400
O	1.42976800	-1.81758900	-1.35613000
O	-0.03514700	-3.40783700	-0.66796600
C	0.87348900	-2.99221200	-1.39808100
C	1.41991000	-3.87462300	-2.51726700
H	1.23492000	-4.92795600	-2.29226600
H	0.89827100	-3.62603400	-3.45010700
H	2.48779900	-3.70379500	-2.67845400

Int10_2

Rh	0.97194500	0.00995700	-0.11529300
C	3.12743800	0.29288900	-0.72350500
C	3.62647400	1.39422500	-1.61301500
C	3.02423100	0.34825000	0.70993300
C	3.47334900	1.49752100	1.56332100
C	2.73127500	-0.99884600	1.20634000
C	2.67776800	-1.37677400	2.65659800
C	2.52266300	-1.82938700	0.10160000
C	2.23660300	-3.30281900	0.10572900
C	2.68068300	-1.00780400	-1.11209300
C	2.65682500	-1.56082800	-2.50939900
H	-4.85829900	-2.64216100	1.52218500
H	-6.27369200	1.68715000	0.31987000
H	-4.39683300	2.66921600	-0.95791600
C	-4.30080000	1.65899800	-0.56774600
H	3.29221200	2.37661100	-1.26395200
H	3.27800300	1.27388900	-2.64393600
H	4.72656500	1.41308100	-1.64156200
H	3.20338500	2.45488300	1.10976500
H	4.56518900	1.48638600	1.69879600
H	3.02398900	1.46039500	2.56048500
H	2.19232200	-2.34597200	2.80651300
H	2.12531300	-0.63695600	3.24638900
H	3.68754400	-1.44339200	3.08745000
H	1.75248200	-3.62578100	1.03298300
H	3.16173500	-3.88906800	-0.00112800
H	1.58678300	-3.59687100	-0.72627800
H	3.58279800	-2.10849800	-2.73759800
H	2.55097700	-0.76754300	-3.25597400
H	1.83120700	-2.26785100	-2.65947900
H	-6.06229400	-0.60694300	1.25357700
N	-0.72445400	-0.80083400	-1.28915100
H	-0.34014400	-1.58014200	-1.82035300
C	-3.10391500	0.98312700	-0.77480500
H	-0.97470500	-0.05984400	-1.94450700
C	-2.98129100	-0.36928100	-0.29027800
C	-4.07999300	-0.92972600	0.45777600
C	-5.25333600	-0.16177300	0.67986400
H	-0.98192600	-3.15622900	-0.25582200
H	-2.87052100	-4.06740900	1.07520900
C	-1.86655000	-1.23711200	-0.53542900
C	-1.84818200	-2.53193800	-0.05082000
C	-2.91735700	-3.04689900	0.70536100
C	-4.01481100	-2.25887400	0.95387900
C	-5.36935600	1.10510000	0.16333900
C	-0.85133400	2.17612200	-1.16853400
C	-0.09193800	1.85531400	0.05559700
C	-2.08446000	1.75754500	-1.53778300
H	-2.46371800	2.17542400	-2.47082700
H	-0.32808200	2.85107800	-1.84251900
O	-0.52755200	1.06882400	0.98386400
O	0.71870300	2.96037700	0.40552000
C	0.54880100	3.41236200	1.74601600
H	-0.48381100	3.74371900	1.92583500
H	1.22068500	4.26687900	1.86590900
H	0.80053600	2.64374600	2.48237300

$Cu_2(OAc)_4$

Cu	-0.00418300	-0.00299900	-1.26289300
O	1.38688500	1.41669300	-1.19725300
O	-1.39069100	-1.42615600	-1.19153000
O	-1.43320100	1.39389700	-1.06560000
O	1.42640200	-1.40070500	-1.07669800
Cu	0.00714600	-0.00622400	1.26307700
O	-1.39902700	1.39842400	1.20108100
O	1.41080800	-1.41107800	1.19014500
O	1.41920300	1.40783900	1.06944500
O	-1.40729400	-1.41902700	1.07531400
C	-1.79613000	-1.82591800	-0.05988000
C	-2.89107800	-2.88247200	-0.06866500
H	-3.85494600	-2.37543100	-0.19469000
H	-2.90448300	-3.43228800	0.87358800
H	-2.75236500	-3.56422300	-0.91039100
C	-1.81913200	1.79346600	0.07395600
C	-2.90167800	2.86285000	0.07632300
C	1.80110800	1.81461500	-0.06853600
C	2.84322900	2.92338100	-0.07500100
C	1.82125200	-1.80373100	0.05763400
C	2.93060500	-2.84518200	0.06518800
H	3.88694700	-2.32533900	0.19634100
H	2.95434700	-3.39091200	-0.87920400
H	2.79897100	-3.53223300	0.90378300
H	2.32409500	3.88144100	0.04604700
H	3.38762300	2.93696400	-1.02049700
H	3.53135400	2.80064900	0.76394300

H	-3.18029600	3.13696400	1.09411000
H	-3.77670400	2.48738900	-0.46341100
H	-2.53417400	3.74337100	-0.46029400

$Cu_2(OAc)_2$

Cu	-0.00034100	-1.27343400	-0.00376600
O	-1.90739700	-1.13176700	0.02136400
O	1.90680400	-1.13231100	-0.03472500
H	-4.32704300	0.00169300	1.06779900
C	-2.48682500	0.00032500	-0.01004200
Cu	0.00034300	1.27334600	-0.00374600
C	-3.99804600	0.00064000	0.02105000
H	-4.39471400	-0.89817300	-0.45626500
O	-1.90679100	1.13215900	-0.03495800
O	1.90737400	1.13161600	0.02149400
C	2.48682100	-0.00050000	-0.00994400
C	3.99804400	-0.00024300	0.02088600
H	4.32726000	0.01148500	1.06749800
H	4.39407600	0.89337300	-0.46671800
H	4.39628200	-0.90100300	-0.45080900
H	-4.39581800	0.89628000	-0.46078700

Int11_2

Rh	1.55857200	0.03351800	0.16566200
C	1.38372400	-1.37371800	1.91441700
C	0.18098300	-2.13594900	2.37449200
C	2.37382400	-1.88147600	0.97413600
C	2.36154700	-3.24512600	0.35513900
C	3.43540300	-0.91982700	0.89957800
C	4.70039400	-1.05265200	0.11299100
C	3.08545900	0.20846900	1.72398000
C	3.93422900	1.41715700	1.96490400
C	1.82147200	-0.09731400	2.37487600
C	1.12984500	0.81279600	3.34078100
C	0.26945600	2.74334600	-0.58307800
O	0.86780300	2.03480100	0.32531700
O	-0.41148900	2.30872000	-1.52334200
C	0.46641800	4.24504100	-0.40363300
H	-0.30467600	-2.66718200	1.55163600
H	-0.56173800	-1.48887200	2.84685800
H	0.48286600	-2.88927000	3.11563700
H	1.34437900	-3.58241000	0.13892700
H	2.81465400	-3.97959800	1.03593400
H	2.92824000	-3.26872500	-0.57991900
H	5.02990500	-0.08230200	-0.26354700
H	4.57972300	-1.72909400	-0.73724700
H	5.49089100	-1.46343800	0.75692700
H	4.31348600	1.80446300	1.01597800
H	4.78363800	1.16900200	2.61666100
H	3.36160700	2.21208400	2.44970000
H	1.72344600	0.92330500	4.25726700
H	0.14443500	0.43426100	3.62451500
H	0.99942400	1.80673100	2.89980600
H	1.50918200	4.49728000	-0.63038900
H	-0.19392300	4.80258400	-1.07199000
H	0.27935300	4.54054100	0.63428800
O	3.89551200	1.88084800	-1.28705400
O	2.24171000	0.41811000	-1.79473100
C	3.15973700	1.29953100	-2.08593700
C	3.25130500	1.57032800	-3.58547000
H	3.33859500	0.63254300	-4.14492800
H	2.33268000	2.06566700	-3.92088200
H	4.10826100	2.21113000	-3.80580500
C	-0.96148500	-1.62764700	-1.22315400
C	-0.42445900	-2.65554300	-1.98728700
C	-1.05618700	-3.90457300	-2.11639600
C	-2.24717000	-4.12792200	-1.47053000
C	-4.69682300	-2.43027700	0.73463300
C	-4.09767400	-1.16737100	0.88911400
C	-2.88727700	-0.83883300	0.29316800
C	-2.20447500	-1.82185000	-0.51900400
C	-2.83820700	-3.11139500	-0.67613700
C	-4.07567300	-3.38227000	-0.03377800
H	0.51014000	-2.47350800	-2.51213900
H	-0.60323300	-4.67420900	-2.73493200
H	-2.76385000	-5.07935800	-1.56346100
H	-5.64177400	-2.64163700	1.22699800
H	-4.58625900	-0.42448800	1.50740500
H	-4.51912600	-4.36571300	-0.16718100
N	-0.19920500	-0.42003300	-1.19114100
H	0.39940300	-0.35710800	-2.01813100
H	-0.71235400	0.47414600	-1.19315400
C	-2.30844300	0.47872300	0.61851600
H	-1.25732100	0.47608900	0.89623900
C	-2.89328900	1.69344600	0.66185700
H	-2.28375600	2.52934800	0.98916500
C	-4.24970100	2.07866400	0.21266900
O	-5.11555400	1.37051700	-0.26735000
O	-4.41204300	3.41453200	0.39064000
C	-5.67357300	3.94617500	-0.03807000
H	-6.49915900	3.47965500	0.50780600
H	-5.63244000	5.01445900	0.18080400
H	-5.81968200	3.78573500	-1.11018500

Int12_2

Rh	-1.35939700	-0.46323700	0.06273600
C	-2.45909100	0.92303300	-1.30091800
C	-1.92518900	1.44238000	-2.59844200
C	-3.16249200	-0.32623200	-1.13834400
C	-3.56278200	-1.25460500	-2.24473200
C	-3.58581600	-0.41925100	0.25457800
C	-4.41089100	-1.52827800	0.82764700
C	-3.08710900	0.71374000	0.94975900
C	-3.29732600	1.05663200	2.39273800
C	-2.35379000	1.53093000	-0.00801300
C	-1.72633600	2.84644900	0.32944300
H	1.08042800	3.01714500	-1.97796100
C	1.92116100	3.39499300	-0.03899200
O	2.52779300	3.14423700	0.98754400
O	1.36097900	4.62243900	-0.26166700
H	-1.25667100	0.71319700	-3.06981100
H	-1.36058100	2.36688500	-2.45929300
H	-2.74615200	1.65157700	-3.29627600
H	-2.85280700	-1.21164600	-3.07653500
H	-4.55038900	-0.98383800	-2.64387500
H	-3.61992000	-2.29283900	-1.90285800
H	-4.23853500	-1.65112600	1.90019500
H	-4.19680100	-2.48376800	0.34018600
H	-5.47916200	-1.31605500	0.68153000
H	-3.49805100	0.16557900	2.99442800
H	-4.15296600	1.73621600	2.51179100
H	-2.42148900	1.55565800	2.81794700
H	-2.50887000	3.59460900	0.51873200
H	-1.08998800	3.22007600	-0.47334300
H	-1.11618800	2.77509800	1.23568100
C	1.55664900	5.58465900	0.78182800
H	2.62200200	5.76609000	0.95392200
H	1.07091600	6.49892300	0.43552300
O	0.14237300	-0.53567600	1.71378300
O	-0.95520100	-2.33188300	1.10539800
C	-0.07687900	-1.77673900	1.85085300
C	0.68281200	-2.60070300	2.85522800
H	-0.00912100	-3.22196500	3.43333000
H	1.36846700	-3.27179800	2.32608500
H	1.25807200	-1.95933800	3.52617000
C	1.21691800	-1.75281400	-1.08202100
C	1.16140900	-3.14487800	-1.22689000
C	2.22438700	-3.99001600	-0.87354600
C	3.36690700	-3.45852300	-0.31780600
C	4.89760200	-0.16406900	0.45995200
C	3.92665800	0.71462300	-0.05414700
C	2.73335300	0.25586600	-0.60188100
C	2.45917300	-1.16281700	-0.62140800
C	3.50399700	-2.05190500	-0.17974500
C	4.69981800	-1.52037500	0.37489000
H	0.23258200	-3.58190900	-1.58745500
H	2.12138000	-5.06494200	-1.00251000
H	4.18337600	-4.09832300	0.00756400

H	5.81517400	0.23744100	0.88187100
H	4.12824200	1.77729400	-0.05835000
H	5.46187900	-2.21543900	0.72022000
N	0.10815300	-0.96637300	-1.40657700
H	1.10106500	5.24804900	1.71819900
H	-0.49567700	-1.55942200	-1.98125900
C	1.90378300	1.20435300	-1.35974400
H	1.46787700	0.77044500	-2.25300500
C	1.64143000	2.52279500	-1.19002000

TS10_2

Rh	1.44772200	-0.35595700	-0.09879500
C	2.16000700	1.53019100	0.84525800
C	1.33195400	2.64098800	1.41178700
C	2.63677700	0.37743600	1.57045500
C	2.42758100	0.10412000	3.02800200
C	3.53348000	-0.36078200	0.68645000
C	4.29534600	-1.58992900	1.06943200
C	3.54647000	0.28591500	-0.57828100
C	4.33425500	-0.11181000	-1.78783200
C	2.66577900	1.44683600	-0.49331200
C	2.43905200	2.44193200	-1.58619100
H	-0.86424900	2.52301300	-2.00448200
C	-1.96182000	2.91349100	-0.18581800
O	-2.47530200	2.55815400	0.88530400
O	-1.75375300	4.26394100	-0.44508000
H	0.57835000	2.28159300	2.11913800
H	0.81841600	3.20727200	0.63216300
H	1.98373700	3.33521900	1.96039300
H	1.46952900	0.49833600	3.37783400
H	3.21985500	0.57997200	3.62299900
H	2.45215700	-0.96790300	3.24499800
H	4.49506400	-2.22956500	0.20605300
H	3.75472300	-2.18360800	1.81151400
H	5.26151300	-1.30922000	1.51075800
H	4.62341100	-1.16543600	-1.75283600
H	5.25440800	0.48423500	-1.85800300
H	3.76649300	0.05042800	-2.70867500
H	2.52310200	1.97834100	-2.57319200
H	3.18985900	3.24258600	-1.52989600
H	1.44925100	2.89884100	-1.51003100
C	-2.22252100	5.15159300	0.56358500
H	-1.75913600	4.94845200	1.53579000
H	-1.94966200	6.15695800	0.22966900
O	0.83132200	-1.32740200	-2.02870100
O	1.11497200	-2.51877900	-0.21098300
C	0.77981000	-2.45255600	-1.44013200
C	0.28350300	-3.67846400	-2.15684400
H	0.74765700	-4.57977800	-1.74830000
H	-0.80056400	-3.75697300	-2.00850700
H	0.47786700	-3.60433100	-3.22968400
C	-1.47786900	-1.07446800	0.79109800
C	-1.22929300	-1.99834400	1.78292500
C	-2.27921100	-2.87056700	2.17988300
C	-3.53861800	-2.81465800	1.61368600
C	-5.20072100	-0.68656200	-1.02398800
C	-4.11288100	0.14147200	-1.40899900
C	-2.88614300	-0.03184300	-0.80408000
C	-2.75649200	-1.02298100	0.18913400
C	-3.82180400	-1.86712400	0.59074200
C	-5.06966600	-1.67050200	-0.06141700
H	-0.25539600	-2.06762500	2.25572500
H	-2.07896200	-3.59922200	2.96168300
H	-4.32129600	-3.48967400	1.95187100
H	-6.16402300	-0.53996300	-1.50674300
H	-4.24845200	0.90394100	-2.17084100
H	-5.92085800	-2.29025200	0.21070500
N	-0.61824000	-0.05717100	0.24821900
H	-3.31022000	5.09052200	0.68516900
H	-0.68207000	0.75786700	0.86259500
C	-1.59200300	0.66510400	-1.14982100
H	-1.08829100	0.15501600	-1.97225200
C	-1.48162400	2.08183000	-1.22933300

TS11_2

Rh	-1.22044200	-0.35678000	0.06205900
C	-2.54160000	-0.26839000	-1.72761600
C	-2.13444700	-0.10662200	-3.15934100
C	-2.70008900	-1.53417200	-1.04029800
C	-2.52201300	-2.89555700	-1.63781300
C	-3.22675300	-1.25756900	0.28117100
C	-3.60039000	-2.28406900	1.30113300
C	-3.31441900	0.16314200	0.43265000
C	-3.81575800	0.91408700	1.62577300
C	-2.90643100	0.77919300	-0.82433000
C	-2.96293000	2.24936800	-1.10418200
H	-0.15418100	2.24719500	-1.88227700
C	0.88112500	2.74587900	-0.07642200
O	1.77195400	2.67279900	0.77293600
O	-0.02166700	3.83166300	-0.03721400
H	-1.38927600	-0.84972800	-3.46184300
H	-1.72259500	0.88565200	-3.35453500
H	-3.00609800	-0.24551700	-3.81334200
H	-1.78549500	-2.89446100	-2.44654700
H	-3.47020200	-3.25534200	-2.06053600
H	-2.19831400	-3.62450700	-0.88893400
H	-3.54313100	-1.88291200	2.31595700
H	-2.95102200	-3.16197500	1.24815500
H	-4.63250200	-2.62130900	1.13250200
H	-3.66251900	0.35240700	2.55094300
H	-4.89215400	1.11304200	1.52792900
H	-3.30516600	1.87514300	1.72828400
H	-2.27857200	2.81600900	-0.46350500
H	-3.98214100	2.62011500	-0.93263000
H	-2.69759000	2.46982300	-2.14065100
C	0.20953800	4.74647800	1.02435300
H	1.19524700	5.22191800	0.94695400
H	-0.56850200	5.51250000	0.94055100
O	-0.41887800	0.73926100	1.92005700
O	-0.27466200	-1.43948600	1.72289900
C	-0.01470400	-0.36558400	2.37237100
C	0.80546300	-0.43819900	3.63314000
H	0.65239000	-1.39050900	4.14803400
H	1.86511500	-0.36180300	3.36114900
H	0.56491600	0.39667100	4.29621300
C	1.80133200	-1.49169900	-0.53094400
C	1.82431300	-2.80004900	-0.10346600
C	3.06160900	-3.32474900	0.36420600
C	4.22452300	-2.57603500	0.40310300
C	5.14088400	0.94137000	-0.65199900
C	3.88443000	1.40317500	-1.12510500
C	2.79913500	0.55866200	-1.05185900
C	2.98357800	-0.72601200	-0.51513000
C	4.22226900	-1.22662800	-0.05105800
C	5.32159900	-0.32987400	-0.13061500
H	0.93084200	-3.41574500	-0.09327800
H	3.08444200	-4.35555500	0.70919600
H	5.14646100	-3.01962600	0.77156300
H	5.99308800	1.61475000	-0.70478600
H	3.78673900	2.40970300	-1.51961800
H	6.30381500	-0.64667100	0.21203500
N	0.72233000	-0.69353200	-1.05583000
H	0.14230400	4.26108400	2.00471500
H	0.33392000	-1.15774600	-1.87752900
C	1.37099600	0.71703200	-1.54259800
H	1.36257400	0.59271500	-2.63515600
C	0.58994400	1.90192300	-1.17349800

Int13_2

Rh	1.32106000	-0.47565600	-0.09403200
C	2.41972300	1.40661500	0.52430000
C	1.89012600	2.73747800	0.95044600
C	2.71078200	0.29998900	1.39973000
C	2.53524400	0.29825000	2.88637100
C	3.39848000	-0.72078500	0.61549500
C	3.95587700	-1.99340800	1.16984000
C	3.43024900	-0.28782200	-0.74066800
C	4.03234700	-1.00497700	-1.90805500

C	2.78204000	1.01992500	-0.80704300
C	2.63365000	1.86772300	-2.03061500
H	-1.29091200	2.61715400	-2.24174900
C	-1.30686300	3.05083700	-0.14317400
O	-1.26042300	2.70878100	1.08499500
O	-1.33539600	4.40601100	-0.45291900
H	0.87171000	2.69230000	1.35775900
H	1.86540000	3.43436800	0.10976900
H	2.54740200	3.15635600	1.72385200
H	1.68207500	0.91295800	3.18700600
H	3.42949000	0.70730700	3.37781100
H	2.38138700	-0.71283000	3.27510200
H	4.07158400	-2.75983100	0.39950800
H	3.31565200	-2.40134300	1.95699600
H	4.94466600	-1.80714000	1.61095200
H	4.20794100	-2.06110800	-1.68872200
H	4.99715800	-0.55267900	-2.17386300
H	3.38568700	-0.94618800	-2.78841800
H	2.69715200	1.26897100	-2.94324100
H	3.42972300	2.62401000	-2.07045200
H	1.66924100	2.38661300	-2.02939900
C	-1.36095600	5.29199100	0.65656700
H	-0.44029200	5.24440200	1.25232800
H	-1.45929100	6.29620500	0.23220400
O	0.51870300	-1.69139900	-1.79042700
O	0.67568100	-2.55196500	0.21879200
C	0.32415500	-2.67018900	-1.00106100
C	-0.35253200	-3.92585600	-1.47800300
H	0.00769000	-4.79357100	-0.91911800
H	-1.43107900	-3.83288200	-1.30148800
H	-0.19031600	-4.07070500	-2.54890000
C	-1.66399300	-0.67495700	0.87466200
C	-1.54179900	-1.38923100	2.04340700
C	-2.67375600	-2.13180000	2.48358900
C	-3.87425300	-2.15339500	1.79419600
C	-5.12605200	-0.45792100	-1.35504200
C	-3.96300000	0.26925400	-1.73361200
C	-2.83099400	0.14787200	-0.95828200
C	-2.88164000	-0.68130900	0.17330100
C	-4.02018000	-1.40520400	0.59178800
C	-5.16876200	-1.27441100	-0.23606400
H	-0.61939500	-1.40660500	2.61408600
H	-2.58424200	-2.70356900	3.40393000
H	-4.71028300	-2.73467600	2.17550400
H	-6.01849800	-0.36219300	-1.96913300
H	-3.98582800	0.90960100	-2.61152200
H	-6.08317900	-1.80497000	0.01836400
N	-0.72462700	0.20604000	0.21071200
H	-2.20891100	5.09425000	1.32185200
H	-0.68013600	1.07793100	0.79011800
C	-1.41867600	0.72497100	-1.08777800
H	-0.93039600	0.21277900	-1.92307500
C	-1.26839200	2.20734700	-1.23848300

Int14_2

Rh	-1.62788100	-0.09403900	-0.07638200
C	-2.36274200	1.99565700	-0.18548200
C	-1.62781900	3.23450100	0.22219400
C	-2.37299900	1.40468600	-1.49452000
C	-1.67445600	1.92223800	-2.71453000
C	-3.39261000	0.34824500	-1.50585000
C	-3.75262200	-0.45606300	-2.71636600
C	-3.91727500	0.23271800	-0.20748800
C	-4.96539400	-0.72122100	0.27645700
C	-3.22978900	1.20846500	0.64657500
C	-3.56829100	1.46698800	2.08272100
H	0.09358800	1.40260500	1.20781300
C	0.78544000	-0.53222300	1.67516900
O	1.45972800	-1.52307900	1.44887500
O	0.35777200	-0.22068100	2.92923800
H	-0.68577200	3.35204700	-0.32107800
H	-1.40594500	3.24439900	1.29292400
H	-2.24246800	4.11908300	0.00610100
H	-0.80280600	2.52974000	-2.45689900
H	-2.35380000	2.55198600	-3.30665900
H	-1.33379000	1.10733500	-3.36066400
H	-4.29614700	-1.36775700	-2.45429500
H	-2.86099100	-0.74629900	-3.28120600
H	-4.38974700	0.13012000	-3.39283900
H	-5.11849500	-1.54603800	-0.42460800
H	-5.92817100	-0.20718700	0.40283900
H	-4.69620200	-1.15101600	1.24638500
H	-3.73888700	0.53324100	2.62740600
H	-4.48653600	2.06646800	2.15995800
H	-2.77008600	2.01035400	2.59549500
C	0.68329500	-1.17845500	3.94505900
H	1.76596500	-1.31284900	4.02536000
H	0.28628600	-0.76871300	4.87602300
O	-1.55157200	-2.00867500	1.03256300
O	-0.72912400	-1.90790200	-0.99491300
C	-0.95431600	-2.58096700	0.06921700
C	-0.48951000	-4.00531800	0.17812200
H	-0.56681700	-4.51213100	-0.78787400
H	0.56421100	-3.99614000	0.47927200
H	-1.06397900	-4.54478000	0.93502200
C	3.01822500	-0.57666600	-1.34110500
C	3.80275700	-1.53640200	-1.96047100
C	5.21019800	-1.46387500	-1.76909300
C	5.83618400	-0.49206200	-1.00420100
C	4.53889500	2.41155600	1.07454000
C	3.13953700	2.27839300	0.86186500
C	2.70370500	1.25552400	0.04283600
C	3.65450000	0.40596400	-0.54203500
C	5.04660500	0.49515900	-0.34501500
C	5.47016800	1.55879500	0.50002300
H	3.37345400	-2.32053500	-2.57754100
H	5.82528800	-2.21618200	-2.25885900
H	6.91819900	-0.48632000	-0.90105600
H	4.89006500	3.21306200	1.72061500
H	2.45244500	2.96661800	1.34836200
H	6.52972000	1.70081800	0.70101000
N	1.65564900	-0.32346900	-1.35835400
H	0.21669100	-2.14444300	3.73168500
H	1.00075100	-1.10092400	-1.35908500
C	1.32377800	0.79600600	-0.43912400
H	0.87168800	1.60496300	-1.03106400
C	0.31502300	0.47289200	0.68000100

TS12_2

Rh	0.80200300	-0.63576200	0.04112500
C	2.80773600	-0.27380800	1.06391500
C	3.09071700	0.76241300	2.10826800
C	2.41005300	-1.63535900	1.32001000
C	2.24970700	-2.28201200	2.66216400
C	2.28733100	-2.28977600	0.04222000
C	1.95790700	-3.73240600	-0.18334100
C	2.62314900	-1.34806600	-0.99458800
C	2.71631200	-1.66118200	-2.45668300
C	2.94907700	-0.09203800	-0.35453500
C	3.44144900	1.13978900	-1.05186700
H	-0.55071900	2.92685800	-2.06955400
C	0.69517600	3.38079800	-0.36060400
O	1.13016700	3.14806600	0.78763200
O	1.06261400	4.51389300	-1.02741600
H	2.55245100	0.55408900	3.03806600
H	2.80727300	1.76238100	1.77082200
H	4.16343100	0.77315000	2.34750100
H	1.92720900	-1.56435600	3.42251100
H	3.19835900	-2.71908300	3.00629000
H	1.50928100	-3.08697400	2.63307600
H	1.37617000	-3.86189400	-1.09832100
H	1.38754400	-4.15394400	0.64885400
H	2.88519700	-4.31490000	-0.27936400
H	1.85266700	-2.24868900	-2.77859300
H	3.62947200	-2.23357400	-2.67337900
H	2.74643200	-0.74771100	-3.05781000
H	2.85235700	1.36321600	-1.94779300
H	4.48491400	1.01141500	-1.37154900

H	3.39549900	2.01301200	-0.39821300
C	1.87709100	5.43319500	-0.29570000
H	2.83652400	4.98653100	-0.01558400
H	2.04533800	6.27632000	-0.96917100
O	-0.53175500	-2.57427400	-2.10701200
O	-0.89853500	-1.85641900	0.01037400
C	-1.17409200	-2.55671400	-1.05214900
C	-2.44484700	-3.39362800	-0.91680100
H	-2.70196200	-3.58775400	0.12757400
H	-3.27768400	-2.84997700	-1.37893800
H	-2.32409300	-4.33776700	-1.45638500
C	-1.81708000	0.66380900	1.36357800
C	-2.21671000	0.39898400	2.65220700
C	-3.58736700	0.06507600	2.85132300
C	-4.50583800	-0.01166500	1.81769200
C	-4.29629400	0.56352500	-1.92959600
C	-2.92611700	0.92106000	-2.06101300
C	-2.15477500	0.94875100	-0.91911600
C	-2.74535200	0.60547500	0.30991300
C	-4.09949300	0.26184500	0.47984200
C	-4.87882700	0.24988100	-0.71025400
H	-1.52949700	0.43138900	3.49230100
H	-3.91908500	-0.14156400	3.86548300
H	-5.53935800	-0.27472300	2.02696300
H	-4.91005500	0.54211000	-2.82620700
H	-2.52052500	1.16153100	-3.03928500
H	-5.93382500	-0.00841600	-0.66390500
N	-0.54119200	0.99124700	0.81197300
H	1.37048000	5.77727500	0.61191700
H	0.03532900	1.70165500	1.28513400
C	-0.74255600	1.36124800	-0.61088800
H	0.00685400	0.26919400	-1.17755700
C	-0.22597200	2.58774200	-1.09365700

TS13_2

Rh	-1.08674800	-0.20919900	0.13386400
C	-2.48173700	-1.64153000	-0.95999000
C	-2.51230000	-1.90724100	-2.43587800
C	-1.73648300	-2.38449100	0.02429200
C	-0.88598000	-3.59341500	-0.23298800
C	-2.08819700	-1.87785700	1.33319900
C	-1.61360300	-2.39494000	2.65900100
C	-3.01274300	-0.80779600	1.14188600
C	-3.67340300	-0.02573200	2.23501700
C	-3.26478600	-0.65140800	-0.28018800
C	-4.26490200	0.27364800	-0.90557700
H	0.00064300	-0.15005700	-2.29502700
C	-0.23154300	1.94971000	-1.88999500
O	0.20198700	2.99055800	-1.41549500
O	-1.12803400	1.94236200	-2.91224300
H	-1.59557300	-2.38950400	-2.78765500
H	-2.65089100	-0.98691100	-3.01071900
H	-3.34655700	-2.57825000	-2.68468100
H	0.00531300	-3.61037500	0.40192900
H	-0.55700400	-3.64864300	-1.27454900
H	-1.45344600	-4.51114900	-0.02364800
H	-1.33977500	-1.56497700	3.31641600
H	-0.73266500	-3.03383400	2.54595000
H	-2.39297900	-2.98964100	3.15575400
H	-2.99810400	0.11776500	3.08126200
H	-4.56556800	-0.55958600	2.59238800
H	-3.99809400	0.95888300	1.88725200
H	-4.38277200	1.19022700	-0.31988300
H	-5.25508600	-0.19972400	-0.97927700
H	-3.96361800	0.56649200	-1.91582400
C	-1.54697400	3.23553700	-3.37265300
H	-0.69429100	3.81632100	-3.73658000
H	-2.24469900	3.04363500	-4.18973600
O	-0.97647600	1.70392200	0.99748700
O	-0.51804700	0.88200000	3.06302900
C	-0.72560600	1.80657900	2.27185600
C	-0.75201400	3.25429400	2.76321800
H	-1.78881100	3.53692700	2.98728300
H	-0.16704000	3.35210600	3.68163100
H	-0.37943100	3.94453700	2.00101200
C	3.19712100	1.04963400	0.37380400
C	4.22575000	1.71749100	1.00661700
C	5.47445800	1.03804400	1.11904200
C	5.70204800	-0.23686200	0.63000300
C	3.53312600	-2.71987300	-1.26727400
C	2.31117200	-1.99934400	-1.33540000
C	2.26778800	-0.75019800	-0.74857700
C	3.42319200	-0.25506300	-0.12122400
C	4.64739300	-0.93679700	-0.03007200
C	4.66642100	-2.22268900	-0.63655000
H	4.10894500	2.72070200	1.40424000
H	6.28802200	1.55962900	1.61693700
H	6.67889500	-0.69949100	0.73985300
H	3.57857400	-3.70219300	-1.73003900
H	1.45059900	-2.43726200	-1.83119200
H	5.57539400	-2.81868500	-0.61350500
N	1.88631300	1.38145500	0.05738000
H	-2.04480300	3.79255800	-2.57369700
H	1.46939300	2.30526100	0.03945200
C	1.22072300	0.32105400	-0.57643000
H	0.51479400	-0.32329300	0.59469000
C	0.11185800	0.57451000	-1.49310700

Int15_2

Rh	0.34514100	0.00038900	-0.42806100
C	-1.46650300	1.16028600	-0.05181900
C	-1.67560800	2.59771100	-0.42259200
C	-1.79747900	0.01331700	-0.85237600
C	-2.41170600	0.02699900	-2.22147100
C	-1.47838400	-1.14981000	-0.07073900
C	-1.70240700	-2.57905500	-0.46407200
C	-1.15043700	-0.70664500	1.29368100
C	-0.85607000	-1.64320600	2.42574900
C	-1.14175800	0.69150100	1.30510000
C	-0.83182600	1.60499000	2.45191000
C	2.88234900	-0.00475900	-0.13973200
O	2.23802400	-1.10078800	-0.19044100
O	2.23919700	1.09261200	-0.17626100
C	4.38782800	-0.00551300	-0.08900600
H	-1.62534400	2.74538400	-1.50484200
H	-0.92040800	3.24338500	0.03689800
H	-2.66060100	2.94860700	-0.08184100
H	-2.11667200	0.91321000	-2.78956000
H	-3.50798200	0.03053900	-2.14137100
H	-2.12355200	-0.85212300	-2.80387700
H	-0.95986900	-3.24080600	-0.00681800
H	-1.64377100	-2.71237600	-1.54778000
H	-2.69494200	-2.92228900	-0.13754100
H	-0.12187400	-2.40306400	2.13586500
H	-1.76549000	-2.17481800	2.73781300
H	-0.46333500	-1.11627500	3.29949400
H	-1.74089700	2.11064900	2.80571000
H	-0.12188400	2.38610600	2.15875300
H	-0.39987500	1.06487000	3.29880800
H	4.77921200	-0.00524800	-1.11396500
H	4.75751900	0.89039900	0.41630000
H	4.75668700	-0.90252200	0.41503700
H	0.67599300	0.00936600	-1.96849700

12a

H	-4.89875000	-0.84692000	0.00022900
H	-2.73967400	3.63837400	0.00018000
C	5.46891000	-0.09733300	0.00026500
H	5.53243600	-0.72924500	-0.89082900
H	6.28054000	0.63249300	0.00056400
H	-0.31263500	3.15135900	-0.00000500
H	-4.43343200	1.86544200	0.00024700
N	0.36675300	-1.06025200	-0.00017700
H	5.53190600	-0.72946100	0.89122000
H	1.11328900	-1.74714500	-0.00015700
C	0.67249300	0.29215400	-0.00020200
H	2.07700000	1.88529400	-0.00034000
C	3.10736900	-0.04184100	-0.00006200

O	3.10209500	-1.27475200	0.00021900
O	4.25984000	0.67353100	-0.00009100
C	1.93798600	0.81154200	-0.00023700
C	-1.01049400	-1.27422100	-0.00012300
C	-1.81158100	-2.39684200	-0.00009100
C	-3.22384300	-2.19056000	0.00005900
C	-3.81619800	-0.93956500	0.00014700
C	-2.41592700	2.60103000	0.00010000
C	-1.02393100	2.33028300	-0.00001700
C	-0.62248300	1.00496000	-0.00013400
C	-1.61167400	0.00376600	-0.00007900
C	-2.99560600	0.22951300	0.00008200
C	-3.37954900	1.59810100	0.00014100
H	-1.40525000	-3.40342300	-0.00012000
H	-3.86100800	-3.07115700	0.00012500

Int1_3

Ir	-1.21461700	-0.09970800	-0.20218100
C	-1.96629700	-0.84436900	1.72289900
C	-1.20732000	-1.63023800	2.74266300
C	-2.11262000	0.58464900	1.68779500
C	-1.51225000	1.55558800	2.65428800
C	-2.97490800	0.92196500	0.56869900
C	-3.48785900	2.28683300	0.22877500
C	-3.40099400	-0.32600700	-0.04710100
C	-4.33414700	-0.44128500	-1.20877600
C	-2.76629000	-1.41387800	0.64007400
C	-2.97015400	-2.87550100	0.38669200
C	0.08450900	-1.20944100	-2.16880000
O	-0.86367900	-0.37916700	-2.37379200
O	0.35020000	-1.50228800	-0.95739600
C	0.85603800	-1.79698900	-3.31187000
H	-0.36192500	-1.06461300	3.13758100
H	-0.82929200	-2.56808400	2.32657900
H	-1.87535800	-1.88124800	3.57799900
H	-0.53173100	1.21842400	2.99623000
H	-2.16892200	1.65907500	3.52798900
H	-1.39742600	2.54567600	2.20489300
H	-3.71293900	2.37803000	-0.83753100
H	-2.76719000	3.06495800	0.49395500
H	-4.41442900	2.48841600	0.78304400
H	-4.22427500	0.39801100	-1.90108400
H	-5.37015200	-0.43850800	-0.84427900
H	-4.17480900	-1.36949300	-1.76295600
H	-3.77950900	-3.25627400	1.02371200
H	-2.06912800	-3.45134500	0.61581700
H	-3.24336500	-3.06925800	-0.65398800
H	1.37838000	-0.99722800	-3.84909000
H	1.58102200	-2.53145000	-2.95626700
H	0.16580100	-2.27082300	-4.01781800
H	-0.72716500	2.69450400	-1.70662100
O	1.57614000	0.11787600	2.04470200
C	2.18160100	0.34858200	1.00406000
H	3.43897000	0.12707300	-1.44992700
N	2.24616700	2.47644300	-0.39225800
C	3.46099200	-0.32463600	0.67045800
C	4.15405200	-0.98235600	1.70288800
C	5.34301700	-1.65084300	1.43202900
C	5.84570200	-1.68200500	0.12619500
C	5.15746800	-1.04168100	-0.90757200
C	3.97110600	-0.36051600	-0.63870700
H	3.75046700	-0.95328400	2.70975200
H	5.87971300	-2.14854600	2.23449400
H	6.77298900	-2.20765400	-0.08463800
H	5.54305600	-1.07452100	-1.92229800
C	1.60277800	1.36119900	0.05156600
N	0.34737100	1.35277000	-0.41678300
C	0.19628400	2.47863700	-1.19197400
C	1.36611200	3.18838800	-1.17148100
C	3.60463400	2.92400300	-0.06453400
H	3.64880200	4.00262900	-0.21855900
H	4.33640300	2.43388500	-0.71010700
H	3.82922200	2.70399000	0.98000000
H	1.64353700	4.12875900	-1.62333100

TS1_3

Ir	-0.64450200	-0.20842500	0.02322000
C	-1.80155800	1.13890900	-1.37029900
C	-1.58851200	2.58239800	-1.69512100
C	-1.25184200	0.03223200	-2.10259800
C	-0.38370800	0.11752000	-3.31981500
C	-1.84446400	-1.19311100	-1.57166000
C	-1.64023000	-2.56515600	-2.13398300
C	-2.72974200	-0.82160100	-0.50529300
C	-3.58339500	-1.74378600	0.30444900
C	-2.67589800	0.61883800	-0.33813700
C	-3.55517900	1.41948100	0.57574200
C	0.08241900	-1.06756200	2.84364400
O	-0.76569600	-1.23901600	1.90779800
O	1.03389000	-0.23042000	2.77844300
C	-0.06210700	-1.89448000	4.09481500
H	-0.61792300	2.75814600	-2.16497400
H	-1.66996100	3.21926400	-0.81302300
H	-2.36320300	2.89760800	-2.40749700
H	0.28958300	0.97803600	-3.27969500
H	-1.00979200	0.22557200	-4.21573900
H	0.21840500	-0.78637100	-3.44692600
H	-1.83820800	-3.34280300	-1.39169000
H	-0.62093500	-2.69630000	-2.50714300
H	-2.32423900	-2.72725500	-2.97791400
H	-3.22784600	-2.77598900	0.25815600
H	-4.60942600	-1.72309800	-0.08645900
H	-3.62279900	-1.43616600	1.35272200
H	-4.54921200	1.55157500	0.12744900
H	-3.14145400	2.41314500	0.76540300
H	-3.69074700	0.91772700	1.53859700
H	0.87735200	-2.42111100	4.29311200
H	-0.25265200	-1.23083000	4.94534400
H	-0.87699600	-2.61408800	4.00115400
H	0.57225400	-3.25146800	0.06596900
O	3.73256200	1.12471500	-1.12753800
C	2.69463800	0.79137300	-0.55450800
H	3.24915300	-3.76923800	-0.43666500
N	3.33077700	-1.63613400	-0.57847800
C	1.78562200	1.80433300	0.05852900
C	2.17454500	3.14449800	-0.08817600
C	1.44885100	4.16490900	0.52182200
C	0.33223900	3.85491800	1.30579900
C	-0.06476200	2.52699600	1.44537200
C	0.62625900	1.46593700	0.81487400
H	3.05896100	3.37217400	-0.67369900
H	1.76476500	5.19772500	0.40478900
H	-0.21938300	4.64637500	1.80608100
H	-0.92017000	2.29121800	2.07301800
C	2.39338000	-0.65222200	-0.43057100
N	1.20434100	-1.21468000	-0.16117200
C	1.38432100	-2.56832400	-0.12783400
C	2.70868100	-2.83640800	-0.38223200
C	4.76068800	-1.49334500	-0.87527400
H	5.21919700	-2.47633300	-0.76143500
H	5.21919200	-0.79003000	-0.17986100
H	4.89961700	-1.13306400	-1.89498200
H	0.79979000	0.50971900	1.70862400

Int2_3

Ir	-0.63356300	-0.07274400	0.01808400
C	-2.01719800	0.78301700	-1.49175800
C	-1.88693500	2.09135300	-2.20554900
C	-1.44718200	-0.48084700	-1.93832100
C	-0.71041800	-0.69805400	-3.22591500
C	-2.06486700	-1.55025900	-1.13465100
C	-1.85937700	-3.01309600	-1.37806200
C	-2.84268400	-0.94587100	-0.13451200
C	-3.62802900	-1.61753900	0.94767700
C	-2.77649400	0.51707300	-0.31224700
C	-3.58420800	1.50004400	0.48021700
C	0.25006400	0.23521500	3.17088300
O	-0.58914000	-0.10854000	2.33022800

O	1.32982900	0.94290300	2.87624800
C	0.13149200	-0.11263000	4.62162500
H	-0.91858400	2.19270700	-2.70227700
H	-2.02055400	2.94235100	-1.53446900
H	-2.66503700	2.14938400	-2.97893100
H	-0.07402800	0.15573700	-3.47403000
H	-1.42354000	-0.83500000	-4.05043200
H	-0.08159200	-1.59219000	-3.18251100
H	-2.17355300	-3.61807900	-0.52349200
H	-0.81161600	-3.24175300	-1.59590000
H	-2.44792400	-3.33309500	-2.24833400
H	-3.37006200	-2.67570700	1.04080400
H	-4.70283000	-1.55094500	0.73192700
H	-3.46189200	-1.13603200	1.91697700
H	-4.62651000	1.50252600	0.13316100
H	-3.19808800	2.51763900	0.37692500
H	-3.59329500	1.24487700	1.54428900
H	1.02431900	-0.66201900	4.93963700
H	0.08072300	0.80632700	5.21547400
H	-0.75955300	-0.71668900	4.79366000
H	0.22560200	-3.00779800	1.19400400
O	3.72177300	0.20721200	-1.65190700
C	2.69992100	0.21594100	-0.96328700
H	2.75063400	-4.05976400	0.73337500
N	3.05406900	-2.15091900	-0.18728500
C	1.97398600	1.47290200	-0.63313700
C	2.71120300	2.65605000	-0.85242900
C	2.20960300	3.89392800	-0.47694000
C	0.95391900	3.95902700	0.13573500
C	0.20432500	2.79749500	0.32466100
C	0.66689000	1.52162600	-0.07177400
H	3.69429900	2.57256300	-1.30459600
H	2.79328200	4.79539300	-0.64019800
H	0.55346700	4.91649200	0.46012300
H	-0.77706800	2.88284400	0.78392900
C	2.25786100	-1.05220900	-0.34288200
N	1.05595600	-1.29663400	0.19812100
C	1.08289100	-2.56608100	0.71022800
C	2.32763600	-3.09985400	0.47786300
C	4.45018200	-2.32571000	-0.60120900
H	4.80522800	-3.26155600	-0.16844100
H	5.05497100	-1.49594400	-0.23493800
H	4.51904400	-2.36773300	-1.68878700
H	1.30311300	1.18787900	1.92088000

Int3_3

Ir	0.55349200	-0.03089100	-0.23646500
C	2.17441700	0.79998800	0.99520000
C	2.16923900	2.10077900	1.73497600
C	1.68529700	-0.47638800	1.52419700
C	1.12345400	-0.69026900	2.89340600
C	2.14121000	-1.54514000	0.62927500
C	1.98107600	-3.00783000	0.90393400
C	2.72413200	-0.93687500	-0.49260500
C	3.30578600	-1.60485000	-1.69715700
C	2.71903200	0.52712600	-0.29034600
C	3.39101500	1.49523000	-1.21357400
C	-1.05985600	-2.57692700	-0.89689400
N	-1.10220800	-1.26508600	-0.49954900
C	-2.31236900	-3.11520500	-0.74514000
C	-4.53852300	-2.31266200	0.06388500
H	1.26440200	2.21811400	2.33732300
H	2.24255800	2.95553800	1.05912200
H	3.03065400	2.13493500	2.41536000
H	0.58706200	0.19320400	3.24945000
H	1.94050300	-0.89552300	3.59938200
H	0.44040200	-1.54439400	2.91572200
H	2.04287400	-3.60632300	-0.00864400
H	1.02864100	-3.22434400	1.39664500
H	2.77948200	-3.34684200	1.57792300
H	2.97898200	-2.64374900	-1.78813400
H	4.40235600	-1.60274200	-1.62807900
H	3.04068600	-1.07431000	-2.61738800
H	4.48106000	1.41935400	-1.09930900
H	3.10678000	2.52842300	-1.00014100
H	3.15593200	1.28181800	-2.26112300
H	-4.81418400	-3.31498000	-0.26562300
H	-5.13495500	-1.57018300	-0.46665900
H	-4.70952200	-2.21159100	1.13588300
H	-0.15287600	-3.04196700	-1.24938100
O	-3.99491600	0.33357900	0.87231000
C	-2.88044000	0.30533300	0.34837200
H	-2.69413500	-4.10336700	-0.95325100
N	-3.11545300	-2.12788700	-0.24091200
C	-2.10746500	1.54366800	0.05848400
C	-2.87732300	2.72441100	0.07309500
C	-2.32238900	3.94701700	-0.28090600
C	-0.97467700	3.99791500	-0.64635200
C	-0.19761100	2.83878500	-0.62023900
C	-0.72359300	1.57877300	-0.26384600
H	-3.92489800	2.65427300	0.34762100
H	-2.93241100	4.84594300	-0.28308500
H	-0.52377800	4.94256800	-0.94083100
H	0.85246500	2.91948300	-0.88072400
C	-2.35774800	-1.00163800	-0.10767800

AcOH

O	0.64114400	1.20465300	0.00000600
C	0.09067100	0.12199300	-0.00002200
C	-1.39501900	-0.11340200	0.00000700
H	-1.92068600	0.84232000	-0.00026500
H	-1.68277800	-0.69439100	-0.88300000
H	-1.68281000	-0.69395800	0.88330800
O	0.78134900	-1.04174600	-0.00001000
H	1.73242300	-0.80877100	0.00008400

TMSCCBr

C	-0.99275200	0.00002900	-0.00057200
C	0.22596000	0.00010700	-0.00082000
Si	2.07979300	0.00002400	-0.00022000
Br	-2.78725500	0.00003700	-0.00002300
C	2.66108400	0.31281000	1.76612600
C	2.66314400	1.37282800	-1.15348300
C	2.66224200	-1.68579500	-0.61152200
H	2.30290000	-0.46426800	2.45216100
H	2.30787100	1.28079200	2.14179200
H	3.75799200	0.31795600	1.81238100
H	2.30762800	2.35607200	-0.82250600
H	2.30914500	1.21549000	-2.17950200
H	3.76014100	1.40734000	-1.18113900
H	2.30659200	-2.49514900	0.03755200
H	3.75915300	-1.72865400	-0.62651000
H	2.30731400	-1.89108800	-1.62870900

TS2_3

Ir	-0.38375800	-0.45514100	0.31744000
C	-0.98690700	-0.90435700	2.42882500
C	-1.48991700	0.08467500	3.42965000
C	-1.81844700	-1.76422100	1.59477500
C	-3.31149200	-1.73057300	1.53753500
C	-0.97188300	-2.71763900	0.94104700
C	-1.39803400	-3.82936400	0.03568100
C	0.38371500	-2.43142000	1.33279500
C	1.58738400	-3.22463000	0.94403600
C	0.38797400	-1.32691600	2.26299300
C	1.55757800	-0.93667400	3.11319400
C	-2.48214100	-0.78082600	-1.90791800
H	5.45568500	-1.15389700	0.10789100
C	-3.53942200	-0.14630200	-2.50774300
C	-4.58491700	2.12039000	-2.40703600
H	-2.41902400	0.55798200	3.10134900
H	-0.75348400	0.86788400	3.62441100
H	-1.69267200	-0.43116800	4.37798600
H	-3.70432900	-0.74211000	1.78723300
H	-3.71668400	-2.44246900	2.26952100
H	-3.68790700	-2.01924100	0.55280900
H	-0.77436500	-3.87032000	-0.86440900
H	-2.44107500	-3.72126600	-0.27122700

H	-1.29651900	-4.79679800	0.54447700
H	1.41297200	-3.82290800	0.04780900
H	1.83939900	-3.91126300	1.76381800
H	2.45396300	-2.57872700	0.77836800
H	1.67956100	-1.67115700	3.92081800
H	1.42021300	0.04223700	3.57616300
H	2.48869600	-0.92593800	2.53872900
H	-5.16449100	1.68585000	-3.22236600
H	-4.08613900	3.02718000	-2.74862200
H	-5.23965300	2.36390200	-1.57006000
H	-2.13176000	-1.79004100	-2.04354100
O	-3.16116700	3.36710900	-0.36009600
C	-2.32080600	2.46514800	-0.30862200
H	-4.24463100	-0.48890000	-3.24979800
N	-3.59023700	1.12088400	-1.99904800
C	-1.07092400	2.59885100	0.47906700
C	-0.84905900	3.90940600	0.96480400
C	0.29084600	4.23774200	1.67689900
C	1.24987400	3.24414900	1.89500200
C	1.04066900	1.95144400	1.41771800
C	-0.12265400	1.57271900	0.72340700
H	-1.60241900	4.65976400	0.75058900
H	0.44160100	5.24944100	2.04239900
H	2.16509800	3.47278000	2.43577900
H	1.81381400	1.21428200	1.59471600
C	-2.56721500	1.25126400	-1.10413100
N	-1.87868700	0.10085500	-1.04846500
C	1.48477000	-0.26267600	-0.69170700
C	2.64153400	0.21596800	-0.70028000
Si	4.36299800	0.87879800	-0.87399800
C	4.45935800	1.79101300	-2.52222600
H	5.45938900	2.22126300	-2.66542300
H	4.25851300	1.12274300	-3.36811100
H	3.73409500	2.61259300	-2.56371200
C	4.73953200	2.06345100	0.54575300
H	4.08164800	2.93927200	0.52344200
H	5.77337400	2.42316200	0.45665500
H	4.63953700	1.58245900	1.52578400
C	5.53292700	-0.60251100	-0.83696700
H	5.32420800	-1.30164300	-1.65543900
H	6.57218000	-0.26486400	-0.94239500
Br	0.76932300	-1.54128800	-2.14767100

Int4_3

Ir	-0.32775500	-0.49288300	0.17449800
C	-0.71015100	-1.55546100	2.25895000
C	-0.93622700	-0.94740900	3.60314200
C	-1.76900300	-2.07603800	1.42551800
C	-3.21688800	-1.97643400	1.76732900
C	-1.17987700	-2.77991600	0.32831900
C	-1.88019100	-3.58295600	-0.71664500
C	0.25886600	-2.70743800	0.47599100
C	1.26273200	-3.43824500	-0.34895000
C	0.55112500	-1.99335300	1.70012800
C	1.88941000	-2.01008100	2.36529300
C	-3.17726300	-0.21605000	-1.07617800
H	4.89769300	-1.32842900	-2.45201800
C	-4.04906300	0.70604700	-1.59112800
C	-4.15879800	3.20230100	-1.74143400
H	-1.76469900	-0.23377500	3.59048800
H	-0.04820500	-0.44679400	3.98915600
H	-1.20045800	-1.75168400	4.30362200
H	-3.48424600	-0.96608900	2.09020800
H	-3.42397700	-2.65094300	2.60956400
H	-3.86181000	-2.26973900	0.93797800
H	-1.56572400	-3.27731200	-1.72061000
H	-2.96568100	-3.49330800	-0.64080300
H	-1.61924200	-4.64180200	-0.59638000
H	0.86825700	-3.69551200	-1.33304100
H	1.53885900	-4.36838900	0.16629900
H	2.17029000	-2.84223800	-0.47632700
H	2.15124300	-3.05471800	2.57716700
H	1.88844800	-1.46932100	3.31267600
H	2.66738600	-1.59891500	1.71523600
H	-5.13427400	2.95429200	-2.16084400
H	-3.54692100	3.70565800	-2.48979800
H	-4.28088200	3.85382200	-0.87610300
H	-3.23889100	-1.28923400	-1.11991500
O	-1.70901700	3.99812700	-0.62634300
C	-1.50940400	2.86667900	-0.18573100
H	-4.98820000	0.58180800	-2.10874200
N	-3.52260500	1.94196200	-1.33830700
C	-0.52144500	2.59703000	0.88419100
C	-0.16630000	3.75157900	1.62044400
C	0.72963500	3.69636700	2.67281600
C	1.31532600	2.46719800	2.98024700
C	0.99173400	1.32996200	2.24325700
C	0.04652900	1.34487600	1.20419700
H	-0.62765100	4.69060100	1.33436400
H	0.97761600	4.59126400	3.23580100
H	2.04173900	2.38683400	3.78489600
H	1.52294600	0.42192500	2.48140000
C	-2.35649400	1.76460700	-0.65967400
N	-2.13417900	0.45411500	-0.48694700
C	1.55606100	-0.03801900	-0.28628600
C	2.72665000	0.22139600	-0.54928100
Si	4.45527000	0.66821200	-0.99855700
C	4.54059200	2.53666900	-1.26457300
H	5.56163400	2.84804700	-1.52173900
H	3.87981700	2.85597400	-2.07989000
H	4.24274200	3.08367100	-0.36154900
C	5.61125300	0.16213400	0.40901100
H	5.34791300	0.66456100	1.34800400
H	6.64908900	0.42923800	0.16979800
H	5.58318300	-0.92000300	0.58815200
C	4.93582500	-0.23994600	-2.58447900
H	4.26499900	0.01804800	-3.41318800
H	5.95762000	0.02134300	-2.88985900
Br	-0.25815500	-0.89949800	-2.37913900

TS3_3

Ir	-0.63245300	-0.47660800	0.11383200
C	-1.48777100	-1.82706800	1.86205500
C	-1.61321500	-1.55674800	3.32694900
C	-2.57047100	-1.65591200	0.93033100
C	-3.91397500	-1.11749000	1.29580900
C	-2.15500300	-2.15780300	-0.34333600
C	-3.01340000	-2.34092500	-1.55087900
C	-0.80484000	-2.70456900	-0.18857700
C	-0.06487200	-3.51843500	-1.19861100
C	-0.40814300	-2.52048500	1.17509800
C	0.80883300	-3.15371100	1.77822500
C	-2.86519300	1.38761000	-0.93575700
H	4.30634700	-2.82270400	-1.12817900
C	-3.06494100	2.66732500	-1.38697400
C	-1.78612100	4.82116700	-1.32463600
H	-2.02523200	-0.56133200	3.51844000
H	-0.66325400	-1.64955100	3.85346900
H	-2.30797000	-2.28971400	3.75888500
H	-3.83526400	-0.23557900	1.93813700
H	-4.45518200	-1.88610200	1.86452400
H	-4.51821400	-0.87055100	0.42151300
H	-2.45531200	-2.13712800	-2.46731900
H	-3.89253700	-1.69297400	-1.52819100
H	-3.36312900	-3.38110800	-1.58579400
H	-0.35983500	-3.26334800	-2.21717100
H	-0.28490600	-4.58149900	-1.02991100
H	1.01438600	-3.37561700	-1.10383700
H	0.75669100	-4.23750400	1.61756200
H	0.87269300	-2.98137900	2.85375700
H	1.72895500	-2.79529000	1.30696800
H	-2.69703700	5.16960200	-1.81198300
H	-0.93204800	4.96118600	-1.98712900
H	-1.62309600	5.37906800	-0.40187300
H	-3.48877000	0.51989800	-1.06531300
O	0.61671800	4.08464600	0.01058500
C	0.11879600	2.99840100	0.30194200
H	-3.88967100	3.11201900	-1.92319300

N	-1.96402000	3.39474700	-1.02909100
C	0.62132300	2.17828100	1.43049400
C	1.16500200	2.93440000	2.48838800
C	1.63141700	2.33538000	3.64779700
C	1.58556200	0.94106000	3.74708000
C	1.09604000	0.17467500	2.69735200
C	0.59792500	0.76298800	1.51593300
H	1.19141600	4.01310900	2.37491800
H	2.02917700	2.93924600	4.45756700
H	1.95772200	0.44008200	4.63664700
H	1.17385100	-0.89822700	2.77177000
C	-1.12154400	2.56462800	-0.35395600
N	-1.66146500	1.33976300	-0.28487600
C	1.35857000	-0.13535500	0.04226200
C	2.54140500	-0.21275600	-0.30516400
Si	4.27532900	-0.32190200	-0.91947900
C	4.56980800	1.10601200	-2.11770000
H	5.58665100	1.06321400	-2.52934600
H	3.86663700	1.06870900	-2.95848100
H	4.44959400	2.07826700	-1.62455900
C	5.46060500	-0.22280300	0.54854200
H	5.35054100	0.72251700	1.09366300
H	6.50149600	-0.29056600	0.20586400
H	5.29122800	-1.04173300	1.25851800
C	4.48442900	-1.97851900	-1.80616900
H	3.78787200	-2.07294600	-2.64814200
H	5.50300700	-2.08143100	-2.20331400
Br	-0.35169200	-0.27285800	-2.46162000

TS4_3

Ir	-1.29517100	-0.08126400	-0.14971900
C	-2.78354600	-0.93837500	1.29029300
C	-2.52228700	-1.62021900	2.59484500
C	-2.98592500	0.48796600	1.12565000
C	-3.02708700	1.49997800	2.22812500
C	-3.42787100	0.71810400	-0.24975800
C	-3.89100000	2.03022100	-0.79925400
C	-3.38615400	-0.52823800	-0.93240000
C	-3.75849800	-0.76336600	-2.36276500
C	-2.95406500	-1.56560400	0.00945500
C	-2.93683800	-3.03866800	-0.27031300
C	-0.43137500	2.66844000	-1.33961500
H	4.73290400	-2.12553800	1.42241800
C	0.40135300	3.73013900	-1.07640000
C	2.10913500	4.29746100	0.66187400
H	-1.85889200	-1.03545600	3.23754700
H	-2.08984200	-2.61263900	2.45965400
H	-3.47630700	-1.73848500	3.12654200
H	-2.34187200	1.24192400	3.04012400
H	-4.04145600	1.54691200	2.64724600
H	-2.77197900	2.50033600	1.86720300
H	-3.81740200	2.06388300	-1.88943700
H	-3.31945900	2.86628800	-0.38654000
H	-4.94469000	2.18995800	-0.53255000
H	-3.51613800	0.09754900	-2.99244100
H	-4.84015400	-0.93865500	-2.43772500
H	-3.25720700	-1.64388800	-2.77333700
H	-3.95123200	-3.45053800	-0.18484200
H	-2.29957900	-3.57335400	0.43811800
H	-2.57721800	-3.25704000	-1.28006900
H	2.27612300	5.12632700	-0.02656400
H	3.03954200	3.74951400	0.81146400
H	1.75435000	4.67444100	1.62162600
H	-1.14448300	2.53851100	-2.13881300
O	1.83638000	2.15842500	2.50407100
C	1.22658000	1.49249000	1.66372600
H	0.55296500	4.66229700	-1.59915900
N	1.10088500	3.42069600	0.05631400
C	1.06293400	0.02186900	1.80460900
C	1.56836700	-0.54412000	2.97648700
C	1.55176200	-1.92844900	3.17029700
C	1.00529100	-2.76907300	2.19067000
C	0.49962800	-2.22276800	1.02133600
C	0.53265300	-0.81394900	0.75479000
H	1.97474600	0.10997900	3.74096500
H	1.95700700	-2.34910400	4.08599900
H	0.97900600	-3.84375900	2.34850600
H	0.09363300	-2.88340600	0.26039900
C	0.70142800	2.18044800	0.46579500
N	-0.23305700	1.71727900	-0.37837000
C	1.66389600	-0.78252700	-0.79248700
C	2.90431100	-0.74912000	-0.91981100
Si	4.72394500	-0.70384600	-0.64523900
C	5.60895000	-0.82117800	-2.31162100
H	6.69799200	-0.81066900	-2.17078600
H	5.35156100	-1.74727300	-2.84012900
H	5.34984400	0.02005300	-2.96620600
C	5.16640300	0.93178900	0.19381700
H	4.91383200	1.78844700	-0.44345800
H	6.24459700	0.97844100	0.39646700
H	4.64266900	1.05299200	1.14944600
C	5.22116200	-2.16863800	0.44169200
H	4.95161700	-3.12446300	-0.02420200
H	6.30664400	-2.17410800	0.60694500
Br	0.18687800	-0.85283400	-2.14357500

TS5_3

Ir	-0.86805200	-0.07697000	-0.14049800
C	-2.24831400	-1.05520000	-1.80600600
C	-1.84261800	-1.89224000	-2.97821800
C	-2.61667400	-1.53952800	-0.52592200
C	-2.67896200	-2.97353800	-0.09456400
C	-3.05354200	-0.39383100	0.28137200
C	-3.73640200	-0.48234900	1.61216200
C	-2.94090600	0.78197700	-0.52919100
C	-3.42142200	2.15453700	-0.17217000
C	-2.37832800	0.39305100	-1.80239000
C	-2.24370400	1.29690200	-2.99183500
C	-0.50204800	-0.78104900	2.84100000
Br	-0.30970300	2.99010300	1.63607600
C	0.24808200	-1.53356100	3.71222900
C	2.17593900	-3.10773800	3.54354500
H	-1.30711800	-2.79520100	-2.67205000
H	-1.21117800	-1.33971300	-3.67718400
H	-2.74146700	-2.20984800	-3.52427000
H	-1.92945600	-3.58322700	-0.60765300
H	-3.66623500	-3.39606500	-0.32542900
H	-2.52309900	-3.07686400	0.98296300
H	-3.62613900	0.44123800	2.18729700
H	-3.35656200	-1.31240800	2.21324600
H	-4.81178100	-0.65262100	1.46374700
H	-3.39966400	2.32904300	0.90620600
H	-4.46046100	2.27464300	-0.50805700
H	-2.82745300	2.93249200	-0.65814800
H	-3.21787400	1.41475600	-3.48621400
H	-1.54615300	0.89773000	-3.73174400
H	-1.90040500	2.29443300	-2.70161200
H	2.04608300	-3.08531500	4.62611200
H	3.18173900	-2.77766900	3.28310500
H	2.02311600	-4.12012200	3.16996300
H	-1.33187200	-0.12562800	3.04811200
O	2.62054200	-3.26898900	0.80149400
C	1.82466200	-2.35928000	0.55459800
H	0.19483200	-1.64476800	4.78468900
N	1.17846600	-2.19840200	2.96811700
C	1.71616500	-1.78280200	-0.81078400
C	2.44444500	-2.47139900	-1.80149100
C	2.48436000	-2.02700900	-3.11680400
C	1.80525500	-0.85286100	-3.45821900
C	1.07963900	-0.16107600	-2.49051400
C	0.97456100	-0.62321400	-1.16013400
H	2.98123300	-3.36678700	-1.50662300
H	3.04932800	-2.57695100	-3.86369300
H	1.84049700	-0.47436200	-4.47657100
H	0.57195000	0.75588300	-2.76745800
C	0.99432600	-1.84531700	1.65781100
N	-0.03307800	-0.98641700	1.57445300
C	0.16494400	1.53162200	0.52799700

C	1.27950400	1.25466100	-0.06875900
Si	3.02044000	1.86742600	-0.49295900
C	3.01827000	2.77719700	-2.14343800
C	4.28981800	0.48307900	-0.47398400
C	3.36395600	3.07948000	0.91593100
H	4.26954900	-0.08409000	0.46374000
H	5.29081600	0.92548500	-0.56861700
H	4.16138500	-0.21894100	-1.30319700
H	2.86130100	2.10621900	-2.99408900
H	3.98924900	3.27055100	-2.28541000
H	2.24444200	3.55365000	-2.17042200
H	2.62841800	3.88878000	0.96200600
H	4.35303200	3.53161400	0.76170000
H	3.37532700	2.57577000	1.88937400

TS6_3

Ir	-0.79927900	-0.14788000	0.24238100
C	-2.57490200	-1.62264700	0.66788600
C	-2.50573900	-3.08864900	0.96293500
C	-2.57691300	-0.57045900	1.62828700
C	-2.51559700	-0.72472100	3.11646900
C	-2.79724400	0.69382300	0.92628000
C	-3.16469900	1.99710400	1.56999500
C	-2.91322200	0.39580400	-0.47151600
C	-3.28119600	1.35738300	-1.55805700
C	-2.74593000	-1.02461100	-0.64449400
C	-2.99092300	-1.75651900	-1.93061600
C	0.23014600	1.65318700	2.51991900
C	2.47384100	3.34886500	-1.17008600
C	1.33308200	1.99193500	3.26514000
C	3.66826000	1.15274300	3.51973100
H	-1.98142400	-3.28996500	1.90108100
H	-2.00189300	-3.64205900	0.16680800
H	-3.52203700	-3.49510500	1.05636600
H	-1.96404100	-1.62143600	3.41033600
H	-3.53338100	-0.80900100	3.52067500
H	-2.04403000	0.13793200	3.59517400
H	-2.76373000	2.85705100	1.02733400
H	-2.82815400	2.05115600	2.60836600
H	-4.25876400	2.09769100	1.58450200
H	-3.01325900	2.38463700	-1.30005200
H	-4.36722000	1.32755500	-1.72226700
H	-2.80019800	1.09945800	-2.50585200
H	-4.06687300	-1.74891500	-2.15216300
H	-2.67810900	-2.80126100	-1.87439900
H	-2.48202300	-1.28453700	-2.77656400
H	3.68068300	1.96493100	4.24778200
H	4.41639100	1.33337600	2.74806600
H	3.88472300	0.20615400	4.01533700
H	-0.73289400	2.13144300	2.48996000
O	3.78280300	-0.96617200	1.72352800
C	2.59357100	-0.85118400	1.41924700
H	1.48412800	2.77087000	3.99736800
N	2.32535400	1.12035500	2.92815300
C	1.92353800	-1.85370400	0.55567500
C	2.55586400	-3.11309800	0.53241700
C	2.05199800	-4.16461700	-0.21821000
C	0.91416700	-3.94996200	-1.00519900
C	0.30822600	-2.70136000	-1.02641700
C	0.75458200	-1.62881600	-0.21777900
H	3.45107300	-3.24309300	1.13092800
H	2.54569000	-5.13175200	-0.20892300
H	0.51188600	-4.75153100	-1.61915800
H	-0.52419300	-2.53860900	-1.69855300
C	1.82001000	0.25755200	1.99177700
N	0.53898600	0.57309700	1.74003300
C	0.39160300	1.17864900	-0.96395800
C	0.82979900	0.02615500	-1.33682900
Br	1.69682100	-0.55436100	-2.92381200
H	2.76425200	3.20045800	-0.12308600
H	2.69926900	4.39082800	-1.43236400
H	-0.19437000	5.18151500	-0.68326700
H	-0.20947700	4.03940500	0.66596500
H	-1.48735400	3.98322900	-0.56848900
H	0.42805400	4.17433500	-3.62658300
H	-0.86124500	2.97010800	-3.45823600
H	0.77721400	2.45601900	-3.88991300
C	-0.41537600	4.14221400	-0.40568800
C	0.20350700	3.15880100	-3.27479700
H	3.11187000	2.70564700	-1.78774700
Si	0.64140300	2.98106200	-1.44617900

Int5_3

Ir	-1.12610700	-0.00626500	0.04542500
C	-3.22138800	0.27756100	1.13620500
C	-3.58490100	1.30964200	2.15625900
C	-3.45247100	0.31346900	-0.24384200
C	-4.15317200	1.37996600	-1.02467800
C	-2.85729100	-0.90436600	-0.83130800
C	-3.03294800	-1.34350300	-2.24929200
C	-2.42214000	-1.76496400	0.27196400
C	-2.00539500	-3.19744200	0.15435100
C	-2.54387200	-0.99362500	1.46232700
C	-2.24766100	-1.44370900	2.85826600
C	-0.71911100	1.84457200	-2.39691600
H	3.28205800	-3.66648600	1.11716100
C	0.11116300	2.80074600	-2.93167700
C	2.13455700	4.05642100	-2.19973000
H	-3.86992100	2.25762800	1.69339000
H	-2.75566400	1.49887100	2.84650000
H	-4.43337000	0.95932600	2.75894900
H	-4.14808100	2.33956000	-0.50113800
H	-5.20059100	1.09152800	-1.18693600
H	-3.70452600	1.52358800	-2.01107300
H	-2.23812500	-2.02813300	-2.55408900
H	-3.03844800	-0.49321300	-2.93705900
H	-3.99440300	-1.86514800	-2.35594000
H	-1.33591800	-3.35311600	-0.69476500
H	-2.89240400	-3.82778700	0.00949200
H	-1.49152200	-3.53686300	1.05716100
H	-3.17148700	-1.80269400	3.33250800
H	-1.86260400	-0.62470000	3.47275400
H	-1.52169800	-2.26008400	2.87595600
H	2.02554100	4.45020100	-3.21093500
H	3.10810200	3.57845200	-2.09084500
H	2.04814800	4.86460200	-1.47318500
H	-1.57013800	1.35751700	-2.84504400
O	2.54179300	3.16964900	0.39390100
C	1.62651800	2.35228200	0.33204600
H	0.09913600	3.29516300	-3.89128100
N	1.06321700	3.07377200	-1.99622800
C	1.33205500	1.52826300	1.56248100
C	1.07032100	2.26626200	2.73284800
C	0.97852400	1.63474000	3.96825300
C	1.19234500	0.25454000	4.05380100
C	1.46781800	-0.48111300	2.90404400
C	1.53567100	0.12797700	1.63652000
H	0.95234900	3.34393300	2.66294000
H	0.76565700	2.21560500	4.86099700
H	1.14454400	-0.24694200	5.01651500
H	1.63030600	-1.55303900	2.97589400
C	0.81698000	2.28492400	-0.90166200
N	-0.27902600	1.53479700	-1.14362000
C	0.66017200	-0.90924500	-0.31064700
C	1.78025400	-0.71933400	0.41321600
Si	3.53976700	-1.39861600	0.08189800
C	4.19445100	-0.75158100	-1.57273900
H	5.21316200	-1.12103500	-1.75046600
H	3.56778100	-1.06670000	-2.41291400
H	4.23478400	0.34518800	-1.57815300
C	4.68592300	-0.75744300	1.44390800
H	4.72239500	0.33859900	1.47129800
H	5.70802700	-1.11355700	1.25774200
H	4.39508300	-1.10657900	2.44147100
C	3.54786900	-3.29116000	0.12070700
H	2.83450700	-3.71159900	-0.59582000
H	4.54524300	-3.67866400	-0.12529400
Br	0.76903600	-1.97716700	-1.96344600

Int6_3

Ir	-1.08863700	0.04231600	-0.00774400
C	-2.78217600	-1.10790200	-1.01811200
C	-2.76115200	-2.54243300	-1.43457900
C	-3.31679700	-0.57752400	0.17831400
C	-3.95058100	-1.34040700	1.29977700
C	-3.10483800	0.86033800	0.14850900
C	-3.64118600	1.80948000	1.16917400
C	-2.55832000	1.22203100	-1.16435300
C	-2.42869100	2.60551300	-1.71992900
C	-2.31189700	0.00667200	-1.86031300
C	-1.85800300	-0.12727200	-3.27879500
C	-0.78418200	-0.43872900	3.00608900
C	2.54398700	2.59857200	1.86104300
C	0.03006000	-0.96916300	3.97839200
C	2.12493900	-2.31362300	4.05095300
H	-2.85581500	-3.21708900	-0.58003800
H	-1.84415300	-2.79295700	-1.97609000
H	-3.60354200	-2.73848700	-2.11221400
H	-3.59652800	-2.37419100	1.33550000
H	-5.04042400	-1.36487400	1.16754900
H	-3.75107300	-0.87774600	2.27044700
H	-3.17143800	2.79179700	1.10764700
H	-3.51876200	1.42273700	2.18537200
H	-4.71882900	1.94137200	0.99592600
H	-2.28643700	3.35106200	-0.93488200
H	-3.35014900	2.86571800	-2.25884100
H	-1.59830200	2.68100400	-2.42694500
H	-2.73554800	-0.12673600	-3.94028800
H	-1.31850700	-1.06168200	-3.44819900
H	-1.21531900	0.70471400	-3.57740700
H	1.90035800	-2.25421800	5.11646900
H	3.09047400	-1.85062300	3.84732800
H	2.15234400	-3.35642400	3.73486000
H	-1.69087100	0.13541400	3.11297000
O	2.78592400	-2.63419700	1.38912100
C	1.77558700	-2.06059200	0.99324400
H	-0.04478000	-0.95368000	5.05529100
N	1.05806300	-1.59628000	3.34095600
C	1.46661400	-2.13083200	-0.48365700
C	1.33237100	-3.42722900	-1.00959400
C	1.25132800	-3.63103100	-2.38393000
C	1.35855000	-2.53962400	-3.25361300
C	1.51789700	-1.25495600	-2.74267100
C	1.54493500	-1.02406400	-1.35669900
H	1.31067800	-4.27490600	-0.33082300
H	1.13851100	-4.63734800	-2.77657000
H	1.32801800	-2.69368600	-4.32850100
H	1.62357300	-0.40982400	-3.41610500
C	0.87231900	-1.44674500	1.98936700
N	-0.25659300	-0.73806700	1.78245000
C	0.75037100	1.08050900	-0.17551600
C	1.66442800	0.35731100	-0.82357300
Br	3.51558900	1.03349000	-1.22652700
H	2.23929500	1.98033100	2.71552700
H	2.82484700	3.58488300	2.25407800
H	-0.00205300	4.31636300	2.18585400
H	-0.72173400	2.71039300	2.33646000
H	-1.17301300	3.77242200	0.98580900
H	1.78706600	5.02123700	-0.25803900
H	0.66065200	4.23353100	-1.37346700
H	2.36348200	3.74452400	-1.34742500
C	-0.34005500	3.44118800	1.61386800
C	1.52467600	4.05996000	-0.71965600
H	3.43426800	2.14571100	1.41619000
Si	1.12459700	2.77915000	0.61628800

TS7_3

Ir	1.17518100	0.16286600	-0.04108800
C	2.24964000	-0.25758200	1.80902500
C	1.88322500	-1.21139700	2.90254200
C	3.27093900	-0.52013000	0.78409900
C	3.94257000	-1.84360800	0.59286200
C	3.48629800	0.66739900	0.06560500
C	4.43367100	0.88795900	-1.07112500
C	2.61396100	1.71376700	0.63195300
C	2.63695300	3.15394500	0.22311100
C	1.93776200	1.16511300	1.76787400
C	1.10233000	1.91935300	2.75376100
C	1.32855900	-2.30536000	-1.80397800
H	-2.68808000	4.10070000	0.17463900
C	0.65607500	-3.38326800	-2.32032200
C	-1.59735700	-4.41153600	-2.03089900
H	1.79257800	-2.23515700	2.52868700
H	0.94319700	-0.93584600	3.38614700
H	2.66998300	-1.20567500	3.66992300
H	3.22956500	-2.67001300	0.67032100
H	4.69625200	-1.98885700	1.37840300
H	4.44955400	-1.91130300	-0.37252000
H	3.97636400	1.48189300	-1.86841400
H	4.78465600	-0.05427200	-1.49912100
H	5.31217600	1.44345400	-0.71581200
H	2.78490000	3.26418000	-0.85415500
H	3.46615500	3.66735500	0.72849900
H	1.70969000	3.66370600	0.49628000
H	1.74805300	2.32349400	3.54478200
H	0.35615000	1.27624200	3.22485300
H	0.58549300	2.75877900	2.28142700
H	-1.09816600	-5.23799900	-2.53787800
H	-2.37515800	-3.99456200	-2.67142600
H	-2.04475000	-4.77033700	-1.10415900
H	2.31957600	-1.94666400	-2.03199900
O	-2.96519100	-2.40959200	-0.63094300
C	-1.90833500	-2.04611600	-0.12770500
H	0.95551200	-4.13544100	-3.03428500
N	-0.58010500	-3.39298600	-1.74231400
C	-1.95643700	-1.44482500	1.25996800
C	-2.06169000	-2.32347100	2.34569100
C	-2.34167600	-1.82915500	3.62013600
C	-2.53808800	-0.45812300	3.80710700
C	-2.42962300	0.42038200	2.72789100
C	-2.13082600	-0.06057900	1.44597100
H	-1.94243600	-3.39233600	2.18825600
H	-2.42377600	-2.51435600	4.45896000
H	-2.77099500	-0.07067100	4.79501800
H	-2.56601800	1.48733700	2.87826700
C	-0.65096600	-2.33968700	-0.86999500
N	0.51797700	-1.66672500	-0.90257700
C	-0.66756200	0.75069700	-0.11251800
C	-1.93086700	0.84733000	0.25841200
Si	-3.36879700	1.80929100	-0.57057300
C	-3.76744900	0.99716400	-2.22844100
H	-4.58351500	1.53555600	-2.72810200
H	-2.90018100	1.00067300	-2.89694400
H	-4.08466000	-0.04393300	-2.09400800
C	-4.87651600	1.69750700	0.55718500
H	-5.17775300	0.66008400	0.74397000
H	-5.72307100	2.20363200	0.07414800
H	-4.71430400	2.18378500	1.52607700
C	-2.86798500	3.61564400	-0.79285700
H	-1.95561800	3.70805400	-1.39135300
H	-3.66508000	4.17221600	-1.30287300
Br	-0.03243700	1.50262200	-2.11726000

Int7_3

Ir	-1.01658200	-0.14384100	0.11703400
C	-1.62774100	-0.07800700	2.27930800
C	-0.92134500	0.61674900	3.40211900
C	-2.82303300	0.43040600	1.60035000
C	-3.42990200	1.77379400	1.85652000
C	-3.29981400	-0.57050600	0.73157500
C	-4.50776300	-0.51972000	-0.14609200
C	-2.40138700	-1.73119700	0.83007000
C	-2.65533300	-3.05532200	0.18004800
C	-1.44379300	-1.45465900	1.87186500
C	-0.48655900	-2.43547100	2.47118300
C	-1.34057400	2.76428200	-0.80606000

H	0.79008100	-3.86931600	-1.48525400
C	-0.70425800	3.87797000	-1.28554500
C	1.67024400	4.58791200	-1.62075400
H	-0.85773300	1.69426700	3.22736600
H	0.09171200	0.23153000	3.54060700
H	-1.47299600	0.46201100	4.33923100
H	-2.66464800	2.54558600	1.97951300
H	-4.01055200	1.73889800	2.78803900
H	-4.10538600	2.07667900	1.05287600
H	-4.26420200	-0.83533800	-1.16532200
H	-4.93439900	0.48514100	-0.18835200
H	-5.27485800	-1.20191900	0.24307100
H	-2.94556300	-2.93107600	-0.86648600
H	-3.47050300	-3.57562800	0.70004100
H	-1.76871400	-3.69295600	0.21651400
H	-0.98529100	-2.95552400	3.29964500
H	0.40272000	-1.94346700	2.87183500
H	-0.17313100	-3.18778500	1.74364700
H	1.20021900	5.56730400	-1.71323200
H	2.07893300	4.27880000	-2.58386200
H	2.47217800	4.63995500	-0.88434000
H	-2.39676500	2.55638200	-0.75196700
O	3.00932700	2.05820400	-1.30611700
C	2.18144400	1.84649800	-0.43155400
H	-1.08879200	4.80659300	-1.67914000
N	0.63824100	3.63985600	-1.18476500
C	2.63089600	1.17868700	0.84883500
C	3.15812000	1.98928800	1.86207200
C	3.78317000	1.40909200	2.96615800
C	3.89139600	0.01877600	3.05512400
C	3.34966200	-0.79448400	2.05909800
C	2.71193200	-0.22238900	0.94992100
H	3.09640400	3.07087800	1.77693300
H	4.19574300	2.04152800	3.74678300
H	4.38719600	-0.43587200	3.90810800
H	3.40609400	-1.87495100	2.14621400
C	0.80900400	2.40738800	-0.62311400
N	-0.39884100	1.85769200	-0.38971000
C	0.72686200	-0.74025100	-0.08367200
C	1.98861800	-1.05939000	-0.07431200
Si	2.75533500	-2.33389200	-1.29124700
C	3.83090400	-1.36874900	-2.50021500
H	4.34398500	-2.06128000	-3.18067900
H	3.23080500	-0.68285600	-3.10962500
H	4.59755900	-0.77953800	-1.98350700
C	3.79008400	-3.55894800	-0.29996700
H	4.62666700	-3.07164500	0.21355900
H	4.21320200	-4.31085600	-0.97953400
H	3.18902600	-4.09009000	0.44783900
C	1.32597600	-3.19445200	-2.16438500
H	0.60161200	-2.47237300	-2.56018500
H	1.69761600	-3.79658600	-3.00345100
Br	-1.58563900	-0.35224400	-2.37549200

TS8_3

Ir	-1.10237100	-0.03190800	-0.19942600
C	-1.56716400	0.06092000	-2.38017700
C	-0.62623700	0.00901600	-3.54493200
C	-2.34998400	-1.05569400	-1.87325300
C	-2.25916400	-2.45097700	-2.40299500
C	-3.23567900	-0.57677800	-0.86766300
C	-4.26288900	-1.35291800	-0.10502700
C	-3.03676200	0.87140400	-0.75293300
C	-3.88062600	1.77798200	0.08739800
C	-2.06085400	1.26221500	-1.73472500
C	-1.68072500	2.66007300	-2.10775400
C	-0.43891700	-2.94193600	0.38406900
H	-0.79594600	3.94613000	0.62182400
C	0.45458600	-3.92488500	0.70096100
C	2.91712300	-4.04570300	1.09535200
H	-0.06666500	-0.93071500	-3.56698000
H	0.09204200	0.83286800	-3.51545700
H	-1.18479600	0.08714800	-4.48771500
H	-1.22472400	-2.74691100	-2.59823000
H	-2.79727000	-2.49649200	-3.35960700
H	-2.71394400	-3.18250300	-1.73229500
H	-4.25632600	-1.07473100	0.95302000
H	-4.09306500	-2.43052000	-0.17532700
H	-5.26476700	-1.14394600	-0.50320000
H	-4.07830600	1.33317400	1.06587600
H	-4.84352000	1.95603700	-0.41006300
H	-3.39634700	2.74400500	0.24714200
H	-2.25785500	2.95844800	-2.99331900
H	-0.62064300	2.74087700	-2.36175600
H	-1.90569100	3.36967600	-1.30953600
H	2.73268200	-5.10978300	0.94411300
H	3.18794500	-3.86152600	2.13619100
H	3.73254200	-3.73236800	0.44220200
H	-1.50878300	-3.00771000	0.28061700
O	3.33346400	-1.24978100	1.70861300
C	2.76603600	-1.13784400	0.63295400
H	0.32673400	-4.98112000	0.88354100
N	1.68346100	-3.32786100	0.75588000
C	3.48039100	-0.35298500	-0.44803400
C	4.71373600	-0.83670200	-0.89384200
C	5.47600900	-0.08754200	-1.79328700
C	5.03188600	1.16345900	-2.23109300
C	3.81271600	1.66594700	-1.78419700
C	3.02918400	0.90716200	-0.90114100
H	5.07935600	-1.79576600	-0.53953200
H	6.42709600	-0.47874400	-2.14211100
H	5.63567600	1.74543700	-2.92063600
H	3.45455300	2.63497900	-2.11591200
C	1.53049000	-2.00128600	0.45203200
N	0.22556000	-1.74835000	0.21832000
C	0.56226900	1.03984400	-0.07012100
C	1.71979400	1.27515700	-0.46743300
Si	1.17930300	2.58903100	1.34996100
C	1.71664200	1.65140200	2.87825400
H	1.77401600	2.35507200	3.72034100
H	0.98137600	0.87964300	3.12683900
H	2.70096200	1.18706100	2.76053300
C	2.45688200	3.86673100	0.81205700
H	3.46350500	3.45382300	0.69696600
H	2.49704200	4.63346200	1.59867800
H	2.17206300	4.36639800	-0.12074000
C	-0.48231000	3.44056400	1.54016300
H	-1.24759200	2.72614100	1.85361200
H	-0.37170900	4.20436900	2.32310500
Br	-1.60019400	-0.13598500	2.33766000

Int8_3

Ir	-1.53460800	-0.27006500	-0.04944900
C	-1.07835500	-2.42221300	0.26721200
C	0.24840300	-3.03102400	0.58879200
C	-2.08352500	-2.01549100	1.20516000
C	-2.00256300	-2.11095900	2.69511100
C	-3.22907500	-1.51765900	0.45055600
C	-4.55083700	-1.12124200	1.03274000
C	-2.94768200	-1.73395400	-0.96333500
C	-3.90021500	-1.48408600	-2.08645700
C	-1.61218400	-2.22848500	-1.08265700
C	-0.90503400	-2.59380400	-2.35050700
C	-1.61855000	1.62672300	2.52136300
H	4.46051500	-2.32896200	2.66732500
C	-0.78728500	2.58663900	3.07101000
C	1.42330700	3.61040800	2.52669900
H	0.60014700	-2.72952300	1.57872300
H	1.00535400	-2.75030200	-0.14761700
H	0.16378400	-4.12619400	0.58038400
H	-0.96814700	-2.09581700	3.04751100
H	-2.45658600	-3.05521300	3.02403400
H	-2.54701100	-1.29782400	3.18301500
H	-5.09148700	-0.43622600	0.37454700
H	-4.43160400	-0.63475400	2.00536400
H	-5.17653900	-2.01175000	1.17983000
H	-4.58604400	-0.66564300	-1.86059800
H	-4.49535800	-2.39242900	-2.25264500

H	-3.37726000	-1.24716500	-3.01539900
H	-1.03658700	-3.66401900	-2.55808200
H	0.16864700	-2.39811300	-2.28117600
H	-1.29897100	-2.03441200	-3.20252900
H	1.39897800	3.85394300	3.58903500
H	1.33659700	4.52623600	1.93937800
H	2.35905200	3.10325600	2.29175100
H	-2.56676800	1.25701600	2.88019600
O	0.48342400	0.51174100	-0.61371600
C	0.89546100	1.50305100	0.03814700
H	-0.87849700	3.16476100	3.97878300
N	0.29140700	2.71729300	2.25038900
C	2.06588200	2.27185200	-0.44382700
C	1.89189000	3.63711600	-0.70930400
C	2.92143000	4.39060400	-1.26975800
C	4.14706800	3.78420200	-1.55157700
C	4.33967200	2.43227800	-1.27927400
C	3.30708500	1.64684700	-0.73137300
H	0.93166700	4.10038500	-0.50268000
H	2.76432900	5.44267000	-1.48649900
H	4.95757400	4.36418100	-1.98289500
H	5.29606500	1.96331500	-1.48615200
C	0.11210500	1.84906700	1.20692500
N	-1.04274300	1.17327600	1.38330300
C	3.58633900	0.27644300	-0.43626300
C	3.94492500	-0.86663700	-0.19231300
Si	4.61660500	-2.55594100	0.17881800
C	3.95238900	-3.77070400	-1.10167300
H	4.36117100	-4.77337300	-0.92023200
H	2.85910400	-3.84569900	-1.06873000
H	4.23836900	-3.47595900	-2.11868500
C	6.49664400	-2.45310100	0.06708100
H	6.82427900	-2.13909800	-0.93141600
H	6.94408700	-3.43506700	0.26910500
H	6.90920300	-1.74336200	0.79429600
C	4.08143400	-3.03868200	1.92190900
H	2.98990800	-3.07675000	2.01781700
H	4.47324300	-4.03111500	2.17977800
Br	-2.38283700	1.67143200	-1.46725400

17a

O	-0.36446400	1.99208100	0.00192100
C	-0.15296900	0.77594200	-0.02174500
H	0.85513200	-1.70749700	0.79092100
N	-2.59934400	0.23276700	0.09521100
C	1.25417100	0.26217900	0.00151900
C	2.26221000	1.15305100	-0.40806800
C	3.60111200	0.77398900	-0.37514700
C	3.95545900	-0.49728900	0.08783400
C	2.96335600	-1.38415700	0.51178300
C	1.61912300	-1.01265300	0.46603100
H	1.97674000	2.14179300	-0.75248200
H	4.36894000	1.46812600	-0.70605200
H	5.00074400	-0.79327900	0.12006700
H	3.23534800	-2.36932100	0.88099400
C	-1.28901600	-0.16051600	-0.09591500
N	-1.22475800	-1.46083100	-0.39726600
C	-2.50825100	-1.90876100	-0.40143200
C	-3.37253500	-0.87487100	-0.09407300
C	-3.12566800	1.55077400	0.45342900
H	-4.19088500	1.43876600	0.66293700
H	-2.98284800	2.25614300	-0.36656100
H	-2.61751800	1.93246100	1.33993200
H	-4.44759200	-0.83444100	0.00570800
H	-2.75557800	-2.93907600	-0.62173600

NaOAc

O	-1.12889800	-0.04724800	0.00000000
C	0.00000000	0.53516800	0.00000000
C	0.03488200	2.06077400	0.00000000
H	-0.97121500	2.48713600	0.00000000
H	0.58011500	2.41881900	0.88124800
H	0.58011500	2.41881900	-0.88124800
O	1.11552500	-0.07510300	0.00000000
Na	-0.02648400	-1.99287500	0.00000000

NaBr

Br	0.00000000	0.00000000	0.61240400
Na	0.00000000	0.00000000	-1.94855700

18a

O	-0.66553100	-0.78891800	-1.27761500
C	-1.42073900	-0.14068400	-0.55266400
H	-3.25293700	1.86429000	-0.47594200
N	-2.98504200	-2.06989600	-0.17978300
C	-1.18056500	1.32041200	-0.30579200
C	0.14244100	1.80666900	-0.12552500
C	0.34396500	3.19195500	0.03271900
C	-0.72576100	4.08178800	-0.01060000
C	-2.02306400	3.60296800	-0.20061700
C	-2.24370900	2.23288600	-0.33625000
H	2.78565200	-2.58919000	1.46731800
H	1.35399500	3.55785500	0.18847200
H	-0.54450300	5.14672700	0.10465500
H	-2.86217600	4.29149800	-0.24047700
C	-2.57576400	-0.78044400	0.09597000
N	-3.34268000	-0.22963300	1.04200700
C	-4.25652900	-1.17691500	1.37879900
C	-4.05114600	-2.32264900	0.63143700
C	-2.43669000	-3.02323900	-1.14539600
H	-3.08962800	-3.89757500	-1.15969600
H	-1.42749700	-3.32151100	-0.85664900
H	-2.40154900	-2.57701800	-2.14018900
H	-4.56407600	-3.27330000	0.60778800
H	-5.01225300	-1.00356600	2.13382300
C	1.28905000	0.95508000	-0.05011800
C	2.31775600	0.30294900	0.05064300
Si	3.85329000	-0.71278200	0.19370900
C	4.80176500	-0.58784200	-1.43284400
H	5.73125300	-1.17021800	-1.38330500
H	4.21168300	-0.97405600	-2.27277500
H	5.07165900	0.45000300	-1.66350000
C	4.89015500	-0.02958900	1.61561500
H	5.16628900	1.01805900	1.44432200
H	5.81888600	-0.60473300	1.72501900
H	4.35147400	-0.08267100	2.56949600
C	3.35503900	-2.50066800	0.53403300
H	2.73494400	-2.90471500	-0.27538400
H	4.24380300	-3.13893600	0.62397900

PhCCBr

C	1.28426800	0.00002200	-0.00002500
C	0.07196700	0.00005900	-0.00003700
H	-1.52401500	2.15434300	0.00000000
Br	3.07646400	-0.00000700	0.00001000
C	-1.35691200	0.00003100	-0.00002300
C	-2.06969100	-1.21561000	-0.00001600
C	-3.46278000	-1.20977400	0.00001200
C	-4.16300900	-0.00004000	0.00002000
C	-3.46284100	1.20973000	0.00000900
C	-2.06975200	1.21563700	-0.00001100
H	-1.52390300	-2.15428900	-0.00000300
H	-4.00305700	-2.15244900	0.00003700
H	-5.24960700	-0.00006600	0.00003000
H	-4.00316600	2.15237800	0.00002800

TS5_3_Ph

Ir	-1.00401100	-0.17033700	0.15051800
C	-2.52457200	-0.09370600	1.91916300
C	-2.29998200	0.53569800	3.26166800
C	-3.13071600	0.51162300	0.78950000
C	-3.67775900	1.90422200	0.69993900
C	-3.22916200	-0.48976900	-0.27615800
C	-3.98504900	-0.32430900	-1.56031800
C	-2.68090800	-1.71164300	0.22732300
C	-2.69747300	-3.03643900	-0.47170700
C	-2.19644900	-1.47147400	1.56967400
C	-1.75409500	-2.53563900	2.53073300

C	-1.07278800	1.70001300	-2.30376100
Br	0.34271200	-2.11479200	-2.51928000
C	-0.58883700	2.89090400	-2.79102800
C	0.97126400	4.66853700	-1.99612800
H	-2.23608900	1.62549100	3.19393500
H	-1.38159100	0.17169400	3.73117900
H	-3.13259800	0.29344600	3.93590000
H	-3.18595600	2.58286800	1.40246900
H	-4.75075300	1.90167700	0.93606300
H	-3.56910900	2.31714400	-0.30756100
H	-3.62821300	-1.01370100	-2.33093100
H	-3.91285500	0.69464600	-1.95095000
H	-5.05232800	-0.53364500	-1.40059100
H	-2.56497000	-2.92693900	-1.55089900
H	-3.66213500	-3.53394500	-0.30125800
H	-1.91275400	-3.70012500	-0.09898000
H	-2.63106100	-3.04792600	2.95043700
H	-1.18799500	-2.11930500	3.36704800
H	-1.13615200	-3.29424500	2.04080900
H	0.79163700	5.02481700	-3.01137900
H	2.03858800	4.50707900	-1.84487900
H	0.61415400	5.40297200	-1.27395900
H	-1.75424500	1.00371300	-2.76415500
O	1.58537300	3.84926900	0.59650400
C	1.06682600	2.74347900	0.42834200
H	-0.76399000	3.40101200	-3.72641100
N	0.24131200	3.40525800	-1.83947700
C	1.27927800	1.63903400	1.40873100
C	2.06876900	1.97306100	2.51755500
C	2.38191600	1.02678500	3.49370600
C	1.91348300	-0.28164100	3.36191900
C	1.13518700	-0.62584500	2.25741500
C	0.76357200	0.31675700	1.26980600
H	2.43607000	2.99008800	2.60313200
H	3.00012200	1.30784500	4.34144900
H	2.16384100	-1.03256400	4.10634100
H	0.80932200	-1.65361800	2.14390700
C	0.26493000	2.52550900	-0.78813500
N	-0.54117400	1.48815200	-1.06378900
C	0.46188700	-1.06100800	-0.89442000
C	1.64918400	-0.80353500	-0.42215900
H	2.88681300	-2.95956500	0.56702000
C	3.05431200	-0.97072300	-0.27300400
C	3.94736800	0.04413800	-0.68758700
C	5.32006800	-0.15926100	-0.60443700
C	5.81893600	-1.36667800	-0.10326100
C	4.94579300	-2.37789500	0.31614700
C	3.57252200	-2.18408000	0.24105100
H	3.55085800	0.97551000	-1.07849100
H	6.00355500	0.61910600	-0.92985900
H	6.89232600	-1.52124600	-0.03839100
H	5.34049800	-3.31330600	0.70132800

TS6_3_Ph

Ir	0.41754900	-0.69787900	0.20759900
C	2.31887200	-2.08648900	0.30487600
C	3.76731800	-1.70741700	0.30273100
C	1.51712700	-2.28684900	1.46083200
C	1.95194900	-2.13586800	2.88709200
C	0.22802400	-2.83150000	1.02791900
C	-0.77835500	-3.48151200	1.93006400
C	0.24873900	-2.92815100	-0.39925500
C	-0.79246800	-3.56263100	-1.26881100
C	1.51952400	-2.42234400	-0.86028500
C	2.00002600	-2.50455300	-2.27732200
C	-1.46734300	-0.18982900	2.60895100
H	-2.76933100	-1.67551000	0.31979500
C	-2.05006900	0.78689000	3.37855700
C	-1.86561800	3.26448000	3.59608700
H	4.00492300	-0.98656900	1.08967800
H	4.08431800	-1.28984600	-0.65431100
H	4.37116400	-2.60698000	0.48493700
H	2.78820500	-1.43788700	2.97977900
H	2.27752700	-3.10573800	3.28670600
H	1.13611800	-1.77602100	3.52130200
H	-1.80408800	-3.36999500	1.56716400
H	-0.72101300	-3.10118700	2.95269900
H	-0.56616300	-4.55865500	1.97775100
H	-1.76544700	-3.60363700	-0.77485700
H	-0.49137100	-4.59287800	-1.50351900
H	-0.90864500	-3.03166200	-2.21791200
H	2.37066500	-3.51886200	-2.48018100
H	2.82086900	-1.81215800	-2.47831800
H	1.19412500	-2.30120200	-2.98805700
H	-2.61901600	3.06644200	4.35950500
H	-2.27399500	3.92524800	2.83160400
H	-0.99260500	3.73529400	4.04834000
H	-1.66874000	-1.24575600	2.60390700
O	0.06902400	3.92872800	1.71232900
C	0.26494000	2.74842200	1.41425900
H	-2.80428400	0.72916200	4.14919700
N	-1.49619200	1.97362800	3.00378100
C	1.38506800	2.35608000	0.52724200
C	2.43608100	3.29323600	0.47414800
C	3.56503700	3.07835000	-0.30174100
C	3.63387600	1.92099700	-1.08650700
C	2.58520000	1.01359600	-1.07988100
C	1.45017800	1.16389800	-0.24475000
H	2.34184100	4.19331000	1.07198400
H	4.37036500	3.80671200	-0.31424700
H	4.49736500	1.73594200	-1.72000500
H	2.62803300	0.16388900	-1.74949800
C	-0.57743300	1.71217100	2.02324500
N	-0.54977500	0.39058200	1.77783200
C	-1.17723700	0.16788100	-0.87035600
C	-0.17041900	0.83213300	-1.34224900
Br	0.16174300	1.62156300	-3.02883100
C	-2.60153300	-0.01435400	-1.04280300
C	-3.31737700	0.83826300	-1.91237100
C	-4.68933300	0.68182100	-2.08389700
C	-5.37684600	-0.32628500	-1.39947400
C	-4.68009600	-1.17657900	-0.53739100
C	-3.30718200	-1.01960300	-0.35572600
H	-2.78829700	1.61616300	-2.45327500
H	-5.22414700	1.34713500	-2.75626500
H	-6.44780500	-0.44632600	-1.53758700
H	-5.20722000	-1.96123400	-0.00136000

Int5_3_Ph

Ir	-1.19480500	-0.06253600	0.03630300
C	-3.37106900	0.54826100	0.77958800
C	-3.83423500	1.88790200	1.25795800
C	-3.48167600	0.01175600	-0.50929000
C	-4.13046100	0.64118200	-1.70045400
C	-2.83567800	-1.31657200	-0.50706400
C	-2.90762800	-2.30288200	-1.62896600
C	-2.47958600	-1.63384600	0.87811900
C	-2.04311100	-2.97222100	1.38655300
C	-2.70791300	-0.45072700	1.63888000
C	-2.51823300	-0.28419600	3.11338000
C	-0.63984800	0.69217300	-2.90813200
Br	0.84590200	-2.60401400	-0.95087500
C	0.19252800	1.40522900	-3.73781700
C	2.07743300	3.01024600	-3.46561000
H	-4.05087400	2.56318200	0.42646600
H	-3.08789000	2.36318100	1.90329800
H	-4.75179300	1.77735300	1.85131700
H	-4.18196900	1.72922400	-1.61080500
H	-5.15707100	0.26293700	-1.79949400
H	-3.60822800	0.39672200	-2.62891300
H	-2.09534700	-3.03059400	-1.57191200
H	-2.86187500	-1.81098200	-2.60497400
H	-3.86038600	-2.84806100	-1.57485400
H	-1.34143000	-3.45258100	0.70078500
H	-2.91786400	-3.62721800	1.49331000
H	-1.56067800	-2.89023500	2.36391800
H	-3.47253200	-0.46907100	3.62571900
H	-2.20293000	0.73143700	3.36856300

H	-1.78157300	-0.98626700	3.51042500
H	2.05952400	2.92129200	-4.55222000
H	3.05614000	2.71848000	-3.08461900
H	1.86899000	4.03895500	-3.17162000
H	-1.42651700	-0.00020300	-3.16095200
O	2.24085100	3.34641600	-0.71208400
C	1.43524600	2.44547800	-0.49186500
H	0.24866500	1.45903700	-4.81456600
N	1.04172700	2.11236200	-2.94036100
C	1.13345900	2.08855700	0.94061700
C	0.79409200	3.18106400	1.76105800
C	0.60415200	3.01552600	3.12812000
C	0.77459900	1.75023500	3.69927100
C	1.12293600	0.66547400	2.89809800
C	1.31980500	0.80594300	1.51083900
H	0.68739400	4.16320100	1.31041000
H	0.33578900	3.86771000	3.74574200
H	0.63477700	1.60886000	4.76731200
H	1.24832900	-0.31577800	3.34592200
C	0.73506500	1.82321800	-1.63553000
N	-0.30089300	0.95843600	-1.61417600
C	0.63355500	-0.95965300	0.08483500
C	1.70231200	-0.39553600	0.68254900
H	3.48904700	-0.56389800	2.75186600
C	3.14267000	-0.78195800	0.62817100
C	3.76900600	-1.07035600	-0.59880900
C	5.12611600	-1.38653900	-0.65627900
C	5.89485600	-1.41509800	0.50981300
C	5.29160300	-1.11785300	1.73347600
C	3.93432600	-0.79898900	1.79070000
H	3.19006700	-1.04274600	-1.51501500
H	5.58535900	-1.60090000	-1.61770000
H	6.95259400	-1.65906300	0.46416800
H	5.87715000	-1.13004400	2.64889100

Int6_3_Ph

Ir	-1.04116100	0.03341600	-0.01949100
C	-3.16497200	-0.67870800	-0.73884300
C	-3.58323100	-2.06673600	-1.10161700
C	-3.32423300	-0.03146300	0.49819500
C	-3.96245600	-0.57439100	1.73818100
C	-2.72496800	1.30497100	0.38236100
C	-2.84541700	2.39633200	1.39762300
C	-2.32859600	1.50209000	-1.01283300
C	-1.93793400	2.80579700	-1.63109700
C	-2.50319600	0.25081200	-1.67382500
C	-2.29217300	-0.01874200	-3.13091500
C	-0.50675300	-0.13628000	3.04222000
H	0.86016200	2.04837300	2.10189900
C	0.30604500	-0.69331900	4.00237000
C	2.14216500	-2.37660800	4.06376800
H	-3.80082700	-2.67224100	-0.21843100
H	-2.81459400	-2.57580700	-1.69210500
H	-4.49174500	-2.02847300	-1.71778800
H	-4.00701300	-1.66656800	1.72951900
H	-4.99012600	-0.19684200	1.82533400
H	-3.42503600	-0.26169100	2.63824100
H	-2.01568800	3.10500600	1.32924800
H	-2.89092700	2.00555100	2.41743200
H	-3.77676900	2.95180500	1.21809700
H	-1.39796700	3.44426300	-0.92849000
H	-2.84665600	3.34122800	-1.93887200
H	-1.31599000	2.66415500	-2.51824600
H	-3.21964700	0.18969100	-3.68203400
H	-2.02669600	-1.06310000	-3.31589300
H	-1.50563800	0.61715000	-3.54554000
H	2.15469800	-2.05080500	5.10441500
H	3.12046700	-2.21524000	3.61194700
H	1.89030200	-3.43601000	4.00611000
H	-1.27248200	0.61307000	3.15538400
O	2.25711900	-3.29186300	1.45442300
C	1.44310800	-2.46197600	1.05715100
H	0.36485100	-0.52644900	5.06736900
N	1.12715000	-1.57476900	3.36870600
C	1.06678500	-2.48940000	-0.39986600
C	0.66074300	-3.74581800	-0.88843500
C	0.46348500	-3.95571600	-2.24842100
C	0.71432700	-2.91821900	-3.15417800
C	1.13548200	-1.67861600	-2.68651500
C	1.30329600	-1.43518300	-1.30996500
H	0.51562600	-4.56143200	-0.18681700
H	0.14023600	-4.92919800	-2.60532700
H	0.58600100	-3.07978000	-4.22080500
H	1.34287900	-0.87361700	-3.38553000
C	0.81469600	-1.55285700	2.03287800
N	-0.18440600	-0.66996200	1.82904900
C	0.85908200	0.83029300	-0.34876700
C	1.69920800	-0.07024800	-0.87076900
Br	3.59811300	0.30263600	-1.22045400
C	1.22670700	2.22801200	-0.01957800
C	1.62803200	3.11524600	-1.03524100
C	1.95389000	4.44002200	-0.74196500
C	1.89708500	4.90537200	0.57413900
C	1.50418900	4.03434400	1.59314900
C	1.16320300	2.71299800	1.29862200
H	1.68169300	2.76099100	-2.06038100
H	2.25653600	5.10842700	-1.54407000
H	2.15630800	5.93556200	0.80325800
H	1.46172500	4.38261200	2.62214600

TS7_3_Ph

Ir	-1.14422300	-0.34817900	-0.00559600
C	-2.36801500	0.09524100	1.76018300
C	-2.27709000	1.28052500	2.67012300
C	-3.37726300	-0.06776400	0.70489400
C	-4.35475200	0.99288500	0.30736400
C	-3.26910800	-1.37285100	0.19039800
C	-4.09847300	-1.99057700	-0.89124000
C	-2.19393500	-2.06822100	0.91952700
C	-1.84962400	-3.51788100	0.76387400
C	-1.72425600	-1.19263800	1.95541000
C	-0.77924900	-1.55291400	3.05754800
C	-1.82815200	1.85149500	-2.01198300
Br	0.11668600	-1.55654400	-2.04659000
C	-1.38206200	2.97445000	-2.66151100
C	0.63824400	4.43371900	-2.55926500
H	-2.37025600	2.21889200	2.11604500
H	-1.33264400	1.29771900	3.21875000
H	-3.09314300	1.24406800	3.40477500
H	-3.90017300	1.98726100	0.32781500
H	-5.19029300	1.00167100	1.02042800
H	-4.76936100	0.81931400	-0.68849100
H	-3.50386600	-2.64186800	-1.53821500
H	-4.58467200	-1.23588900	-1.51470400
H	-4.88550500	-2.61021600	-0.44022100
H	-1.94438400	-3.84422200	-0.27475400
H	-2.53055500	-4.12928500	1.37097800
H	-0.82793900	-3.72302200	1.09341100
H	-1.35296300	-1.94361300	3.90858300
H	-0.21205500	-0.68692500	3.40535900
H	-0.07457200	-2.32807700	2.74665600
H	-0.01803100	5.09592500	-3.12493800
H	1.46433100	4.09854800	-3.18738300
H	1.03253500	4.96508700	-1.69300800
H	-2.72943600	1.28158000	-2.17223300
O	2.39069000	2.84203300	-1.01689000
C	1.41614600	2.38974300	-0.42901900
H	-1.82771000	3.57048200	-3.44341100
N	-0.16564300	3.28451700	-2.12676500
C	1.58489300	2.01241900	1.02708800
C	1.48877200	3.03357500	1.98106400
C	1.87377700	2.79424000	3.30048600
C	2.37351000	1.54091100	3.66912300
C	2.45544100	0.51619300	2.72767600
C	2.05718700	0.74123800	1.40160000
H	1.13425600	4.01765900	1.68634600
H	1.80008500	3.59039500	4.03573600
H	2.68725200	1.35914700	4.69302100

H	2.82079100	-0.46516600	3.01558100
C	0.11421400	2.36936600	-1.14871300
N	-0.90178500	1.48685500	-1.07224200
C	0.75095100	-0.51108500	0.05733500
C	2.02527100	-0.37676100	0.38751100
H	4.54560300	0.57763400	0.33900900
C	3.23888700	-1.10099400	-0.03777900
C	3.18044100	-2.43678000	-0.47344700
C	4.34016900	-3.09936000	-0.87018700
C	5.57540100	-2.44616400	-0.83208200
C	5.64351600	-1.12222100	-0.39219100
C	4.48614600	-0.45394100	0.00592900
H	2.22754600	-2.95361900	-0.49460300
H	4.27980700	-4.13255500	-1.20157400
H	6.47821900	-2.96747900	-1.13845800
H	6.59885100	-0.60556200	-0.35906400

Int7_3_Ph

Ir	-0.99627900	-0.32082300	0.10240000
C	-1.78293900	-0.01420600	2.18977200
C	-1.38875700	1.05198300	3.16364800
C	-3.01082400	0.00235900	1.39174200
C	-3.97083800	1.14886600	1.36107800
C	-3.13094900	-1.23834700	0.73472800
C	-4.23656300	-1.69759800	-0.15832200
C	-1.96822700	-2.06393900	1.09492500
C	-1.80994000	-3.50759100	0.73083200
C	-1.20674900	-1.33903100	2.08116900
C	-0.08192700	-1.88542800	2.90153300
C	-2.00628300	2.16542300	-1.40238700
Br	-1.33089600	-1.11176000	-2.31060700
C	-1.63208200	3.30553100	-2.06258500
C	0.51173000	4.54363100	-2.43691500
H	-1.55744200	2.05167600	2.75312900
H	-0.33804600	0.97144800	3.45110200
H	-1.99516800	0.95907800	4.07473900
H	-3.44824100	2.10869200	1.31549200
H	-4.56688800	1.14608300	2.28351800
H	-4.66198500	1.08565600	0.51747600
H	-3.84496200	-2.23337900	-1.02736700
H	-4.84634000	-0.86425300	-0.51473300
H	-4.88883000	-2.38699400	0.39439600
H	-2.09182000	-3.68730400	-0.30975900
H	-2.45920800	-4.12290200	1.36778800
H	-0.78024100	-3.84509700	0.87102800
H	-0.50011800	-2.35768600	3.80019800
H	0.60630800	-1.10181800	3.22539900
H	0.48505600	-2.64562100	2.35897100
H	-0.17523000	5.33875200	-2.72795400
H	1.06145400	4.18886400	-3.31003900
H	1.21239700	4.92618300	-1.69459500
H	-2.97657600	1.69943200	-1.34789800
O	2.41506800	2.51112600	-1.58681300
C	1.58338400	2.27658700	-0.72235200
H	-2.20265700	4.01701200	-2.64012400
N	-0.28626800	3.45186600	-1.86760200
C	2.05166500	2.00205100	0.68891500
C	2.19997100	3.08757100	1.56222000
C	2.83850500	2.91134900	2.78947400
C	3.33423600	1.65325500	3.14845900
C	3.15993000	0.56273100	2.29870000
C	2.51443200	0.72761300	1.06340800
H	1.83943300	4.07068500	1.27151300
H	2.96092400	3.75721600	3.45958200
H	3.84195500	1.51882100	4.09923400
H	3.51292700	-0.42210200	2.58994500
C	0.13982200	2.42790800	-1.07477600
N	-0.90450100	1.62926600	-0.78482200
C	0.84383200	-0.46659600	0.07207200
C	2.15728400	-0.45034700	0.20029800
H	4.82484400	-0.10351500	-0.14122800
C	3.12536200	-1.42134400	-0.35039800
C	2.69868700	-2.69003000	-0.78460000
C	3.60964900	-3.59088100	-1.32932500
C	4.96070100	-3.24634900	-1.44118000
C	5.39217000	-1.99173500	-1.00613500
C	4.48288400	-1.08141300	-0.46596600
H	1.65284600	-2.96852000	-0.68551300
H	3.26591500	-4.56675000	-1.66150700
H	5.67074600	-3.95254000	-1.86256100
H	6.43962200	-1.71521300	-1.09049500

TS8_3_Ph

Ir	1.14525500	-0.14287800	0.14043000
C	2.28130500	0.79289800	1.81337000
C	1.74361500	1.65176100	2.91514100
C	2.49443800	-0.62531300	1.88367800
C	2.19828000	-1.49584700	3.06517800
C	3.22605900	-1.03490400	0.68852100
C	3.83970300	-2.38165100	0.44054900
C	3.41207900	0.12025200	-0.12289300
C	4.16618900	0.17317500	-1.41167900
C	2.78070600	1.25758000	0.52824500
C	2.89108200	2.68520100	0.08590900
C	0.38413200	-3.14165500	0.29269100
C	-1.10783400	4.75727600	0.22754600
C	-0.52213200	-4.13080100	0.04405100
C	-2.90433100	-4.20070000	-0.74231900
H	0.95531900	1.14831300	3.48173700
H	1.34964000	2.59624300	2.53494600
H	2.55636100	1.89056600	3.61449300
H	1.37031400	-1.09853300	3.65840800
H	3.08164900	-1.54989500	3.71608200
H	1.94651100	-2.51644000	2.76563200
H	3.68580100	-2.72012500	-0.58846100
H	3.44113700	-3.14005900	1.11946900
H	4.92306600	-2.33223900	0.61350100
H	4.22705300	-0.81040100	-1.88321500
H	5.18982600	0.52081800	-1.21415000
H	3.70446500	0.86404800	-2.12013800
H	3.81971000	3.13290200	0.46539500
H	2.05623800	3.28667200	0.45601200
H	2.90371200	2.76354200	-1.00458500
H	-2.80162500	-5.24905900	-0.46085600
H	-3.04331700	-4.12424100	-1.82272100
H	-3.76966500	-3.77935600	-0.22670100
H	1.41169800	-3.23508700	0.59406800
O	-2.93871100	-1.36502600	-1.94998600
C	-2.61529900	-1.28476400	-0.77943600
H	-0.45135800	-5.20606300	0.10690400
N	-1.67996300	-3.50425600	-0.33746500
C	-3.52418000	-0.57602800	0.19726500
C	-4.84886500	-1.01070500	0.29698700
C	-5.72772700	-0.38167700	1.18262000
C	-5.30104100	0.69698900	1.96218700
C	-3.98910600	1.15175500	1.86253600
C	-3.09615400	0.51779600	0.98470100
H	-5.19226200	-1.84199000	-0.31041400
H	-6.75259800	-0.73295800	1.25649100
H	-5.99223000	1.18496000	2.64233200
H	-3.64952100	2.00322000	2.44345100
C	-1.46237100	-2.15663600	-0.30167600
N	-0.19789600	-1.90869000	0.08130300
C	-0.54315100	0.91362100	0.38815000
C	-1.74226000	0.92257400	0.80738000
H	-1.54804100	1.64152800	-2.06848700
C	-1.46601100	4.91212200	-1.11597300
C	-1.62780000	3.79408200	-1.94574500
C	-1.43166500	2.51617700	-1.43970800
H	-0.64147700	3.34422000	1.79002000
H	-1.00182400	5.62720600	0.86856200
Br	0.76742600	-0.09557800	-2.40383400
H	-1.63248400	5.90780700	-1.51734700
H	-1.91819600	3.92510700	-2.98389700
C	-1.04211400	2.35085100	-0.08880400
C	-0.90183800	3.48273500	0.74612700

Int8_3_Ph

Ir	-1.48678500	-0.44316100	-0.06584600
C	-0.76658800	-2.55137900	0.04005000
C	0.62202300	-3.03917900	0.30269400
C	-1.80514500	-2.36321700	1.00893600
C	-1.69656500	-2.60197000	2.48086800
C	-3.00772400	-1.93126600	0.30566800
C	-4.36339400	-1.75553300	0.91671000
C	-2.71458300	-1.97279900	-1.12376300
C	-3.70349700	-1.73204100	-2.21732000
C	-1.33101900	-2.28909900	-1.28492800
C	-0.58591000	-2.43180500	-2.57547200
C	-1.68682700	1.18217300	2.68688800
Br	-2.65746400	1.50026600	-1.22869600
C	-0.98819100	2.22302700	3.27298300
C	0.99863200	3.62891200	2.70328500
H	0.94011700	-2.81966300	1.32499200
H	1.34073200	-2.59318900	-0.38898400
H	0.66068900	-4.12825400	0.16457400
H	-0.67470000	-2.45827200	2.84132100
H	-1.98700900	-3.63817400	2.70036800
H	-2.36265000	-1.94724000	3.04873100
H	-4.98638400	-1.08003400	0.32525600
H	-4.29694200	-1.35468900	1.93190600
H	-4.87664600	-2.72493500	0.97281600
H	-4.45917400	-1.00099600	-1.92438000
H	-4.21275200	-2.67766100	-2.44830500
H	-3.21910800	-1.37606900	-3.12882500
H	-0.54983300	-3.48913200	-2.86961400
H	0.44465200	-2.07769900	-2.48107600
H	-1.06624600	-1.87282400	-3.38218600
H	0.98157600	3.81563500	3.77709600
H	0.75203100	4.54826400	2.16962500
H	1.98995900	3.28229600	2.41151600
H	-2.54193300	0.64036200	3.06112200
O	0.37677400	0.66831300	-0.62928000
C	0.65945400	1.66141800	0.08595100
H	-1.11624600	2.71091000	4.22796200
N	0.00449800	2.58802900	2.41481300
C	1.65359600	2.65636000	-0.38346500
C	1.22592800	3.97808300	-0.56937400
C	2.08133700	4.92993400	-1.12125700
C	3.38308300	4.56755000	-1.47519200
C	3.82724800	3.26272000	-1.27922300
C	2.97552900	2.28048900	-0.73704800
H	0.20768000	4.25057500	-0.30638100
H	1.73101500	5.94583600	-1.27550100
H	4.05813000	5.30414400	-1.90098000
H	4.84414700	2.98571300	-1.53778000
C	-0.09475800	1.77815800	1.31614200
N	-1.11588800	0.91216700	1.48903600
C	3.49070300	0.97172800	-0.50252000
C	4.02250500	-0.10267800	-0.29165300
H	5.92993600	-1.25552700	-1.77865800
C	4.65034800	-1.35945400	-0.04022100
C	4.28994200	-2.12723900	1.08658000
C	4.91280100	-3.34920300	1.33032900
C	5.89872400	-3.82347800	0.46009000
C	6.26326700	-3.06789800	-0.65822200
C	5.64830800	-1.84390700	-0.91065000
H	3.52983400	-1.75228800	1.76529400
H	4.63042600	-3.93159000	2.20308900
H	6.38253400	-4.77689200	0.65362600
H	7.02998400	-3.43286000	-1.33600100

18a_Ph

O	0.72836400	-0.76274700	1.30031000
C	1.54342100	-0.21831100	0.55449700
H	3.61666000	1.53069400	0.45629900
N	2.81450700	-2.34193500	0.13252500
C	1.49049100	1.26090600	0.30821300
C	0.23835100	1.91343500	0.13908500
C	0.21737900	3.31414400	-0.01956200
C	1.39346300	4.05736300	0.01258000
C	2.62050200	3.41501000	0.19014500
C	2.66277600	2.02788400	0.32535300
H	-4.46922100	1.81848900	-0.58738700
H	-0.73804900	3.80807900	-0.16715900
H	1.35062600	5.13682800	-0.10261500
H	3.54202200	3.98911100	0.22059700
C	2.58525600	-1.00488400	-0.12388800
N	3.39657900	-0.55889700	-1.08802900
C	4.15790800	-1.62290400	-1.45526000
C	3.81274800	-2.73532500	-0.70878700
C	2.15729300	-3.21805500	1.10332800
H	2.67059900	-4.18078100	1.08496400
H	1.10641600	-3.35428100	0.84319300
H	2.22032400	-2.78872500	2.10426400
H	4.18422900	-3.74996700	-0.70572400
H	4.91067400	-1.55005200	-2.22949700
C	-1.00202600	1.21246400	0.07385600
C	-2.09852400	0.69175800	-0.01565700
C	-3.35872100	0.03013100	-0.10001200
C	-3.44699100	-1.35926700	0.12859600
C	-4.67740200	-2.00661000	0.04811500
C	-5.83522000	-1.28538200	-0.25947400
C	-5.75755200	0.09179700	-0.48745500
C	-4.53176200	0.74894000	-0.40997100
H	-2.54529500	-1.91457100	0.36886400
H	-4.73368700	-3.07705400	0.22662600
H	-6.79321000	-1.79436600	-0.32154500
H	-6.65495000	0.65583400	-0.72703900

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C	-0.59850700	-0.00014500	0.00000600
C	0.61202500	-0.00022000	-0.00006400
C	2.08732700	-0.00000400	-0.00014600
Br	-2.39686100	-0.00002000	-0.00001900
C	2.59618300	-1.13445900	-0.91890500
C	2.59552300	-0.22860700	1.44186300
C	2.59537700	1.36334400	-0.52287200
H	2.24911800	-0.99517000	-1.94862000
H	2.24749500	-2.11240700	-0.56934600
H	3.69256000	-1.14214800	-0.92360100
H	2.24764100	-1.18973000	1.83606000
H	2.24754300	0.56358800	2.11379600
H	3.69190900	-0.22992200	1.45152200
H	2.24726600	1.54946500	-1.54478700
H	3.69176800	1.37260000	-0.52633700
H	2.24728000	2.18496400	0.11267200

TS5_3_tBu

Ir	0.92849400	0.08752200	0.04126800
C	2.97009000	1.30711200	-0.24964700
C	3.15286900	2.78793900	-0.36849900
C	3.08086500	0.51761100	0.90215300
C	3.42186500	0.96552300	2.28778000
C	2.77178200	-0.87756900	0.52495600
C	3.00345900	-2.07131300	1.39636800
C	2.63145800	-0.92182500	-0.93213200
C	2.58768800	-2.16354700	-1.76606200
C	2.64142000	0.42662200	-1.38714800
C	2.57217400	0.88881100	-2.80888100
C	0.00089000	-0.29735800	2.95047500
Br	-0.44828400	-3.04630500	0.10144100
C	-1.01691800	-0.03357200	3.83735600
C	-3.12715800	1.29438000	3.82464900
H	3.18389900	3.27458100	0.60949400
H	2.35016500	3.24651700	-0.95577900
H	4.09658500	3.01115100	-0.88383100
H	3.27272500	2.04082600	2.41582400
H	4.47531700	0.74220400	2.50387400
H	2.82076500	0.44514000	3.03956500
H	2.34791100	-2.89992900	1.11900900
H	2.84346300	-1.84105000	2.45303100
H	4.04413000	-2.40694800	1.28579900
H	1.91422900	-2.91012100	-1.33899200
H	3.59250200	-2.60268000	-1.82225800
H	2.25623500	-1.94888500	-2.78507600

H	3.59063800	1.02184000	-3.19932100
H	2.05813500	1.84984300	-2.90055100
H	2.06190300	0.16297300	-3.44642100
H	-3.19664300	0.84773800	4.81706500
H	-3.99586000	1.01114000	3.22994400
H	-3.08657800	2.38064900	3.90562400
H	0.86989600	-0.92090600	3.08116500
O	-3.09800900	2.53276400	1.34782400
C	-2.11242200	1.89987900	0.97764600
H	-1.17777800	-0.36079400	4.85357600
N	-1.89969400	0.78483600	3.20093100
C	-1.59715400	2.13031600	-0.41482300
C	-1.40941200	3.48017400	-0.78374500
C	-1.05168600	3.81948300	-2.08407800
C	-0.89906900	2.81983100	-3.05352300
C	-1.09770600	1.48279800	-2.71077600
C	-1.45040800	1.14589300	-1.40105000
H	-1.55368300	4.25548500	-0.03721600
H	-0.90454900	4.86271100	-2.34823100
H	-0.63233400	3.08370600	-4.07332500
H	-0.99265300	0.70484900	-3.46015100
C	-1.42454100	1.01289600	1.93486700
N	-0.25548500	0.35438300	1.77999600
C	-0.59584500	-1.15468200	-0.46814000
C	-1.72757400	-0.74429200	-1.03371000
C	-3.04655600	-1.36928200	-1.48355100
C	-2.76377800	-2.48804000	-2.51514400
C	-3.97372000	-0.32846100	-2.13874100
C	-3.78651300	-1.95791100	-0.25754300
H	-4.20289400	0.49575700	-1.45463100
H	-4.91883600	-0.81069400	-2.41468700
H	-3.53664600	0.09543500	-3.04837000
H	-2.28307700	-2.07986900	-3.41194300
H	-3.70381800	-2.96318200	-2.82127800
H	-2.10890000	-3.25900600	-2.10091800
H	-3.17614800	-2.69942600	0.26355300
H	-4.71478900	-2.44403000	-0.58172100
H	-4.05171700	-1.16867700	0.45571700

TS6_3_tBu

Ir	0.74736300	0.06177300	-0.23110300
C	2.20596700	-0.74904100	-1.89290500
C	1.85139400	-1.46453500	-3.15891000
C	2.37477500	0.65559400	-1.74395100
C	2.23866000	1.68794700	-2.82057200
C	2.84839100	0.91891800	-0.38531100
C	3.45298100	2.20893600	0.08406200
C	2.96517300	-0.34570700	0.28355900
C	3.61050900	-0.59122300	1.61093800
C	2.52881600	-1.37458600	-0.62317800
C	2.68183800	-2.84466900	-0.36707200
C	0.01891000	3.05284300	-0.19422100
C	-1.42767200	1.00319600	3.60509400
C	-1.01583300	3.94992900	-0.29319900
C	-3.45634600	3.84419300	-0.79624900
H	1.23001700	-0.84660800	-3.81285700
H	1.31665100	-2.39743400	-2.96609000
H	2.76789600	-1.71606300	-3.70969200
H	1.57852300	1.35019100	-3.62384700
H	3.22292500	1.89574600	-3.26145400
H	1.84893500	2.63289500	-2.43163800
H	3.28624900	2.38681200	1.14940400
H	3.07759000	3.06768500	-0.47792500
H	4.53959200	2.17446400	-0.07667200
H	3.53316400	0.27364500	2.27305300
H	4.67970600	-0.79336000	1.45491000
H	3.18521400	-1.46241800	2.11579400
H	3.74701000	-3.11077600	-0.40815600
H	2.16801200	-3.44962500	-1.11694500
H	2.31473400	-3.12987000	0.62353000
H	-3.33988900	4.91954500	-0.65586000
H	-4.16183500	3.44781500	-0.06600900
H	-3.82525400	3.63729200	-1.80070700
H	1.04645300	3.23918300	0.06317000
O	-3.90040000	1.14245800	-1.24369600
C	-2.70932000	0.85784100	-1.09860400
H	-1.04118700	5.02141400	-0.16390400
N	-2.13411500	3.23630900	-0.60556800
C	-2.20458100	-0.50439600	-1.39053500
C	-3.03970200	-1.26604300	-2.23328000
C	-2.71539100	-2.56378900	-2.59752100
C	-1.55207900	-3.14048900	-2.07423700
C	-0.74246100	-2.41585700	-1.21011400
C	-1.00557700	-1.06575700	-0.87889600
H	-3.94970000	-0.80218700	-2.59856500
H	-3.36604000	-3.12796200	-3.25904200
H	-1.28667300	-4.16478100	-2.32284900
H	0.10960100	-2.90932700	-0.76110900
C	-1.77346200	1.91880700	-0.70282300
N	-0.45803300	1.79749900	-0.45462700
C	-0.15360800	0.05665400	1.70543200
C	-0.82484200	-0.87718600	1.12871600
Br	-1.84905400	-2.32883100	1.78391100
H	-1.89180600	1.77880900	2.98630500
H	-1.36312500	1.38124100	4.63238400
H	0.96050400	2.26835200	4.14977000
H	0.43826400	2.70721400	2.51563300
H	1.87533200	1.69333600	2.74745700
H	0.65180100	-0.05170700	5.04681600
H	1.60890700	-0.70974600	3.70722000
H	-0.01635700	-1.34171700	4.02687600
C	0.86863900	1.90283300	3.12041200
C	0.59703200	-0.43489800	4.02071700
H	-2.08436900	0.12721200	3.60514800
C	-0.01265800	0.64498200	3.09344800

Int5_3_tBu

Ir	0.98695500	0.05634900	-0.08700100
C	3.01159400	0.08054900	-1.33790600
C	3.20362800	0.56363100	-2.74078100
C	3.23961800	0.78532600	-0.14867500
C	3.77420500	2.17436500	-0.00294900
C	2.83648100	-0.08637600	0.97311100
C	3.08512700	0.21084100	2.41708900
C	2.54116700	-1.41238700	0.42347700
C	2.35625800	-2.66688300	1.21827200
C	2.54191000	-1.27693700	-0.99433500
C	2.33960900	-2.36488700	-2.00090100
C	0.35239700	2.79200000	1.22493500
H	-2.51455800	-3.80541900	0.66321400
C	-0.60444500	3.77338000	1.33297700
C	-2.82133500	4.25884100	0.30417700
H	3.31344000	1.65012400	-2.78516400
H	2.36256800	0.27583100	-3.38058200
H	4.10788200	0.11562200	-3.17404600
H	3.63335100	2.76309000	-0.91316000
H	4.85175200	2.13394800	0.20722300
H	3.30602500	2.70746300	0.82914000
H	2.42817500	-0.37770900	3.06115200
H	2.93070200	1.27003500	2.64432800
H	4.12570700	-0.03712300	2.66967800
H	1.70496900	-2.50171600	2.07981000
H	3.32944500	-3.01632800	1.58722100
H	1.91845500	-3.46240900	0.60990100
H	3.31735200	-2.74612300	-2.32657300
H	1.81847800	-2.00174300	-2.89109900
H	1.77483200	-3.20320100	-1.58664100
H	-2.70759800	5.14360800	0.93135500
H	-3.70700400	3.69946800	0.60591000
H	-2.92170700	4.55522700	-0.74000300
H	1.28515100	2.69035200	1.75591000
O	-3.24040500	2.09799000	-1.39006000
C	-2.14757300	1.60282100	-1.12819600
H	-0.64011800	4.66786700	1.93641700
N	-1.61723800	3.43896300	0.48544500
C	-1.70603700	0.39140500	-1.91467500
C	-1.55705000	0.57847900	-3.30089100
C	-1.30488800	-0.50417100	-4.13746400

C	-1.22715100	-1.79228600	-3.59655800
C	-1.38571400	-1.98556100	-2.22658700
C	-1.62743900	-0.90677200	-1.35506600
H	-1.65204100	1.57783100	-3.71617200
H	-1.18633600	-0.34803300	-5.20579800
H	-1.04301300	-2.64556000	-4.24346100
H	-1.32488600	-2.98797100	-1.81310700
C	-1.27939900	2.26154000	-0.13135500
N	-0.06915500	1.86597300	0.31720800
C	-0.65799800	-0.80772200	0.79457300
C	-1.78231300	-1.14159000	0.13084100
C	-3.13367400	-1.70500100	0.65926400
C	-3.78849200	-0.69299800	1.62859400
H	-4.73390800	-1.09904500	2.00963900
H	-3.14746800	-0.46869900	2.48329900
H	-4.01463300	0.24792600	1.11287100
C	-4.13841000	-1.93368800	-0.49139300
H	-4.33788400	-1.01397300	-1.05280000
H	-5.08978100	-2.27700000	-0.06809700
H	-3.79948000	-2.69664200	-1.19943900
C	-2.91445500	-3.06304100	1.36461600
H	-2.21741500	-2.97843600	2.20083100
H	-3.86766100	-3.44622400	1.75016100
Br	-0.53725900	-0.95541900	2.75353900

Int6_3_tBu

Ir	-1.03746000	-0.03969600	-0.04068600
C	-2.61584600	-0.11105300	1.63175300
C	-2.46240000	0.41476400	3.02165700
C	-3.20946700	0.54240900	0.53101800
C	-3.81781700	1.90988100	0.50953500
C	-3.11575200	-0.35441700	-0.61587000
C	-3.78115400	-0.10243100	-1.92967800
C	-2.57515100	-1.63568800	-0.15346400
C	-2.57554300	-2.92970500	-0.90615100
C	-2.20825400	-1.46287800	1.21046600
C	-1.70811500	-2.52997000	2.13052000
C	-0.82032900	2.69166300	-1.44843000
C	1.92237700	-0.28221700	-3.15151100
C	-0.00338500	3.78055000	-1.64358000
C	2.19555400	4.56968800	-0.77290700
H	-2.51090700	1.50611500	3.05317600
H	-1.51734400	0.09468100	3.47044400
H	-3.27136300	0.02298300	3.65350400
H	-3.42158000	2.54292000	1.30805200
H	-4.90450300	1.83606700	0.65118300
H	-3.64856000	2.41707900	-0.44475300
H	-3.42851600	-0.78047600	-2.70787800
H	-3.63673000	0.92797000	-2.26826200
H	-4.86256800	-0.26086600	-1.81103500
H	-2.55988100	-2.78011200	-1.98731900
H	-3.49338600	-3.48333400	-0.66371700
H	-1.72631000	-3.55994100	-0.62938100
H	-2.56531500	-3.03709500	2.59520800
H	-1.09180600	-2.12197600	2.93448900
H	-1.12615800	-3.28359600	1.59396000
H	1.94521100	5.40307800	-1.42997600
H	3.12835700	4.10728100	-1.09478900
H	2.30489500	4.92475300	0.25230300
H	-1.77370300	2.46501900	-1.89883100
O	2.97013500	2.54792600	0.96038100
C	1.92295300	1.92699900	0.80419300
H	-0.12011100	4.65531600	-2.26542900
N	1.09595400	3.60146300	-0.85887200
C	1.64988400	0.76887700	1.73601000
C	1.62762800	1.09379600	3.10425600
C	1.62478100	0.09483700	4.07249800
C	1.69381900	-1.24838400	3.68325600
C	1.73510600	-1.57978800	2.33327500
C	1.69150400	-0.58706200	1.33797300
H	1.63580200	2.13833400	3.40178900
H	1.60250100	0.36073500	5.12533800
H	1.72283500	-2.03340100	4.43379900
H	1.80598200	-2.61988000	2.02959800
C	0.94717300	2.41366000	-0.18970300
N	-0.22362900	1.85251700	-0.55139700
C	0.70193600	-0.83055000	-0.98433900
C	1.70108300	-0.96259600	-0.10098100
Br	3.51249300	-1.72054000	-0.49851800
H	1.70527200	0.78888900	-3.06152900
H	1.98657600	-0.51748300	-4.22143600
H	-0.36171500	-0.93880600	-4.32653200
H	-0.74545100	0.30909400	-3.13239700
H	-1.34896500	-1.34518000	-2.92128400
H	1.08745600	-2.83891000	-3.81795600
H	0.22681800	-3.23354200	-2.32033000
H	1.97834200	-2.97113700	-2.29102600
C	-0.49738700	-0.75035900	-3.25407400
C	1.04261100	-2.63376400	-2.74082100
H	2.89950800	-0.47059200	-2.70572700
C	0.79505300	-1.12455800	-2.50381900

TS7_3_tBu

Ir	-1.06085600	-0.02946400	-0.02359800
C	-1.91815300	-0.00524000	1.98862400
C	-1.30623300	0.51093600	3.25380000
C	-2.93951100	0.70818200	1.20922200
C	-3.35761900	2.12065500	1.47294900
C	-3.41973600	-0.15837900	0.21263000
C	-4.46140000	0.12499900	-0.82419600
C	-2.72659000	-1.45054200	0.35976800
C	-3.05106100	-2.67860400	-0.43277500
C	-1.88649200	-1.38139500	1.51690700
C	-1.16095400	-2.52356400	2.15572100
C	-0.89129900	2.80169600	-1.12688900
Br	-0.34103800	-0.89285400	-2.48532100
C	-0.06779300	3.84474600	-1.46868700
C	2.35518500	4.38240400	-1.23840500
H	-1.05498900	1.57233400	3.17287000
H	-0.39938000	-0.03782400	3.51782600
H	-2.02104500	0.39963000	4.08105800
H	-2.49840700	2.75661300	1.70568800
H	-4.02734600	2.14712800	2.34308200
H	-3.89441100	2.55516600	0.62642200
H	-4.17214100	-0.26776300	-1.80389200
H	-4.65455400	1.19583100	-0.92552800
H	-5.40597200	-0.36104100	-0.54489900
H	-3.28394100	-2.43508000	-1.47240100
H	-3.93109500	-3.17296400	0.00054200
H	-2.22525700	-3.39394800	-0.42453500
H	-1.83586900	-3.03434900	2.85537700
H	-0.29026200	-2.18290800	2.71963100
H	-0.82984800	-3.25685200	1.41572100
H	1.98562800	5.36026600	-1.54856600
H	3.01291000	3.97174500	-2.00469700
H	2.90600600	4.47914200	-0.30256100
H	-1.94568500	2.67354900	-1.31418900
O	3.42998500	1.95409700	-0.38446100
C	2.34716900	1.63232100	0.09129900
H	-0.27142400	4.78299900	-1.96270300
N	1.18809100	3.51098400	-1.05417900
C	2.34686600	0.70904800	1.28991900
C	2.63530200	1.28198500	2.53552700
C	2.83804300	0.46885200	3.65020000
C	2.76352800	-0.92093600	3.52103100
C	2.47233900	-1.49419700	2.28359300
C	2.26955700	-0.68943900	1.15172900
H	2.71505000	2.36176200	2.62770900
H	3.06231500	0.91879300	4.61305400
H	2.92372200	-1.55892000	4.38555400
H	2.39316400	-2.57251700	2.19235800
C	1.12404600	2.28369200	-0.44778700
N	-0.14991000	1.84161200	-0.49310800
C	0.64419900	-0.85490100	-0.38970500
C	1.88362200	-1.26598800	-0.19361000
C	2.84668900	-2.09224800	-1.08188700
C	2.14255500	-3.37842300	-1.56229500
C	4.11509000	-2.48927500	-0.30364700

C	3.27532600	-1.23516400	-2.29446500
H	2.41203000	-0.92820300	-2.89009200
H	3.94826300	-1.81571700	-2.93712000
H	3.80766400	-0.33395800	-1.97130100
H	3.89464500	-3.14923900	0.54164000
H	4.65548100	-1.61496500	0.07415000
H	4.78673500	-3.03168200	-0.97874100
H	1.85514800	-4.01065400	-0.71364000
H	2.81988200	-3.95693000	-2.20189300
H	1.24207400	-3.14911700	-2.13738000

Int7_3_tBu

Ir	-0.94479300	-0.12816100	0.07441600
C	-1.44428300	-0.51161800	2.22642600
C	-0.60503500	-0.19836500	3.42597500
C	-2.58999700	0.28572000	1.78120300
C	-2.99304700	1.58904800	2.39569200
C	-3.23770400	-0.41159900	0.74337100
C	-4.46496500	-0.00659900	-0.00555000
C	-2.50207200	-1.66216900	0.49965500
C	-2.97171900	-2.74946500	-0.41620000
C	-1.46890000	-1.76355500	1.49868800
C	-0.63047700	-2.96837000	1.78526900
C	-0.90898000	2.92605800	-0.10473600
H	0.55956200	-3.19294800	-2.24350600
C	-0.15022200	4.04165300	-0.34196900
C	2.28082700	4.53522000	-0.63876400
H	-0.38124100	0.87023600	3.48875000
H	0.33852700	-0.74878300	3.41226700
H	-1.14651800	-0.47967500	4.33933700
H	-2.12471600	2.22351400	2.59604600
H	-3.48824200	1.39983600	3.35744400
H	-3.69153100	2.14158900	1.76280800
H	-4.31323100	-0.09902000	-1.08540800
H	-4.75196300	1.02425600	0.21444400
H	-5.29989400	-0.66236600	0.27401100
H	-3.35129300	-2.33750500	-1.35470800
H	-3.78579300	-3.31075100	0.06146100
H	-2.16877000	-3.45200600	-0.65081500
H	-1.15783000	-3.60138200	2.51117100
H	0.33482000	-2.69666200	2.21834800
H	-0.45594900	-3.56497300	0.88677600
H	1.91941100	5.55467300	-0.50236300
H	2.65087800	4.40357100	-1.65602900
H	3.08495300	4.33766100	0.07052400
H	-1.98017500	2.83602300	-0.03257400
O	3.32949800	1.90548200	-0.98005900
C	2.47369300	1.54054100	-0.18577900
H	-0.42403400	5.07793100	-0.47129800
N	1.15148000	3.63058200	-0.39237900
C	2.83049100	0.48259100	0.83375000
C	3.45601900	0.91133400	2.01188100
C	3.97383700	-0.02259000	2.90809700
C	3.86814600	-1.38845900	2.63022400
C	3.22691700	-1.82077400	1.47044800
C	2.71058000	-0.89142400	0.55218800
H	3.55108100	1.97413600	2.21803700
H	4.46325500	0.31520900	3.81694000
H	4.27033800	-2.11922600	3.32602000
H	3.11219600	-2.88236600	1.28091500
C	1.18074300	2.28436900	-0.15986600
N	-0.08012200	1.84067500	0.01498200
C	0.67741800	-0.86756100	-0.44155000
C	1.89148300	-1.31528900	-0.64341800
C	2.40232400	-2.06688000	-1.88694900
C	3.32728900	-1.11911400	-2.67992300
H	3.73261100	-1.64752700	-3.55130900
H	2.78003600	-0.24035900	-3.03720700
H	4.16938500	-0.77272800	-2.07137100
C	3.18929700	-3.32774700	-1.48201300
H	4.08786000	-3.08376300	-0.90631300
H	3.50952900	-3.85539600	-2.38830500
H	2.57358300	-4.01685400	-0.89244100
C	1.20232300	-2.47175900	-2.76232400
H	0.58908600	-1.60431800	-3.03256000
H	1.55717800	-2.94085000	-3.68700900
Br	-1.67124200	0.37935300	-2.33150900

TS8_3_tBu

Ir	1.07628600	-0.00284700	-0.14726700
C	1.74958500	-0.12955800	-2.27790100
C	0.93385800	0.01516700	-3.52658400
C	2.60702600	0.90678600	-1.70555900
C	2.74846300	2.28662600	-2.26686100
C	3.33244400	0.34692300	-0.62864800
C	4.34768400	1.02018300	0.23861500
C	2.96033600	-1.06873000	-0.51601900
C	3.65590500	-2.05100900	0.37541600
C	2.05909700	-1.36806800	-1.60218800
C	1.58997000	-2.72355800	-2.02887900
C	0.21642000	2.95348400	-0.13512500
H	0.74917300	-3.56892600	0.78111100
C	-0.74380100	3.90940700	0.03184100
C	-3.19750900	3.89816900	0.53758200
H	0.45870000	0.99904300	-3.58443500
H	0.15014500	-0.74523600	-3.58334600
H	1.57384000	-0.09710700	-4.41260100
H	1.79372000	2.68759400	-2.61757300
H	3.42166800	2.24681000	-3.13424200
H	3.18144200	2.98563600	-1.54669900
H	4.17267400	0.78349400	1.29246900
H	4.31922800	2.10683200	0.12509600
H	5.35628900	0.67565500	-0.02571600
H	3.77001400	-1.65191400	1.38706900
H	4.65805900	-2.26809600	-0.01837400
H	3.10900500	-2.99417000	0.44000100
H	2.20709600	-3.05920000	-2.87318300
H	0.54960500	-2.70990100	-2.36380700
H	1.69194500	-3.46212400	-1.23107600
H	-3.13371000	4.92203300	0.16829300
H	-3.39750300	3.90637700	1.61090700
H	-4.00668800	3.38399900	0.01569900
H	1.27168600	3.08335300	-0.29909100
O	-3.24534500	1.19628500	1.77330300
C	-2.80358100	0.99870000	0.65348600
H	-0.70048100	4.98756000	-0.00021700
N	-1.91551500	3.24062500	0.26474400
C	-3.57246100	0.09097000	-0.27625500
C	-4.88853100	0.43662400	-0.59012300
C	-5.65320800	-0.40064100	-1.40695100
C	-5.12040000	-1.59658300	-1.89786200
C	-3.81593200	-1.96214900	-1.57785000
C	-3.03387900	-1.12262100	-0.76497900
H	-5.31487000	1.35610100	-0.20142500
H	-6.67274200	-0.11951000	-1.65374000
H	-5.72430400	-2.24298300	-2.52723700
H	-3.39262400	-2.89134700	-1.94502400
C	-1.65708000	1.89911700	0.22053000
N	-0.34881000	1.70104300	-0.03182000
C	-0.54537900	-1.11806900	0.02196600
C	-1.68577700	-1.37648300	-0.41080100
C	-1.08446500	-2.61124200	1.44799700
C	-1.65387300	-1.78132900	2.56824900
H	-1.74017500	-2.44291300	3.44456800
H	-0.98668100	-0.95756800	2.83109900
H	-2.65319700	-1.40149000	2.34306700
C	-1.98559200	-3.72002000	0.94595700
H	-3.01948000	-3.40418500	0.79212700
H	-1.99210000	-4.49063500	1.73113100
H	-1.60103600	-4.18619200	0.03430400
C	0.33397900	-3.08244700	1.66645500
H	0.98654100	-2.27618400	2.00116200
H	0.27978200	-3.84082000	2.46393200
Br	1.40040400	0.42415300	2.38586700

Int8_3_tBu

Ir	1.45089500	0.14267000	-0.04222900
C	1.54371400	2.33547300	0.38736600

C	0.44243500	3.23210300	0.85442800
C	2.50472800	1.65946900	1.20719400
C	2.57313200	1.69970900	2.69999600
C	3.42267600	0.94327900	0.32975400
C	4.66077300	0.21989200	0.76179100
C	3.07677400	1.29532200	-1.04404800
C	3.84699500	0.89439900	-2.25978000
C	1.89308200	2.09244100	-1.01348000
C	1.18055500	2.68122200	-2.19090800
C	1.24655200	-1.80459600	2.48115100
H	-4.18361000	2.77596100	2.39631400
C	0.27422900	-2.62856600	3.01811900
C	-2.09574600	-3.22362200	2.50452200
H	0.14436000	3.00532700	1.88123900
H	-0.43651900	3.15075000	0.20944700
H	0.78121700	4.27665100	0.82551300
H	1.58341900	1.82320200	3.14774100
H	3.19069900	2.55326800	3.01044000
H	3.03124400	0.79637400	3.11056700
H	4.96166300	-0.53465800	0.03085100
H	4.51898100	-0.27818500	1.72504100
H	5.48978800	0.93188800	0.87189400
H	4.29312600	-0.09557200	-2.14789400
H	4.65727300	1.61887000	-2.41949700
H	3.21770100	0.88724400	-3.15213200
H	1.56488400	3.69005200	-2.39214000
H	0.10635900	2.76586500	-2.00509700
H	1.32553100	2.07915000	-3.09131300
H	-2.10656000	-3.48185000	3.56357400
H	-2.16938600	-4.13257900	1.90498600
H	-2.93370700	-2.56337600	2.28328600
H	2.25601800	-1.63085200	2.82039500
O	-0.70994800	-0.20540800	-0.54133600
C	-1.26496200	-1.14705300	0.07755100
H	0.28509300	-3.25383800	3.89856100
N	-0.83119100	-2.53153200	2.22780100
C	-2.53954600	-1.71969700	-0.41452900
C	-2.56271900	-3.08848400	-0.72396600
C	-3.69251300	-3.67297300	-1.29078900
C	-4.82368800	-2.89119500	-1.53515400
C	-4.81949400	-1.53481500	-1.22217400
C	-3.68140700	-0.91606600	-0.66824100
H	-1.67647800	-3.69063800	-0.54707500
H	-3.68675400	-4.72940300	-1.54079600
H	-5.71288900	-3.33780100	-1.97054600
H	-5.70202700	-0.92996500	-1.40376600
C	-0.52938500	-1.65981400	1.21717500
N	0.73092000	-1.20474800	1.38150600
C	-3.75691900	0.47340000	-0.34101600
C	-3.95902200	1.64415200	-0.08467600
C	-4.23858800	3.05910600	0.22231100
C	-3.55284300	3.96021300	-0.83078800
H	-3.77200900	5.01249400	-0.61467600
H	-2.46554700	3.82685100	-0.81842600
H	-3.91490700	3.73331500	-1.83939900
C	-5.76830700	3.28491100	0.17939600
H	-6.17314300	3.05240500	-0.81156100
H	-5.99349000	4.33368400	0.40555400
H	-6.28058200	2.65662700	0.91624200
C	-3.70309900	3.39743500	1.63262400
H	-2.62068000	3.24079000	1.69344500
H	-3.91190900	4.44838800	1.86447100
Br	1.79802800	-1.90579000	-1.52031500

18a_tBu

O	-0.44342300	-0.82654500	-1.28761000
C	-1.12736500	-0.10401200	-0.56211800
H	-2.73620900	2.08077600	-0.54069400
N	-2.86364500	-1.87670000	-0.17660700
C	-0.73745900	1.32348800	-0.31176300
C	0.62532100	1.66573500	-0.09827000
C	0.96486700	3.02389100	0.06107600
C	-0.00286500	4.02186800	-0.01554700
C	-1.33862200	3.68268100	-0.23864600
C	-1.69790400	2.34260500	-0.37424300
H	2.62414000	-2.43878600	1.49306700
H	2.00327800	3.28319600	0.24362100
H	0.28709100	5.06254900	0.10085400
H	-2.09917300	4.45553200	-0.30385400
C	-2.34242100	-0.62527500	0.08527600
N	-3.06341300	0.00512800	1.01766900
C	-4.06188700	-0.85150300	1.35829600
C	-3.95493600	-2.02152300	0.62832600
C	-2.38740300	-2.89232300	-1.11648600
H	-3.10518900	-3.71437200	-1.11247500
H	-1.40465900	-3.25868300	-0.81558600
H	-2.31557900	-2.47469800	-2.12166700
H	-4.54918200	-2.92391300	0.61467100
H	-4.80508400	-0.59980000	2.10366900
C	1.66944600	0.69269400	0.00834400
C	2.61141300	-0.06553900	0.12427400
C	3.73012500	-1.01905200	0.23898100
C	4.50939200	-1.04847700	-1.09721400
H	5.33673600	-1.76486600	-1.02824400
H	3.86043500	-1.35251600	-1.92578000
H	4.92657600	-0.06331000	-1.33346200
C	4.67304500	-0.57586800	1.38106800
H	5.08924100	0.41878800	1.18620100
H	5.50570200	-1.28347300	1.47402200
H	4.14267800	-0.54291100	2.33920300
C	3.16794500	-2.42697700	0.54203900
H	2.48220800	-2.75423100	-0.24706800
H	3.98962200	-3.15039800	0.60660300

22a

C	-2.70109700	-0.07030100	0.08563000
C	-3.16012700	-0.23599600	-1.22441100
C	-4.29218300	0.46692900	-1.63180600
C	-4.95272700	1.31373200	-0.73632100
C	-4.48629900	1.46231100	0.57092900
C	-3.35181200	0.76677400	0.99258700
H	-2.64182100	-0.90055300	-1.90782800
H	-4.66065900	0.35159100	-2.64694000
H	-5.83586300	1.85775000	-1.05962900
H	-5.00381900	2.11759700	1.26553600
H	-2.97496900	0.86510100	2.00481200
S	-1.26264300	-0.98964100	0.63060000
N	-0.07573100	-0.20584700	-0.31485500
H	-0.10677900	0.80671100	-0.15175300
H	5.63656400	0.90721600	-0.06737700
C	1.27549500	-0.63398100	-0.28828800
C	1.67931300	-1.94851300	-0.43241400
C	3.05599800	-2.27355500	-0.43214400
C	4.02535500	-1.30330000	-0.31149600
C	4.11231300	2.41533300	0.07324100
C	2.71573900	2.64438100	0.08344900
N	1.81921500	1.68268700	-0.02628500
C	2.25959700	0.40096000	-0.15639200
C	3.64519600	0.05716100	-0.17829500
C	4.57131300	1.12472000	-0.05588300
H	0.93817300	-2.73088000	-0.54048300
H	3.34197300	-3.31640000	-0.53730900
H	5.08088500	-1.56165800	-0.32014500
H	4.79730200	3.25224700	0.16727500
H	2.33187600	3.65797600	0.18746900
O	-1.06886400	-0.74066800	2.06657000
O	-1.34131100	-2.37561300	0.15273700

25a

C	2.69202600	0.22441600	-0.03245100
C	2.75663400	-1.12437500	-0.41561700
C	3.97430600	-1.80442300	-0.39378200
C	5.13809500	-1.14838300	0.01159800
C	5.08283000	0.19682200	0.38515600
C	3.86935400	0.87939200	0.35676000
H	1.87102400	-1.64972300	-0.76318100
H	4.01338500	-2.84604300	-0.70059800
H	6.08489700	-1.68155200	0.03007200

H	5.98630200	0.71400700	0.69683700
H	3.81112600	1.92654300	0.63453900
C	1.42653800	1.03717500	-0.03642900
N	0.26213800	0.30893200	-0.01192000
H	0.31255100	-0.70055800	0.08682200
H	-5.43777600	-0.75153300	0.06293400
C	-1.05773100	0.76502900	-0.03436100
C	-1.45406700	2.09048900	-0.11295500
C	-2.82970600	2.41959100	-0.13194100
C	-3.80898800	1.45384500	-0.07251400
C	-3.92806000	-2.27760300	0.15180200
C	-2.53432300	-2.51801700	0.16354000
N	-1.62926700	-1.55917200	0.10398800
C	-2.05646400	-0.26822400	0.02780900
C	-3.43905600	0.08617600	0.00898900
C	-4.37433800	-0.97817400	0.07455900
H	-0.70284100	2.86618800	-0.15575300
H	-3.10741500	3.46834500	-0.19403500
H	-4.86244400	1.72035200	-0.08644700
H	-4.62086300	-3.11189200	0.20297700
H	-2.15883200	-3.53837500	0.22404300
O	1.45481200	2.26668700	-0.04795900

26a

Rh	1.06334600	-0.89017400	-0.70197600
Rh	-1.06344100	-0.89029900	0.70194200
O	0.03253200	-2.21443200	-1.92708500
O	-1.56016400	-2.60200100	-0.39046600
C	-0.98514000	-2.84351200	-1.49410200
C	-1.55949700	-3.93283300	-2.36262200
H	-0.82014700	-4.29705200	-3.07904800
H	-1.92490600	-4.75803400	-1.74525200
H	-2.41234400	-3.51513900	-2.90962600
C	0.37514400	2.94511500	-3.51369700
H	3.64666800	2.97824100	0.66628000
H	3.43502200	4.98494400	-0.71210300
H	1.91957100	5.05338100	-2.68096400
H	-1.00952200	1.71571300	-4.61466800
H	-0.66521200	-0.26049200	-3.11472000
O	2.93223400	-0.89944000	2.17017100
C	2.98993800	2.95063800	-0.18988400
C	2.85513900	4.10745300	-0.98625800
O	1.56006300	-2.60208100	0.39020200
O	-0.03249800	-2.21461000	1.92700100
C	0.98524900	-2.84353300	1.49397100
C	1.55991300	-3.93255000	2.36267000
H	1.92911700	-4.75611400	1.74541700
H	2.41014200	-3.51326200	2.91254000
H	0.81955000	-4.29935700	3.07674300
C	2.01711200	4.15572100	-2.07777900
C	-0.31298600	1.78491000	-3.78635800
C	-0.12486900	0.66356100	-2.95779300
N	0.70449500	0.69224800	-1.91949500
C	1.40755300	1.82936500	-1.61681900
C	-4.84957400	-0.48544000	-0.39055600
C	-5.93226500	0.34171300	-0.08493800
C	-6.98174800	-0.16908200	0.68155200
C	-6.94475800	-1.49050500	1.12997100
C	-5.85933300	-2.31071600	0.80820600
C	-4.80372400	-1.81383500	0.04431800
H	-5.95684100	1.36133200	-0.45286200
H	-7.82975800	0.46608500	0.92230800
H	-7.76388900	-1.88448400	1.72545900
H	-5.83592500	-3.34272000	1.14757900
H	-3.95630600	-2.44105300	-0.21306200
S	-3.46441300	0.18392200	-1.33265000
N	-2.29736700	0.54899600	-0.19243400
O	-3.95234100	1.39610800	-2.01563300
H	-0.24184200	3.82871600	4.13224600
C	-2.28203400	1.78158300	0.48227400
C	-2.98997800	2.95053100	0.19012900
C	-2.85495400	4.10738200	0.98640900
C	-2.01672900	4.15568300	2.07777500
C	0.31318100	1.78466900	3.78634900
C	0.12481500	0.66326500	2.95791700
N	-0.70455400	0.69202700	1.91961900
C	-1.40746300	1.82922700	1.61690400
C	-1.26619700	3.00335600	2.41340600
C	-0.37477000	2.94496300	3.51361700
H	-3.64683600	2.97818200	-0.66593700
H	-3.43488000	4.98486600	0.71231800
H	-1.91900200	5.05338100	2.68087200
H	1.00976000	1.71544500	4.61462000
H	0.66494900	-0.26089000	3.11493500
O	-2.93242500	-0.89934600	-2.17024000
C	1.26650500	3.00345400	-2.41343300
C	4.84944500	-0.48560100	0.39051300
C	5.93221300	0.34149900	0.08503500
C	6.98168100	-0.16929900	-0.68147700
C	6.94459200	-1.49066100	-1.13005700
C	5.85908300	-2.31081800	-0.80842600
C	4.80349000	-1.81393700	-0.04451200
H	5.95681800	1.36106700	0.45308700
H	7.82975600	0.46582400	-0.92212900
H	7.76369900	-1.88464400	-1.72557500
H	5.83560300	-3.34278900	-1.14789600
H	3.95605600	-2.44115100	0.21285900
S	3.46431500	0.18384700	1.33265400
N	2.29730600	0.54908000	0.19258500
O	3.95240900	1.39591600	2.01576600
H	0.24243400	3.82881900	-4.13244200
C	2.28204800	1.78169900	-0.48216700

26b

Rh	-0.86899400	0.83907400	0.90920000
Rh	0.83779700	-0.93096400	0.83926700
O	0.19227100	1.60609700	2.54655200
O	1.86428100	0.09497200	2.30225100
C	1.31089000	1.10246600	2.85965200
C	2.07424400	1.76441800	3.98559800
H	2.40968600	2.75600300	3.66049300
H	1.41350600	1.90811000	4.84618700
H	2.94028200	1.16803300	4.27862500
C	-3.55387300	0.81672100	-2.47603600
C	-4.57409600	1.70965000	-2.86759700
C	-4.94180900	2.78011400	-2.08517400
C	-3.82286600	4.28996800	1.14375400
C	-2.79909600	3.37056600	1.45751300
N	-2.51545600	2.33360000	0.69045600
C	-3.22063600	2.11332800	-0.45861500
H	-3.27354200	0.02059000	-3.15146100
C	-4.54151700	4.10690500	-0.01449100
O	-1.93685400	-0.30461600	2.23957800
O	-0.28649900	-1.85372500	2.36297800
C	-1.39184500	-1.34803900	2.72775700
C	-2.13831400	-2.02354800	3.85719900
H	-1.97515700	-1.45406900	4.78025200
H	-3.21285900	-2.02571200	3.65507700
H	-1.77788700	-3.04331300	4.00747800
H	-5.06948100	1.53806600	-3.81971200
H	-5.72888000	3.46297500	-2.39228000
H	-4.01915500	5.12505800	1.80863500
H	-2.19355000	3.48747500	2.35234400
O	-0.39726300	-1.91525700	-0.61392000
C	2.96671200	2.52168500	-0.85430500
C	3.28069500	3.54414100	-1.75176600
C	4.34440600	4.39861200	-1.45764100
C	5.08082600	4.22410900	-0.28431400
C	4.75730200	3.19375100	0.60234700
C	3.69425900	2.33495000	0.32372600
H	2.70735700	3.65931200	-2.66524600
H	4.59863900	5.19709700	-2.14890900
H	5.91172600	4.88812100	-0.06203200
H	5.33589500	3.05256100	1.51100000
H	3.44005900	1.52637200	1.00124400
S	1.55519600	1.45711800	-1.21788500
N	1.92013200	-0.03748500	-0.67845300
O	1.31377500	1.54844300	-2.66503900

H	5.30800900	-4.77255900	-0.77073000
C	2.93061100	-0.81106300	-1.27251200
C	3.66739500	-0.47909400	-2.40635200
C	4.69395400	-1.32124300	-2.88452600
C	5.00826000	-2.50778400	-2.26187200
C	3.77117300	-4.43637200	0.68970300
C	2.75454600	-3.54907600	1.10448100
N	2.49885900	-2.41527400	0.47721300
C	3.23400100	-2.05812300	-0.61843800
C	4.27604400	-2.90024800	-1.11423300
C	4.52184000	-4.11070900	-0.41577700
H	3.44642300	0.42891900	-2.95225100
H	5.23916100	-1.01443800	-3.77306500
H	5.79808900	-3.15177800	-2.63790400
H	3.94007900	-5.35662300	1.23991900
H	2.13182800	-3.77385900	1.96651700
O	0.44156000	1.98455500	-0.34186100
C	-4.25786200	3.00753500	-0.86554300
C	-2.91507500	-2.48821700	-1.02455500
C	-3.93396300	-2.66442200	-1.96446100
C	-4.99355500	-3.52243100	-1.66575700
C	-5.02485200	-4.20336000	-0.44826000
C	-3.98712600	-4.03883400	0.47290100
C	-2.92612700	-3.17994000	0.19003400
H	-3.88956000	-2.16286100	-2.92327100
H	-5.78812300	-3.66373700	-2.39282100
H	-5.85037900	-4.87258900	-0.22214700
H	-3.99710400	-4.58721700	1.41061900
H	-2.10025400	-3.07218500	0.88247900
S	-1.56122600	-1.34816900	-1.38755300
N	-1.88970800	0.12012400	-0.74328300
O	-1.41504600	-1.32368200	-2.84908300
H	-5.32884100	4.80079500	-0.29843900
C	-2.88158500	0.96730100	-1.26540000

26c

Rh	0.73079200	0.98121800	-0.21587100
Rh	-0.71488500	-0.95642800	0.26801400
O	0.34867200	1.64628200	1.71423000
O	-1.02080500	-0.11035600	2.15343400
C	-0.40175100	0.95568700	2.47272100
C	-0.54824300	1.43545100	3.89973400
H	-0.56819400	2.52779700	3.93604500
H	-1.44751700	1.02173200	4.36138700
H	0.32371000	1.09519300	4.47167000
C	4.83589600	0.59816800	1.07406000
C	5.92598500	1.49313500	1.02111100
C	5.81710200	2.73710800	0.44215200
C	3.12173100	4.73307600	-1.20753500
C	2.07507700	3.79101700	-1.10427500
N	2.24116100	2.60296100	-0.55259200
C	3.46016000	2.24287600	-0.05337700
H	4.97853100	-0.35777100	1.56056400
C	4.35984900	4.40461800	-0.70682800
O	0.99712100	0.15909500	-2.11823200
O	-0.30420600	-1.64117700	-1.64975400
C	0.40463700	-0.92551600	-2.42518700
C	0.52996800	-1.39613300	-3.85712600
H	-0.35242400	-1.05395300	-4.41184400
H	1.41955900	-0.97533000	-4.33116500
H	0.55321300	-2.48797200	-3.90117200
H	6.87107100	1.17702000	1.45447800
H	6.66173500	3.41921100	0.40554800
H	2.93401000	5.69550600	-1.67284800
H	1.07891600	4.01376500	-1.47753300
O	1.06628000	-1.93871000	0.96695200
C	-3.57674400	2.38959200	-0.16938200
C	-3.69010800	2.19046000	1.20891700
C	-4.55724400	3.00489100	1.93667300
C	-5.29234100	4.00345500	1.29234000
C	-5.16783500	4.19034400	-0.08577700
C	-4.30720100	3.38040300	-0.82794000
H	-3.12326800	1.40385100	1.69630700
H	-4.66094600	2.85507400	3.00756000
H	-5.96694600	4.63363000	1.86538900
H	-5.74275000	4.96381300	-0.58698600
H	-4.20813800	3.50416900	-1.90094100
S	-2.42266900	1.38883400	-1.12545100
N	-2.43274700	-0.10441600	-0.47018900
O	-1.06488000	1.98377700	-0.85005900
H	-5.15740200	-5.10873800	0.72924100
C	-3.55305500	-0.94677000	-0.57742600
C	-4.76412400	-0.63824600	-1.19121600
C	-5.84521600	-1.54573000	-1.17303900
C	-5.75237800	-2.77412700	-0.55896500
C	-3.11725100	-4.70323800	1.25915500
C	-2.07499300	-3.75412400	1.17941600
N	-2.22784000	-2.57934900	0.59630800
C	-3.42782100	-2.24145400	0.03915200
C	-4.53205600	-3.14692100	0.05694700
C	-4.33478100	-4.39849800	0.69671500
H	-4.89181800	0.30467300	-1.70660400
H	-6.76958300	-1.25284800	-1.66366500
H	-6.59002200	-3.46564600	-0.54851500
H	-2.94142900	-5.65364200	1.75297200
H	-1.09338700	-3.96047600	1.59791900
O	-2.85545400	1.44743400	-2.53109700
C	4.57227200	3.13784300	-0.10281700
C	3.52739300	-2.41457800	0.13883800
C	4.20520400	-3.46710300	0.75798000
C	4.99766300	-4.31110700	-0.02073500
C	5.10967700	-4.09689700	-1.39620500
C	4.43034600	-3.03613600	-2.00040700
C	3.63027400	-2.18730200	-1.23559600
H	4.12018000	-3.61216500	1.82956700
H	5.53026700	-5.13249600	0.45008400
H	5.73161900	-4.75404700	-1.99781200
H	4.52494100	-2.86432300	-3.06884700
H	3.10640900	-1.35426700	-1.69246400
S	2.45276900	-1.37505700	1.14620600
N	2.46019200	0.11143900	0.47609500
O	2.96615500	-1.43181300	2.52413700
H	5.18774000	5.10725300	-0.76206200
C	3.59759300	0.93647300	0.53475300

27a

Rh	0.94368300	-1.17805300	-0.85174100
Rh	-0.94365100	-1.17718200	0.85196900
O	-0.29539700	-2.48644600	-1.92424500
O	-1.65113000	-2.84339200	-0.16367500
C	-1.26156600	-3.07758200	-1.34850800
C	-2.01751600	-4.12542800	-2.12756500
H	-1.45200400	-4.45079000	-3.00313500
H	-2.24377800	-4.98202300	-1.48596500
H	-2.96888800	-3.68981800	-2.45318800
C	-0.06974000	2.84249300	-3.31137500
H	3.79381700	2.48201900	0.32484100
H	3.40932900	4.61339900	-0.81515300
H	1.64679500	4.85894800	-2.54688200
H	-1.65389300	1.72986200	-4.25279500
H	-1.17254100	-0.35246600	-2.93729000
O	3.23441100	-0.90061700	1.66835900
C	3.02159000	2.53437300	-0.43314000
C	2.79229900	3.76129300	-1.08836700
O	1.65056300	-2.84411900	0.16451200
O	0.29530200	-2.48523700	1.92507600
C	1.26110700	-3.07722900	1.34962000
C	2.01683800	-4.12470600	2.12937200
H	2.24363200	-4.98143500	1.48814900
H	2.96793600	-3.68878600	2.45539600
H	1.45094500	-4.44991400	3.00475600
C	1.81150000	3.90830600	-2.04852200
C	-0.83449100	1.72066600	-3.54170100
C	-0.56434300	0.53644100	-2.82707800
N	0.42838300	0.46709800	-1.94650400
C	1.22291700	1.55925500	-1.71047200
C	-4.84888900	0.08804900	-0.25804500
C	-5.80763300	0.21813400	-1.27351600

C	-7.14443800	0.45256100	-0.95717000
C	-7.54266000	0.53437300	0.37985100
C	-6.59756800	0.38369600	1.39748700
C	-5.25633500	0.16931000	1.08153300
H	-5.48975600	0.12789200	-2.30747500
H	-7.87779600	0.56214000	-1.75189600
H	-8.58662700	0.70785500	0.62787100
H	-6.90514600	0.43104500	2.43880000
H	-4.52477900	0.04796700	1.87448700
C	-3.42876900	-0.23849300	-0.64853500
N	-2.39230700	0.12823800	0.20254600
O	-3.23411900	-0.89985800	-1.66867300
H	0.27137800	3.77284600	3.83810600
C	-2.27731600	1.39587600	0.75388300
C	-3.02159300	2.53499800	0.43247200
C	-2.79240900	3.76206400	1.08746400
C	-1.81160500	3.90934200	2.04757300
C	0.83471600	1.72226500	3.54100900
C	0.56461700	0.53786900	2.82665600
N	-0.42816500	0.46824000	1.94616300
C	-1.22280600	1.56028700	1.70993800
C	-0.99228400	2.79935600	2.37171100
C	0.06983000	2.84397300	3.31051100
H	-3.79380100	2.48243600	-0.32550900
H	-3.40951500	4.61406900	0.81411200
H	-1.64699500	4.86007900	2.54578900
H	1.65416300	1.73168400	4.25205000
H	1.17287600	-0.35098700	2.93699500
C	2.27738700	1.39512200	-0.75431200
C	0.99232200	2.79817300	-2.37250400
C	4.84898800	0.08792900	0.25801700
C	5.80756700	0.21868400	1.27356100
C	7.14433000	0.45344500	0.95730000
C	7.54270800	0.53489800	-0.37969600
C	6.59780900	0.38355400	-1.39740700
C	5.25660200	0.16884500	-1.08154500
H	5.48960700	0.12868900	2.30752100
H	7.87754700	0.56356500	1.75208000
H	8.58665200	0.70864700	-0.62762900
H	6.90551900	0.43062100	-2.43869300
H	4.52517300	0.04701000	-1.87455300
C	3.42893400	-0.23907500	0.64828700
N	2.39243100	0.12762900	-0.20269600
H	-0.27133000	3.77124400	-3.83916600

27b

Rh	-1.03757700	-0.63230700	-1.12268400
Rh	1.03752100	0.63217000	-1.12285100
O	-0.22117500	-1.73646300	-2.73508900
O	1.80316800	-0.74099400	-2.48671700
C	1.00639600	-1.58438300	-3.01413200
C	1.59159600	-2.51565400	-4.05560000
H	0.89418800	-2.63296100	-4.89008000
H	2.55241900	-2.14569300	-4.41945300
H	1.73989500	-3.50543300	-3.60677600
C	-3.18999300	0.33563700	2.43295500
C	-4.31524200	-0.24635800	3.05337200
C	-5.06507000	-1.21320300	2.42114900
C	-4.88478800	-3.13580600	-0.77517300
C	-3.71299200	-2.54724600	-1.30135300
N	-3.06324800	-1.57501900	-0.68857400
C	-3.52374900	-1.09702500	0.50762000
H	-2.62437300	1.08159600	2.97649300
C	-5.35196700	-2.70232000	0.44280500
O	-1.80338600	0.74061400	-2.48662600
O	0.22090600	1.73610900	-2.73536700
C	-1.00666700	1.58397100	-3.01425100
C	-1.59212300	2.51508700	-4.05571300
H	-2.55240200	2.14434900	-4.42021700
H	-1.74166600	3.50453400	-3.60655400
H	-0.89437900	2.63341000	-4.88976400
H	-4.58506600	0.08325000	4.05315400
H	-5.93646300	-1.65272900	2.89872000
H	-5.38313100	-3.92741700	-1.32570800
H	-3.29186100	-2.88996800	-2.24286800
O	0.04630200	1.94431800	0.17380100
C	1.74419000	-2.83109200	1.37608100
C	0.99438800	-3.57195400	2.29978000
C	1.55233000	-4.69009600	2.91937500
C	2.85073800	-5.09377800	2.59992400
C	3.59217900	-4.37315200	1.66014100
C	3.04589400	-3.24238600	1.05477300
H	-0.02209800	-3.26643700	2.52827700
H	0.96929000	-5.25173800	3.64438400
H	3.28134100	-5.97087500	3.07592300
H	4.59697100	-4.69208100	1.39626400
H	3.62136100	-2.68299400	0.32326800
C	1.10678600	-1.68039300	0.65491300
N	1.71294400	-0.50739100	0.44016800
C	-2.80303900	-0.02402100	1.14491400
H	6.23532800	3.14826000	0.89320400
C	2.80300300	0.02422600	1.14482000
C	3.18985100	-0.33519400	2.43296000
C	4.31507800	0.24687800	3.05335100
C	5.06499000	1.21357800	2.42099700
C	4.88499100	3.13561000	-0.77569700
C	3.71318600	2.54701400	-1.30182800
N	3.06336900	1.57491300	-0.68891400
C	3.52377900	1.09710900	0.50738300
C	4.67153800	1.66867600	1.13781000
C	5.35208000	2.70231700	0.44239000
H	2.62417600	-1.08104000	2.97659400
H	4.58482200	-0.08255600	4.05321200
H	5.93637400	1.65315700	2.89854000
H	5.38340500	3.92709900	-1.32634700
H	3.29211100	2.88960100	-2.24342400
O	-0.04626800	-1.94434100	0.17403200
C	-4.67152100	-1.66852000	1.13807400
C	-1.74403100	2.83125400	1.37587500
C	-3.04567900	3.24267000	1.05448200
C	-3.59186400	4.37353800	1.65976000
C	-2.85038500	5.09413400	2.59953000
C	-1.55204000	4.69033000	2.91906800
C	-0.99418800	3.57209100	2.29957100
H	-3.62116800	2.68329700	0.32297600
H	-4.59660600	4.69256200	1.39581000
H	-3.28091400	5.97130700	3.07545500
H	-0.96897100	5.25195000	3.64407000
H	0.02225900	3.26647400	2.52812500
C	-1.10673900	1.68044200	0.65479500
N	-1.71292000	0.50744000	0.44023000
H	-6.23521600	-3.14822700	0.89365100

27c

Rh	-0.69351400	-0.99873700	-0.02261500
Rh	0.68980600	1.00018100	-0.02582200
O	-0.75708800	-0.84736700	-2.10360500
O	0.76036600	0.83865200	-2.10602500
C	0.00626400	-0.00913200	-2.67933900
C	0.04624900	-0.05049700	-4.19216000
H	-0.92681700	-0.34491500	-4.59344900
H	0.34562300	0.91850000	-4.59809000
H	0.78232000	-0.80049500	-4.50741600
C	-4.66674100	0.02835700	1.11558300
C	-5.78577400	-0.75021600	1.47862800
C	-5.79660700	-2.11703900	1.31012200
C	-3.37679900	-4.73841000	0.20576800
C	-2.27776200	-3.89599500	-0.07419500
N	-2.33367500	-2.58241400	0.04607100
C	-3.49568400	-1.98539300	0.45055100
H	-4.70131700	1.09730700	1.28175700
C	-4.54627800	-4.17131700	0.65391000
O	-0.52831600	-1.00105300	2.05699200
O	0.51001000	1.01646900	2.05234700
C	-0.01057900	0.00944800	2.62839400
C	0.02032600	0.00326600	4.14185100
H	-0.74715100	-0.66127000	4.54456300
H	1.00190800	-0.35409900	4.47711800

H	-0.11537700	1.01673900	4.52862000
H	-6.65155100	-0.24782200	1.90179400
H	-6.66453500	-2.71155800	1.58180900
H	-3.27640700	-5.81222500	0.08327100
H	-1.32541800	-4.31088700	-0.39416300
O	-1.15765200	2.02976100	-0.25629400
C	3.45371300	-2.29355600	-0.54653500
C	3.56379900	-3.58687400	-0.01780300
C	4.60436400	-4.42386300	-0.42047800
C	5.52503300	-3.98698500	-1.37569400
C	5.40382200	-2.70796400	-1.92468100
C	4.37778400	-1.86051700	-1.50819400
H	2.83222200	-3.92862800	0.70800900
H	4.69033700	-5.42040200	0.00454800
H	6.33020800	-4.64287300	-1.69631900
H	6.10847500	-2.36893300	-2.67930700
H	4.28470500	-0.86637900	-1.93528900
C	2.28041000	-1.43747300	-0.16605200
N	2.38004100	-0.13673900	0.14226300
C	-3.53358700	-0.54812600	0.54856200
H	5.40044900	4.79416700	0.89451400
C	3.53003700	0.55264600	0.55279100
C	4.66323800	-0.02120900	1.12238300
C	5.78188000	0.75919900	1.48273900
C	5.79211300	2.12536300	1.30899400
C	3.37238800	4.74132600	0.19165600
C	2.27393500	3.89738500	-0.08606900
N	2.33007200	2.58434600	0.03990300
C	3.49179900	1.98948300	0.44844200
C	4.63658500	2.76893600	0.79981200
C	4.54155000	4.17654400	0.64348700
H	4.69819800	-1.08956600	1.29247700
H	6.64777600	0.25881500	1.90803700
H	6.65968900	2.72127300	1.57874200
H	3.27179000	5.81456600	0.06443400
H	1.32190400	4.31058800	-0.40911200
O	1.15576000	-2.02930200	-0.24375600
C	-4.64099800	-2.76305000	0.80426500
C	-3.45561200	2.29479700	-0.55821600
C	-4.37913900	1.86133200	-1.52011600
C	-5.40589300	2.70805700	-1.93625400
C	-5.52827300	3.98671000	-1.38666700
C	-4.60800400	4.42403200	-0.43127000
C	-3.56673500	3.58776700	-0.02890000
H	-4.28478000	0.86755400	-1.94774700
H	-6.11017700	2.36880300	-2.69112100
H	-6.33405400	4.64200600	-1.70699400
H	-4.69489500	5.42030000	-0.00578300
H	-2.83566200	3.92966800	0.69735800
C	-2.28261100	1.43887700	-0.17681100
N	-2.38342600	0.13904500	0.13496100
H	-5.40562400	-4.78759300	0.90673300

$Rh_2(OAc)_4$

Rh	0.00031300	-0.00270600	-1.19698100
Rh	-0.00311600	-0.00010500	1.19804000
O	-1.42902400	-1.49792300	-1.13260800
O	-1.43497800	-1.49219900	1.13418100
C	-1.84061400	-1.90879400	0.00088600
C	-2.92559600	-2.95710000	-0.00225300
H	-2.79577000	-3.63740500	-0.84747000
H	-2.92837100	-3.51298900	0.93756600
H	-3.89673400	-2.45969500	-0.11492500
O	1.42944600	1.49198700	1.13453000
O	1.42940500	1.49303600	-1.13225300
C	1.83805400	1.90621900	0.00147800
C	2.92271400	2.95492100	-0.00135000
H	3.89369300	2.45844000	-0.11923100
H	2.78987000	3.63799200	-0.84392400
H	2.92835400	3.50772200	0.94024300
O	-1.49467600	1.42669600	-1.13687600
O	-1.49560600	1.43197400	1.12991200
O	1.49493800	-1.43305200	-1.12788200
O	1.48777000	-1.43339800	1.13884800
C	1.90637100	-1.84049200	0.00722700
C	2.98221100	-2.89842900	0.00073400
H	2.61468400	-3.78791500	-0.52222100
H	3.85431100	-2.53112300	-0.55038800
H	3.27310000	-3.16439300	1.01819600
C	-1.90879000	1.83802600	-0.00476000
C	-2.95693900	2.92318200	-0.00414800
H	-3.50999900	2.92697300	-0.94559700
H	-3.63982100	2.79258400	0.83893100
H	-2.45987100	3.89413500	0.11146200

AcOH

O	0.64390200	1.20230300	0.00001200
C	0.09134900	0.12338200	0.00002000
C	-1.39576500	-0.11104800	0.00002200
H	-1.91892400	0.84584600	-0.00051600
H	-1.68510700	-0.69205100	-0.88241800
H	-1.68545300	-0.69152400	0.88264000
O	0.77974000	-1.04386900	0.00001400
H	1.72684400	-0.80375000	-0.00016700

Int1_4

Rh	-1.13246900	-0.87313600	0.65696900
Rh	1.13287600	-0.87329900	-0.65682800
O	-0.16449500	-2.20580500	1.90502800
O	1.57663700	-2.54241500	0.51665300
C	0.90489200	-2.79743100	1.56004500
C	1.42239700	-3.87720300	2.47991400
H	0.60754200	-4.32143500	3.05610700
H	1.94370300	-4.64886500	1.90747900
H	2.13783600	-3.42289700	3.17500400
O	-4.27003800	0.28366300	1.91418800
O	-3.02084000	-1.57385900	2.10685200
C	-3.95173000	-0.87547400	2.49078000
C	-4.84794400	-1.22600300	3.64517000
H	-4.52917200	-2.16701600	4.09460700
H	-4.81908000	-0.42700200	4.39431000
H	-5.88206200	-1.31096600	3.29394400
O	4.26970200	0.28396400	-1.91400100
O	3.02101100	-1.57392600	-2.10626000
O	-1.57590400	-2.54280200	-0.51584700
O	0.16506500	-2.20643300	-1.90448800
C	-0.90423200	-2.79808400	-1.55920400
C	-1.42161200	-3.87825200	-2.47867000
H	-1.94386000	-4.64917900	-1.90611700
H	-2.13618800	-3.42400800	-3.17469600
H	-0.60655200	-4.32336600	-3.05389600
C	3.95177400	-0.87540700	-2.49028900
C	4.84810900	-1.22600600	-3.64455900
H	5.88224100	-1.31059200	-3.29328400
H	4.52960500	-2.16722100	-4.09375900
H	4.81903700	-0.42719200	-4.39389000
C	4.74518700	-0.25103300	1.24717900
C	5.84654500	0.60757300	1.23533100
C	7.08753500	0.11401300	0.82983400
C	7.21913300	-1.22204800	0.44635100
C	6.11021100	-2.07310000	0.47165400
C	4.86380000	-1.59432000	0.87581900
H	5.73321700	1.63891900	1.55103100
H	7.95074600	0.77363900	0.82001700
H	8.18786900	-1.60295100	0.13403400
H	6.21494900	-3.11541900	0.18277200
H	3.99490200	-2.24406200	0.89517300
S	3.13874400	0.38401100	1.76600700
N	2.29294200	0.63562700	0.33177600
O	3.38997000	1.64583900	2.48654800
H	0.33915700	3.88866600	-4.05801400
C	2.08519700	1.92309400	-0.21777300
C	2.56256500	3.15761000	0.22548800
C	2.34148200	4.33790000	-0.51549700
C	1.67130300	4.33448600	-1.71725900
C	0.04538500	1.76951200	-3.88996900
C	0.23433800	0.64080600	-3.06947300
N	0.84372000	0.72178700	-1.89287600

C	1.34895900	1.91963100	-1.45091700
C	1.16616800	3.10972900	-2.21526900
C	0.49250600	2.99561300	-3.45776600
H	3.10977800	3.21806400	1.15310800
H	2.73198700	5.27060400	-0.11663500
H	1.52312200	5.24586300	-2.28903000
H	-0.47279500	1.65199700	-4.83535800
H	-0.13482000	-0.33683200	-3.34770700
O	2.48417600	-0.70353000	2.50317100
H	3.67832500	0.39492700	-1.12969300
C	-4.74504000	-0.25173100	-1.24733300
C	-5.84640400	0.60686900	-1.23578500
C	-7.08739500	0.11343400	-0.83013600
C	-7.21899400	-1.22250300	-0.44622600
C	-6.11007300	-2.07356400	-0.47125500
C	-4.86366200	-1.59490600	-0.87555600
H	-5.73308600	1.63810900	-1.55183500
H	-7.95060900	0.77305900	-0.82053900
H	-8.18773200	-1.60330400	-0.13379100
H	-6.21481500	-3.11579900	-0.18206700
H	-3.99477100	-2.24466600	-0.89473900
S	-3.13853700	0.38306300	-1.76625500
N	-2.29290400	0.63519500	-0.33200200
O	-3.38958700	1.64459900	-2.48736400
H	-0.34049600	3.88984000	4.05718900
C	-2.08580800	1.92283000	0.21735000
C	-2.56385200	3.15704100	-0.22604500
C	-2.34326300	4.33756300	0.51472000
C	-1.67295700	4.33467200	1.71641000
C	-0.04572200	1.77079900	3.88944500
C	-0.23417600	0.64187700	3.06913900
N	-0.84367400	0.72238500	1.89256300
C	-1.34947200	1.91992600	1.45044300
C	-1.16721500	3.11023400	2.21459500
C	-0.49344000	2.99662800	3.45707400
H	-3.11116600	3.21710700	-1.15363300
H	-2.73424800	5.27001300	0.11573400
H	-1.52514800	5.24621400	2.28801500
H	0.47253000	1.65368000	4.83484700
H	0.13546900	-0.33553700	3.34750800
O	-2.48392500	-0.70480900	-2.50287100
H	-3.67879500	0.39454700	1.12981100

TS1_4

Rh	1.01262200	-0.35645000	-1.12769500
Rh	-1.33541200	-0.78034400	-0.04365800
O	-2.63700300	-2.50012200	-2.26792900
O	-0.92468600	-1.09817800	-2.06545300
C	-1.59629600	-1.95422400	-2.73800400
C	-1.16009800	-2.27432600	-4.13800600
H	-0.07149200	-2.23533300	-4.22174000
H	-1.53359400	-3.25376200	-4.44220100
H	-1.58471500	-1.51706800	-4.80872100
C	0.97024200	4.23255000	-2.54481700
H	4.50255700	2.22477700	0.88180400
H	4.73368800	4.53964300	0.13695400
H	3.11655700	5.56358900	-1.44533500
H	-0.79896500	3.74745700	-3.67225000
H	-0.86095100	1.38687800	-2.84644800
O	2.26086700	-1.38027200	1.75452200
C	3.78519500	2.61247200	0.17313000
C	3.90621200	3.95251100	-0.25275700
O	1.36395800	-2.39145800	-0.75211800
O	-0.57155700	-2.70958300	0.36534900
C	0.56894600	-3.08834800	-0.05587300
C	1.01797900	-4.47844600	0.33060300
H	1.59324600	-4.93508600	-0.47922600
H	1.67674100	-4.39155700	1.20307400
H	0.16753600	-5.11153600	0.59241700
C	3.01443500	4.52891600	-1.13170600
C	-0.03372800	3.39988000	-2.98634200
C	-0.07402700	2.06485200	-2.53889700
N	0.83320500	1.58155200	-1.69655500
C	1.83126400	2.39173900	-1.21957900
C	-4.33967300	-0.40888600	-0.12785600
C	-5.60627400	-0.35880900	0.43753800
C	-6.02499200	-1.44387400	1.21744900
C	-5.17392700	-2.53192200	1.43075900
C	-3.89824300	-2.54983200	0.85993700
C	-3.45375300	-1.49204000	0.04599800
H	-6.24143100	0.50933500	0.29127700
H	-7.01403800	-1.43125400	1.66754000
H	-5.50599500	-3.36376700	2.04676200
H	-3.24104000	-3.40007800	1.02686800
H	-2.92046700	-1.99940900	-1.13574700
S	-3.65184400	1.00510800	-1.01087200
N	-2.15517600	1.12320000	-0.25524400
O	-4.49986400	2.18233200	-0.75997000
H	-0.99904200	1.29942400	5.45376100
C	-2.11453900	1.81725600	0.97730200
C	-2.45147400	3.15264700	1.15486100
C	-2.35614500	3.75428300	2.42931100
C	-1.91891100	3.05025000	3.53194000
C	-0.76231800	-0.44360700	4.22429600
C	-0.87226100	-0.96585800	2.91956200
N	-1.29986000	-0.22517900	1.90697900
C	-1.64934700	1.08813200	2.10708500
C	-1.55010200	1.68864900	3.39374000
C	-1.09116300	0.87214700	4.45887600
H	-2.79930900	3.72936200	0.30700100
H	-2.63145400	4.80032900	2.53193500
H	-1.84485900	3.52365000	4.50674800
H	-0.40033300	-1.08743200	5.01845900
H	-0.59525700	-1.98536000	2.68234000
O	-3.38864400	0.61533600	-2.40725700
C	1.94573200	3.74837100	-1.63662500
C	4.69436900	-0.98073900	0.80330400
C	5.90033600	-0.47879500	1.29354600
C	7.10087200	-1.03550000	0.84592500
C	7.08639600	-2.08303500	-0.07544200
C	5.86998300	-2.58348200	-0.55082200
C	4.66448200	-2.03827700	-0.11177800
H	5.89462000	0.32540800	2.02136900
H	8.04474600	-0.65154300	1.22304300
H	8.02203000	-2.51309100	-0.42267700
H	5.85988100	-3.40461800	-1.26265200
H	3.71371200	-2.42586100	-0.46529800
S	3.13919300	-0.26659400	1.37490400
N	2.47452100	0.46607800	0.02158000
O	3.47325800	0.74224300	2.39512900
H	1.02614200	5.26467400	-2.88109000
C	2.74415700	1.80697900	-0.28618100

Int2_4

Rh	1.00080000	-0.36123600	-1.05543400
Rh	-1.39633200	-0.70847400	0.14145300
O	-2.57391400	-2.58283400	-2.49080500
O	-0.94689300	-1.16898200	-1.91293300
C	-1.45660100	-1.94629800	-2.74334400
C	-0.85823100	-2.19619400	-4.08518700
H	0.17098300	-1.83672600	-4.11297300
H	-0.90003700	-3.26196000	-4.32640700
H	-1.45318900	-1.65887100	-4.83423600
C	1.09388900	4.15522900	-2.68508700
H	4.67326200	2.16464600	0.70358300
H	4.97761900	4.42318900	-0.17796700
H	3.34173100	5.43643400	-1.74794700
H	-0.74656600	3.69996400	-3.70536500
H	-0.87943100	1.39251400	-2.75904200
O	2.32004200	-1.28653900	1.84743500
C	3.94686900	2.54708000	0.00102200
C	4.10947000	3.85478900	-0.50189600
O	1.27766200	-2.39787400	-0.57145500
O	-0.58748600	-2.58720000	0.69297100
C	0.52554900	-3.01411300	0.23520800
C	0.98483100	-4.37124400	0.71811300
H	1.47460300	-4.91952200	-0.09146000
H	1.72521100	-4.21496000	1.51165600

H	0.15428800	-4.95525600	1.12009900
C	3.20775900	4.42514800	-1.37537800
C	0.03345700	3.35073300	-3.03689100
C	-0.04651100	2.04302300	-2.51979300
N	0.87446200	1.55389400	-1.69358600
C	1.92802600	2.34256100	-1.30227100
C	-4.33547400	-0.55738500	-0.18813200
C	-5.69506400	-0.85236800	-0.09449600
C	-6.07278100	-2.02439800	0.56282900
C	-5.09684600	-2.86719400	1.10423100
C	-3.73668900	-2.54687500	1.00769800
C	-3.33221200	-1.37471700	0.35493400
H	-6.43553400	-0.17745900	-0.51471500
H	-7.12511900	-2.27899000	0.65343000
H	-5.39698600	-3.77954900	1.61428400
H	-2.98979100	-3.20725000	1.44030000
H	-2.92474900	-2.30276200	-1.60978400
S	-3.72477600	0.90151000	-1.04224100
N	-2.27978400	1.13682800	-0.21845400
O	-4.66680000	2.01960800	-0.87327700
H	-1.03048300	1.81064500	5.42322200
C	-2.30791000	1.91263900	0.96063000
C	-2.74915700	3.22663400	1.05566400
C	-2.67682900	3.92008700	2.28342300
C	-2.15339200	3.33573000	3.41837100
C	-0.69906500	0.00329700	4.31515600
C	-0.81512400	-0.62663400	3.05995200
N	-1.33099300	0.00528100	2.01418200
C	-1.76964400	1.30346900	2.12709200
C	-1.68124000	2.00091400	3.36428000
C	-1.12255000	1.30436700	4.46616600
H	-3.15498600	3.71591400	0.17934000
H	-3.03394100	4.94547900	2.32150200
H	-2.09273500	3.88297600	4.35447200
H	-0.25923100	-0.54896000	5.13825500
H	-0.47096400	-1.63795900	2.88625200
O	-3.35629800	0.50553900	-2.41742700
C	2.08537800	3.67000800	-1.79460800
C	4.71973700	-1.04635300	0.76763000
C	5.96655300	-0.60738900	1.21412700
C	7.12018300	-1.23871200	0.74266900
C	7.01951700	-2.29644200	-0.16152800
C	5.76298300	-2.73340000	-0.59320900
C	4.60364200	-2.11391600	-0.12888900
H	6.02680200	0.20830100	1.92642600
H	8.09505100	-0.90352000	1.08615800
H	7.91859600	-2.78415400	-0.52876800
H	5.68563000	-3.56265300	-1.29143300
H	3.62210400	-2.45206600	-0.44746900
S	3.22513400	-0.23152700	1.36954200
N	2.52833100	0.46484300	0.02352900
O	3.65444200	0.80265300	2.32843400
H	1.18269600	5.16519600	-3.07708600
C	2.85218300	1.76686600	-0.37269000

Int3_4

C	-4.84639300	-0.71932800	1.04957200
C	-4.44180600	-1.91090700	0.44078300
C	-3.09280000	-2.25880300	0.41503300
C	-2.16864800	-1.39196400	1.00607000
C	-2.55179500	-0.19510200	1.61645800
C	-3.90689800	0.13445100	1.63164500
H	-5.90050900	-0.45637300	1.07084800
H	-5.17534800	-2.57328700	-0.00916100
H	-2.76238800	-3.18505700	-0.04072500
H	-4.22401000	1.06172000	2.09914300
C	-3.33200600	0.44800500	-2.96918400
H	-3.60409700	-0.38172700	-3.62480000
H	-4.14504100	0.63653000	-2.25989400
H	-3.20246400	1.35954500	-3.56281900
S	-0.45687200	-1.89230200	1.06348200
O	-0.38541000	-3.34145600	0.83815500
N	0.29351400	-1.10982100	-0.38729800
H	-0.29523700	-1.35315500	-1.23186800
C	1.69653500	-1.47321500	-0.45814100
C	2.62612200	-0.46642700	-0.08076400
C	2.14572100	-2.73019200	-0.80735800
C	4.01194600	-0.77309700	0.00714000
C	3.52912100	-3.02541000	-0.75963200
H	1.43521200	-3.49647700	-1.09529100
C	2.99908800	1.75542500	0.51765200
C	4.88678500	0.26573400	0.41758200
C	4.44042200	-2.08120100	-0.34145600
H	3.86377300	-4.01928900	-1.04018700
C	4.37945300	1.51633900	0.68602300
H	2.57490700	2.74350500	0.65613800
H	5.95050500	0.06265400	0.50553400
H	5.49884500	-2.31963400	-0.28467600
H	5.02133100	2.33230200	1.00014800
N	2.15410900	0.80568100	0.14369100
Rh	0.19188800	1.00978800	-0.49488100
O	0.24222700	3.10617100	-0.56480000
C	-0.32712600	3.35882200	0.56399400
O	-0.63683400	2.43259800	1.35129900
O	-1.65995900	1.08469500	-1.42949200
C	-2.04971500	0.13812800	-2.21289500
O	-1.47850000	-0.96255900	-2.39015500
C	-0.63668700	4.80194800	0.88896600
H	-1.61893300	5.05574300	0.47135000
H	-0.67546200	4.95266000	1.97088300
H	0.10182500	5.47145900	0.43959900
H	-1.81439900	0.46942500	2.05062600
O	0.21163000	-1.28875300	2.21691500

Int4_4

C	2.21169500	1.61609400	0.09762900
C	2.17860900	2.88892500	0.67134700
C	2.89503700	3.12280600	1.84618500
C	3.63364700	2.09380500	2.43417500
C	3.66525100	0.82684600	1.84512500
C	2.95517800	0.57873900	0.67008800
H	1.61739600	3.68447400	0.19370600
H	2.88052600	4.11139500	2.29667500
H	4.19250200	2.28126900	3.34712900
H	4.25186700	0.03069300	2.29543800
H	2.98254100	-0.39677200	0.19528000
S	1.26074800	1.29131600	-1.39736500
N	-0.15686300	0.58065500	-0.86503700
Rh	-0.13802800	-1.39092000	-0.24298100
H	-5.49441600	0.48346800	1.35695600
C	-1.30364800	1.29355600	-0.50655800
C	-1.59867600	2.64738700	-0.67954000
C	-2.84303300	3.17407400	-0.27200500
C	-3.82850300	2.39508400	0.29701800
C	-4.20072200	-1.22129800	1.19659300
C	-2.92931500	-1.67115000	0.79362100
N	-2.03262400	-0.84479400	0.26754000
C	-2.32117100	0.48342200	0.09356000
C	-3.58411800	1.01372200	0.48614500
C	-4.52146000	0.11036800	1.04790800
H	-0.87673800	3.29848000	-1.15122600
H	-3.02145100	4.23490700	-0.42673700
H	-4.78337200	2.81672600	0.59596600
H	-4.90331800	-1.93046200	1.62069100
H	-2.62675600	-2.70749700	0.90272600
O	0.98110500	2.58915700	-2.03495700
O	1.97046400	0.25651900	-2.15459400
O	1.76663200	-2.40868800	-0.51869700
O	0.03609500	-3.42604800	0.35392500
C	1.26358900	-3.46459400	-0.01902600
C	2.05807000	-4.72982700	0.11029000
H	1.70851100	-5.45180400	-0.63753700
H	3.12005000	-4.53567200	-0.05301000
H	1.90144800	-5.17514300	1.09766700

TS2_4

C	-4.15525900	-1.98311700	-1.28158800
C	-3.04688700	-2.45299100	-0.57264900

C	-2.13365900	-1.53190300	-0.07104600
C	-2.24985200	-0.13793400	-0.25370500
C	-3.36568600	0.28765700	-1.00090400
C	-4.30694900	-0.61401300	-1.50248800
H	-4.88465400	-2.68743600	-1.67127100
H	-2.09904400	0.88031000	0.69812200
H	-3.51261600	1.35196800	-1.16757300
H	-5.15870300	-0.24652300	-2.06871500
H	-3.16509400	4.48938900	1.30891100
H	-1.69788000	4.49761600	2.29101800
H	-1.62022100	5.07430500	0.60791900
O	-0.38690900	-3.53887100	0.20624900
S	-0.65970100	-2.18761000	0.72625400
O	-0.72604800	-2.01834700	2.18645600
N	0.42779800	-1.05795600	0.06455700
C	1.81452400	-1.21488200	0.08970900
C	2.53244400	-0.01180200	-0.20289200
C	2.53739600	-2.37638500	0.33704600
C	3.95238700	0.00136100	-0.25756100
C	3.94939600	-2.35550500	0.28893400
H	2.01920100	-3.30274000	0.55170800
C	2.40545400	2.26814300	-0.68806800
C	4.57651300	1.23886200	-0.55558200
C	4.65392000	-1.20690100	-0.00324300
H	4.48491000	-3.28019200	0.48470500
C	3.80888000	2.36315900	-0.77040200
H	1.76700600	3.13330300	-0.83445300
H	5.66086200	1.28758700	-0.60933000
H	5.73931400	-1.20888100	-0.04071100
H	4.26294400	3.32212700	-0.99639000
N	1.79050800	1.12327600	-0.41891500
Rh	-0.26319500	0.75375800	-0.25150600
O	-0.81870600	2.76127700	-0.00148100
C	-1.75945600	2.93694900	0.84473400
O	-2.42248000	1.98359500	1.35987000
C	-2.08169600	4.34437600	1.27523400
H	-2.88083900	-3.51710900	-0.43763400

Int5_4

C	2.13588900	-1.62056200	-0.09999000
C	3.27148300	-2.43000000	-0.16454200
C	4.48766100	-1.83885000	-0.50224300
C	4.53445800	-0.46827300	-0.77602300
C	3.37775500	0.31350600	-0.71321000
C	2.13166600	-0.24171700	-0.36712500
H	3.20799600	-3.49629500	0.03580000
H	5.38852500	-2.44321700	-0.55951500
H	5.48127300	-0.00655400	-1.04759400
H	3.44749800	1.37256600	-0.95260900
H	1.38039900	1.54075700	1.62067800
S	0.58892300	-2.39563800	0.36562800
N	-0.44209900	-1.07962700	-0.00784000
Rh	0.33281900	0.67482500	-0.35620900
H	-5.68241100	1.37523600	-0.25337200
C	-1.82871600	-1.19236600	0.06534800
C	-2.56021100	-2.35373800	0.29939800
C	-3.96995800	-2.31299400	0.35505100
C	-4.67089800	-1.14039600	0.17281100
C	-3.83665500	2.44261400	-0.51447300
C	-2.43250200	2.32617300	-0.53826300
N	-1.80420800	1.17341800	-0.34997500
C	-2.54254200	0.03887300	-0.12680500
C	-3.96526900	0.06611500	-0.07624400
C	-4.59735200	1.31793800	-0.28189800
H	-2.05132700	-3.30102300	0.42806000
H	-4.50585600	-3.23941700	0.54148800
H	-5.75618700	-1.12259100	0.21322000
H	-4.29568700	3.41233900	-0.67648400
H	-1.80404900	3.19397100	-0.71599200
O	0.30018300	-3.53864900	-0.51919900
O	0.53930200	-2.64568000	1.81736900
O	1.74069800	2.45050800	1.81165100
O	1.11291000	2.69721700	-0.32875000
C	1.62907500	3.15590300	0.70173200
C	2.17328000	4.54620100	0.78836000
H	2.01352100	5.07377200	-0.15212000
H	1.68826200	5.08467100	1.60939500
H	3.24484200	4.50457900	1.01324500

Int6_4

Rh	1.31006600	0.75082800	0.63667400
Rh	-1.67391200	0.08615100	-0.13234900
O	0.79221100	2.28422300	2.13791700
O	2.84180200	3.13462400	1.80658100
C	1.64695600	3.15040500	2.37067700
C	1.40646900	4.30487900	3.29289900
H	0.53551500	4.11180900	3.92027300
H	2.28860100	4.49400400	3.91073300
H	1.22220100	5.20332900	2.69130300
C	2.50895500	-2.63058500	3.82739400
H	3.88389300	-2.86913700	-1.29534000
H	4.65153500	-4.61157600	0.24162100
H	4.03518000	-4.57863400	2.65020500
H	1.40318300	-1.46735100	5.26243800
H	0.80043400	0.29081900	3.58954100
O	2.00924200	0.61285400	-2.73627300
C	3.62136500	-2.79363500	-0.25092100
C	4.04941600	-3.79878800	0.64023000
O	0.84083500	2.26507500	-0.76116400
O	-1.18653400	1.60279000	-1.53730500
C	-0.12294300	2.30859700	-1.57242400
C	-0.00278600	3.29128000	-2.71985900
H	0.42902500	4.23325500	-2.36978500
H	0.68781400	2.86197500	-3.45463000
H	-0.96450800	3.47736200	-3.20183400
C	3.71357500	-3.78945000	1.97680100
C	1.74376100	-1.56235400	4.23661500
C	1.39587300	-0.56830400	3.30397500
N	1.77434500	-0.62407700	2.02841600
C	2.51559000	-1.69052700	1.58241200
C	-4.32910600	-1.18648100	-0.35307100
C	-5.55088800	-1.58304900	-0.89993600
C	-5.91371900	-1.08993100	-2.15219100
C	-5.04953100	-0.22687500	-2.83357700
C	-3.82273000	0.15383500	-2.27720100
C	-3.45640100	-0.31754400	-1.01470300
H	-6.18943200	-2.27601800	-0.35929000
H	-6.85825200	-1.38591800	-2.59984900
H	-5.32872600	0.15179300	-3.81408800
H	-3.16141400	0.82125300	-2.81929800
H	2.85994700	2.33703600	1.19888800
S	-3.78165700	-1.77464700	1.24705100
N	-2.10714000	-1.59293200	1.04784000
O	-4.17586900	-3.18384300	1.40721700
H	0.70575600	-4.33173700	-3.26222200
C	-1.46015100	-2.73862300	0.51533700
C	-1.38312800	-3.96822300	1.15379300
C	-0.76161900	-5.06871000	0.52228300
C	-0.21844300	-4.96293900	-0.74080600
C	0.14430000	-2.26210000	-3.30784400
C	-0.42731400	-1.19940900	-2.57868900
N	-0.89221300	-1.36919900	-1.35137000
C	-0.85792400	-2.60850800	-0.76305400
C	-0.25978100	-3.71994600	-1.42055300
C	0.24310200	-3.50589100	-2.72856800
H	-1.82784300	-4.08646000	2.13426700
H	-0.72414100	-6.01839600	1.04857200
H	0.24512500	-5.81704000	-1.22596500
H	0.52719900	-2.06670000	-4.30283800
H	-0.47867800	-0.19829600	-2.98225400
O	-4.20836100	-0.82606800	2.29191800
C	2.92258000	-2.72709700	2.47457500
C	4.38313100	0.87565700	-1.60742000
C	5.66272100	0.33048800	-1.48046100
C	6.72753300	1.16544000	-1.13550200
C	6.51227700	2.52962000	-0.92986100
C	5.22941600	3.06604300	-1.07303200
C	4.15553900	2.24153300	-1.41163600

H	5.82344400	-0.72549400	-1.66691300
H	7.72633200	0.74896300	-1.03796300
H	7.34491900	3.17645200	-0.66676200
H	5.06400500	4.12998600	-0.92601400
H	3.15358200	2.64100600	-1.52919700
S	2.99368400	-0.20645200	-2.01414700
N	2.30270000	-0.65921200	-0.56477700
O	3.56961900	-1.36317300	-2.72939500
H	2.80008800	-3.41008700	4.52655300
C	2.85006600	-1.71311000	0.18901800
H	-4.05753800	1.21313400	1.05039400
C	-2.12040100	1.37057800	1.79852200
H	-1.22744800	1.96740300	1.93537100
C	-3.13930800	1.79469800	0.98639700
Si	-3.34088600	3.56679600	0.32532700
H	-2.26256300	0.53569500	2.47868700
C	-1.78194700	4.58800300	0.65712500
C	-4.74816700	4.24923300	1.40075700
C	-3.89130400	3.67428100	-1.47563900
H	-0.86636300	4.11253900	0.29222200
H	-1.66012200	4.76175300	1.73370500
H	-1.86218800	5.57262200	0.17814600
H	-4.11517600	4.71790100	-1.73436300
H	-4.80382000	3.09146000	-1.64740800
H	-3.12396300	3.30885800	-2.16303600
H	-4.50399800	4.21009400	2.46948000
H	-5.67777600	3.68468800	1.25496800
H	-4.95838200	5.29718700	1.14811400

TS3_4

Rh	-1.27114900	-0.84853800	0.74488600
Rh	1.24859400	-0.22749200	-0.36147800
O	-0.37246400	-1.96570000	2.37556400
O	-0.66745000	-4.07554900	1.63255600
C	-0.35672900	-3.19043700	2.56095800
C	0.03339700	-3.79146900	3.87809000
H	0.24325200	-3.00738100	4.60594700
H	-0.77164500	-4.43742400	4.24484000
H	0.92172600	-4.41881500	3.74455000
C	-2.31164800	2.79706100	3.68475400
H	-4.57031800	2.19333500	-1.08124100
H	-5.30590500	4.00735600	0.37728800
H	-4.28628400	4.37006400	2.61559800
H	-0.81855100	1.97925300	5.00295900
H	-0.24865900	0.11356500	3.43139800
O	-2.36883000	-1.13727400	-2.49251800
C	-4.12172400	2.28266900	-0.10339500
C	-4.52983800	3.33747400	0.73919900
O	-0.98694700	-2.57257400	-0.49815400
O	0.67226400	-1.72442400	-1.76650200
C	-0.22257100	-2.57936200	-1.53037800
C	-0.42360800	-3.69898300	-2.52132600
H	-0.58735500	-4.64775900	-2.00075800
H	-1.32411800	-3.47513200	-3.10312600
H	0.42817900	-3.78648900	-3.19869500
C	-3.97094500	3.54740200	1.98052300
C	-1.33742500	1.89777300	4.05357000
C	-1.00465600	0.84587200	3.17996200
N	-1.60048200	0.69248000	2.00060300
C	-2.56047700	1.58362500	1.59169700
C	3.85979900	1.17036200	-0.63686900
C	4.70807100	2.01970900	-1.34105500
C	4.95150200	1.76080200	-2.69210400
C	4.32264600	0.67742800	-3.31662600
C	3.45263400	-0.14894600	-2.60297500
C	3.20060700	0.08336700	-1.23983000
H	5.15731500	2.87104800	-0.83888300
H	5.61933800	2.40594300	-3.25600900
H	4.49988400	0.48481100	-4.37198300
H	2.94996000	-0.97043800	-3.10642900
H	-0.85806700	-3.60262500	0.76643700
S	3.38400900	1.52850300	1.05387300
N	1.71473000	1.38172700	0.90494800
O	3.81495300	2.89675800	1.38803800
H	-1.29937000	4.52003900	-3.00536200
C	1.07025600	2.57698800	0.47913800
C	1.04625500	3.74849400	1.22321300
C	0.41978500	4.91094300	0.72054400
C	-0.19178600	4.92278400	-0.51499900
C	-0.79148100	2.44978300	-3.26020400
C	-0.18016200	1.32623500	-2.66233800
N	0.39107100	1.38565200	-1.47157900
C	0.40477200	2.56633200	-0.77961900
C	-0.21293900	3.74127600	-1.29823500
C	-0.81560400	3.64498800	-2.57874400
H	1.53335400	3.77233300	2.19014200
H	0.42912500	5.81194200	1.32790000
H	-0.66443900	5.82281900	-0.89839200
H	-1.25649500	2.34296300	-4.23410000
H	-0.18831800	0.35571700	-3.14443400
O	3.85043200	0.43521300	1.92694000
C	-2.95804100	2.66711000	2.43002000
C	-4.67756000	-1.35288500	-1.22404400
C	-5.99134600	-0.88132900	-1.24214700
C	-7.01876900	-1.70974000	-0.78474900
C	-6.73071600	-2.99338700	-0.31906200
C	-5.41183000	-3.45748600	-0.31373900
C	-4.37714900	-2.63936200	-0.76555700
H	-6.20516000	0.10976100	-1.62614600
H	-8.04438200	-1.35137900	-0.80000400
H	-7.53352100	-3.63606800	0.03227300
H	-5.18873500	-4.46196700	0.03621400
H	-3.35016200	-2.98889500	-0.77432400
S	-3.33714000	-0.28219400	-1.79050500
N	-2.59022200	0.29390200	-0.41723400
O	-3.96643000	0.80429400	-2.56581800
H	-2.59380000	3.61568900	4.34177200
C	-3.13240400	1.37759100	0.29342100
H	2.36883100	-1.54537400	1.76064700
C	3.21478100	-1.72989300	-0.23508900
Si	5.05394300	-2.06817600	0.28155200
C	2.16613800	-1.83038700	0.73402600
H	2.98159500	-2.28992500	-1.14103900
H	1.46018300	-2.64523200	0.60828200
C	5.13354200	-2.52767000	2.11071300
C	6.39056700	-0.80600000	-0.12593200
C	5.41208900	-3.63035600	-0.74254400
H	6.34401800	0.07239800	0.52325500
H	6.36334400	-0.47148900	-1.16776500
H	7.36524100	-1.28642300	0.03878300
H	4.45249000	-3.35088600	2.35909200
H	4.88878600	-1.67257400	2.74720900
H	6.15020200	-2.85745700	2.36425500
H	6.40176800	-4.03266100	-0.48823800
H	5.41132800	-3.42270800	-1.82044600
H	4.68072800	-4.42758700	-0.55807300

TS4_4

Rh	-1.20034500	-0.77431000	0.84787400
Rh	1.35464400	-0.07827500	-0.12659800
O	-0.36766700	-1.67222000	2.62919500
O	-0.42244800	-3.85684400	2.06785100
C	-0.26489100	-2.87018800	2.92904800
C	0.07517300	-3.31290700	4.32071600
H	0.01505500	-2.47204200	5.01241600
H	-0.59896200	-4.11435400	4.63812100
H	1.09477700	-3.71615700	4.33068600
C	-2.70170200	3.03461300	3.34938000
H	-4.55339600	1.83078300	-1.47687300
H	-5.53742300	3.69353700	-0.24224200
H	-4.71417300	4.33490700	2.01433000
H	-1.24254900	2.46605600	4.82775500
H	-0.43231400	0.51466600	3.48517200
O	-2.00933300	-1.41775000	-2.42155800
C	-4.19033000	2.03961400	-0.48208000
C	-4.74055400	3.12499500	0.23083500
O	-0.71779900	-2.57900400	-0.19796600
O	1.01997200	-1.76170200	-1.38226000

C	0.13658600	-2.63045700	-1.15788600
C	0.05060600	-3.82787000	-2.07244900
H	-0.09263100	-4.74444000	-1.49097600
H	-0.82905600	-3.69640500	-2.71107600
H	0.94030000	-3.91912400	-2.69714400
C	-4.29140200	3.48829200	1.48128600
C	-1.68929500	2.25563700	3.86164400
C	-1.22080200	1.15758600	3.11672500
N	-1.72097200	0.84856400	1.92389100
C	-2.71148100	1.62019800	1.37092500
C	3.88197700	1.49617800	-0.35679200
C	4.71868700	2.31109700	-1.11099300
C	5.07904900	1.90142500	-2.39844700
C	4.56940500	0.70785500	-2.91786600
C	3.72670100	-0.09865500	-2.14974200
C	3.36947600	0.27365800	-0.84282700
H	5.05568300	3.26069100	-0.70702800
H	5.73747900	2.52275900	-2.99897500
H	4.82685600	0.40507800	-3.92990600
H	3.32535000	-1.01525100	-2.57041700
H	-0.58339500	-3.47580100	1.15039700
S	3.19719100	2.09019600	1.20071500
N	1.57558900	1.73138600	0.93756200
O	3.46164500	3.53619400	1.29027400
H	-1.34959300	4.04404800	-3.57007900
C	0.84807700	2.78426600	0.31681100
C	0.62913200	4.02044400	0.90802600
C	-0.06775300	5.03843900	0.21921700
C	-0.55247500	4.84204200	-1.05620900
C	-0.59626300	2.03464500	-3.53107500
C	0.06194800	1.06068100	-2.74899600
N	0.49235800	1.31190300	-1.52481200
C	0.31412800	2.55580200	-0.98364600
C	-0.36918700	3.58739400	-1.69061300
C	-0.82166100	3.28368100	-3.00016700
H	1.01485300	4.20793700	1.90264000
H	-0.21493700	5.99520200	0.71295700
H	-1.07919800	5.63270700	-1.58337900
H	-0.93967300	1.77081800	-4.52538800
H	0.20712600	0.05044600	-3.11347100
O	3.66857900	1.24560200	2.31549500
C	-3.24915900	2.73787500	2.07592800
C	-4.39439600	-1.69156300	-1.31300300
C	-5.73008100	-1.31090400	-1.45492300
C	-6.73502900	-2.16655200	-0.99821700
C	-6.40331000	-3.38858400	-0.41141300
C	-5.06247400	-3.76377000	-0.28428700
C	-4.04985800	-2.91734100	-0.73446800
H	-5.97637200	-0.37013700	-1.93379900
H	-7.77680700	-1.87819000	-1.10859000
H	-7.18833600	-4.05296600	-0.06020500
H	-4.80435800	-4.72147200	0.16012900
H	-3.00586300	-3.19979400	-0.64928100
S	-3.08618800	-0.57890200	-1.87623700
N	-2.48890900	0.16884700	-0.51237700
O	-3.72371300	0.38522400	-2.79401900
H	-3.08869900	3.88411400	3.90619900
C	-3.16683600	1.25737800	0.06116600
H	2.15510600	-1.01759800	2.22778900
C	3.53883700	-1.16707900	0.57577000
C	2.28582300	-1.43153200	1.23101000
H	1.82683100	-2.40638000	1.08010000
H	4.15174700	-0.49300100	1.17021600
Si	4.62620600	-2.59721800	-0.09026500
C	3.74798700	-3.79517600	-1.25455900
H	4.41878100	-4.63464400	-1.48212600
H	2.84517200	-4.21660300	-0.79942400
H	3.46364400	-3.33374500	-2.20519700
C	6.23102800	-1.95696300	-0.85580000
H	6.98655400	-2.75379800	-0.84370400
H	6.11603700	-1.62705500	-1.89252900
H	6.63915400	-1.11426500	-0.28401100
C	5.06604800	-3.51855700	1.51023900
H	5.73861800	-4.35983900	1.29637700
H	5.57574400	-2.86541100	2.22938800
H	4.17577400	-3.92367300	2.00623100

TS5_4

Rh	-1.10837600	-0.88058600	0.36095100
Rh	1.43870900	-0.21268200	-0.67945500
O	-0.43581400	-2.61620900	1.47383000
O	-1.33950500	-4.22965700	0.17973000
C	-0.85452600	-3.77374600	1.31795300
C	-0.89471300	-4.75962100	2.44792100
H	-0.17368000	-4.48470900	3.21876300
H	-1.90096900	-4.73721200	2.88638600
H	-0.70565200	-5.77452900	2.09150500
C	-1.56830600	1.66276500	4.40439900
H	-4.11740300	2.88929300	-0.08765800
H	-4.58448200	4.16046600	1.94649800
H	-3.42137900	3.65977600	4.08525800
H	-0.09481900	0.33499800	5.24249300
H	0.17945200	-0.93994500	3.10722500
O	-2.44001000	-0.02017400	-2.67093100
C	-3.61826800	2.60418800	0.82630600
C	-3.86941900	3.34334500	2.00105200
O	-1.11234900	-2.12994900	-1.37046700
O	0.59638700	-1.10932200	-2.42127700
C	-0.38921600	-1.89427600	-2.40317300
C	-0.76675900	-2.60462100	-3.67888600
H	-1.04105300	-3.64376800	-3.47210000
H	-1.64547900	-2.10169300	-4.09688000
H	0.04592800	-2.57151500	-4.40716300
C	-3.22923600	3.07449200	3.19073200
C	-0.67608200	0.61567000	4.37042500
C	-0.50985800	-0.10949100	3.17582600
N	-1.18637100	0.18613100	2.06989600
C	-2.06232500	1.24245300	2.06051600
C	4.07487500	1.14911500	-0.97063900
C	4.85399300	2.16493400	-1.51491500
C	4.85167100	2.35017500	-2.89945900
C	4.04649500	1.53967000	-3.70712300
C	3.26224900	0.53296700	-3.14513600
C	3.26735600	0.30508000	-1.75795300
H	5.43436500	2.80691700	-0.85954300
H	5.46327300	3.13060000	-3.34319700
H	4.02880800	1.69519300	-4.78290900
H	2.64184400	-0.09163500	-3.78161500
H	-1.28783000	-3.50942800	-0.51963600
S	3.90344100	0.97384700	0.80491000
N	2.22280500	0.90146200	0.93181800
O	4.47325900	2.16711600	1.45196700
H	-0.83602700	5.29602100	-1.42998000
C	1.62593600	2.19584200	0.98803100
C	1.77947200	3.06401200	2.05832100
C	1.21535700	4.35974000	2.02410000
C	0.50115000	4.80395700	0.93183700
C	-0.55121300	3.38751300	-2.37022800
C	-0.01211000	2.09113700	-2.21845700
N	0.65341400	1.72809600	-1.13608000
C	0.84562400	2.62522900	-0.12192500
C	0.30118100	3.94098600	-0.17550000
C	-0.40649100	4.30061600	-1.35105900
H	2.36159200	2.74914400	2.91604500
H	1.36242500	5.01575900	2.87769000
H	0.08242000	5.80622300	0.90637700
H	-1.09884300	3.62938700	-3.27424200
H	-0.16213900	1.32612500	-2.97108600
O	4.43793800	-0.34004100	1.20240100
C	-2.29695400	2.01056800	3.23925900
C	-4.67026600	-0.36201900	-1.28792200
C	-5.89393200	0.23481000	-0.97841200
C	-6.98668500	-0.57520600	-0.66159100
C	-6.85345800	-1.96444000	-0.66117500
C	-5.62657700	-2.55110700	-0.98577800
C	-4.52751300	-1.75299400	-1.30127000
H	-5.99197500	1.31401800	-1.00399700
H	-7.94247800	-0.11721000	-0.42230500

H	-7.70681300	-2.59131400	-0.41678600
H	-5.52709500	-3.63320500	-1.00118100
H	-3.57249700	-2.19463300	-1.56524400
S	-3.23736800	0.67629200	-1.65125800
N	-2.33043200	0.71538600	-0.25324100
O	-3.76194100	2.01203400	-1.99629000
H	-1.72237500	2.23508400	5.31551700
C	-2.71737000	1.53514500	0.82035600
C	3.33316000	-1.57986300	-1.37003400
C	2.40751400	-2.16765500	-0.42058000
H	1.65534600	-2.78141400	-0.91972900
H	4.36976300	-1.50047200	-1.05626800
H	3.21793900	-1.88109400	-2.40837800
Si	3.09434900	-3.11930600	1.08542800
C	2.41096100	-4.89046700	0.85311400
H	2.54323900	-5.48963700	1.76397400
H	1.35140500	-4.93123700	0.57889600
H	2.95876300	-5.40387100	0.05115900
C	2.63179100	-2.51111300	2.81370300
H	1.57225300	-2.68655300	3.02291200
H	3.21858900	-3.04908600	3.57081700
H	2.84089300	-1.44365600	2.92127800
C	4.97382900	-3.35842200	0.96800100
H	5.27206800	-3.74184400	-0.01695100
H	5.53352600	-2.44048300	1.16227000
H	5.28840600	-4.10780300	1.70778300

TS6_4

Rh	-1.05424000	-0.77935600	0.43655100
Rh	1.61804800	-0.26197500	-0.37103100
O	-0.70038900	-2.52162500	1.72750700
O	-1.88727100	-3.96266800	0.45855600
C	-1.36172100	-3.56310800	1.60372400
C	-1.64200100	-4.48498000	2.75286400
H	-1.28562100	-4.05221100	3.68759700
H	-2.71930800	-4.67284600	2.81559600
H	-1.15171400	-5.44967400	2.58233400
C	-1.83282400	1.97433800	4.28034100
H	-3.84488400	3.06212800	-0.50995400
H	-4.48794100	4.43677800	1.40604700
H	-3.58521700	3.99802800	3.68011700
H	-0.49414200	0.65253400	5.32808200
H	-0.05807000	-0.74634000	3.29700600
O	-2.10646900	-0.09837100	-2.74720100
C	-3.45891500	2.80389800	0.46509800
C	-3.81193400	3.60200100	1.57355500
O	-0.94213300	-2.13347400	-1.19492700
O	1.06023300	-1.49483900	-2.00966200
C	-0.02629400	-2.13128500	-2.08763100
C	-0.29543900	-2.92944900	-3.34014700
H	-0.73008000	-3.90226700	-3.09221100
H	-1.03185500	-2.37786400	-3.93576400
H	0.61366200	-3.06596900	-3.92868900
C	-3.31689400	3.36765800	2.83741900
C	-0.97323100	0.90473000	4.38789200
C	-0.71188300	0.11520600	3.25259700
N	-1.25968100	0.37783500	2.06991200
C	-2.09169200	1.45811400	1.91803500
C	4.16845500	1.31196800	-0.53590000
C	5.01242900	2.23177000	-1.14765500
C	5.24062100	2.12579500	-2.52280000
C	4.60540500	1.11894900	-3.25663800
C	3.75205700	0.20798900	-2.63015400
C	3.52033500	0.28657800	-1.24883200
H	5.46833400	3.02117600	-0.55788100
H	5.90311400	2.82973900	-3.01832500
H	4.77375600	1.04379800	-4.32816800
H	3.26321700	-0.56963300	-3.21044400
H	-1.60692000	-3.33706900	-0.27404100
S	3.75487600	1.42626100	1.20507700
N	2.08301000	1.17463900	1.11475000
O	4.10249700	2.77564100	1.67997800
H	-0.68109700	4.88336000	-2.46616800
C	1.38981400	2.39525200	0.85332100
C	1.29985600	3.43195800	1.76948000
C	0.68750200	4.65666500	1.41829200
C	0.17556700	4.86648300	0.15569800
C	-0.13572600	2.87838000	-3.00094400
C	0.40165100	1.66097600	-2.52956400
N	0.84091700	1.51808300	-1.29248700
C	0.80400400	2.57805800	-0.42980200
C	0.22934300	3.82581800	-0.80617700
C	-0.23890400	3.94571900	-2.13942800
H	1.73383900	3.30624100	2.75416400
H	0.64042300	5.44884200	2.16053800
H	-0.27239600	5.81828600	-0.11607000
H	-0.49168700	2.93910200	-4.02343400
H	0.44420400	0.78291400	-3.16221100
O	4.34838300	0.28011700	1.91794900
C	-2.42598500	2.28509100	3.03090600
C	-4.43164600	-0.29569700	-1.50139200
C	-5.63655900	0.34659300	-1.20587300
C	-6.76405100	-0.42194400	-0.90979500
C	-6.68596100	-1.81573000	-0.91830200
C	-5.47931700	-2.44787100	-1.23121400
C	-4.34541000	-1.69036000	-1.52435600
H	-5.69481200	1.42859000	-1.22717900
H	-7.70486500	0.07171000	-0.68213100
H	-7.56726400	-2.40985900	-0.69183600
H	-5.42189400	-3.53284400	-1.25467300
H	-3.40477400	-2.16466500	-1.78115700
S	-2.95312100	0.68772000	-1.83898300
N	-2.13788600	0.82304000	-0.38780000
O	-3.43089700	2.00154200	-2.31225600
H	-2.06260700	2.59426800	5.14310600
C	-2.60106400	1.70844500	0.60233100
C	3.66925900	-1.49140400	-0.38782500
C	2.69403300	-1.91917700	0.58446100
H	4.63576200	-1.16764300	-0.01451800
H	3.72589200	-2.05242100	-1.31841600
H	2.91422400	-1.51362000	1.57418100
Si	2.51984200	-3.80569400	0.73564100
C	2.05126500	-4.20916600	2.52646600
H	1.18770100	-3.63663200	2.87388400
H	1.83887600	-5.27813200	2.65924000
H	2.89288000	-3.96541000	3.18794300
C	1.44617600	-4.72625800	-0.52336500
H	1.60612700	-5.80652800	-0.40454200
H	0.37426200	-4.54474200	-0.42306600
H	1.73968100	-4.47266300	-1.54903600
C	4.27125100	-4.51164900	0.48490100
H	5.00539500	-4.02599200	1.13985400
H	4.28823600	-5.58559800	0.71589000
H	4.62476600	-4.39884900	-0.54824200

TS7_4

C	0.72274300	2.70261400	-0.01214100
C	0.96563700	3.95987600	-0.55163200
C	2.07924800	4.15204500	-1.37404600
C	2.90865300	3.07053500	-1.67548500
C	2.65976300	1.81394100	-1.12152500
C	1.56441600	1.59208300	-0.26557800
H	0.26365000	4.76532800	-0.35960700
H	2.28131000	5.13405800	-1.79166200
H	3.76200300	3.20632300	-2.33476500
H	3.34073200	0.99352800	-1.33189700
H	1.23841300	-4.22130600	0.95798600
S	-0.83880800	2.43697000	0.84933100
N	-1.28193200	1.10522100	-0.04515300
Rh	0.34408500	-0.16506400	-0.45350100
H	-4.53643600	-3.63136000	-0.76128400
C	-2.49367700	0.44558000	0.11708500
C	-3.69256600	0.99546000	0.56654900
C	-4.87128700	0.22345100	0.60309500
C	-4.89271700	-1.08936700	0.18068200
C	-2.43088800	-3.55135300	-1.17540800
C	-1.27560100	-2.74748200	-1.11880100
N	-1.29172400	-1.49201100	-0.68417500

C	-2.48843000	-0.93283300	-0.28757100
C	-3.69630900	-1.69332800	-0.28110900
C	-3.63029700	-3.03112000	-0.74612300
H	-3.72076300	2.03591800	0.86951400
H	-5.78536900	0.69056100	0.95986200
H	-5.81021700	-1.67053100	0.19217400
H	-2.35172500	-4.56939800	-1.54232100
H	-0.31204600	-3.14070400	-1.42106200
O	-0.57200500	2.08518900	2.26307900
O	-1.72020300	3.59842900	0.61551200
H	2.78054200	-4.83588200	0.35048700
H	4.55158200	-0.95995400	-0.69117600
H	3.39544400	-1.73599600	-1.79138700
H	4.71350600	-2.67213400	-1.07540500
H	4.50904400	-1.61749600	2.38722200
H	4.75882800	-3.32071600	1.97496600
H	3.40395500	-2.84826700	3.01199600
C	1.98790500	0.38665700	1.12388300
H	1.53707300	0.92892900	1.95251200
C	1.59566100	-1.02556200	0.99149400
Si	2.88954100	-2.35413600	0.60000800
H	0.88977700	-1.35290100	1.76237800
H	3.05063900	0.59552500	1.02379900
C	3.98103300	-1.87895800	-0.87442300
C	2.05428000	-4.01837700	0.25298100
C	3.99141500	-2.55142800	2.13379400
H	1.64296400	-4.07527300	-0.76195500

TS8_4

C	-2.75754600	-0.81952500	0.13424200
C	-3.92276100	-1.53179000	-0.12977800
C	-4.80423400	-1.07149400	-1.11068600
C	-4.48244600	0.07157900	-1.84636900
C	-3.31315400	0.78056300	-1.57212800
C	-2.42159300	0.36460800	-0.56493700
H	-4.11048600	-2.45953400	0.40186500
H	-5.72218800	-1.61558600	-1.31282400
H	-5.15098500	0.42123100	-2.62874000
H	-3.09981100	1.69367500	-2.12372200
H	3.06459300	4.30741800	0.59336900
S	-1.53403100	-1.57847300	1.22377200
N	-0.26192200	-1.40602100	0.16490600
Rh	-0.30199100	0.41305700	-0.85192200
H	5.32430800	-1.59022800	-1.31925800
C	0.99999900	-1.95480000	0.33753400
C	1.34125900	-3.06568000	1.10566500
C	2.66143000	-3.56103900	1.10687300
C	3.65584400	-2.98539500	0.34363500
C	3.94650600	-0.09734200	-2.01372100
C	2.62945600	0.39182300	-1.91220300
N	1.70777300	-0.18128700	-1.14435700
C	2.03429900	-1.31439200	-0.42928700
C	3.35761400	-1.84765000	-0.44821900
C	4.31063200	-1.20044700	-1.27479000
H	0.57637800	-3.56679700	1.68762400
H	2.88652100	-4.43141300	1.71743000
H	4.66433200	-3.38830400	0.33527600
H	4.65402900	0.41158400	-2.65996900
H	2.32138000	1.27900600	-2.45504900
O	-1.35586400	-0.74408100	2.43366400
O	-1.89808700	-2.99176900	1.44512700
H	2.03151700	4.43527500	-0.83453100
H	-0.24187300	5.33484100	1.19404100
H	0.86138700	5.06072700	2.55072600
H	-0.71525200	4.25931500	2.51782100
H	0.67246800	1.26768900	2.68887300
H	2.03226800	2.33686500	3.06788700
H	2.19161500	1.11004700	1.80312900
C	-1.66709900	1.85889800	0.33424300
H	-1.65841400	1.50504900	1.36372800
C	-0.40543200	2.39905600	-0.19287200
H	-0.56483500	3.04277200	-1.07163500
Si	0.90736000	3.10056000	0.97738800
H	-2.55608900	2.44565900	0.11600600
C	1.50075800	1.83517700	2.24836100
C	0.12989900	4.57358700	1.89214500
C	2.36484300	3.75058000	-0.04356800
H	2.93121200	2.94094200	-0.51837100

TS9_4

C	1.37202600	1.69019900	-0.43622000
C	2.06180400	2.72540100	-1.05588600
C	3.00568600	2.42796400	-2.04411900
C	3.20101600	1.10106700	-2.43471600
C	2.50970900	0.06615600	-1.80013200
C	1.58956100	0.32845400	-0.76589100
H	1.82277900	3.75365500	-0.80188000
H	3.55428900	3.23058200	-2.52820300
H	3.89759200	0.86826600	-3.23626000
H	2.68466700	-0.96145600	-2.10553400
H	3.00687800	-3.12053200	2.63341800
S	-0.03300800	2.11397500	0.61791500
N	-1.10572900	1.06500200	-0.11339100
Rh	-0.21586800	-0.73916300	-0.69486100
H	-6.05289100	-1.95633700	-0.03457300
C	-2.43986500	0.94936400	0.25709500
C	-3.22933100	1.93287300	0.84931700
C	-4.59560600	1.70341400	1.10994200
C	-5.20802300	0.51337700	0.77736000
C	-4.19011300	-2.73675200	-0.76241700
C	-2.81982600	-2.46502100	-0.94349900
N	-2.26630600	-1.30472200	-0.60884600
C	-3.05435000	-0.31111700	-0.06671900
C	-4.44532200	-0.51973000	0.17627900
C	-4.99414700	-1.77245500	-0.19853700
H	-2.78938100	2.89328600	1.09325400
H	-5.17468200	2.49743100	1.57391400
H	-6.26489400	0.35075300	0.96790800
H	-4.58520800	-3.70267900	-1.05957200
H	-2.15440000	-3.21408100	-1.36060500
O	0.24442400	1.71728000	2.01847900
O	-0.38478900	3.53071000	0.39627100
H	2.96087400	-1.56725500	3.48308700
H	4.63883400	-1.79541300	-1.14002900
H	3.75508700	-3.19878500	-0.50809200
H	5.29137900	-2.71952900	0.21355200
H	5.39225400	0.24572500	1.68543000
H	3.85416900	1.07982000	1.94266200
H	4.53087700	0.95189400	0.31048400
C	1.62208200	-0.97440800	0.72225100
H	1.23071500	-0.36019000	1.53707000
C	0.78450600	-2.14203100	0.46788000
H	1.21571200	-2.96744600	-0.10746000
H	0.11383400	-2.47311300	1.26133100
Si	3.50081500	-1.22819700	1.04816100
C	4.36312500	-2.33030900	-0.22576100
C	3.48991500	-2.13879100	2.71048700
C	4.39607700	0.41790600	1.25642000
H	4.51594000	-2.30033700	3.06681000

TS10_4

C	1.61404800	1.44814900	-0.58585500
C	2.33675300	2.50234500	-1.13163500
C	3.20913000	2.27354000	-2.19939100
C	3.29880600	0.99298000	-2.74227100
C	2.56750300	-0.06030700	-2.18921800
C	1.71599300	0.11708800	-1.07782900
H	2.17939000	3.50443900	-0.74508100
H	3.78397400	3.09460600	-2.61756000
H	3.94193300	0.80526100	-3.59819500
H	2.67603700	-1.05201600	-2.62137700
H	3.62583400	-3.69721600	1.22643900
S	0.33963700	1.88969600	0.61954700
N	-0.89841800	1.09787100	-0.14759400
Rh	-0.26565800	-0.74255400	-0.97171700
H	-6.11334100	-1.41949900	0.10252100
C	-2.20240300	1.07888700	0.33126200
C	-2.83484300	2.07467400	1.07296300

C	-4.19336100	1.95681300	1.43004000
C	-4.95300200	0.86992300	1.04959600
C	-4.40126900	-2.30676200	-0.84146600
C	-3.02684100	-2.15578400	-1.11118300
N	-2.33265400	-1.08956800	-0.72786300
C	-2.96985100	-0.07855100	-0.04121800
C	-4.35273400	-0.17254100	0.29991500
C	-5.05634900	-1.32520400	-0.13311500
H	-2.27695300	2.95893300	1.36006400
H	-4.64823800	2.75678800	2.00818300
H	-6.00384000	0.79664400	1.31430900
H	-4.91569700	-3.19822000	-1.18506800
H	-2.47609900	-2.92621600	-1.64111500
O	0.65819400	1.28139400	1.93231400
O	0.16965000	3.35788000	0.61295600
H	4.85687000	-2.79467800	2.11976500
H	3.41009800	1.18686300	1.71778300
H	4.47842900	0.50689800	0.47173900
H	4.81883200	0.22317200	2.18412000
H	2.74121800	-1.28957800	3.92802800
H	1.60706100	-2.43789800	3.20722400
H	1.25771000	-0.69144100	3.16975200
C	1.80944000	-1.52218500	-0.05851500
Si	2.98727100	-1.26591000	1.46263500
C	0.55248000	-2.23666000	0.18037800
H	0.44267600	-3.20710100	-0.31532700
H	0.10676300	-2.21395300	1.17461200
H	2.37883400	-2.03482600	-0.83398600
C	4.01170900	0.31545200	1.44455900
C	4.16623800	-2.74294800	1.26767800
C	2.04956200	-1.44155400	3.08841900
H	4.77582300	-2.66486200	0.35815200

23a

C	-1.36172400	-0.79776000	0.00063300
H	-1.41112200	-1.89144300	0.00092200
C	-2.52860100	-0.14021800	0.00044900
H	-2.58138800	0.94800300	0.00020800
H	-3.49112000	-0.65292800	0.00051300
Si	0.34549000	-0.00077400	0.00007400
C	0.18509300	1.88396400	-0.00091700
C	1.28756500	-0.56768200	-1.54193500
C	1.28867600	-0.56622600	1.54194400
H	0.78888600	-0.24031100	-2.46268900
H	1.37074400	-1.66127200	-1.58475800
H	2.30761000	-0.16213400	-1.55688900
H	0.79129500	-0.23737100	2.46285800
H	2.30901100	-0.16135400	1.55512600
H	1.37116900	-1.65982200	1.58595000
H	-0.34711900	2.25204800	0.88492400
H	-0.34798900	2.25109600	-0.88660700
H	1.17711800	2.35386500	-0.00163700

Int7_4

Rh	1.15711200	-1.01903000	-0.55786200
Rh	-0.94548700	-0.01664800	0.70696100
O	0.09263600	-2.37971600	-1.89186400
O	0.34780500	-4.34068700	-0.80761400
C	0.00945700	-3.61746500	-1.85261700
C	-0.45990200	-4.41039900	-3.03585400
H	-0.99172600	-3.76576200	-3.73633800
H	0.41423100	-4.84110800	-3.54041800
H	-1.09846200	-5.23795900	-2.71634100
C	1.75422500	2.17964400	-4.08403400
H	4.51792400	2.30313900	0.44539100
H	5.00193500	3.93782900	-1.30371300
H	3.75001300	3.95359100	-3.45026300
H	0.17047400	1.14234500	-5.11089200
H	-0.14308000	-0.50861400	-3.25561500
O	2.64005600	-0.86392100	2.52149900
C	3.96877000	2.24499100	-0.48180600
C	4.23261700	3.19365100	-1.49259100
O	1.03038700	-2.52363300	0.93643000
O	-0.42781400	-1.38910300	2.21946900
C	0.36844800	-2.33768300	2.03205400
C	0.59849900	-3.33320700	3.13903200
H	0.66788100	-4.34977900	2.73954900
H	1.55497300	-3.09359800	3.61672000
H	-0.19592600	-3.27828500	3.88587900
C	3.54440700	3.21114600	-2.68496800
C	0.79170000	1.20547200	-4.22402000
C	0.60278100	0.27217900	-3.18873300
N	1.32644400	0.30414200	-2.07429800
C	2.28498700	1.26732700	-1.89497900
C	-4.00911800	1.20588000	0.43247500
C	-4.60354100	2.35213500	0.97941300
C	-5.26271800	2.29876900	2.20276500
C	-5.31447900	1.08595700	2.89070800
C	-4.72048500	-0.04728500	2.34380900
C	-4.05773400	-0.04189300	1.09770000
H	-4.54335700	3.28141500	0.42494400
H	-5.72336000	3.19299000	2.61277100
H	-5.81336800	1.01994500	3.85410400
H	-4.76811100	-0.98444100	2.89333800
H	0.64909200	-3.73391500	-0.06059900
S	-3.10084700	1.49188000	-1.11065100
N	-1.49890200	1.49565800	-0.63344100
O	-3.51716500	2.82094100	-1.59731000
H	1.62078200	5.13565400	2.72197800
C	-0.88649300	2.74220500	-0.37362600
C	-0.91170600	3.83064400	-1.24285300
C	-0.29256800	5.05311300	-0.90669200
C	0.37720800	5.22021900	0.28601000
C	1.21522500	3.09294400	3.24346700
C	0.62119300	1.88966700	2.80542000
N	-0.02512100	1.79115000	1.65554200
C	-0.14287200	2.88589900	0.84493300
C	0.47053500	4.13025300	1.18614700
C	1.14981600	4.20017200	2.42960400
H	-1.43082000	3.74004200	-2.18687200
H	-0.35145500	5.87551200	-1.61515800
H	0.84688800	6.16589200	0.54271800
H	1.73521700	3.11698000	4.19542800
H	0.70171600	0.97981900	3.39155900
O	-3.33491000	0.35184000	-2.01526700
C	2.53790900	2.24071800	-2.90553900
C	4.76012300	-1.30247200	1.00457800
C	6.04941700	-0.84481600	0.72579400
C	7.00484500	-1.74887600	0.25637200
C	6.67100900	-3.09183800	0.07370400
C	5.37932700	-3.53952400	0.36612200
C	4.41557700	-2.64709400	0.83439000
H	6.30297000	0.19630900	0.89115500
H	8.01187700	-1.40239400	0.04105000
H	7.41877800	-3.79233400	-0.28805200
H	5.12365100	-4.58813000	0.23881800
H	3.41244200	-2.98296000	1.07571500
S	3.50930000	-0.13835400	1.58828800
N	2.59375100	0.24696400	0.24105700
O	4.23123200	1.04007300	2.09890700
H	1.92112100	2.91392100	-4.86781000
C	2.99687100	1.25593400	-0.65320200
H	-2.20090800	-1.34397500	-1.16416400
C	-3.53606800	-1.38900300	0.59967700
Si	-4.92334300	-2.32543200	-0.42339800
C	-2.15909100	-1.47886400	-0.08844300
H	-3.46350100	-1.99622800	1.51060000
H	-1.73560200	-2.46496600	0.13377600
C	-4.25395600	-3.04146100	-2.04275000
C	-6.40893700	-1.22351900	-0.81517600
C	-5.50485300	-3.77144200	0.66336000
H	-6.12629400	-0.38114700	-1.45602800
H	-6.88002400	-0.81773600	0.08751300
H	-7.17214800	-1.80484000	-1.35030800
H	-3.40412900	-3.71501100	-1.87999600
H	-3.93513100	-2.24603100	-2.72423800
H	-5.03918100	-3.62088500	-2.54705100
H	-6.27503500	-4.36568900	0.15370500

H	-5.93727400	-3.42697300	1.61168700
H	-4.67819300	-4.45174400	0.90747800

Int8_4

Rh	1.09910900	0.98328400	0.57576500
Rh	-1.09960000	-0.15706400	-0.42462800
O	0.16181800	2.17418000	2.14442300
O	-0.03733100	4.18056700	1.13574500
C	-0.10291400	3.38614700	2.18180900
C	-0.55938000	4.04802500	3.44710300
H	-0.20697400	3.48838000	4.31513200
H	-0.21394400	5.08370500	3.49039300
H	-1.65666900	4.05479100	3.46043900
C	2.46571400	-2.35356700	3.74711800
H	4.43768000	-2.03518000	-1.17030900
H	5.28814000	-3.74434700	0.35988100
H	4.41655100	-3.95827100	2.67801500
H	1.02192500	-1.47929500	5.08479500
H	0.31249500	0.24800600	3.42111100
O	2.29970400	1.27614700	-2.62974800
C	4.04753600	-2.07192700	-0.16468900
C	4.52568400	-3.05985400	0.72242800
O	0.59627200	2.53221900	-0.79606100
O	-0.87278000	1.28493500	-1.95417600
C	-0.15682900	2.30569500	-1.82134600
C	-0.14989000	3.34925200	-2.90742500
H	-0.24753300	4.35111700	-2.47619700
H	0.81604100	3.29807200	-3.42071100
H	-0.95177700	3.17367300	-3.62654600
C	4.04828400	-3.18723700	2.00780200
C	1.48926300	-1.45267600	4.10635400
C	1.07866300	-0.47705100	3.17977400
N	1.60689600	-0.39702100	1.96282500
C	2.57349600	-1.28500900	1.56634100
C	-3.84870800	-1.55787900	-0.13299900
C	-4.21884300	-2.64771400	-0.93063900
C	-4.78483900	-2.43827500	-2.18598500
C	-4.96743500	-1.13404500	-2.64465500
C	-4.62007100	-0.05418400	-1.83389400
C	-4.07301800	-0.22013400	-0.54895700
H	-4.05968100	-3.65274100	-0.55669000
H	-5.07387800	-3.28730900	-2.79902600
H	-5.39399800	-0.95276200	-3.62770000
H	-4.78959500	0.95140900	-2.20255900
H	0.21093000	3.64356100	0.31972400
S	-2.92694700	-1.99125300	1.38168200
N	-1.34497900	-1.79924100	0.87054700
O	-3.24231100	-3.40379300	1.66509500
H	1.65876800	-4.86790500	-3.10856200
C	-0.67120100	-2.96283900	0.43165700
C	-0.54547600	-4.12434400	1.18862100
C	0.10423300	-5.26648200	0.67338000
C	0.65973700	-5.27420400	-0.58808600
C	1.06810500	-2.82155400	-3.38148000
C	0.42996800	-1.71642800	-2.77797600
N	-0.10440100	-1.77619700	-1.56990600
C	-0.05156700	-2.94189100	-0.85947500
C	0.59813500	-4.10195400	-1.38136600
C	1.15692900	-4.00291700	-2.68144300
H	-0.97499800	-4.15780000	2.18102900
H	0.16292200	-6.15553000	1.29595300
H	1.15459100	-6.15815900	-0.98126300
H	1.49455500	-2.71573900	-4.37357200
H	0.37916300	-0.75443100	-3.27735400
O	-3.19850000	-1.01705000	2.45091000
C	3.04270300	-2.29724800	2.45451000
C	4.40015800	1.79268300	-1.09645000
C	5.71974700	1.43649600	-0.80805500
C	6.56080200	2.37411600	-0.20561900
C	6.08648100	3.65200900	0.09660800
C	4.76780000	4.00065800	-0.20903700
C	3.91597100	3.07204400	-0.80757300
H	6.08398800	0.44847700	-1.06642900
H	7.58934500	2.10581200	0.01943200
H	6.74617500	4.37940800	0.56185200
H	4.40361700	5.00080900	0.01078000
H	2.89197000	3.32959100	-1.05552100
S	3.29145600	0.56164900	-1.81682900
N	2.47968500	-0.12274000	-0.52331600
O	4.14885200	-0.42875200	-2.49158900
H	2.80079400	-3.11907600	4.44200900
C	3.07453000	-1.15233000	0.23351100
H	-2.02960500	1.21714900	1.64397000
C	-3.78994200	0.96216500	0.37888200
H	-4.16416700	0.63653600	1.35570400
C	-2.27051400	1.23514100	0.58170300
Si	-4.77398600	2.58623900	0.10537800
H	-1.97937000	2.20730500	0.16867200
C	-6.63961700	2.24852300	0.11092000
C	-4.31041000	3.55468500	-1.46316500
C	-4.35897400	3.69978500	1.58518900
H	-4.77237300	3.15592000	-2.37415900
H	-3.22634700	3.57392500	-1.62820600
H	-4.64285000	4.59705700	-1.36691300
H	-6.95086500	1.74602700	1.03565800
H	-6.95264900	1.61247800	-0.72543800
H	-7.20712300	3.18592600	0.04042000
H	-5.01534100	4.57960000	1.61066800
H	-3.32732000	4.06786300	1.52891100
H	-4.47895200	3.17299300	2.54029400

Int9_4

Rh	1.02924200	-0.90850900	-0.38481400
Rh	-1.38639700	-0.18313600	0.64060200
O	0.39394400	-2.60986600	-1.57288300
O	1.33364400	-4.24680100	-0.33558900
C	0.84774300	-3.76054500	-1.45853500
C	0.93070900	-4.69341800	-2.62942100
H	0.23831100	-4.38294200	-3.41272600
H	1.95291500	-4.65414300	-3.02799600
H	0.72802500	-5.72264600	-2.32484800
C	1.58004700	1.75790500	-4.34130800
H	4.06200800	2.81339800	0.22890800
H	4.56115200	4.15736500	-1.74801600
H	3.43268600	3.73632000	-3.92261200
H	0.11994600	0.46283300	-5.25213200
H	-0.20363600	-0.87626100	-3.16403800
O	2.36688800	-0.18979400	2.68379400
C	3.57425300	2.56354200	-0.70108100
C	3.84505300	3.34523000	-1.84412300
O	1.03500700	-2.21792600	1.27659100
O	-0.60755400	-1.14486300	2.36793900
C	0.32091400	-1.98582400	2.32479700
C	0.65393800	-2.78041900	3.56143000
H	0.85429700	-3.82564700	3.30523300
H	1.56501500	-2.36118900	4.00164800
H	-0.15466000	-2.72575400	4.29277400
C	3.22397500	3.12111600	-3.05238900
C	0.68466900	0.71286100	-4.36029000
C	0.49112400	-0.04843400	-3.19301400
N	1.14712100	0.21046800	-2.06640400
C	2.03038100	1.25739500	-2.00524200
C	-3.92716500	1.00508600	1.13456100
C	-4.10342200	2.24978000	1.75355500
C	-4.01563000	2.35942000	3.13709600
C	-3.72992200	1.22538000	3.90481800
C	-3.57284200	-0.00931100	3.28754900
C	-3.67974900	-0.17055700	1.88975500
H	-4.31329100	3.11761500	1.13851900
H	-4.16460300	3.32371300	3.61477700
H	-3.65038000	1.30279300	4.98576100
H	-3.38688900	-0.89258800	3.89186100
H	1.23916000	-3.56259600	0.39765200
S	-3.86265900	1.02255100	-0.68122200
N	-2.19962000	0.96606500	-0.93077200
O	-4.44343900	2.30171800	-1.12433500
H	0.81697700	5.45891700	1.32764500
C	-1.61011900	2.26180700	-0.99953300

C	-1.80745000	3.11739300	-2.07293900
C	-1.27221300	4.42507900	-2.06873900
C	-0.54512000	4.89673500	-0.99670400
C	0.59940100	3.55995400	2.30541300
C	0.09352200	2.24619700	2.17914400
N	-0.57485100	1.84146300	1.11430200
C	-0.81118900	2.71819600	0.09253900
C	-0.30333500	4.05146900	0.11590400
C	0.41515000	4.45013400	1.27306900
H	-2.40590600	2.77949600	-2.91124200
H	-1.45490900	5.06852200	-2.92519400
H	-0.15082200	5.90936100	-0.98954600
H	1.15136800	3.83226600	3.19839400
H	0.27200100	1.50166100	2.94734000
O	-4.46778700	-0.21256300	-1.19935500
C	2.28800200	2.06405300	-3.15273300
C	4.61251900	-0.46501100	1.30750900
C	5.83548700	0.15194400	1.03804200
C	6.93634300	-0.63790000	0.69898600
C	6.81121800	-2.02639000	0.63706700
C	5.58468900	-2.63375000	0.92326500
C	4.47753500	-1.85612600	1.26055600
H	5.92714400	1.22957500	1.11101700
H	7.89179400	-0.16464000	0.49023700
H	7.67092300	-2.63736200	0.37557400
H	5.49194900	-3.71603900	0.89228200
H	3.52305200	-2.31503900	1.49645700
S	3.16996800	0.54736800	1.70089700
N	2.28032900	0.62841600	0.28633300
O	3.67770800	1.87521400	2.09335100
H	1.75284400	2.36012900	-5.22945100
C	2.67080300	1.49827400	-0.74769000
Si	-3.05906000	-2.95010100	-1.15810600
C	-3.71723800	-1.59326400	1.31017100
H	-4.66453100	-1.67796500	0.77345800
C	-2.51417300	-1.97673300	0.40177900
H	-3.77389300	-2.27243000	2.16896200
H	-1.89020700	-2.68269800	0.96231200
C	-2.34375500	-4.71807300	-0.96020100
C	-2.58895400	-2.27790300	-2.86880000
C	-4.93303900	-3.29409100	-1.18779200
H	-5.14508200	-4.00301200	-2.00101900
H	-5.53073700	-2.39604300	-1.36595200
H	-5.28699900	-3.76503900	-0.26130700
H	-2.94652700	-5.27543500	-0.22967300
H	-1.31214800	-4.75647600	-0.59524200
H	-2.39084600	-5.28260900	-1.90147600
H	-1.57559800	-2.57396400	-3.15580000
H	-2.65904100	-1.18719200	-2.88664200
H	-3.28009600	-2.67056900	-3.62681400

Int10_4

Rh	-1.02444300	-0.86039800	0.56247100
Rh	1.29315500	-0.31886900	-0.58207700
O	-0.40750500	-2.49780300	1.88631000
O	-1.82846600	-4.01070900	1.00214400
C	-1.05034600	-3.55677300	1.96525900
C	-1.03845800	-4.39878500	3.20475500
H	-0.18493800	-4.13554900	3.83087700
H	-1.96211300	-4.20553000	3.76567600
H	-1.01873100	-5.46228500	2.95390500
C	-1.15690200	2.25033500	4.21363000
H	-3.54038400	3.13160600	-0.44741700
H	-3.78240700	4.76441300	1.35414500
H	-2.69632400	4.42930800	3.56478900
H	0.12233500	0.87051800	5.26101400
H	0.21905600	-0.72335600	3.33547200
O	-2.39261200	-0.37822700	-2.52627200
C	-3.07673000	2.92320400	0.50477500
C	-3.20112900	3.86655600	1.54717400
O	-1.20217700	-2.31277200	-0.95632100
O	0.71418800	-1.77248300	-2.01200600
C	-0.38551600	-2.38180600	-1.94787000
C	-0.81076200	-3.23486800	-3.11585100
H	-1.31768000	-4.14207800	-2.77482400
H	-1.53014100	-2.65328300	-3.70396300
H	0.04063000	-3.49474800	-3.74757500
C	-2.60172400	3.69073100	2.77432800
C	-0.42352700	1.09392400	4.35093100
C	-0.36007200	0.18796700	3.27646200
N	-0.99534300	0.41324000	2.13204300
C	-1.72463700	1.55966800	1.95430000
C	4.19263800	1.26074700	0.46211400
C	4.81234600	2.40061400	-0.05848700
C	5.72932700	2.27750200	-1.10138300
C	6.01456500	1.01307300	-1.61630900
C	5.40637900	-0.11690000	-1.06821000
C	4.48182300	-0.03011400	-0.01481000
H	4.56993400	3.37173300	0.35828100
H	6.21323000	3.16235800	-1.50542900
H	6.72482200	0.90110200	-2.43133700
H	5.67048200	-1.10056300	-1.44875200
H	-1.70310000	-3.45202500	0.18130900
S	2.84193900	1.53092600	1.62057800
N	1.53918800	1.43537400	0.58791200
O	3.03289400	2.88116600	2.18457000
H	-0.37779500	4.33977300	-4.10452300
C	1.09057400	2.61659900	-0.04239500
C	0.98221300	3.87232100	0.55911400
C	0.57635600	5.00731000	-0.17369300
C	0.24102500	4.93174700	-1.50757100
C	-0.04934600	2.21883400	-4.06132300
C	0.30073200	1.12679000	-3.24075100
N	0.63455200	1.27201600	-1.96826700
C	0.66273200	2.51541700	-1.40688300
C	0.26886500	3.67020200	-2.14947300
C	-0.08044300	3.47904500	-3.51048200
H	1.23843100	3.98491700	1.60160500
H	0.53085000	5.96272100	0.34295400
H	-0.05950600	5.81234700	-2.06854300
H	-0.31636500	2.04555800	-5.09865700
H	0.29019700	0.11134900	-3.62050900
O	2.74989900	0.41872300	2.57959400
C	-1.83616900	2.52152900	2.99978600
C	-4.56938300	-0.31366500	-1.03058800
C	-5.68628700	0.43586000	-0.65440400
C	-6.81987200	-0.22548500	-0.17764300
C	-6.83445600	-1.61851400	-0.08677200
C	-5.71600500	-2.35866800	-0.48070300
C	-4.57645400	-1.70949600	-0.95557200
H	-5.67381200	1.51560700	-0.75022000
H	-7.69396900	0.35027000	0.11379500
H	-7.72044000	-2.12876500	0.28124600
H	-5.73352100	-3.44395200	-0.42706400
H	-3.70438800	-2.26907900	-1.27600000
S	-3.07968900	0.53160600	-1.60367000
N	-2.11445800	0.70638500	-0.24349200
O	-3.50997400	1.84378200	-2.11639000
H	-1.21680900	2.97127100	5.02473000
C	-2.34880500	1.74457700	0.68049000
H	2.02438400	-1.80764000	1.48315900
C	3.96176500	-1.30526600	0.63342100
H	4.17304900	-1.23079700	1.70292300
C	2.45719900	-1.77392400	0.48069900
H	4.63455000	-2.07912800	0.25039300
Si	2.65367100	-3.56676300	-0.17298900
C	3.44399000	-3.60773300	-1.90239900
C	1.18575800	-4.77912500	-0.19773200
C	3.84526700	-4.48355200	1.01545100
H	3.69103200	-4.63876400	-2.18879400
H	4.37574000	-3.03112500	-1.95243300
H	2.76580600	-3.19959300	-2.65930200
H	0.28169400	-4.45127300	-0.71068300
H	0.90799400	-5.07718100	0.82044300
H	1.52437700	-5.69488400	-0.70177600
H	3.87537800	-5.55161600	0.75929900
H	3.50386200	-4.41271700	2.05721900
H	4.87840500	-4.11959900	0.98945400

TS11_4

Rh	-1.40245600	-0.75368200	0.81824600
Rh	1.01028400	-0.46462800	-0.25924700
O	-0.81864800	-1.56588500	2.63798500
O	1.05540200	-2.68018100	2.09335200
C	0.09244300	-2.42426400	2.86288300
C	0.02514900	-3.16624700	4.18081500
H	-0.95392600	-3.05592200	4.65093500
H	0.24850400	-4.22513000	4.02170600
H	0.79307900	-2.76414800	4.85237500
C	-2.27247400	3.46058100	2.96584100
H	-4.63215000	2.00073200	-1.55655100
H	-5.25096700	4.11410300	-0.50608700
H	-4.18147900	4.87719300	1.60499100
H	-0.81142000	2.85555700	4.42969500
H	-0.34037300	0.68867500	3.26698300
O	-2.61387400	-1.62630200	-2.30670500
C	-4.15780000	2.27016100	-0.62524700
C	-4.50152800	3.49650500	-0.01788400
O	-1.26616900	-2.65240500	-0.04554200
O	0.42381400	-2.10100900	-1.43410300
C	-0.49466100	-2.88171400	-1.02707700
C	-0.69321300	-4.17699300	-1.77495000
H	-0.98313900	-4.97368400	-1.08439400
H	-1.50851900	-4.03472800	-2.49259400
H	0.21126300	-4.46068300	-2.31749400
C	-3.91396100	3.92847600	1.14934900
C	-1.34033200	2.60949200	3.51527600
C	-1.06293700	1.39009100	2.87230700
N	-1.67488400	1.03407000	1.74758500
C	-2.60027800	1.85999500	1.16434400
C	4.15529400	1.22085800	0.10459800
C	4.86162000	2.41140700	-0.12311800
C	5.51967900	2.64048400	-1.32662800
C	5.42031900	1.68690800	-2.33828700
C	4.73550900	0.49866300	-2.10370600
C	4.12072400	0.19295500	-0.87060700
H	4.86082600	3.16677100	0.65337400
H	6.06780600	3.56530400	-1.48107100
H	5.87742500	1.86006300	-3.30897500
H	4.68288500	-0.24023800	-2.89841400
H	1.31587600	-1.75360100	1.09204800
S	3.04410200	1.29546400	1.54209900
N	1.54870400	1.27115100	0.79365500
O	3.30036500	2.58947000	2.20184900
H	-1.04479100	3.96924300	-3.68070900
C	1.09630600	2.45353600	0.15986500
C	1.22896300	3.75720700	0.63837800
C	0.76522700	4.86217500	-0.10823000
C	0.14575700	4.71007200	-1.32897600
C	-0.85917000	1.83822600	-3.50288100
C	-0.41863100	0.78561000	-2.67559900
N	0.17646900	1.00789900	-1.51288500
C	0.39525700	2.28577800	-1.07719500
C	-0.05817700	3.40476500	-1.83803000
C	-0.69179300	3.13633700	-3.07780200
H	1.71966300	3.92725700	1.58516000
H	0.91060500	5.85752100	0.30363600
H	-0.19532300	5.56689200	-1.90290300
H	-1.34934200	1.60510900	-4.44170900
H	-0.58101300	-0.25242400	-2.94027200
O	3.15498900	0.10689100	2.39859800
C	-2.93687800	3.10937700	1.76505100
C	-4.90029100	-1.49955600	-0.97655000
C	-6.20172800	-1.01210700	-1.10473700
C	-7.24567700	-1.68843700	-0.46926700
C	-6.98404500	-2.83713500	0.27877100
C	-5.67641800	-3.31966500	0.39122300
C	-4.62447300	-2.65440600	-0.23704400
H	-6.39305700	-0.12943500	-1.70463400
H	-8.26272900	-1.31847400	-0.56525300
H	-7.79921200	-3.36144100	0.77012900
H	-5.47505800	-4.22068600	0.96435600
H	-3.60605600	-3.02359600	-0.16450700
S	-3.54040400	-0.62019700	-1.77216800
N	-2.74600000	0.17570800	-0.53181200
O	-4.14217800	0.32258500	-2.73458700
H	-2.50909000	4.40870900	3.44167900
C	-3.20676200	1.41697400	-0.05809600
H	3.08123400	-1.71236000	1.31951200
C	3.60279600	-1.23765000	-0.75076100
Si	5.20810600	-2.38177500	-0.48476700
C	2.64195700	-1.76609000	0.32903600
H	3.23267800	-1.53497800	-1.74117800
H	2.42165800	-2.80177000	0.07292800
C	4.66868100	-4.16966800	-0.18135900
C	6.17234700	-1.72575900	0.99914900
C	6.31145800	-2.38742800	-2.02379500
H	5.52993600	-1.56773500	1.87271600
H	6.66771200	-0.77363700	0.77801300
H	6.95175800	-2.44479700	1.28405800
H	4.01060300	-4.54641400	-0.97465900
H	4.15182400	-4.30032300	0.77521000
H	5.55646700	-4.81628500	-0.16511000
H	7.12772700	-3.10530500	-1.86340400
H	6.77061100	-1.41552100	-2.22960500
H	5.77339700	-2.70946900	-2.92405200

TS12_4

Rh	-1.24521800	-0.82300200	0.61132900
Rh	0.84358700	-0.12263200	-0.81700100
O	-0.15284400	-1.69234700	2.14302600
O	1.66392000	-2.58999000	1.14996800
C	0.86809700	-2.43859100	2.12547000
C	1.17903400	-3.21027600	3.38809400
H	0.33022200	-3.20839300	4.07454400
H	1.45735800	-4.23795800	3.13728600
H	2.04004300	-2.74273800	3.88014000
C	-2.05498500	3.13051100	3.23507400
H	-4.96239000	1.85197100	-1.01554700
H	-5.50752100	3.86902800	0.25416400
H	-4.19217100	4.53464400	2.25539900
H	-0.37208800	2.51250500	4.42833200
H	0.04783500	0.47516600	3.03392900
O	-3.00385400	-1.63986600	-2.25998200
C	-4.37395500	2.08833300	-0.14211700
C	-4.67726200	3.25440100	0.59217600
O	-1.06360600	-2.61189600	-0.44736200
O	0.22928200	-1.70223000	-2.05258400
C	-0.48225800	-2.64300800	-1.57511900
C	-0.65687200	-3.88528900	-2.41213800
H	-0.64822900	-4.77519400	-1.77623300
H	-1.63367400	-3.82876200	-2.90478100
H	0.12249500	-3.95881300	-3.17331500
C	-3.95332500	3.63265000	1.70004800
C	-1.01658500	2.29777400	3.58308600
C	-0.77137400	1.14655200	2.81271500
N	-1.51891300	0.83563200	1.75779700
C	-2.56477000	1.63955500	1.38302800
C	4.17386700	1.43148800	0.47575700
C	4.80319900	2.67270800	0.32164000
C	5.89624900	2.80803700	-0.53031400
C	6.33993200	1.69637200	-1.24121200
C	5.72202800	0.45915000	-1.05760200
C	4.64154200	0.26771100	-0.18060600
H	4.43248900	3.52599900	0.87725900
H	6.38376800	3.77232800	-0.64127300
H	7.17639000	1.78097600	-1.92981100
H	6.09967200	-0.39117100	-1.61307900
H	1.75899900	-1.68283700	0.25604700
S	2.63263600	1.47570800	1.42230000
N	1.46379500	1.55849600	0.23595600
O	2.65449100	2.70208600	2.24075900
H	-1.94859000	4.32694400	-3.55125700
C	0.95529800	2.76530200	-0.26338400
C	1.25192300	4.07250500	0.13201300
C	0.65334300	5.18171500	-0.50129200

C	-0.24827300	5.04277700	-1.53301400
C	-1.74840400	2.19369500	-3.43217500
C	-1.14355000	1.12963700	-2.73497800
N	-0.31211100	1.34015000	-1.72218500
C	0.00200500	2.61373600	-1.32796700
C	-0.59220600	3.74106200	-1.96957900
C	-1.48440500	3.48642700	-3.04192000
H	1.94244700	4.24377300	0.94386200
H	0.92747800	6.17493300	-0.15494300
H	-0.69163800	5.90556900	-2.02124200
H	-2.42593700	1.97127100	-4.24936900
H	-1.35239200	0.09544200	-2.97928000
O	2.44761000	0.20490200	2.13931200
C	-2.86760800	2.82530200	2.11557000
C	-4.88394000	-1.86441400	-0.40191300
C	-6.18684200	-1.47648500	-0.08202400
C	-6.95593900	-2.29722500	0.74524700
C	-6.42401600	-3.48808700	1.24284000
C	-5.12122400	-3.86851900	0.90814300
C	-4.34187200	-3.05992600	0.08082100
H	-6.59556000	-0.55954800	-0.49174200
H	-7.97261500	-2.00614700	0.99461600
H	-7.02664400	-4.12429100	1.88540800
H	-4.71174900	-4.80160400	1.28575700
H	-3.33000100	-3.34595100	-0.18832800
S	-3.87520100	-0.78663200	-1.44057800
N	-2.88857100	0.05798500	-0.38529000
O	-4.80598300	0.10985800	-2.15203600
H	-2.26209000	4.03127500	3.80698900
C	-3.32606600	1.24324300	0.23465400
H	2.62724700	-2.33221200	-1.18554200
C	4.04012300	-1.12106300	0.02394000
Si	5.24662000	-2.62018100	-0.20753800
C	2.73385100	-1.31531200	-0.79049600
H	3.78027000	-1.20085600	1.08458900
H	2.79047300	-0.68564900	-1.70450700
C	4.45067600	-4.14817500	0.57866400
C	6.87975300	-2.30572000	0.70593100
C	5.57779100	-3.04877800	-2.02936000
H	6.69737400	-2.04070000	1.75546200
H	7.47646200	-1.49999000	0.26490700
H	7.49780800	-3.21340800	0.70354300
H	3.49242200	-4.41391300	0.12067500
H	4.26921300	-4.00662300	1.65004200
H	5.12282900	-5.00980000	0.46636800
H	6.09216000	-4.01713100	-2.09188800
H	6.20657300	-2.32157600	-2.55609300
H	4.64361300	-3.14433200	-2.59684900

TS13_4

Rh	-0.98214000	0.93943400	-0.54507400
Rh	1.32338600	0.15360100	0.59320000
O	-0.14375500	2.28502800	-1.89613300
O	1.42954000	3.23323200	-0.61554800
C	0.59107400	3.25916500	-1.56950300
C	0.43084600	4.54706800	-2.34008800
H	0.21792400	4.33703100	-3.39162300
H	-0.43025800	5.08887600	-1.92860100
H	1.31617900	5.17836900	-2.24839300
C	-1.98156100	-1.96764400	-4.23806100
H	-4.75063000	-2.00097700	0.28677900
H	-5.48109600	-3.39454300	-1.57825300
H	-4.23288700	-3.44413100	-3.72852500
H	-0.25788100	-1.11128300	-5.20523200
H	0.31071200	0.32154000	-3.23168300
O	-2.49672500	0.75379700	2.56142200
C	-4.19146800	-1.95987800	-0.63557700
C	-4.59882800	-2.77424200	-1.71356600
O	-0.89799300	2.40863100	0.93674900
O	0.71135100	1.40472600	2.15752400
C	-0.18640300	2.28747900	1.98052300
C	-0.43796500	3.26638500	3.10126400
H	-0.58093900	4.27276100	2.69667300
H	-1.36096800	2.97263100	3.61292100
H	0.38564100	3.26607300	3.81813100
C	-3.91395900	-2.80975600	-2.90682900
C	-0.87751500	-1.14884100	-4.31571700
C	-0.54516800	-0.33967300	-3.21465300
N	-1.26454100	-0.34283200	-2.09716600
C	-2.35967000	-1.15896300	-1.97592000
C	3.61367900	-1.77997700	1.00838400
C	3.49801200	-3.05117500	1.57291900
C	3.34604400	-3.18630300	2.95363200
C	3.28554100	-2.04751900	3.75919900
C	3.42799100	-0.78384600	3.18932000
C	3.60645900	-0.60882700	1.80465200
H	3.52447500	-3.92205100	0.92737200
H	3.26786800	-4.17634900	3.39385500
H	3.15674400	-2.14385600	4.83376000
H	3.43815500	0.09706300	3.82601800
H	1.86776900	2.11703700	-0.22763600
S	3.46135300	-1.67388000	-0.79421100
N	1.83030000	-1.27803700	-0.90276800
O	3.74421000	-3.01317800	-1.33729800
H	-1.82389900	-4.64984600	2.16032100
C	0.99459200	-2.42502800	-0.77930300
C	0.93742300	-3.45487800	-1.70777200
C	0.15489700	-4.60599000	-1.46167400
C	-0.56560400	-4.75213500	-0.29466300
C	-1.15145900	-2.71203200	2.79000600
C	-0.41409700	-1.56540900	2.42397600
N	0.22399200	-1.48572000	1.26760200
C	0.20189100	-2.54004700	0.39522000
C	-0.55468900	-3.71452400	0.67119400
C	-1.23582400	-3.76955600	1.91402500
H	1.52770200	-3.38566000	-2.61297300
H	0.14015200	-5.39559000	-2.20800100
H	-1.14706600	-5.64971700	-0.10356800
H	-1.66858600	-2.72204500	3.74280500
H	-0.37491600	-0.68841200	3.05679200
O	4.24510000	-0.54772400	-1.31819200
C	-2.76341700	-1.99799900	-3.05691100
C	-4.64314300	1.32035300	1.11294800
C	-5.98008300	0.94154900	0.98287900
C	-6.91812100	1.88947200	0.56701800
C	-6.51814400	3.19752000	0.29155400
C	-5.17747100	3.56714500	0.43811500
C	-4.23030500	2.63100300	0.85060100
H	-6.28144500	-0.07231500	1.22079600
H	-7.96137700	1.60351800	0.46487200
H	-7.25077900	3.93238800	-0.03106900
H	-4.86913200	4.58950700	0.23628000
H	-3.18779800	2.90731300	0.97492700
S	-3.41535900	0.09779900	1.62253300
N	-2.54132200	-0.25749900	0.23796400
O	-4.16025500	-1.07821000	2.11273500
H	-2.26612600	-2.59911800	-5.07572000
C	-3.07317500	-1.12736000	-0.73182400
Si	4.21423100	2.62210400	-0.88517900
C	4.06894100	0.75143700	1.27544300
H	4.95924000	0.52696500	0.69097600
C	3.13559100	1.71277900	0.46456900
H	4.40667300	1.31051000	2.15521200
H	2.83489600	2.48068500	1.18759800
C	4.28403000	4.48029500	-0.47239700
C	3.61959100	2.36286000	-2.67213000
C	6.04103500	2.09003200	-0.83525000
H	6.59853600	2.73553200	-1.52879000
H	6.19330100	1.05542800	-1.15768700
H	6.50380700	2.21624200	0.15172200
H	4.82433000	4.65122300	0.46869500
H	3.29050800	4.92608100	-0.37056400
H	4.82483900	5.03041700	-1.25499500
H	3.00726600	3.19249800	-3.04334600
H	3.04695600	1.43468100	-2.76491200
H	4.48268400	2.27334600	-3.34436900

TS14_4

Rh	-1.21860500	-0.61058300	0.78455800
Rh	1.02568200	-0.35868800	-0.55943300
O	-0.35956800	-1.36097300	2.51237300
O	1.42942500	-2.56974100	1.85895600
C	0.58170800	-2.18334400	2.71334600
C	0.71910400	-2.73759900	4.11472200
H	-0.19425800	-2.58493200	4.69297800
H	0.96729700	-3.80189000	4.07453500
H	1.54841200	-2.22133300	4.61307600
C	-1.69569600	3.71198300	2.84600700
H	-4.42991800	2.26925100	-1.46580500
H	-4.81435800	4.47316400	-0.47790800
H	-3.57310000	5.21983600	1.54353100
H	-0.18158600	3.05706900	4.23096200
H	0.07141900	0.82882100	3.11794800
O	-2.88404300	-1.56669600	-2.11077000
C	-3.88168500	2.54094300	-0.57674800
C	-4.09213700	3.81317300	-0.00421200
O	-1.19529100	-2.53198900	-0.05321200
O	0.32771600	-2.01557300	-1.63072200
C	-0.56585900	-2.77278900	-1.12495800
C	-0.90806700	-4.03681300	-1.87561600
H	-1.27970500	-4.80247200	-1.19037400
H	-1.70897100	-3.79518500	-2.58273600
H	-0.04836600	-4.41385100	-2.43377200
C	-3.40829400	4.23663400	1.11286700
C	-0.79091800	2.81576000	3.36685000
C	-0.63947800	1.55867900	2.75447100
N	-1.34807300	1.20583000	1.68691000
C	-2.25692500	2.07340900	1.13763700
C	4.39138100	1.20115100	0.52832400
C	5.45016100	2.02436300	0.92230500
C	6.67914800	1.96214100	0.26838300
C	6.84027000	1.07996300	-0.79684100
C	5.77795000	0.26747500	-1.19219700
C	4.53338900	0.29106000	-0.54404900
H	5.29437800	2.71984700	1.73922800
H	7.49591400	2.60318000	0.58715500
H	7.78767100	1.02109000	-1.32544400
H	5.91503000	-0.41378900	-2.02811600
H	1.69309800	-1.85573700	0.80067200
S	2.85410000	1.41131400	1.46930500
N	1.66157100	1.42354300	0.32667500
O	2.95976700	2.70957500	2.16203000
H	-1.05447000	3.82221400	-4.20569900
C	1.34539200	2.57023600	-0.42079600
C	1.73149900	3.89136700	-0.18901300
C	1.31116800	4.93359700	-1.04245400
C	0.50518700	4.70813100	-2.13636600
C	-1.06713900	1.72519500	-3.75168700
C	-0.62652100	0.73633600	-2.84986500
N	0.11953900	1.03593200	-1.79617600
C	0.50231400	2.32903100	-1.55458500
C	0.08388100	3.38604900	-2.41625800
C	-0.72012000	3.03801700	-3.53133400
H	2.35686500	4.12497200	0.66012900
H	1.64311900	5.94352700	-0.81611800
H	0.19327700	5.51856700	-2.78856400
H	-1.68519100	1.43248100	-4.59343100
H	-0.90321500	-0.30383500	-2.96582000
O	2.64561300	0.22803100	2.31829400
C	-2.46126800	3.36663300	1.70489600
C	-4.86301500	-1.32564800	-0.36456300
C	-6.12997600	-0.76369100	-0.19428100
C	-7.03161300	-1.37336800	0.68045000
C	-6.66687300	-2.53090700	1.37024000
C	-5.39878300	-3.08875500	1.18277800
C	-4.48759400	-2.49001700	0.31289000
H	-6.40732200	0.12464900	-0.75067000
H	-8.02068700	-0.94451400	0.81611500
H	-7.37233400	-3.00302500	2.04868100
H	-5.11929700	-3.99650400	1.71074200
H	-3.50122700	-2.91451500	0.15582400
S	-3.68011500	-0.51498500	-1.46157900
N	-2.64716800	0.33947200	-0.46871800
O	-4.46453500	0.37564900	-2.33865900
H	-1.83060000	4.69242700	3.29548200
C	-2.97765100	1.63199000	-0.01989900
Si	3.25909300	-3.47514700	-0.59531100
C	3.47458900	-0.67114100	-1.05742100
H	3.90566500	-1.20747000	-1.90858300
C	2.87229300	-1.66528500	-0.03400300
H	2.69165600	-0.06349500	-1.61018100
H	3.38514200	-1.50040700	0.91680800
C	2.23570400	-4.86144700	0.18646600
C	5.06499800	-3.77624200	-0.08166600
C	3.14594400	-3.64252100	-2.48588400
H	3.15874700	-4.70509900	-2.76275300
H	3.98880500	-3.17329400	-3.00940000
H	2.22087100	-3.20662400	-2.87763000
H	1.15642300	-4.74548500	0.05072500
H	2.41988800	-4.93303700	1.26251000
H	2.52857600	-5.81747900	-0.26944400
H	5.17733300	-3.74885100	1.00992000
H	5.75351300	-3.03004600	-0.49803300
H	5.40939600	-4.76244800	-0.42118300

Int11_4

Rh	1.61428400	-1.14003800	-0.19495400
Rh	-0.01396200	-0.13689800	1.49430600
O	0.20184100	-2.65447000	-0.35612500
O	-0.90296600	-2.01699700	1.49708000
C	-0.66987100	-2.83142700	0.55814700
C	-1.45142400	-4.12063200	0.51483000
H	-0.76946900	-4.96658000	0.65640400
H	-2.21919700	-4.13598800	1.28983300
H	-1.91750100	-4.23232000	-0.46893500
C	0.40784500	1.08063800	-4.28311800
H	4.76219400	2.31378700	-1.51101000
H	4.29852200	3.48173700	-3.60460500
H	2.27541500	2.96944700	-4.95607200
H	-1.32241900	-0.19986300	-4.30530000
H	-0.70606500	-1.30593600	-2.14386400
O	4.18884300	-0.18769600	1.85170400
C	3.87848400	2.04222100	-2.06794400
C	3.59888900	2.71843100	-3.27391500
O	2.31747500	-2.25377800	1.43368000
O	1.25723600	-0.94860200	2.92444900
C	2.07423000	-1.87480000	2.61866600
C	2.82067600	-2.54747400	3.74189900
H	3.01323700	-3.59566100	3.49868700
H	3.78585500	-2.04118900	3.85748100
H	2.26767900	-2.47296900	4.68076200
C	2.48000700	2.44382800	-4.02808400
C	-0.41296700	0.09219100	-3.79290000
C	-0.07787800	-0.54157400	-2.58218700
N	1.01413700	-0.21424300	-1.89897200
C	1.85975500	0.76281700	-2.35920700
C	-4.17960600	0.73100700	0.66838700
C	-3.92866600	1.21903100	1.95479600
C	-4.98188100	1.53463800	2.80937100
C	-6.29170800	1.35789200	2.36699800
C	-6.53413100	0.85487700	1.09110200
C	-5.49801100	0.51192100	0.20302600
H	-2.90568800	1.35755600	2.28298300
H	-4.77631200	1.91663200	3.80513500
H	-7.12813900	1.60536200	3.01538400
H	-7.56209400	0.71395300	0.76949300
C	-5.84514100	-0.08496900	-1.14793700
S	-2.75503400	0.37763500	-0.40922700
N	-1.41584100	0.96863100	0.39357700
O	-2.96536500	1.11165900	-1.67537800
H	1.98079600	5.39552600	1.98979200
C	-1.12936600	2.34568300	0.35617500
C	-1.86376000	3.37094200	-0.24288700
C	-1.45088600	4.71692700	-0.14988400
C	-0.31445000	5.08996800	0.53257200
C	2.32948700	3.34361100	2.51416800

C	1.86067000	2.02322500	2.38200000
N	0.76393400	1.73525200	1.68878800
C	0.04884400	2.72944200	1.07250900
C	0.46262600	4.09066200	1.16630000
C	1.63807300	4.36736500	1.90819300
H	-2.75740500	3.14129200	-0.80423400
H	-2.06045000	5.47237600	-0.63849500
H	-0.00694900	6.12936900	0.59888600
H	3.23596400	3.52500700	3.08113500
H	2.38690400	1.18493500	2.81857200
O	-2.61543100	-1.08415000	-0.51604900
C	1.58022500	1.44902300	-3.57680100
C	5.63269800	-0.93940800	-0.23141600
C	6.70370000	-0.52232000	-1.02322700
C	7.52728300	-1.48393600	-1.61266000
C	7.27830500	-2.84165300	-1.40698000
C	6.20700100	-3.24548400	-0.60423300
C	5.37668800	-2.29650300	-0.00923100
H	6.89655500	0.53583800	-1.16002600
H	8.36546200	-1.16872700	-2.22792800
H	7.92226700	-3.58672800	-1.86632200
H	6.02045900	-4.30252400	-0.43490700
H	4.54716600	-2.59728800	0.62313900
S	4.54604200	0.29424800	0.51034300
N	3.15486000	0.26954200	-0.41608300
O	5.23805000	1.59305400	0.41774700
H	0.17016800	1.59298600	-5.21166700
C	3.02764900	1.04719700	-1.57878700
C	-6.78690900	0.82437300	-1.96944200
Si	-6.51028700	-1.89765900	-1.01974000
H	-4.92982600	-0.18538600	-1.73523700
H	-7.75552800	0.98136100	-1.48276800
H	-6.98471900	0.38828700	-2.95609400
H	-6.33267300	1.80967600	-2.13229400
C	-5.67026700	-2.82458900	0.39605200
C	-6.11152700	-2.75456300	-2.66212800
C	-8.38951900	-1.92372000	-0.76182800
H	-4.58010600	-2.73283600	0.33244000
H	-5.92297200	-3.89283600	0.36684400
H	-5.97730700	-2.44071200	1.37638200
H	-8.69381100	-1.42876100	0.16860100
H	-8.74614600	-2.96087300	-0.70331900
H	-8.92976400	-1.44373700	-1.58709400
H	-6.55687800	-2.23353100	-3.51919500
H	-6.49335000	-3.78371000	-2.67305100
H	-5.02861700	-2.80332500	-2.83230800

Int12_4

Rh	1.67278000	-0.88247700	-0.75789400
Rh	-0.13300500	-0.72777600	1.03176000
O	0.30054500	-2.08037400	-1.75785900
O	-1.00611000	-2.34331100	0.05266700
C	-0.67175200	-2.62023400	-1.13667500
C	-1.48195600	-3.64653100	-1.88621100
H	-0.82946100	-4.28750800	-2.48543200
H	-2.07633200	-4.24957500	-1.19681700
H	-2.15983700	-3.11793900	-2.56562100
C	0.85465600	3.05951300	-3.38775400
H	4.91445300	2.64363300	0.00472700
H	4.66413000	4.67393300	-1.32719500
H	2.78207300	4.95338600	-2.92735800
H	-0.86674200	2.02034300	-4.16017900
H	-0.46305300	0.00073900	-2.73748700
O	4.00134200	-1.10320900	1.74287300
C	4.09313200	2.70431300	-0.69288800
C	3.93448200	3.87895000	-1.45781900
O	2.21695300	-2.65047300	0.20765000
O	0.99018800	-2.16690500	2.02875300
C	1.84632800	-2.86780800	1.40137700
C	2.48033000	-4.02227900	2.13376700
H	2.66610500	-4.85317300	1.44785300
H	3.44534200	-3.68384600	2.52774200
H	1.85352400	-4.35249100	2.96488900
C	2.89539200	4.04332500	-2.34588500
C	-0.01204400	1.99592900	-3.49290500
C	0.20828200	0.84851200	-2.70855600
N	1.23397300	0.76317200	-1.86763900
C	2.11842900	1.80244100	-1.73464700
C	-3.85017400	-0.42166300	0.80286700
C	-3.40403100	-0.50536800	2.12585200
C	-4.14982200	-1.18341100	3.08727600
C	-5.35404600	-1.77779800	2.71576700
C	-5.80278500	-1.67558200	1.40120600
C	-5.08209900	-0.99126400	0.40478800
H	-2.46834500	-0.03748700	2.41177300
H	-3.78944700	-1.24330700	4.11014600
H	-5.94929400	-2.31665000	3.44819100
H	-6.74614900	-2.14044700	1.13039100
C	-5.65873300	-0.90504000	-0.99603500
S	-2.81763000	0.46807700	-0.40683200
N	-1.39320900	0.80631900	0.37613500
O	-3.54745600	1.70084800	-0.76888800
H	1.76626900	3.93652100	4.10328400
C	-1.11436700	2.04925900	0.97440800
C	-1.72469200	3.28387500	0.74551300
C	-1.31953000	4.43818300	1.44841300
C	-0.29846700	4.41534900	2.37257700
C	2.03234700	1.83681500	3.74799200
C	1.58732800	0.72643100	3.00595400
N	0.59487900	0.82340800	2.12762700
C	-0.03437500	2.02517000	1.91514500
C	0.37194000	3.19414200	2.62330400
C	1.43378300	3.06040900	3.55264000
H	-2.52803800	3.35676200	0.02856100
H	-1.83736100	5.37057800	1.23933300
H	0.00218700	5.31027300	2.90933700
H	2.85187200	1.70854500	4.44638400
H	2.05214700	-0.24629800	3.10036700
O	-2.50873100	-0.45699700	-1.51169200
C	1.95527700	2.99607700	-2.49734000
C	5.66468500	-0.84173000	-0.29630800
C	6.78143400	-0.12360000	-0.72762200
C	7.67361300	-0.72526500	-1.61761200
C	7.44795100	-2.02845000	-2.06336400
C	6.33046900	-2.73985500	-1.61640400
C	5.43055700	-2.15123800	-0.72856600
H	6.95669400	0.88084600	-0.35873300
H	8.54722100	-0.17497000	-1.95582100
H	8.14623500	-2.49373500	-2.75376100
H	6.16171800	-3.75889200	-1.95376200
H	4.56288300	-2.69578100	-0.36968100
S	4.49080200	-0.06239000	0.82933600
N	3.20348200	0.40535900	-0.12966100
O	5.17109100	1.10126800	1.42682100
H	0.70659300	3.95917400	-3.97950800
C	3.19800700	1.63702100	-0.80594800
C	-5.92245100	-2.30268300	-1.60224500
Si	-7.21317200	0.23975000	-1.11906500
H	-8.30859100	1.32115400	-3.09682500
H	-5.00163000	-2.89864300	-1.62351300
H	-6.28190900	-2.21669300	-2.63453400
H	-6.67070700	-2.87375300	-1.04200900
C	-8.77921800	-0.64253100	-0.51179900
C	-7.43675300	0.66988500	-2.95159700
C	-6.97037500	1.82792700	-0.12491600
H	-8.96335200	-1.58225900	-1.04667700
H	-9.65549700	-0.00142400	-0.67733600
H	-8.74697000	-0.86773200	0.56107800
H	-6.91414900	1.63090700	0.95254900
H	-7.80900200	2.51742200	-0.28984200
H	-6.04638500	2.33955900	-0.41507800
H	-7.59153100	-0.22169000	-3.57198100
H	-6.56200100	1.20089000	-3.34748100
H	-4.93084800	-0.41821200	-1.64941900

Int13_4

Rh	-1.57473800	-1.19006200	0.12072500
Rh	-0.04566600	0.14880600	-1.41950600

O	-0.02349100	-2.57313800	0.15900800
O	1.06669200	-1.60415500	-1.55190500
C	0.90566600	-2.53666400	-0.71081600
C	1.89404100	-3.67429400	-0.71981500
H	1.42705500	-4.59921800	-0.37330300
H	2.31287600	-3.81055700	-1.71970000
H	2.71245700	-3.41822700	-0.03750900
C	-0.60173000	0.76422600	4.40835400
H	-4.94545600	1.96659200	1.60581900
H	-4.59056900	3.01534000	3.78509400
H	-2.57948400	2.50795000	5.15624700
H	1.19167400	-0.42723900	4.39027100
H	0.69024600	-1.40298000	2.14032600
O	-4.26007100	-0.36296000	-1.83959500
C	-4.06507700	1.70036600	2.17076700
C	-3.84869000	2.30660700	3.42621400
O	-2.13966100	-2.18353200	-1.62823400
O	-1.18010400	-0.65544600	-2.96863200
C	-1.90853600	-1.67940200	-2.76794600
C	-2.55720300	-2.32489600	-3.96564700
H	-2.62058500	-3.40728600	-3.82591900
H	-3.57708900	-1.93338200	-4.05366900
H	-2.00807800	-2.09466500	-4.88121500
C	-2.73711100	2.03410500	4.19189100
C	0.28092000	-0.14557600	3.87324300
C	0.00752200	-0.71096400	2.61384200
N	-1.08685500	-0.39623500	1.92843600
C	-1.99621800	0.49679500	2.43519300
C	3.66573900	0.77153000	-1.23279100
C	3.11022800	1.35970000	-2.36961700
C	3.82856500	1.40440400	-3.56518900
C	5.10856100	0.86181600	-3.60854200
C	5.66775600	0.29671100	-2.46035200
C	4.97659200	0.23859700	-1.24386200
H	2.11934700	1.79752200	-2.32494200
H	3.38590200	1.86103000	-4.44585500
H	5.68167900	0.88181900	-4.53173800
H	6.67202500	-0.10921900	-2.51083900
C	5.61640900	-0.36316700	0.00324100
S	2.68637700	0.72594300	0.30146200
N	1.16543600	1.24812900	-0.11731200
O	3.33590900	1.64989200	1.25347600
H	-2.64682400	5.44095500	-1.37990000
C	0.73602000	2.57928400	0.04642300
C	1.28806200	3.58404400	0.84339900
C	0.71951500	4.87461200	0.88993400
C	-0.40895000	5.20772700	0.17418400
C	-2.72326700	3.44896600	-2.17514500
C	-2.10866300	2.18305400	-2.17489000
N	-1.01663900	1.93492500	-1.45959000
C	-0.44693400	2.91717000	-0.68869700
C	-1.02234600	4.22094600	-0.63376100
C	-2.18667100	4.45668900	-1.40679200
H	2.17080800	3.37539900	1.42795100
H	1.19774200	5.61933800	1.52071700
H	-0.83682400	6.20484000	0.21795200
H	-3.61815200	3.59969400	-2.76889200
H	-2.51278000	1.35230600	-2.73858000
O	2.57483200	-0.68201900	0.72018000
C	-1.77826200	1.11595800	3.70095400
C	-5.50301000	-1.44705000	0.23366300
C	-6.54091100	-1.23578700	1.14325000
C	-7.18071500	-2.33929800	1.71154800
C	-6.78552700	-3.63330000	1.36799000
C	-5.75242400	-3.83057300	0.44684400
C	-5.10416600	-2.73787300	-0.12806400
H	-6.84837000	-0.22552700	1.38922600
H	-7.99069700	-2.18480800	2.41908200
H	-7.28621400	-4.48918400	1.81249900
H	-5.45375400	-4.83799300	0.16988800
H	-4.30324700	-2.87691500	-0.84731300
S	-4.63029500	-0.02772000	-0.45844100
N	-3.21494100	0.08531100	0.42185100
O	-5.49343400	1.14966400	-0.25093400
H	-0.40978900	1.22531600	5.37369000
C	-3.15858200	0.77567300	1.64494200
C	7.09501000	-0.76715000	-0.10642000
H	7.69864500	0.08896800	-0.44205600
H	5.01860000	-1.23076400	0.30550900
H	7.22497800	-1.54636000	-0.87172700
Si	7.86480900	-1.41114800	1.51364400
H	5.49558000	0.36128600	0.81699700
C	7.74244500	-0.09105300	2.86635500
C	9.69041800	-1.79952600	1.18320100
C	6.97913400	-2.98673900	2.08206600
H	10.23813200	-0.90868700	0.84927600
H	9.81010600	-2.56725300	0.40782800
H	10.19052500	-2.16891400	2.08793600
H	8.21589900	0.84963100	2.55670100
H	8.24341600	-0.42107500	3.78580300
H	6.70172300	0.13665000	3.12750800
H	5.92456000	-2.80047000	2.32097900
H	7.44826000	-3.40001800	2.98440200
H	7.00917800	-3.76825000	1.31171300

24a

C	1.70558300	1.66295100	0.05322000
C	2.57188400	0.54647000	-0.00307500
C	3.75800800	0.65798300	0.74621500
C	4.06189300	1.78466900	1.50616500
C	3.17977800	2.86452400	1.54803200
C	2.00017700	2.80190300	0.81393500
C	2.31939400	-0.71049000	-0.81282800
H	4.46442100	-0.16649200	0.72419600
H	4.99276800	1.81739200	2.06616200
H	3.40739300	3.74723900	2.13797000
H	1.30191900	3.63096200	0.81515600
S	0.19271200	1.77560700	-0.92058500
N	-0.72771300	0.54734600	-0.17150000
H	-0.78133100	0.71439600	0.83926800
H	-6.27546700	-0.94951800	0.75965200
C	-2.01196700	0.18698300	-0.64946700
C	-2.32143800	-0.03761800	-1.97834300
C	-3.62504100	-0.44688600	-2.34510400
C	-4.60896000	-0.65050000	-1.40384900
C	-4.90298300	-0.38978500	2.31525400
C	-3.58067200	0.03430100	2.58744100
N	-2.66808200	0.21858500	1.65231900
C	-3.01625600	-0.00914800	0.35578300
C	-4.32129200	-0.44074500	-0.03045700
C	-5.26849000	-0.62430000	1.00961300
H	-1.56429700	0.10447600	-2.73957900
H	-3.84034300	-0.60674000	-3.39791200
H	-5.60552300	-0.97077900	-1.69568200
H	-5.60624700	-0.52149400	3.13166700
H	-3.27203200	0.22758300	3.61352000
O	-0.40680100	3.09804300	-0.68711500
O	0.42613200	1.35685800	-2.31001400
H	1.35109300	-0.62055900	-1.30908600
Si	2.13338500	-2.31914500	0.24462100
C	3.37318700	-0.87234900	-1.93505700
H	3.17302500	-1.76953700	-2.53254800
H	4.39297200	-0.95621300	-1.54339200
H	3.34743700	-0.01318600	-2.61616600
C	1.18530200	-3.56620500	-0.82038300
C	1.16173200	-1.98709000	1.83413800
C	3.81663800	-3.06972200	0.69111300
H	1.70971000	-3.79760800	-1.75595700
H	0.18791100	-3.19287800	-1.08444700
H	1.04919000	-4.51435700	-0.28379900
H	0.15341700	-1.60972100	1.62647000
H	1.66373900	-1.25637800	2.47982400
H	1.05154500	-2.91273300	2.41441700
H	3.67090200	-4.02190300	1.21862000
H	4.41263000	-2.42842300	1.35171700
H	4.42146100	-3.28560400	-0.19819300

Int1_S_5

C	-4.55342900	2.28777600	1.11924900
C	-3.50104000	1.48014700	0.69149900
C	-3.61822200	0.72376600	-0.48435400
C	-4.81264300	0.80059000	-1.22280200
C	-5.86791100	1.59751900	-0.78783000
C	-5.74148200	2.34358800	0.38686300
C	-2.56548100	-0.19361000	-1.02509500
O	-2.64800100	-0.61786500	-2.17078000
N	-1.52384300	-0.64418100	-0.14915400
C	-0.99412800	-1.93405900	-0.43428100
C	0.31113500	-2.16983400	0.06879900
C	-1.66944300	-3.00864800	-0.99433400
C	0.92069200	-3.45728700	0.06415400
C	-1.07782000	-4.28916000	-1.03926700
C	2.16349800	-1.20662300	1.12743500
C	2.20944200	-3.56516400	0.64326400
C	0.17748200	-4.51725200	-0.52016100
C	2.81753400	-2.45271600	1.18203200
N	0.96490600	-1.08288700	0.57770200
Cl	0.86264400	-6.13262400	-0.58587400
H	-4.44203500	2.87807700	2.02411300
H	-2.57729300	1.48594100	1.25132500
H	-4.89925400	0.21960800	-2.13414400
H	-6.78734000	1.63768500	-1.36473200
H	-6.56184800	2.96933800	0.72698000
H	-2.66583400	-2.88471200	-1.39573700
H	-1.63265800	-5.10857400	-1.48293100
H	2.61737100	-0.30227300	1.50999000
H	2.70771600	-4.52801200	0.66068100
H	3.79940000	-2.51334600	1.63685300
Co	0.00961700	0.55860600	0.21204800
C	-0.28947600	1.73989400	-1.73851100
O	0.39428300	0.65507100	-1.64840100
O	-0.84001800	2.09743900	-0.64216800
C	-0.47612500	2.46195300	-3.02610300
H	-0.71297000	3.50993600	-2.83576700
H	0.42643400	2.37791800	-3.63406900
H	-1.30927700	1.99896000	-3.56784500
O	1.60653500	1.63934400	0.71775600
S	2.48333700	2.69442000	0.04673400
O	3.02107500	3.62801300	1.04230000
O	1.93319000	3.25578300	-1.19459400
C	3.94600000	1.67400900	-0.49342700
F	4.54171800	1.11992800	0.57396500
F	3.55575800	0.69404700	-1.31832700
F	4.83041200	2.44862100	-1.12756900
C	-1.11164600	0.10985300	2.89317000
O	-0.40615600	0.80828600	2.13092300
O	-1.91577500	-0.82198700	2.46392200
H	-1.89459500	-0.80588600	1.43108900
C	-1.09822100	0.33392900	4.37357700
H	-2.06560000	0.74796900	4.67859700
H	-0.97181200	-0.62309200	4.88795100
H	-0.30016500	1.02338400	4.64706700

Int1_T_5

C	3.00424500	2.89504700	-1.54617900
C	1.71067000	2.42339900	-1.32304600
C	0.77896900	3.22520200	-0.64637200
C	1.15420200	4.51212500	-0.22051200
C	2.44737300	4.97533800	-0.44057800
C	3.37718900	4.16478600	-1.10121200
C	-0.61702100	2.80521300	-0.35200200
O	-1.50095600	3.62616800	-0.13090000
N	-0.88746500	1.41067200	-0.21256400
C	-2.18193700	0.96855700	-0.21339300
C	-2.44759900	-0.26943700	0.48621800
C	-3.25111300	1.58171300	-0.89463300
C	-3.73325200	-0.87432300	0.45502700
C	-4.52184100	1.00215100	-0.91272100
C	-1.58862100	-1.99437200	1.78827100
C	-3.89309600	-2.10753900	1.13258400
C	-4.76703600	-0.19699100	-0.26070400
C	-2.81857500	-2.67459000	1.78540100
N	-1.41639300	-0.82494600	1.17823700
Cl	-6.36528400	-0.88336600	-0.33516200
H	3.71769000	2.26739800	-2.07110600
H	1.40489800	1.46879400	-1.73613600
H	0.42441500	5.13016100	0.29161800
H	2.73267100	5.96567400	-0.09765600
H	4.38724200	4.52628000	-1.27306300
H	-3.08186400	2.49554100	-1.44575200
H	-5.32134000	1.48616100	-1.46186400
H	-0.72118400	-2.40075000	2.29973500
H	-4.85857800	-2.60038000	1.12848000
H	-2.91070900	-3.62367800	2.30063400
Co	0.38907800	0.06429600	0.20492900
C	-0.27132200	-0.62795800	-2.48672900
O	-0.08554100	-1.02839900	-1.25886500
O	-0.22867900	0.54225700	-2.87803900
C	-0.56103100	-1.77744000	-3.44402800
H	-0.70191000	-1.40121400	-4.45887100
H	0.27126600	-2.48803000	-3.42345500
H	-1.45891700	-2.31605100	-3.12292500
O	1.60668500	-1.37348700	0.80734300
S	3.02479200	-1.58308900	0.29052100
O	3.98987600	-1.74662500	1.38744300
O	3.38803900	-0.68430400	-0.81630400
C	2.89521900	-3.27693800	-0.47399000
F	2.42136000	-4.15483000	0.41978300
F	2.08145300	-3.26236200	-1.53521400
F	4.10956800	-3.67955500	-0.87143600
C	0.87727200	1.30005300	2.84119900
O	1.21765700	1.16987100	1.65758000
O	-0.21744400	0.75315100	3.33715700
H	-0.67147500	0.23730600	2.62573500
C	1.68808400	2.07929400	3.82755700
H	1.03485700	2.68169000	4.46350500
H	2.22761600	1.37484200	4.47116700
H	2.40717400	2.70878900	3.30410200

Int2_S_5

C	3.14582100	2.32133200	-0.34742300
C	1.85166500	1.99297800	-0.76845300
C	0.85918100	2.98697900	-0.86684300
C	1.18232100	4.31396500	-0.57528000
C	2.47611400	4.63859300	-0.16072500
C	3.45422700	3.64547500	-0.03678700
C	-0.56648200	2.62254200	-1.15198900
O	-1.33597100	3.34089700	-1.78199000
N	-0.93708300	1.47515700	-0.46902800
C	-2.20837800	0.88443700	-0.50621000
C	-2.27317500	-0.30316100	0.27291400
C	-3.36965700	1.33049200	-1.11918400
C	-3.47869900	-1.02351600	0.48265000
C	-4.57694400	0.61499000	-0.94570800
C	-1.04105100	-1.80192500	1.59583200
C	-3.40891500	-2.16748400	1.31629300
C	-4.64139200	-0.51817700	-0.16443400
C	-2.20594100	-2.54296600	1.87615700
N	-1.09566800	-0.72621600	0.82638100
Cl	-6.17579300	-1.34636500	0.03830700
H	3.90524800	1.54790300	-0.30707400
H	1.70558500	1.02505300	-1.26368200
H	0.41562500	5.07810200	-0.65507500
H	2.72159500	5.67091600	0.07120300
H	4.45808500	3.90929200	0.28199900
H	-3.35369300	2.22949900	-1.71822500
H	-5.47471200	0.97894900	-1.43336100
H	-0.06469300	-2.08896900	1.96602800
H	-4.30687000	-2.74441700	1.50733100
H	-2.13224700	-3.41342400	2.51748800
Co	0.39069300	0.25705000	0.15614200
C	0.25097600	-0.49443400	-2.61041900
O	0.22661800	-0.84200300	-1.34052200
O	0.41169800	0.64099000	-3.04675500
C	0.06783100	-1.70181900	-3.51900600
H	0.13387800	-1.39012700	-4.56272300

H	0.83657200	-2.44826100	-3.30069100
H	-0.90629300	-2.16581400	-3.33282600
O	1.72336400	-0.99737500	0.90770200
S	2.99689800	-1.55927100	0.27528600
O	4.07473500	-1.65091100	1.26783900
O	3.31475400	-0.97482900	-1.03581200
C	2.52346100	-3.33506000	-0.04760300
F	2.05082600	-3.88570400	1.07988500
F	1.58617100	-3.43074600	-0.99442000
F	3.60591800	-4.01426500	-0.44180800
C	0.08509500	2.00257700	2.57683700
O	0.71598000	1.15372800	1.92572200
O	-0.99166900	2.60509300	2.11972800
H	-1.14137300	2.29166400	1.18768600
C	0.50894200	2.42219100	3.94876900
H	0.78946400	3.48060100	3.92922500
H	-0.33273100	2.31630300	4.64002000
H	1.35291100	1.81999500	4.28305500

TS1_S_5

C	3.00151700	2.14589200	-0.18815700
C	1.66044500	1.92445000	-0.55795600
C	0.81603700	3.05228500	-0.72768200
C	1.29672300	4.34983400	-0.58393700
C	2.63442400	4.54086900	-0.22183500
C	3.48213900	3.44531400	-0.02011300
C	-0.62732200	2.77598500	-0.99884200
O	-1.40159700	3.56133800	-1.54373100
N	-0.96986600	1.54978900	-0.45891500
C	-2.22787100	0.93667400	-0.52954700
C	-2.28818300	-0.29365000	0.19010300
C	-3.38208400	1.40277000	-1.14150600
C	-3.49375200	-1.03570000	0.32275300
C	-4.58367200	0.66571300	-1.03837100
C	-1.08821500	-1.83868500	1.46797800
C	-3.43672900	-2.22512500	1.09227200
C	-4.64702800	-0.51107800	-0.32548100
C	-2.24750100	-2.61608800	1.66783900
N	-1.11975300	-0.72403300	0.75719200
Cl	-6.17527600	-1.37230100	-0.21305900
H	3.67613000	1.30177000	-0.08929200
H	1.60178200	1.17081800	-1.57989200
H	0.62927600	5.19345300	-0.73186400
H	3.01837000	5.54933900	-0.09653700
H	4.52017200	3.60951700	0.25426200
H	-3.36437100	2.33607700	-1.68623100
H	-5.47527200	1.04520300	-1.52562800
H	-0.12445000	-2.13213200	1.86659100
H	-4.33352000	-2.82062600	1.22229900
H	-2.18270000	-3.52059600	2.26172000
Co	0.41645400	0.38018000	0.13042400
C	0.79508800	-0.43511700	-2.56815100
O	0.23407300	-0.66939400	-1.44027700
O	1.52171100	0.56566000	-2.79649400
C	0.55955300	-1.46119600	-3.64912900
H	0.91500200	-1.09188300	-4.61156300
H	1.10628100	-2.37083400	-3.38004500
H	-0.50288400	-1.71188900	-3.70441100
O	1.75181800	-0.89921100	0.88454300
S	2.95882700	-1.63569300	0.32139300
O	3.99366500	-1.81694200	1.34804800
O	3.38136400	-1.16678200	-1.00615300
C	2.28625700	-3.35289300	0.04417300
F	1.75112900	-3.82683700	1.18016900
F	1.33971100	-3.35516800	-0.90302100
F	3.27665100	-4.16627200	-0.33699200
C	-0.05289300	1.92108800	2.65376100
O	0.65130600	1.18081600	1.95137800
O	-1.16961700	2.47491900	2.22626200
H	-1.28375500	2.22757800	1.27286100
C	0.31486700	2.25869100	4.06448000
H	0.49251800	3.33641200	4.14237900
H	-0.51969200	2.01256200	4.72819200
H	1.20867700	1.71137100	4.36154200

TS1_T_5

C	2.76000500	2.33694900	-0.37598800
C	1.43963100	2.01909300	-0.75939600
C	0.48980100	3.06989600	-0.83887900
C	0.85176700	4.39426900	-0.61734900
C	2.17171200	4.68516400	-0.25895200
C	3.11972100	3.66164600	-0.13266300
C	-0.93076500	2.68514500	-1.06379600
O	-1.80642400	3.44022300	-1.47530800
N	-1.12959800	1.37342300	-0.65430800
C	-2.37050900	0.72203000	-0.61133600
C	-2.32849300	-0.52274400	0.08093800
C	-3.58554100	1.14940000	-1.13048300
C	-3.48404100	-1.32937700	0.26424700
C	-4.74175400	0.35309600	-0.97171900
C	-0.97976600	-2.02581300	1.25365300
C	-3.32128600	-2.53241800	0.99494200
C	-4.70123500	-0.84672600	-0.29592600
C	-2.08068000	-2.87293100	1.49024300
N	-1.11036000	-0.89566400	0.57759100
Cl	-6.17225800	-1.78686000	-0.11874000
H	3.50764000	1.55237800	-0.33729500
H	1.43216000	1.25040500	-1.74047700
H	0.10378200	5.17739300	-0.69502400
H	2.46238100	5.71454000	-0.06988500
H	4.14211200	3.90391700	0.14191800
H	-3.64853800	2.09118200	-1.65607900
H	-5.67945900	0.70122700	-1.39068700
H	0.01671400	-2.26888800	1.60198100
H	-4.17677200	-3.17767900	1.16068100
H	-1.93366900	-3.78704900	2.05384600
Co	0.33364100	0.34283300	-0.05962300
C	1.04130100	-0.60071000	-2.75402700
O	0.46219900	-0.92718900	-1.66710900
O	1.52871000	0.54455800	-2.97784800
C	1.15752900	-1.66884800	-3.82031900
H	1.58169500	-1.26350000	-4.73996100
H	1.80134700	-2.46791200	-3.43762600
H	0.17319700	-2.10327200	-4.01884400
O	1.74008700	-0.73205800	0.87934400
S	3.12301900	-1.26528100	0.52612200
O	4.03532100	-1.19273300	1.67462500
O	3.62387100	-0.81114800	-0.77966100
C	2.78575000	-3.08638500	0.30903500
F	2.18258200	-3.57718600	1.40427800
F	1.99672500	-3.30762400	-0.74687700
F	3.94143100	-3.73393000	0.12906500
C	-0.30978600	2.05261000	2.76767200
O	0.42154600	1.39016000	2.04166800
O	-1.55366400	2.40752800	2.42248400
H	-1.73516900	2.06331800	1.52631400
C	0.08119600	2.55516300	4.12677200
H	0.03689700	3.64904100	4.13985000
H	-0.62884700	2.18808700	4.87452500
H	1.08886700	2.22000400	4.37044500

Int3_S_5

C	2.98333300	2.01557900	0.25763200
C	1.61974700	1.89411900	-0.02072400
C	0.94478400	2.97911300	-0.60980900
C	1.61421400	4.16032400	-0.94450700
C	2.97705500	4.27047000	-0.66927200
C	3.65465500	3.20493500	-0.06790500
C	-0.51199800	2.79490200	-0.84775400
O	-1.21932600	3.55558900	-1.50500900
N	-0.95539300	1.65403600	-0.17575700
C	-2.21818300	1.06376500	-0.36407800
C	-2.33403900	-0.26097600	0.16153100
C	-3.34000600	1.64405300	-0.93947200
C	-3.56793000	-0.97432400	0.13652600
C	-4.56272400	0.93853600	-0.99242900
C	-1.23978700	-2.02090600	1.22527100
C	-3.57765800	-2.26940300	0.71420000

C	-4.68190200	-0.32731500	-0.46561800
C	-2.42500100	-2.78504100	1.26286500
N	-1.20054000	-0.81299000	0.69047200
Cl	-6.23607000	-1.15098500	-0.54014700
H	3.53298200	1.20486600	0.72440100
H	2.20110400	1.11168800	-1.88709500
H	1.06205600	4.97272000	-1.40869600
H	3.51188800	5.18208800	-0.91941100
H	4.71553000	3.29507700	0.15082800
H	-3.27856500	2.64409100	-1.34342200
H	-5.42427300	1.41402000	-1.44887400
H	-0.30661200	-2.40422800	1.62183000
H	-4.49711500	-2.84422300	0.71933300
H	-2.41028200	-3.77153100	1.71256000
Co	0.42431600	0.42477000	0.34816000
C	0.99458900	-0.18287400	-2.53749600
O	0.37437400	-0.31254800	-1.46796600
O	1.97166400	0.66832000	-2.73751100
C	0.65915700	-1.04556200	-3.71405800
H	1.05519500	-0.62233600	-4.63763000
H	1.11529700	-2.02761200	-3.54387300
H	-0.42213100	-1.18066500	-3.77939600
O	1.74952300	-0.96090300	0.94221500
S	2.89957500	-1.71911900	0.30331500
O	3.95272100	-2.02158400	1.28110200
O	3.31482300	-1.19598000	-1.00820000
C	2.12372200	-3.36980100	-0.07667600
F	1.62288600	-3.92165800	1.03909500
F	1.12743900	-3.23053000	-0.96479500
F	3.04209700	-4.19456300	-0.58898400
C	-0.14721600	1.71160000	2.92303600
O	0.48785800	0.88162500	2.24674100
O	-1.05153000	2.51358000	2.41758700
H	-1.11549800	2.32104400	1.43170400
C	0.08922500	1.85742900	4.39389100
H	0.47858200	2.86092700	4.59576700
H	-0.86017400	1.75720900	4.92847100
H	0.80014500	1.10763500	4.73915500

Int3_T_5

C	2.75456700	2.20594100	0.33629200
C	1.40994300	2.02369300	0.03458100
C	0.66773800	3.03796600	-0.57665100
C	1.27514500	4.24850000	-0.92667600
C	2.62501700	4.43908400	-0.63718900
C	3.35564600	3.42705200	-0.00424700
C	-0.76925100	2.75441700	-0.81659300
O	-1.53251900	3.46929400	-1.45943200
N	-1.11296600	1.55856400	-0.17813000
C	-2.34481300	0.90382400	-0.34874600
C	-2.36499800	-0.45634700	0.09311900
C	-3.52010600	1.44720200	-0.85040800
C	-3.55389300	-1.24199200	0.05215600
C	-4.70079400	0.67452000	-0.91317200
C	-1.13930000	-2.21860000	1.00653600
C	-3.46955000	-2.57152500	0.53420300
C	-4.72580400	-0.62822900	-0.47160900
C	-2.27201800	-3.05519100	1.01411000
N	-1.18574000	-0.97305300	0.55890900
Cl	-6.22704300	-1.54068300	-0.55922100
H	3.34384300	1.43460800	0.81707300
H	2.89154900	-0.20590800	-1.96064600
H	0.68221400	5.01893800	-1.41217100
H	3.11062900	5.37524800	-0.89677500
H	4.40599600	3.58305500	0.22784000
H	-3.53221900	2.47118900	-1.19412000
H	-5.60355700	1.12554900	-1.31072000
H	-0.17618200	-2.56809300	1.36024300
H	-4.35291200	-3.20026200	0.52164800
H	-2.18597400	-4.06846800	1.38976900
Co	0.34905300	0.40742200	0.36022400
C	1.18908700	-0.01387900	-2.80763000
O	0.54770200	-0.20790900	-1.77124500
O	2.50721500	0.02906000	-2.85101400
C	0.53719800	0.18680700	-4.14667900
H	0.85036200	1.14922600	-4.56436600
H	0.86822000	-0.59400500	-4.83884900
H	-0.54752200	0.16104100	-4.04521200
O	1.75687300	-0.94192000	0.96122800
S	3.06514800	-1.55912800	0.52978300
O	3.94173900	-1.89041200	1.65516500
O	3.70595800	-0.86047300	-0.61212600
C	2.51943700	-3.19569800	-0.17302700
F	1.90289100	-3.91598800	0.77426500
F	1.66917400	-3.00304500	-1.18852300
F	3.57946900	-3.87552800	-0.61468900
C	-0.35487200	1.64401300	3.15041000
O	0.32262900	0.82253700	2.52641200
O	-1.25856400	2.42077600	2.57058600
H	-1.27350500	2.20977300	1.59941600
C	-0.22974900	1.85620200	4.62987400
H	0.08782500	2.88630100	4.82276400
H	-1.20499900	1.71773700	5.10678100
H	0.49625100	1.15960400	5.04808000

MECP_5

C	2.92854300	2.08007200	0.22857300
C	1.56958900	1.94661800	-0.05521200
C	0.87552900	2.99787500	-0.67368000
C	1.53403700	4.17552300	-1.03919900
C	2.89402900	4.30899000	-0.76090300
C	3.58387600	3.26979800	-0.12764800
C	-0.57835800	2.78635700	-0.90456100
O	-1.29770000	3.52377700	-1.57350900
N	-0.99152200	1.63936000	-0.22451100
C	-2.24613400	1.02890500	-0.39277100
C	-2.34133000	-0.28719000	0.15973600
C	-3.37414500	1.57418700	-0.98952600
C	-3.56207200	-1.02252100	0.14387900
C	-4.58380500	0.84594200	-1.03525200
C	-1.22171500	-2.01160400	1.26038400
C	-3.55248100	-2.30572300	0.74612800
C	-4.68408200	-0.40899200	-0.47980100
C	-2.39349200	-2.79290400	1.30940100
N	-1.20035300	-0.81231400	0.70226300
Cl	-6.22149600	-1.26220000	-0.54766600
H	3.48349300	1.28949900	0.72162200
H	2.21336800	1.03156000	-1.99507900
H	0.97285600	4.96699800	-1.52858000
H	3.41805400	5.22040300	-1.03270400
H	4.64202800	3.38049200	0.09475600
H	-3.32623100	2.56423300	-1.41888400
H	-5.44918600	1.29458900	-1.51086700
H	-0.28301500	-2.37189200	1.66612300
H	-4.46175700	-2.89638400	0.75737800
H	-2.36501200	-3.77028900	1.77794000
Co	0.41003400	0.43804000	0.35349900
C	1.02988200	-0.28213400	-2.64859400
O	0.41931400	-0.40431100	-1.58100500
O	2.00303200	0.58684600	-2.84617300
C	0.72438600	-1.15290400	-3.82963600
H	1.12606900	-0.73226700	-4.75197500
H	1.18808600	-2.12961100	-3.64880500
H	-0.35435400	-1.30217700	-3.90819100
O	1.77122700	-0.92853200	0.96084700
S	2.94622800	-1.67520300	0.35531300
O	3.99088700	-1.94113300	1.35302100
O	3.37204300	-1.16367600	-0.95730500
C	2.19718300	-3.34358800	-0.00172400
F	1.69264400	-3.87648200	1.12204400
F	1.20893900	-3.23774500	-0.90164600
F	3.13154900	-4.16766700	-0.48588700
C	-0.18280300	1.79909900	3.01138900
O	0.46976400	0.95506500	2.38380100
O	-1.09158700	2.57154700	2.44670600
H	-1.13668300	2.34265700	1.47629300
C	0.00230000	2.02803300	4.48095300
H	0.36254900	3.04909900	4.64511600

H	-0.95920600	1.93083900	4.99415900
H	0.71930200	1.31388300	4.88499200

Int2_S_ent2_5

C	-3.77469500	0.98481200	0.33626300
C	-2.42972500	1.11696100	0.70344700
C	-1.80568000	2.37757000	0.65362700
C	-2.54144000	3.50343500	0.27601900
C	-3.88370100	3.36601500	-0.08221800
C	-4.49786600	2.10830300	-0.06326100
C	-0.33187900	2.49933200	0.88631200
O	0.19230400	3.48821100	1.39527600
N	0.34876400	1.42741400	0.33817600
C	1.73778400	1.24440000	0.39411300
C	2.15327700	0.02421200	-0.21008500
C	2.71146600	2.10799800	0.87345100
C	3.52456200	-0.30636900	-0.38952600
C	4.07906600	1.77716800	0.74275400
C	1.45644900	-1.94143900	-1.27859400
C	3.81809500	-1.51279100	-1.07150300
C	4.48059600	0.61585900	0.12179900
C	2.79245500	-2.30943300	-1.52968800
N	1.15972600	-0.82236800	-0.63336000
Cl	6.19526600	0.27352100	-0.04820600
H	-4.25064100	0.01118100	0.39274600
H	-2.01267600	0.30087200	1.33566600
H	-2.05202700	4.47182900	0.24518500
H	-4.45190900	4.24112300	-0.38399300
H	-5.54241600	2.01049500	-0.34352800
H	2.42271300	3.04138200	1.33444500
H	4.82439000	2.46475000	1.12742300
H	0.62681800	-2.56826400	-1.57928200
H	4.85163200	-1.79803700	-1.23240300
H	2.99047400	-3.23152900	-2.06366400
Co	-0.56631700	-0.25708800	0.02075000
C	-0.53120600	-0.93136700	2.81694300
O	0.10634500	-0.84678900	1.67660000
O	-1.69174300	-0.57800400	3.02502800
C	0.32863600	-1.55287600	3.90859600
H	-0.16297100	-1.44093900	4.87657600
H	0.46758300	-2.61841200	3.69470100
H	1.31771400	-1.08702600	3.93249300
C	-0.85467400	1.01699000	-2.65611000
O	-1.19338900	0.14525500	-1.83763100
O	-0.01818400	1.98929900	-2.36915500
H	0.22268400	1.90946400	-1.40326000
C	-1.38927300	1.03540900	-4.05394600
H	-1.98820500	1.94103900	-4.19712600
H	-0.55692300	1.07462700	-4.76323300
H	-2.00138300	0.15289000	-4.23566000
I	-1.97564900	-2.56128600	-0.22269500

TS1_S_ent2_5

C	-3.59423800	0.87759700	0.09025700
C	-2.24523100	1.05798600	0.45552700
C	-1.73830000	2.38358400	0.47981000
C	-2.55346500	3.48098100	0.21529000
C	-3.89328300	3.27175400	-0.12498800
C	-4.40948900	1.97374500	-0.19692400
C	-0.26946300	2.55937900	0.69247300
O	0.24971900	3.57765100	1.14749800
N	0.40339800	1.45256800	0.20519400
C	1.78502700	1.23771900	0.29863200
C	2.18917200	-0.04542900	-0.17714900
C	2.76291100	2.12680200	0.72070400
C	3.56157500	-0.41175500	-0.27496300
C	4.12680900	1.76401800	0.66246700
C	1.49473800	-2.09362500	-1.05494400
C	3.85569100	-1.68803500	-0.81619600
C	4.52066200	0.54002600	0.17123800
C	2.83033600	-2.51349900	-1.21847700
N	1.19052700	-0.90993800	-0.54605600
Cl	6.23463500	0.15317200	0.09082500
H	-4.00776500	-0.12579600	0.07334900
H	-2.03323900	0.40286400	1.53342200
H	-2.13365300	4.48187300	0.24975900
H	-4.53370400	4.12218900	-0.34137200
H	-5.45044200	1.81956100	-0.46660500
H	2.47848300	3.10438200	1.08277600
H	4.87481700	2.47342500	0.99958600
H	0.66251300	-2.73585000	-1.31774200
H	4.88877900	-2.00294200	-0.91203000
H	3.02849100	-3.49131400	-1.64247200
Co	-0.60419600	-0.19092600	-0.00352500
C	-0.73895000	-0.56741100	2.80286700
O	-0.02203600	-0.67805500	1.75096100
O	-1.88719700	-0.04600300	2.81149500
C	-0.16525600	-1.13410900	4.07822100
H	-0.61155400	-0.64462600	4.94540300
H	-0.40314600	-2.20351900	4.11720500
H	0.92107100	-1.02530500	4.09121600
C	-0.72861300	0.85372500	-2.77761000
O	-1.10877400	0.04350700	-1.91650000
O	0.09235700	1.84764800	-2.52152600
H	0.29813300	1.82691500	-1.54239800
C	-1.19318000	0.76659700	-4.19830100
H	-1.79045900	1.65351700	-4.43534000
H	-0.32778100	0.76254500	-4.86776600
H	-1.79092700	-0.13222600	-4.34515200
I	-2.02037500	-2.53077900	-0.10240900

Int2_S_ent3_5

C	-4.05769100	-0.30357700	-0.18250700
C	-2.74680500	-0.47966800	-0.63274700
C	-2.22295700	-1.76762100	-0.83356300
C	-3.04082500	-2.88015500	-0.61752400
C	-4.35411300	-2.70494600	-0.17636700
C	-4.86101800	-1.42091100	0.05082200
C	-0.77531100	-1.97332100	-1.16769000
O	-0.37694700	-2.90993100	-1.85632400
N	0.03804900	-1.09028700	-0.47799500
C	1.43765800	-1.07402200	-0.54876900
C	2.00800600	-0.03305400	0.23783100
C	2.30027000	-1.94591100	-1.19815500
C	3.40878800	0.11822400	0.42087300
C	3.69880000	-1.79761100	-1.05312700
C	1.54288900	1.81859800	1.60830300
C	3.84005200	1.16986500	1.26776100
C	4.24358000	-0.80903400	-0.26331400
C	2.91609800	2.00065100	1.86495300
N	1.12886700	0.83309800	0.82853000
Cl	5.98869600	-0.69393900	-0.09670300
H	-4.44340000	0.70177700	-0.04998200
H	-2.23379000	0.39794500	-1.04883400
H	-2.63590800	-3.87422100	-0.77909000
H	-4.98311900	-3.57350900	-0.00362600
H	-5.88390900	-1.29331600	0.39261600
H	1.90120900	-2.74584400	-1.80478800
H	4.35452600	-2.49035800	-1.56945500
H	0.77515100	2.47424000	2.00018100
H	4.90077200	1.31534500	1.43934600
H	3.22612600	2.80964600	2.51608400
Co	-0.64999700	0.58587000	0.20949100
C	-0.34331600	1.27659700	-2.55179500
O	-0.06849300	1.53623300	-1.29395400
O	-1.04282900	0.35743300	-2.96838700
C	0.30043100	2.29455000	-3.48522000
H	0.14150900	1.99628200	-4.52308700
H	-0.14752900	3.27963200	-3.31576600
H	1.37176700	2.37959100	-3.28024100
O	-1.23727200	2.24026600	0.96462100
C	-1.03302100	-1.18640800	2.59563200
O	-1.26758800	-0.12844800	1.98881300
O	-0.33205300	-2.17162900	2.07852000
H	-0.10039200	-1.91710100	1.14148300
C	-1.55015200	-1.43549200	3.97789400
H	-2.31400500	-2.21974800	3.93550500
H	-0.73921300	-1.79713900	4.61649900

H	-1.98258900	-0.52366000	4.38839000
C	-1.97380900	3.14399500	0.40358900
O	-2.08228600	4.30628300	0.77825600
O	-2.69833800	2.68804100	-0.67030900
H	-3.21240400	3.44874000	-0.99244200

TS1_S_ent3_5

C	-3.77175200	-0.27291300	-0.09112600
C	-2.45383200	-0.51336500	-0.52240200
C	-2.08612100	-1.84520800	-0.84614300
C	-3.00761700	-2.88715900	-0.79137900
C	-4.31263900	-2.61915600	-0.36554800
C	-4.69228500	-1.31958700	-0.01027600
C	-0.64694000	-2.09107400	-1.17797500
O	-0.23834900	-3.04142000	-1.84652600
N	0.13447400	-1.14653500	-0.54239000
C	1.52740000	-1.03664000	-0.62428600
C	2.05040100	0.01937600	0.18331200
C	2.42097900	-1.83703700	-1.32158400
C	3.44678800	0.25546900	0.31382700
C	3.81109600	-1.60254600	-1.21964600
C	1.52532800	1.78745900	1.62021800
C	3.84450200	1.31437200	1.16946000
C	4.31474200	-0.59667900	-0.42476800
C	2.89298000	2.06599600	1.82394500
N	1.13493000	0.80022800	0.83351800
Cl	6.05585900	-0.36646700	-0.32131500
H	-4.07725900	0.74347600	0.13623600
H	-2.13173700	0.27470900	-1.48203100
H	-2.69990200	-3.89419400	-1.05712700
H	-5.03658900	-3.42734900	-0.30891500
H	-5.70988000	-1.12569400	0.31731300
H	2.05179000	-2.64735500	-1.93442400
H	4.49282800	-2.23786700	-1.77484100
H	0.73365300	2.37476500	2.07218700
H	4.89985200	1.52609800	1.30119900
H	3.17679700	2.87955000	2.48185600
Co	-0.71966400	0.41426100	0.21341800
C	-0.80715100	1.53529600	-2.39246800
O	-0.17577500	1.46019200	-1.28503700
O	-1.85926600	0.88942000	-2.64771100
C	-0.25571700	2.48761900	-3.42545300
H	-0.49140800	2.13252000	-4.43050500
H	-0.73735500	3.46176100	-3.28113100
H	0.82160900	2.61176700	-3.30366700
O	-1.38862700	1.98611000	1.09943800
C	-0.81488000	-1.44529000	2.56576100
O	-1.20192600	-0.42188900	1.98423100
O	-0.00557300	-2.32749300	2.01437700
H	0.16593000	-2.03049300	1.08075000
C	-1.24361700	-1.77590000	3.96185300
H	-1.80540800	-2.71571200	3.95450300
H	-0.35944800	-1.92482300	4.58941800
H	-1.86178000	-0.97488900	4.36560800
C	-2.08422800	2.99148600	0.69450100
O	-2.21552500	4.05729200	1.29283700
O	-2.73392800	2.79086600	-0.50068000
H	-3.22908100	3.61104100	-0.67062100

Int2_S_ent4_5

C	3.15851600	2.04365100	-1.29178700
C	1.95759500	1.41990700	-1.64849600
C	0.91896200	2.15812900	-2.24654000
C	1.10736900	3.51485000	-2.51778100
C	2.31026700	4.13320800	-2.16689600
C	3.32973600	3.40459900	-1.54584500
C	-0.43040900	1.55007400	-2.47362800
O	-1.15610000	1.83559900	-3.41250900
N	-0.83483900	0.79077500	-1.36069200
C	-2.02798800	0.03135000	-1.31671800
C	-2.08272400	-0.81638800	-0.17965900
C	-3.12577700	0.07358700	-2.15917100
C	-3.23050000	-1.58245600	0.15479700
C	-4.27080400	-0.70345000	-1.86411400
C	-0.90364900	-1.60281000	1.69401000
C	-3.16756400	-2.35515200	1.34051400
C	-4.33463300	-1.49691700	-0.74003100
C	-2.02104500	-2.35313800	2.10724100
N	-0.95545400	-0.86529200	0.59516300
Cl	-5.79219900	-2.41225800	-0.40654000
H	3.95870100	1.45206200	-0.86069700
H	1.95612100	0.32421300	-1.68678500
H	0.30533600	4.08188800	-2.97931100
H	2.44927300	5.19014600	-2.37359300
H	4.26151400	3.89350000	-1.27888200
H	-3.11552100	0.70788400	-3.03372900
H	-5.12091000	-0.65726700	-2.53575700
H	0.03659300	-1.61556300	2.23064300
H	-4.02455000	-2.94952800	1.63693400
H	-1.95348700	-2.93615400	3.01813300
Co	0.51269900	-0.00256400	-0.24969100
C	0.72786300	-1.68971300	-2.54640800
O	0.64847300	-1.55985100	-1.23373400
O	0.72522200	-0.77751800	-3.36296100
C	0.83924700	-3.15478900	-2.94027800
H	0.98232100	-3.23159000	-4.01925400
H	1.67719700	-3.61861600	-2.41339200
H	-0.07227800	-3.68724800	-2.64980800
O	1.81965100	-0.69804200	1.03699600
S	3.21204400	-1.29434900	0.79943400
O	4.13768900	-0.87913300	1.85850000
O	3.66203400	-1.19688400	-0.59622600
C	2.91881900	-3.10859500	1.12637900
F	2.30224100	-3.25815600	2.30731000
F	2.16114400	-3.66002900	0.17480100
F	4.09446000	-3.74253300	1.16594000
O	0.54186400	1.59163700	1.13875400
O	-1.41759600	2.85401900	0.26852700
H	-1.26084400	2.06900000	-0.38979000
C	-1.34474900	2.38045100	2.90643000
S	-0.31218000	2.78073800	1.39191500
F	-2.20591900	3.36819000	3.10855000
F	-1.99769600	1.23920300	2.70234300
F	-0.52539300	2.25860300	3.94203300
O	0.31983500	4.06372700	1.61819200

TS1_S_ent4_5

C	2.99489400	1.93979200	-1.05038200
C	1.74973500	1.41504500	-1.44950100
C	0.86280300	2.26385600	-2.16373000
C	1.21558300	3.56357000	-2.50890900
C	2.46067000	4.05694500	-2.10129300
C	3.34304500	3.25283100	-1.37186200
C	-0.49725400	1.71629100	-2.45090000
O	-1.20866400	2.04979300	-3.38997600
N	-0.86783500	0.85393400	-1.41459800
C	-2.03292900	0.05530300	-1.39811000
C	-2.08022900	-0.82821300	-0.28212000
C	-3.11152600	0.08955500	-2.26538200
C	-3.21299000	-1.64302800	-0.01078200
C	-4.23671100	-0.73340200	-2.02603000
C	-0.94176400	-1.62761600	1.59478300
C	-3.15957700	-2.45626500	1.14887700
C	-4.29636400	-1.56625100	-0.93131800
C	-2.03887900	-2.43802600	1.95048900
N	-0.97210300	-0.85748600	0.52017400
Cl	-5.72949200	-2.54655700	-0.66912100
H	3.70837700	1.30217400	-0.53925100
H	1.91945300	0.33484200	-2.08843600
H	0.51974000	4.18651700	-3.06257400
H	2.74245100	5.07524900	-2.35290800
H	4.30739000	3.64846400	-1.06723300
H	-3.10103300	0.75395400	-3.11779700
H	-5.07199900	-0.69380100	-2.71655300
H	-0.02521700	-1.61857600	2.17208300
H	-4.00366800	-3.09018300	1.39647900
H	-1.97811200	-3.04970800	2.84322800
Co	0.54140600	0.11643400	-0.34062100

C	1.34120400	-1.59667300	-2.45336500
O	0.62328100	-1.42943800	-1.39927000
O	2.05332800	-0.70163400	-2.96739900
C	1.30015300	-2.98077400	-3.05089500
H	1.78480300	-2.98669700	-4.02752900
H	1.82866700	-3.65899900	-2.37305900
H	0.26618200	-3.32492600	-3.13334500
O	1.83974900	-0.59271300	0.96856900
S	3.16705600	-1.33877600	0.86217500
O	4.07007700	-0.96362400	1.95627100
O	3.71229300	-1.38763600	-0.50112500
C	2.66044000	-3.08948400	1.25654200
F	2.06188600	-3.13546800	2.45600300
F	1.80664700	-3.56016800	0.33779800
F	3.74174300	-3.87351700	1.28221100
O	0.46956600	1.64603400	1.13221600
O	-1.57202800	2.82930500	0.33058300
H	-1.38739900	2.08569100	-0.35204600
C	-1.42148000	2.29026000	2.95201500
S	-0.43682600	2.78014000	1.43196300
F	-2.29460900	3.25089100	3.22360800
F	-2.05858200	1.14817300	2.71274100
F	-0.57138500	2.13773900	3.95894700
O	0.12557700	4.09186500	1.67950400

Int2_S_ent5_5

C	3.19338500	-0.98740800	2.10345900
C	1.79681800	-1.06083800	1.99016600
C	1.14888900	-2.31188400	2.03719400
C	1.89843300	-3.47358000	2.24520500
C	3.28592600	-3.38996800	2.36695000
C	3.93569300	-2.15141600	2.28387700
C	-0.32081300	-2.42648300	1.77106400
O	-1.06167600	-3.17117600	2.40369900
N	-0.70510700	-1.70105000	0.65265000
C	-2.03703400	-1.53905100	0.22568500
C	-2.14468000	-0.63242900	-0.85894800
C	-3.18382000	-2.18052800	0.66555600
C	-3.36479900	-0.39628300	-1.54518100
C	-4.41878600	-1.93195700	0.02372400
C	-0.96259900	0.81997300	-2.27997600
C	-3.32212800	0.48300900	-2.65540500
C	-4.51309700	-1.07923700	-1.05399500
C	-2.13050700	1.06532900	-3.02827000
N	-0.99141900	0.00647100	-1.23491500
Cl	-6.06450600	-0.83726900	-1.83477600
H	3.68202200	-0.02017400	2.07253200
H	1.22281200	-0.13828500	2.07457100
H	1.39415800	-4.43353200	2.29051300
H	3.86616200	-4.29498600	2.52064100
H	5.01598200	-2.09913900	2.37768600
H	-3.13351300	-2.87839700	1.48855200
H	-5.30661400	-2.44005500	0.38366100
H	-0.01231300	1.27516200	-2.53076700
H	-4.23117000	0.68796900	-3.20963300
H	-2.07151200	1.73178000	-3.88063500
O	-0.53310600	0.80182800	1.30690600
S	-0.66806400	2.35065700	1.33697700
O	-0.91650100	2.94575200	0.02112000
O	0.31045900	2.97340000	2.23083600
C	-2.30309700	2.41511700	2.23490400
F	-3.24881700	1.81657300	1.50354400
F	-2.21176200	1.80526600	3.41880300
F	-2.64163300	3.69357700	2.42448500
O	1.47805500	-1.29241700	-1.19359900
C	1.34971200	-2.42017800	-1.71420200
Co	0.40266100	-0.26701500	0.02773100
O	0.39036300	-3.25249500	-1.40066800
H	-0.14536900	-2.84827400	-0.66208900
C	2.31157100	-2.89191400	-2.75470300
H	2.71862800	-3.86429500	-2.46239300
H	1.77499600	-3.02640800	-3.70017200
H	3.11020800	-2.16231000	-2.87993000
O	1.63838400	1.23593600	-0.24690200
S	2.50615300	1.82512900	-1.36135500
O	2.70364300	3.26271300	-1.16093600
O	2.13210800	1.35521600	-2.70448500
C	4.18252900	1.07697500	-1.02111700
F	4.60321900	1.43758400	0.19815000
F	4.14482500	-0.25834900	-1.08442200
F	5.05006800	1.52866800	-1.93143400

TS1_S_ent5_5

C	2.72809100	1.51108500	1.47494900
C	1.33515400	1.40447700	1.26922500
C	0.47164900	1.97146400	2.24312500
C	0.96336900	2.71611400	3.30802700
C	2.34917800	2.85810900	3.45311000
C	3.22721100	2.24950100	2.55081100
C	-0.97710200	1.62896800	2.12814200
O	-1.88569300	2.26035600	2.65816400
N	-1.11856800	0.43742600	1.42339500
C	-2.35433200	-0.11267900	1.03224000
C	-2.23450200	-1.18416700	0.10086800
C	-3.61685600	0.23091300	1.49168100
C	-3.36679000	-1.92880200	-0.33547700
C	-4.75274200	-0.48197900	1.04809100
C	-0.78045600	-2.47129500	-1.19561800
C	-3.13106500	-2.99919900	-1.23425900
C	-4.63703800	-1.53524500	0.16980100
C	-1.84822200	-3.27337900	-1.64952600
N	-0.97334000	-1.46516700	-0.35654000
Cl	-6.08100500	-2.40357300	-0.33057700
H	3.40779200	1.06738000	0.75547400
H	1.27509300	2.09590700	0.09881400
H	0.27565500	3.14885200	4.02820500
H	2.74523200	3.43338100	4.28491800
H	4.29975300	2.35299400	2.68564000
H	-3.73211400	1.04111700	2.19675600
H	-5.73075100	-0.19588000	1.41939200
H	0.23298300	-2.63551900	-1.54357400
H	-3.96584200	-3.59391400	-1.58806200
H	-1.64147700	-4.08691500	-2.33549900
O	-0.52367700	1.05832100	-1.11845100
S	0.13038200	2.20932500	-1.84505000
O	0.49780100	2.00227300	-3.23661700
O	1.22151600	2.79474200	-0.95224700
C	-1.21667600	3.50609900	-1.80441600
F	-2.27613300	3.04882400	-2.46592000
F	-1.54720300	3.75191100	-0.53749400
F	-0.76826900	4.61928500	-2.37723100
O	1.19951500	-1.33720400	1.43382800
C	0.88013900	-1.81898900	2.53929600
Co	0.33704600	-0.06011700	0.28296600
O	-0.17843900	-1.44303500	3.20929600
H	-0.64236000	-0.72534500	2.68395000
C	1.71994700	-2.87405400	3.18455000
H	2.13614100	-2.47815100	4.11703400
H	1.09253200	-3.73328400	3.44001600
H	2.52308400	-3.17389900	2.51371400
O	1.91791000	-0.24827800	-0.94779800
S	2.76679700	-1.15298400	-1.81977600
O	3.80191300	-0.38242800	-2.51703200
O	1.99591000	-2.13058900	-2.60656300
C	3.70603900	-2.19392500	-0.58547600
F	4.19540500	-1.43483900	0.40361200
F	2.90822000	-3.13298200	-0.05566100
F	4.72415700	-2.80236100	-1.20323400

Int2_S_ent6_5

C	3.17902200	2.27349200	-0.32598600
C	1.88536900	1.96003800	-0.76333200
C	0.90266600	2.96589700	-0.85777300
C	1.23544700	4.28632500	-0.54858400
C	2.52860000	4.59407200	-0.11925900
C	3.49651200	3.59047900	0.00301300
C	-0.52639800	2.61963200	-1.14905000
O	-1.28454100	3.34336500	-1.78547000

N	-0.91369600	1.48072100	-0.46022400
C	-2.19118800	0.90074600	-0.50073300
C	-2.26860000	-0.28487700	0.27917600
C	-3.34578400	1.35663800	-1.11825700
C	-3.48052600	-0.99532900	0.48461400
C	-4.55989900	0.65187200	-0.94818900
C	-1.05236300	-1.79701500	1.60301400
C	-3.42265400	-2.14094300	1.31682800
C	-4.63680700	-0.48007900	-0.16628500
C	-2.22446500	-2.52812900	1.87889200
N	-1.09688600	-0.71901000	0.83626400
Cl	-6.17839300	-1.29471000	0.03167200
H	3.93073600	1.49253700	-0.28904100
H	1.73968800	1.00202100	-1.27459800
H	0.47649000	5.05847500	-0.62491700
H	2.78126800	5.62141000	0.12657900
H	4.49953800	3.84161800	0.33422100
H	-3.31984700	2.25468300	-1.71845500
H	-5.45273000	1.02314400	-1.43930300
H	-0.07919600	-2.09394300	1.97351400
H	-4.32586000	-2.71079600	1.50417600
H	-2.15962900	-3.40080000	2.51810900
Co	0.40100800	0.24914200	0.16820800
C	0.21755100	-0.48256400	-2.58321900
O	0.22477500	-0.85046300	-1.33381600
O	0.42101300	0.63121900	-3.05538800
O	1.71488200	-1.02456200	0.91040500
S	2.97757000	-1.60540800	0.26879000
O	4.04150000	-1.75382700	1.26934100
O	3.32184300	-0.98788900	-1.02036200
C	2.46066300	-3.35780000	-0.11492100
F	1.90679600	-3.91048800	0.97471600
F	1.58172700	-3.40153900	-1.11507800
F	3.54299800	-4.06659200	-0.45636800
C	0.11059900	1.98651400	2.57314500
O	0.73001600	1.12741600	1.92098900
O	-0.95442900	2.60661500	2.11800100
H	-1.11069700	2.29916400	1.18419000
C	0.54460600	2.39351400	3.94507900
H	0.84262500	3.44715500	3.92804100
H	-0.29776100	2.29942700	4.63718200
H	1.37890300	1.77604500	4.27555900
O	-0.04661000	-1.55607700	-3.37567900
H	-0.01049300	-1.22607000	-4.29086600

TS1_S_ent6_5

C	3.02373500	2.09809400	-0.14196800
C	1.67861000	1.89684800	-0.51329000
C	0.85385000	3.04080200	-0.68243300
C	1.35655700	4.32994700	-0.54537100
C	2.69857800	4.49854900	-0.18650500
C	3.52761000	3.38957700	0.01862900
C	-0.59399000	2.78764900	-0.95417900
O	-1.35548700	3.58631000	-1.49669800
N	-0.95468900	1.56389700	-0.41914700
C	-2.21831100	0.96238300	-0.50751100
C	-2.29311300	-0.28086800	0.18786300
C	-3.36437500	1.45024300	-1.11716800
C	-3.50592600	-1.01469100	0.29883300
C	-4.57320800	0.72250500	-1.03462600
C	-1.11301100	-1.86542200	1.43594500
C	-3.46325200	-2.22094600	1.04246300
C	-4.65106600	-0.46689000	-0.34465100
C	-2.28020100	-2.63610000	1.61368600
N	-1.13152900	-0.73439000	0.75094100
Cl	-6.18745100	-1.31595600	-0.25692700
H	3.68461300	1.24375000	-0.03929500
H	1.63828900	1.18066800	-1.58116900
H	0.70390700	5.18463800	-0.69556400
H	3.10028500	5.50063300	-0.06585100
H	4.56864300	3.53688900	0.29097800
H	-3.33511500	2.39300300	-1.64481600
H	-5.45844600	1.11930200	-1.51964700
H	-0.15363500	-2.17729700	1.83126200
H	-4.36598500	-2.81090500	1.15534800
H	-2.22630800	-3.55466500	2.18667700
Co	0.41931200	0.36783400	0.14912800
C	0.78625300	-0.37553300	-2.55986000
O	0.22464700	-0.64952900	-1.45373600
O	1.53775800	0.61251300	-2.78607700
O	1.74052300	-0.93875500	0.87378100
S	2.93396400	-1.67954600	0.28584600
O	3.97724300	-1.88795900	1.29873000
O	3.34848800	-1.18947600	-1.03685500
C	2.23558800	-3.38194200	-0.01329700
F	1.71493400	-3.87039400	1.12399900
F	1.27608100	-3.35112100	-0.94267800
F	3.21042700	-4.19987400	-0.42527000
C	-0.03383500	1.86164700	2.68481700
O	0.66208800	1.12335400	1.96970100
O	-1.13972800	2.43984200	2.26698300
H	-1.25633900	2.21325600	1.30751300
C	0.34065100	2.16547300	4.10103000
H	0.54583700	3.23696700	4.19615600
H	-0.50094400	1.93021600	4.75965300
H	1.22001900	1.59099300	4.38972000
O	0.51464000	-1.23563200	-3.54650100
H	0.99929600	-0.94229300	-4.33928000

Int4_S_5

C	1.71552400	-3.88373500	-2.33552800
C	0.70548300	-3.18761000	-1.66856100
C	0.34729600	-3.54529100	-0.35989600
C	0.99007300	-4.62891600	0.25796200
C	2.00623400	-5.31261100	-0.40337900
C	2.37373200	-4.93862100	-1.70100400
C	-0.76631500	-2.86751600	0.37040900
O	-1.48456000	-3.49696300	1.14525800
N	-0.98178600	-1.51896900	0.05399700
C	-2.23856000	-0.93097000	0.19681100
C	-2.26617700	0.42302800	-0.24379600
C	-3.44494300	-1.49964900	0.59695900
C	-3.46101200	1.18597200	-0.33689700
C	-4.64226400	-0.75431800	0.53193000
C	-0.97164300	2.18258000	-1.08526500
C	-3.34748400	2.50172300	-0.84604500
C	-4.66277700	0.54618800	0.07641700
C	-2.11487100	2.98784500	-1.23094300
N	-1.05622000	0.94828400	-0.60145600
Cl	-6.18398300	1.41814500	0.00518200
H	1.98074700	-3.60666600	-3.35177500
H	0.17064700	-2.39262800	-2.17974100
H	0.69160400	-4.91511100	1.26148800
H	2.51319000	-6.13760800	0.08896900
H	3.16404900	-5.47584400	-2.21783000
H	-3.47370500	-2.52063400	0.94732100
H	-5.56781700	-1.22530100	0.84487000
H	0.01542900	2.53633800	-1.35012300
H	-4.23432700	3.11927800	-0.93515100
H	-2.00749700	3.98840800	-1.63320900
Co	0.38252200	-0.21968200	-0.07299700
C	1.38423100	-0.60992500	1.95062100
O	0.45225600	0.25986000	1.72675900
O	1.69951100	-1.28928500	0.92579200
C	1.97162100	-0.79880400	3.30359100
H	2.95404800	-1.26559400	3.21681200
H	2.04773600	0.16289600	3.81516600
H	1.31416200	-1.45284300	3.88817100
O	1.73101600	1.01946900	-0.76147000
S	3.03987400	1.61297300	-0.22516900
O	4.07440400	1.62153200	-1.26288300
O	3.40458300	1.15476800	1.12099700
C	2.53928400	3.39361200	-0.00353400
F	2.12373400	3.90778000	-1.17102300
F	1.53683000	3.48258900	0.88067800
F	3.57689700	4.10546900	0.44012700

Int5_5

C	-3.57901900	-1.68090600	-2.04748600
C	-2.46836800	-1.36177000	-1.26938400
C	-2.42088300	-1.75390700	0.07893400
C	-3.49272900	-2.47398600	0.63503600
C	-4.60313600	-2.78135800	-0.14351600
C	-4.64702600	-2.38530500	-1.48491500
C	-1.25140500	-1.48302700	0.93839800
O	-1.06891700	-1.98225400	2.03568600
N	-0.28695300	-0.53391600	0.43717100
C	1.01470900	-0.85128700	0.35092100
C	1.87402500	0.24961200	-0.02151600
C	1.60869200	-2.12351700	0.54217400
C	3.26425700	0.09404800	-0.20564400
C	2.97985100	-2.28833000	0.36699600
C	1.95805100	2.51898300	-0.53021700
C	4.00121700	1.24370700	-0.57520000
C	3.80037100	-1.22011700	0.00208500
C	3.34538100	2.44924600	-0.73814200
N	1.25169300	1.44467100	-0.18186600
Cl	5.49656800	-1.49676300	-0.20188800
O	-1.21764700	3.20261500	0.02270900
C	-2.41274000	2.84340100	0.33071500
O	-2.56854400	1.59209400	0.54807600
C	-3.52894100	3.82659900	0.45596900
H	-3.61165000	-1.38241100	-3.09078100
H	-1.63725900	-0.82121200	-1.71207700
H	-3.43950800	-2.77796400	1.67500900
H	-5.43382100	-3.32951800	0.29034800
H	-5.51381700	-2.62875400	-2.09252700
H	0.99954500	-2.97027800	0.83235400
H	3.42294500	-3.26624900	0.51558900
H	1.40659200	3.44598600	-0.64189600
H	5.07210100	1.17450700	-0.72800300
H	3.88587000	3.34450300	-1.02189200
H	-3.51027800	4.25602300	1.46479300
H	-3.39747400	4.63931500	-0.26205500
H	-4.49003600	3.33092300	0.30675600
Co	-0.65781600	1.35639400	0.19060500

Int6_5

C	1.23680900	4.05504100	-2.45789400
C	1.33996600	2.99006500	-1.56747100
C	1.66951000	3.22837600	-0.22231900
C	1.90706300	4.54261800	0.22006300
C	1.80117400	5.60202000	-0.67340700
C	1.46477200	5.35959000	-2.01071900
C	1.79833900	2.13668500	0.75264100
O	2.17602300	2.24364200	1.90243800
N	1.41892100	0.80484000	0.27652600
C	2.28884800	-0.21037300	0.28255600
C	1.72915900	-1.47401900	-0.13406000
C	3.67170100	-0.15809700	0.60221900
C	2.50851100	-2.64137400	-0.24826100
C	4.44800400	-1.30375500	0.50345700
C	-0.20296700	-2.56951300	-0.83482500
C	1.85542000	-3.81629600	-0.68549700
C	3.89997100	-2.52452400	0.08888300
C	0.50553800	-3.77195700	-0.98151200
N	0.40384900	-1.45671200	-0.42023800
Cl	4.92272400	-3.90391900	-0.01486500
H	0.98168400	3.86949900	-3.49640600
H	1.17469900	1.97492200	-1.91350400
H	2.16560100	4.71273800	1.25969200
H	1.97777200	6.61728400	-0.33243400
H	1.38208200	6.19004500	-2.70566400
H	4.12083400	0.77161700	0.92827200
H	5.50199500	-1.25796500	0.75138900
H	-1.26065500	-2.49589200	-1.05012800
H	2.41159000	-4.74095500	-0.78734200
H	-0.02070300	-4.65526200	-1.32282900
Co	-0.39634500	0.27342800	-0.01180200
C	-1.20978000	1.26826800	1.88313500
O	-0.81295100	0.04039300	1.80467400
O	-1.06328200	1.90178100	0.78339300
C	-1.72708800	1.86906700	3.13492000
H	-2.51368800	2.58718800	2.89446200
H	-2.10377800	1.09051400	3.80026400
H	-0.90661900	2.39981600	3.63237700
O	-2.04786100	-0.25465400	-0.78694200
S	-3.53888000	-0.00075300	-0.43064700
O	-4.26588600	0.47047300	-1.60745700
O	-3.72584200	0.68127000	0.85234100
C	-4.07969600	-1.76189500	-0.13957700
F	-3.81454600	-2.50762800	-1.21988400
F	-3.41484200	-2.26520200	0.90559300
F	-5.38686200	-1.79240600	0.10851300

OTf-

S	0.90918100	-0.00014300	0.00011400
O	1.24405700	1.13292500	0.89513400
O	1.24411800	-1.34173000	0.53398300
O	1.24607000	0.20848000	-1.42828200
C	-0.94972700	-0.00003600	-0.00014700
F	-1.43366000	1.16172800	-0.47703500
F	-1.43465600	-0.99352600	-0.76778700
F	-1.43418300	-0.16763600	1.24397600

Ag_2CO_3

C	0.21160900	2.07589300	0.00025200
O	1.30969900	1.34075300	-0.00263000
Ag	1.39847900	-0.78127000	0.00038200
O	0.30361800	3.32261500	-0.00092800
Ag	-1.53215900	-0.53548700	-0.00051900
O	-0.98665300	1.51566400	0.00418000

$Ag_2CO_3^{\cdot -}$

C	2.08247900	0.59703600	-0.00002100
O	1.80042400	-0.69422800	-0.00045000
Ag	-0.26604300	-1.48695400	0.00006500
O	3.28587800	0.96674400	0.00002400
Ag	-1.05707300	1.10775100	-0.00006200
O	1.12514400	1.50752400	0.00042700

Int7_S_5

H	-3.23634700	3.56374600	-0.98924600
H	-0.76137100	3.15168000	-0.99692200
C	4.93061700	-2.03325200	-0.16971700
C	2.55025400	-1.68730400	-0.04839300
C	2.71218600	-0.31656900	-0.30650300
C	3.99593900	0.19229000	-0.49903000
C	5.10110400	-0.67035600	-0.43278100
H	5.79527400	-2.68916600	-0.11712500
H	4.15262800	1.24840900	-0.70191000
H	6.10179800	-0.27243600	-0.58491800
C	1.14511600	-2.15568800	0.10990800
O	0.81401300	-3.31909600	0.34629700
N	0.27759700	-1.09285600	-0.08116500
C	-1.75335400	0.10986500	-0.20719200
C	-3.17025700	0.25175500	-0.16383800
C	-2.85119000	2.57643700	-0.76021500
C	-1.46074100	2.35304500	-0.77101500
N	-0.93528200	1.16625900	-0.50124000
C	3.64722200	-2.54888200	0.02150100
H	3.48540900	-3.60583500	0.21658600
C	-1.10334500	-1.14159300	0.04366000
C	-1.90125800	-2.23825700	0.35631600
H	-1.43944400	-3.19605200	0.54822400
C	-3.30566300	-2.10849100	0.41383400
H	-3.90361800	-2.97959800	0.66047400
C	-3.69940400	1.53420400	-0.45304600
H	-4.77308900	1.68558400	-0.43256200
C	-3.92893300	-0.90632400	0.16107800
Cl	-5.68587200	-0.80794300	0.24087100
O	1.78682600	2.44247000	-0.52270600
C	1.76805100	2.48455100	0.74795000
O	1.33020300	1.41796100	1.31928300
C	2.24112600	3.65641100	1.54602500
H	3.29641800	3.50643800	1.80271800

H	2.15280000	4.57130200	0.95672800
H	1.67227400	3.74056100	2.47462000
Co	1.02843400	0.59462300	-0.35292200

Int7_T_5

H	-3.12475400	3.67792200	-0.70914700
H	-0.66362900	3.17835700	-0.69563100
C	4.81403100	-2.28084400	-0.17942800
C	2.45051700	-1.85521100	-0.02466800
C	2.67681900	-0.48427700	-0.19883900
C	3.97159400	-0.00359100	-0.37816900
C	5.03922300	-0.91203200	-0.36788700
H	5.65321500	-2.97067600	-0.17148200
H	4.16279200	1.05315300	-0.53647100
H	6.05361200	-0.54706000	-0.50818300
C	1.02866500	-2.26795300	0.11445800
O	0.64212100	-3.42455400	0.27619100
N	0.21599000	-1.14660800	0.01936300
C	-1.77735700	0.12926400	-0.12197100
C	-3.18914700	0.31634500	-0.11425700
C	-2.77787000	2.66513200	-0.53840800
C	-1.39686200	2.39620100	-0.52923800
N	-0.91935300	1.17656000	-0.32287500
C	3.51487100	-2.75992300	-0.00954400
H	3.31338100	-3.81891600	0.12779700
C	-1.17606600	-1.15477000	0.06921600
C	-2.01775300	-2.24257300	0.27313700
H	-1.59416500	-3.22567500	0.41829000
C	-3.41979800	-2.07144400	0.29069700
H	-4.05162200	-2.93789800	0.45463800
C	-3.66745000	1.63228500	-0.32864400
H	-4.73591000	1.81809200	-0.32954100
C	-3.99594800	-0.83529400	0.10369100
Cl	-5.74884900	-0.68279800	0.13374100
O	1.80685400	2.31111000	-0.70524600
C	2.00531500	2.66388400	0.51705100
O	1.69380600	1.85639900	1.43485400
C	2.62677800	4.00383500	0.81264700
H	3.71760000	3.90766900	0.75441700
H	2.31442600	4.74546900	0.07379700
H	2.36348700	4.33333500	1.81956800
Co	1.03133000	0.54097400	-0.19379700

AcOH

C	-0.09184600	0.12269900	-0.00004300
O	-0.64384100	1.20420300	-0.00011800
O	-0.77932000	-1.04352700	0.00009400
H	-1.72836100	-0.81362800	0.00014500
C	1.39639800	-0.11134500	0.00001200
H	1.68338200	-0.69155500	0.88300700
H	1.68328000	-0.69325100	-0.88188600
H	1.91967200	0.84490500	-0.00088600

TfOH

S	0.85179800	-0.14354600	-0.06153600
O	1.21873800	-1.27751800	0.76723200
O	1.25417300	-0.02440600	-1.45639200
O	1.27368300	1.18966500	0.75620400
H	1.45532900	1.92081500	0.13014800
C	-1.01223300	0.01258200	0.00192100
F	-1.41404700	0.02165700	1.26821700
F	-1.37915500	1.14176700	-0.59966100
F	-1.53829200	-1.03025700	-0.63449500

I_2

I	0.00000000	0.00000000	1.43288600
I	0.00000000	0.00000000	-1.43288600

Int8_S_5

H	-3.25627300	-1.74390600	-3.60950000
H	-1.14076400	-0.45557600	-3.21384700
C	2.74961700	4.11943100	1.71722600
C	0.90487900	2.59016500	1.48048500
C	1.23772900	2.35350800	0.13659400
C	2.33879300	3.00605400	-0.41388100
C	3.09199700	3.88228000	0.38043600
H	3.34161600	4.80431800	2.31733900
H	2.62303500	2.84128000	-1.44926100
H	3.95399100	4.38645400	-0.04998200
C	-0.25746500	1.84845200	2.01172900
O	-0.75437300	1.97963000	3.12097200
N	-0.74541400	0.94291000	1.02058800
C	-2.41398400	-0.22732900	-0.18737700
C	-3.64583000	-0.92660000	-0.32015900
C	-3.05278200	-1.32583800	-2.63024700
C	-1.86018100	-0.60846400	-2.41586400
N	-1.55699400	-0.07744200	-1.23994300
C	1.65051300	3.47036700	2.27482900
H	1.36502000	3.62953300	3.31105300
C	-2.00288300	0.34430400	1.06035700
C	-2.85135100	0.22380400	2.15745400
H	-2.56089500	0.64337400	3.10954900
C	-4.08532700	-0.44347600	2.03192800
H	-4.73427000	-0.51948700	2.89727100
C	-3.94464800	-1.47841300	-1.59048200
H	-4.87301100	-2.01959800	-1.73483100
C	-4.47434000	-1.00995700	0.83575200
Cl	-6.01201500	-1.84523700	0.74550000
O	0.61492000	1.50723700	-2.56082900
C	-0.20632600	2.48096200	-2.59531500
O	-0.88217300	2.65826300	-1.51727300
C	-0.36271800	3.38171100	-3.77710600
H	0.34271600	4.21546200	-3.67956300
H	-0.13126400	2.83931900	-4.69623600
H	-1.37482400	3.78997500	-3.81548200
Co	-0.00824100	1.16441300	-0.70860600
I	1.18306400	-0.96103700	0.71728200
I	3.27481200	-2.95946000	-0.23941900

Int8_T_5

H	3.23868200	0.29503200	3.32719900
H	0.86132500	-0.39925800	2.93200900
C	-5.41557900	0.42631600	-1.60005000
C	-3.09693000	1.01109000	-1.31642800
C	-3.01176900	0.22627800	-0.14975300
C	-4.14533700	-0.46153300	0.28592900
C	-5.33763700	-0.35854700	-0.43863200
H	-6.35028400	0.49211300	-2.14881800
H	-4.10693400	-1.07889700	1.17828800
H	-6.21832200	-0.89753000	-0.09798000
C	-1.87427400	1.70930000	-1.73365300
O	-1.73248500	2.42702500	-2.71285800
N	-0.82869500	1.43126200	-0.79436400
C	1.24440400	1.52439000	0.30103900
C	2.58135900	1.96948000	0.43469000
C	2.70322600	0.66355900	2.46000400
C	1.37236000	0.26859600	2.24702200
N	0.66810900	0.69014200	1.20031300
C	-4.29307700	1.11451300	-2.04419300
H	-4.32226300	1.72756900	-2.94051400
C	0.41153800	1.94009400	-0.81336700
C	0.97226200	2.81734400	-1.78008700
H	0.36624300	3.13650600	-2.61531400
C	2.28523800	3.25554300	-1.64928900
H	2.70134700	3.92384300	-2.39448500
C	3.31091600	1.51288800	1.55593500
H	4.33809000	1.82825500	1.69816000
C	3.08179900	2.85172100	-0.57735900
Cl	4.70946200	3.43880400	-0.48041300
O	-1.84280200	-0.42344300	2.41490600
C	-2.13072300	0.76272400	2.78858500
O	-1.92675300	1.67785600	1.91485100
C	-2.69758500	1.06982600	4.13794100
H	-3.78674600	0.94943000	4.09877600
H	-2.30304000	0.37206400	4.88010500
H	-2.47284700	2.10001800	4.42152200
Co	-1.28735600	0.32444500	0.67123900
I	-0.67730700	-1.95979000	-0.60533100

I	2.60432200	-2.90420300	-0.35169300

TS2_T_5

H	2.82576100	-3.79561300	1.28298700
H	0.55474000	-2.75614600	1.11545900
C	-3.37841600	3.89401400	-0.21947400
C	-1.22107100	2.83280900	-0.27695300
C	-1.76931000	1.61967900	0.17582900
C	-3.13671400	1.55288900	0.44427800
C	-3.93068000	2.68684800	0.24053000
H	-4.01584000	4.76056800	-0.36763100
H	-3.58344500	0.63607600	0.81164100
H	-4.99703900	2.63280500	0.44597600
C	0.21998400	2.84081300	-0.52417600
O	0.90469600	3.77053800	-0.92114000
N	0.76349100	1.54153100	-0.22371000
C	2.33460100	-0.16394800	0.18478400
C	3.65964700	-0.66217100	0.24391000
C	2.72559000	-2.76370300	0.96696500
C	1.44737700	-2.18794200	0.87838500
N	1.25995800	-0.92786200	0.49401500
C	-2.01698100	3.97311000	-0.47869300
H	-1.55769000	4.89220200	-0.83121800
C	2.06108600	1.20511700	-0.21301800
C	3.16046300	2.04393600	-0.54466500
H	2.97172400	3.06488400	-0.84100600
C	4.45868200	1.55293300	-0.48797700
H	5.28718200	2.20377700	-0.74317300
C	3.83412400	-2.00527800	0.64779200
H	4.83029100	-2.42836800	0.70598700
C	4.71868500	0.23661700	-0.10599600
Cl	6.36300700	-0.30599700	-0.05404800
O	-1.94396500	-0.16614500	2.87376600
C	-0.92751800	0.49916500	3.06397400
O	-0.07840100	0.83183100	2.12264000
C	-0.53823900	1.03537500	4.43346700
H	-0.68295300	2.12146500	4.45491500
H	-1.16155900	0.57595400	5.20307800
H	0.51774900	0.83908400	4.64155200
Co	-0.45563000	0.25641100	0.37558300
I	-0.87630600	-0.61525300	-2.20839900
I	-2.37442400	-2.46766900	0.12974800

Int9_T_5

H	3.10083500	-3.84310700	-0.30569700
H	0.75588800	-3.00135200	-0.26362900
C	-3.72473700	3.48465000	0.73867100
C	-1.50669000	2.57396000	0.50256300
C	-2.00526000	1.26703300	0.32524000
C	-3.39258000	1.09420000	0.35873100
C	-4.23687900	2.19086900	0.56366700
H	-4.39673800	4.32314600	0.89564100
H	-3.83613500	0.11515500	0.22120200
H	-5.31260400	2.03316300	0.58583100
C	-0.05530400	2.74813600	0.45857600
O	0.55991900	3.79989600	0.57110300
N	0.57665800	1.47776700	0.26966200
C	2.28822300	-0.13000600	0.12808700
C	3.65445000	-0.51199900	0.11379800
C	2.91198700	-2.78310100	-0.18065300
C	1.58818700	-2.31538300	-0.15654700
N	1.28187800	-1.02880800	-0.00580000
C	-2.35144900	3.67810100	0.70657200
H	-1.91286600	4.66365400	0.83421400
C	1.89892500	1.25921800	0.27934600
C	2.92468200	2.23441700	0.41700200
H	2.64886200	3.27201300	0.52872400
C	4.26241600	1.85737600	0.40871500
H	5.03143000	2.61368500	0.51731700
C	3.94970900	-1.88424100	-0.04530600
H	4.98043600	-2.21881900	-0.06115300
C	4.63327900	0.52274000	0.26173500
Cl	6.32136900	0.12093700	0.26051300
O	-1.77828900	-1.97192000	2.53583200
C	-1.02922100	-1.00953400	2.84025800
O	-0.46418600	-0.17888400	2.05271200
C	-0.76287400	-0.78040200	4.32271600
H	-1.29759100	0.12195200	4.63791900
H	-1.10584600	-1.62991000	4.91444800
H	0.30601400	-0.61421900	4.48147200
Co	-0.57840800	-0.02375600	0.13146200
I	-0.65033800	0.23862200	-2.55305300
I	-2.07868900	-2.21148100	-0.09501800

TS3_T_5

H	3.16411200	-3.65516400	-1.26211000
H	0.82337500	-2.85289900	-0.97222000
C	-3.71175700	2.89582000	1.48779000
C	-1.46654400	2.35950400	0.77503300
C	-1.97195400	1.24821100	0.05657300
C	-3.36096900	1.01358200	-0.00187500
C	-4.21633400	1.81730000	0.74640600
H	-4.39217800	3.53304200	2.04451200
H	-3.76138100	0.21047000	-0.60769100
H	-5.28355000	1.61722400	0.73376100
C	0.01106600	2.54276900	0.85870600
O	0.54350100	3.58574100	1.25455000
N	0.63288300	1.40002200	0.45886700
C	2.38045900	-0.11460300	-0.01251100
C	3.75082400	-0.48824000	-0.14344700
C	2.98412200	-2.64737100	-0.90501600
C	1.65775700	-2.20064800	-0.74480800
N	1.36282500	-0.98390300	-0.30880800
C	-2.33974500	3.16121100	1.50505500
H	-1.92752400	3.97588700	2.09278800
C	1.99827900	1.18881400	0.42891800
C	3.00103800	2.09950900	0.75251500
H	2.73106300	3.08958400	1.08999900
C	4.35813000	1.73772800	0.63395600
H	5.12133000	2.46482500	0.89034100
C	4.02511600	-1.79978100	-0.60319900
H	5.05381300	-2.12359800	-0.71545000
C	4.72932000	0.48502400	0.19799200
Cl	6.44035000	0.08864700	0.06704000
O	-1.66877500	-2.35822400	2.30100100
C	-0.91217300	-1.43229100	2.70931100
O	-0.36179700	-0.52020800	2.01830700
I	-1.05927900	0.97340000	-2.30713200
C	-0.62348600	-1.40572700	4.20423000
H	-0.93475800	-0.43741700	4.60770200
H	-1.14682700	-2.21082200	4.72097600
H	0.45567000	-1.50503300	4.35707700
Co	-0.46581500	-0.10930000	0.10377000
I	-1.97174700	-2.33185600	-0.30109900

Int10_T_5

H	-4.04861100	3.25284200	-1.18512400
H	-1.58183700	3.17817400	-0.80500500
C	4.24197800	-2.58231900	1.28791600
C	1.91082300	-1.99070100	0.85889200
C	2.17198800	-2.06876500	-0.51847800
C	3.44863900	-2.38482700	-0.98692600
C	4.48499900	-2.62806100	-0.08554600
H	5.03965000	-2.78326100	1.99612700
H	3.63549000	-2.45163900	-2.05249000
H	5.47513000	-2.86427500	-0.46403200
C	0.60447900	-1.67954500	1.51969200
O	0.29591300	-2.20917800	2.57710000
N	-0.24395100	-0.70974300	0.92438300
C	-2.33037500	0.17123600	0.29825400
C	-3.73506600	0.11558900	0.10443300
C	-3.59778900	2.36070000	-0.76616500
C	-2.20890800	2.33237600	-0.55248700
N	-1.59306500	1.26904000	-0.03981900
C	2.96737200	-2.27687700	1.74571600
H	2.75932600	-2.23631500	2.80937300
C	-1.59862900	-0.92158500	0.86055400
C	-2.30324200	-2.08031900	1.21193100

H	-1.78466700	-2.92595600	1.64273900
C	-3.69150600	-2.15086700	1.02709600
H	-4.21927100	-3.05388600	1.31225400
C	-4.36127900	1.25838400	-0.44542100
H	-5.43313100	1.26075400	-0.60742600
C	-4.39751200	-1.08793000	0.49121700
Cl	-6.12687400	-1.22613700	0.29602800
O	0.38545100	1.96986100	2.48256900
C	1.57652100	1.55216500	2.47964700
O	1.98456300	0.89126100	1.44985900
C	2.53643700	1.82434100	3.60382700
H	3.16970200	2.67669000	3.33071400
H	1.99197100	2.06974300	4.51752900
H	3.18669700	0.96126000	3.76670900
Co	0.29847800	1.06113800	0.50592700
I	0.66350900	-1.86663800	-2.04129300
I	1.31999300	2.98740900	-1.05355500

Int11_D_5

H	-3.42083000	-3.61334800	0.02523700
H	-0.94831200	-3.18670300	-0.04591700
C	4.63792400	2.20025700	-0.73962000
C	2.26618400	1.82452000	-0.55779000
C	2.46123100	0.43431400	-0.43917400
C	3.76427200	-0.06497800	-0.47834100
C	4.84103500	0.81486400	-0.62733100
H	5.48813600	2.86657000	-0.85188600
H	3.94847700	-1.13124100	-0.38743400
H	5.85411000	0.42033300	-0.65387300
C	0.87929400	2.30043200	-0.51436800
O	0.49238900	3.45844600	-0.59054500
N	-0.00077000	1.17719300	-0.37705700
C	-1.97871300	-0.08015700	-0.26263000
C	-3.38813900	-0.21612300	-0.22530300
C	-3.04691600	-2.59928200	-0.05688900
C	-1.66150700	-2.37087300	-0.09753000
N	-1.14847800	-1.14828400	-0.19848100
C	3.34679600	2.71031400	-0.70576400
H	3.15627700	3.77659500	-0.78995900
C	-1.34213200	1.21984900	-0.36424700
C	-2.17212300	2.36931500	-0.43357800
H	-1.71401900	3.34449100	-0.50953000
C	-3.55719100	2.23699100	-0.40037100
H	-4.17918200	3.12335400	-0.45285400
C	-3.91286900	-1.52458000	-0.12033900
H	-4.98566700	-1.67630900	-0.08912400
C	-4.16325700	0.98595400	-0.29845900
Cl	-5.89645800	0.89742900	-0.26055300
O	1.57888700	-2.31566200	-0.68415300
C	1.39732700	-2.09329500	-1.92796300
O	0.88240700	-0.95953200	-2.22233000
Co	0.81659900	-0.52361600	-0.30441500
I	0.99478000	-0.51227600	2.36859300
C	1.79041000	-3.08036900	-2.98340800
H	2.85547600	-2.95109800	-3.20957700
H	1.64137000	-4.10015600	-2.62054800
H	1.21795400	-2.91180000	-3.89772300

TS4_D_5

H	3.40558300	3.58788100	0.89169700
H	0.95067400	3.13465300	0.61015000
C	-4.43598400	-1.68643700	-1.51715000
C	-2.13125700	-1.63314800	-0.78961800
C	-2.39862000	-0.41745600	-0.11088400
C	-3.69317900	0.13478900	-0.09814300
C	-4.69658500	-0.48778700	-0.83579700
H	-5.23487500	-2.17910900	-2.06319800
H	-3.89823600	1.03994400	0.46195100
H	-5.69070800	-0.05162000	-0.86432100
C	-0.71251400	-2.10941400	-0.87777700
O	-0.40004000	-3.26171600	-1.19691000
N	0.11746600	-1.06993600	-0.59265500
C	2.09025800	0.14000500	-0.16294300
C	3.49884300	0.30277300	-0.03217300
C	3.06871800	2.60185800	0.59186100
C	1.68906900	2.35853400	0.43906600
N	1.22436600	1.17305300	0.07408900
C	-3.15639900	-2.24998900	-1.50236900
H	-2.93173600	-3.15428500	-2.06025500
C	1.49898100	-1.10568400	-0.54292500
C	2.34203900	-2.18270500	-0.79797500
H	1.91892600	-3.13434800	-1.08782100
C	3.74003700	-2.03466200	-0.67546500
H	4.37904600	-2.88766100	-0.87841200
C	3.96665800	1.58319500	0.35761300
H	5.03212900	1.75145900	0.46966100
C	4.30791800	-0.83444600	-0.30504500
Cl	6.05997900	-0.71162500	-0.17163200
O	-1.42576000	2.44712600	-0.23891100
C	-1.31191600	2.48800200	-1.51523600
O	-0.82953700	1.45169900	-2.07804100
Co	-0.68193700	0.61640100	-0.24252000
I	-1.44345700	-0.22143000	2.21215600
C	-1.75586700	3.68630100	-2.29986800
H	-2.84536300	3.65119500	-2.41776100
H	-1.50528500	4.60351900	-1.76070700
H	-1.29556700	3.68785700	-3.28963400

Int12_D_5

H	4.36858000	3.26709800	1.42041300
H	1.89595100	3.37688500	0.97495300
C	-4.12970800	-0.38794600	-2.48586400
C	-2.09791500	-0.90118300	-1.24029500
C	-2.87391400	-1.00269400	-0.08354000
C	-4.25408500	-0.79985300	-0.10719800
C	-4.88112400	-0.48489900	-1.31337100
H	-4.61329600	-0.15300200	-3.42956500
H	-4.83870400	-0.88997400	0.80175000
H	-5.95555500	-0.32573100	-1.33132500
C	-0.62869200	-1.25559400	-1.32116200
O	-0.35353700	-2.34157600	-1.84386800
N	0.27536700	-0.34994300	-0.83248800
C	2.45707900	0.33317400	-0.17059900
C	3.85850100	0.18599900	0.03926700
C	3.86079500	2.42205600	0.96961800
C	2.47701900	2.49529400	0.72773400
N	1.81319600	1.48485900	0.17980300
C	-2.75573600	-0.60689600	-2.44552400
H	-2.16891900	-0.55474100	-3.35857500
C	1.63888400	-0.68709000	-0.74654900
C	2.28005100	-1.86642200	-1.11905500
H	1.71168200	-2.66574100	-1.56660000
C	3.66927600	-2.03379300	-0.92083200
H	4.12969500	-2.96875600	-1.22261200
C	4.54626900	1.27625800	0.62696400
H	5.61341300	1.19939200	0.80349700
C	4.44381400	-1.04565100	-0.35956500
Cl	6.17041900	-1.31007900	-0.13828600
O	-0.49311300	3.28976800	0.33663900
C	-1.70707100	3.12137700	-0.06588300
O	-1.98517600	1.98950000	-0.56471200
Co	-0.06094800	1.47419100	-0.23870400
I	-1.99322400	-1.52275000	1.81805000
C	-2.71419500	4.22406700	0.05406100
H	-2.76680300	4.56117000	1.09420000
H	-2.39109100	5.07735400	-0.55207400
H	-3.69648600	3.88680500	-0.27976700

TS5_T_5

H	-3.52938500	1.08223100	3.73977300
H	-1.48585100	-0.27934700	3.21040600
C	2.18842900	-4.29493600	-1.84192700
C	0.85372200	-2.28379400	-1.76098700
C	1.50900300	-1.89011200	-0.56404000
C	2.49939100	-2.72783500	-0.02125100
C	2.81824500	-3.93285800	-0.64530200
H	2.45765200	-5.22337100	-2.33600300
H	3.02367400	-2.42941200	0.88062500

H	3.57257400	-4.58196900	-0.21103600
C	-0.34407200	-1.53125500	-2.23066700
O	-0.75078100	-1.50141700	-3.38100700
N	-0.99099600	-0.94954000	-1.12446800
C	-2.59142300	0.16742400	0.14499400
C	-3.75902100	0.94144100	0.34226000
C	-3.29390100	0.83870200	2.71037200
C	-2.14852500	0.07493900	2.42899300
N	-1.81555800	-0.25235700	1.18280600
C	1.20039400	-3.47868000	-2.39441200
H	0.66845100	-3.77496500	-3.29315100
C	-2.14220200	-0.21924800	-1.16145300
C	-2.89293700	0.18419900	-2.27812200
H	-2.57410200	-0.09741000	-3.27166500
C	-4.05284500	0.94779500	-2.09755600
H	-4.62567600	1.25529900	-2.96494100
C	-4.10000000	1.27107500	1.67454200
H	-4.98623100	1.86218700	1.87552200
C	-4.48415500	1.32092600	-0.83135000
Cl	-5.93324100	2.26921100	-0.67810700
O	0.37269700	-1.73483900	2.33994700
C	-0.18434500	-2.90095900	2.35177600
O	-0.83955400	-3.25660500	1.33622300
C	-0.04276800	-3.76736200	3.57329300
H	1.01008000	-3.83532100	3.86307600
H	-0.58496600	-3.30985000	4.40839100
H	-0.44477300	-4.76393000	3.38441300
Co	-0.25508800	-1.27948100	0.55696300
I	1.98165100	0.38704500	-0.19736200
I	2.89457700	3.53945800	0.19811200

Int13_T_5

H	4.18227300	-0.76753500	2.72503500
H	1.68738400	-0.94760600	2.94799600
C	-5.12900400	1.91883900	-1.38067300
C	-2.75489100	1.69685500	-0.84457300
C	-2.83581900	0.32181100	-1.13996700
C	-4.04687300	-0.23653900	-1.55093700
C	-5.19080700	0.55412000	-1.66646500
H	-6.01352700	2.54195200	-1.46698900
H	-4.10343900	-1.29445000	-1.78286400
H	-6.12519000	0.09852000	-1.98122500
C	-1.54723000	2.47028800	-0.43475700
O	-1.49147600	3.68673800	-0.54351500
N	-0.45417700	1.77104300	0.15584500
C	1.80928100	1.36965600	0.61681300
C	3.19730200	1.53854400	0.41674700
C	3.53843400	-0.14422900	2.11603900
C	2.14468500	-0.25469600	2.25096700
N	1.31448900	0.48795300	1.52222600
C	-3.92201700	2.47715300	-0.98423000
H	-3.85092000	3.53654300	-0.76470600
C	0.82396000	2.10140700	-0.13912900
C	1.28354800	3.00504500	-1.12532800
H	0.57676200	3.56667600	-1.72051600
C	2.65051300	3.18867800	-1.32637500
H	2.98772100	3.88939600	-2.08150300
C	4.06730900	0.75000800	1.20549400
H	5.14032700	0.84489700	1.08551900
C	3.59484700	2.48602800	-0.58100100
Cl	5.27930000	2.76138000	-0.88300800
O	-0.97373400	-0.72164900	3.07116000
C	-2.22575700	-0.45350000	2.96775600
O	-2.53680500	0.38115800	2.05127600
C	-3.24689100	-1.10729600	3.84042000
H	-3.49843900	-2.08663500	3.41613100
H	-2.83985700	-1.26666300	4.84175100
H	-4.15412100	-0.50185200	3.88484000
Co	-0.62145600	0.48565000	1.59461800
I	-1.17522100	-1.07388500	-1.04466900
I	1.62376100	-3.46093000	-0.82268400

BBr_3

B	0.00103700	-0.00000600	-0.00008900
Br	-0.95239500	1.64582800	0.00000400
Br	-0.95022500	-1.64708000	0.00000400
Br	1.90247200	0.00125200	0.00000400

32a-^{t}Bu

C	3.51177700	-1.01178400	0.00011400
C	3.96670800	0.30786600	0.00005100
C	3.04638300	1.36297800	-0.00005000
C	1.68031800	1.10011500	-0.00014000
C	1.21336400	-0.22471900	-0.00010400
C	2.14163800	-1.27559100	0.00012600
H	5.03300900	0.51633800	0.00013500
H	3.39940500	2.39059300	-0.00007200
H	0.95612000	1.90852200	-0.00020100
C	-2.55397500	0.04777200	0.00008500
H	1.78342700	-2.30239800	0.00020700
H	4.22181300	-1.83408600	0.00023800
C	-0.22814400	-0.53744700	-0.00013000
H	-0.46403800	-1.60826200	-0.00034200
N	-1.11865300	0.37391100	0.00019800
C	-2.89930200	-1.44793800	0.00041000
C	-3.13855300	0.71449600	-1.25775600
C	-3.13897300	0.71545000	1.25726600
H	-3.98741100	-1.57077700	0.00021900
H	-2.50722100	-1.95561800	0.88917500
H	-2.50674200	-1.95588200	-0.88804800
H	-4.22810100	0.59945500	-1.28172900
H	-2.72361700	0.25889300	-2.16430400
H	-2.90016100	1.78335900	-1.27239100
H	-4.22855100	0.60060300	1.28102400
H	-2.90042900	1.78427800	1.27122100
H	-2.72437700	0.26041800	2.16425200

32a-^{i}Pr

C	-3.27747200	-0.95342200	-0.00050200
C	-3.67038500	0.38603600	-0.00030200
C	-2.70250600	1.39763500	0.00005500
C	-1.35002500	1.07230000	0.00020600
C	-0.94551400	-0.27326200	0.00001000
C	-1.92125400	-1.28045000	-0.00035200
H	-4.72584100	0.64370300	-0.00041900
H	-3.00780900	2.44036200	0.00022100
H	-0.59086100	1.84791400	0.00049500
C	2.79754000	-0.29607600	0.00008200
H	-1.61066700	-2.32248400	-0.00050100
H	-4.02497100	-1.74173600	-0.00077600
C	0.47731500	-0.65205400	0.00020500
H	0.67454300	-1.73542600	-0.00005900
N	1.42413600	0.20183600	0.00020800
H	2.81096700	-1.39960700	-0.00012000
C	3.49985900	0.20460500	1.26595300
C	3.49985600	0.20508400	-1.26560200
H	2.99568200	-0.16701800	-2.16452800
H	3.49406200	1.30090100	-1.29900400
H	4.54085400	-0.13695600	-1.28707300
H	4.54086200	-0.13742700	1.28727000
H	2.99570400	-0.16785900	2.16474000
H	3.49404500	1.30040800	1.29978000

32a-Me

C	2.30865900	1.05654900	-0.00018600
C	2.79818700	-0.25066300	-0.00007000
C	1.90639300	-1.32991500	0.00014000
C	0.53387800	-1.10365300	0.00021000
C	0.03216900	0.20881200	0.00008200
C	0.93228000	1.28429000	-0.00008400
H	3.86957900	-0.43090800	-0.00012800
H	2.28639400	-2.34778900	0.00024800
H	-0.16666600	-1.93255800	0.00037000
C	-3.68968400	-0.03482800	-0.00004700
H	0.54738400	2.30125100	-0.00016200
H	2.99672800	1.89723600	-0.00033900
C	-1.41411900	0.48357300	0.00012500
H	-1.69097600	1.54946200	0.00038000

N	-2.29637500	-0.43737600	-0.00020000
H	-3.83680100	1.05689400	0.00006900
H	-4.18888600	-0.45840500	-0.88083700
H	-4.18872100	-0.45853900	0.88078200

L1

C	1.20841800	0.65580900	0.00000000
C	1.17153800	-0.73838300	0.00000000
C	-0.07035800	-1.37306800	0.00000000
C	-1.22089900	-0.58380700	0.00000000
N	-1.20186600	0.75750000	0.00000000
C	0.00000000	1.35329800	0.00000000
H	2.09053100	-1.31762800	0.00000000
H	-0.15105400	-2.45559900	0.00000000
H	-2.20468600	-1.04977200	0.00000000
H	2.15027600	1.19558500	0.00000000
H	-0.00420200	2.44182100	0.00000000

L2

C	0.56855200	1.20051800	-0.00585000
C	-0.18465200	0.00070200	-0.03486300
C	0.56862700	-1.19943300	-0.02278400
C	1.95406700	-1.13474900	0.00052200
N	2.67449400	0.00031900	0.01938000
C	1.95400300	1.13547800	0.01696700
N	-1.55078800	-0.00053100	-0.07435300
H	0.08454900	-2.16786500	-0.03234400
H	2.52470900	-2.06267800	0.00666200
H	0.08472100	2.16901900	0.00328200
H	2.52452200	2.06326400	0.03826200
C	-2.28212000	1.25479100	0.01383400
C	-2.27746500	-1.25653900	0.04324700
H	-2.02068600	-1.94084400	-0.77419800
H	-3.34736100	-1.05284700	-0.00924100
H	-2.06868100	-1.76504700	0.99500700
H	-1.97116900	1.94652400	-0.77723600
H	-2.13628000	1.75298300	0.98315500
H	-3.34633200	1.05436600	-0.11497200

L3

C	1.20026400	1.13217400	-0.00001800
C	0.00002600	1.83878100	0.00000200
C	-1.20025100	1.13217500	0.00001600
C	-1.15913600	-0.26691400	-0.00000200
N	-0.00000600	-0.94839200	-0.00001800
C	1.15910300	-0.26695500	-0.00002200
H	0.00000400	2.92549200	0.00001700
H	-2.15448200	1.64958600	0.00004300
C	-2.41952200	-1.09204900	0.00000200
C	2.41951500	-1.09205900	0.00001800
H	2.15452900	1.64951900	-0.00001900
H	-3.31333300	-0.46155700	0.00000900
H	-2.45266800	-1.74342400	0.88156000
H	-2.45267300	-1.74340600	-0.88157000
H	3.31329600	-0.46152900	-0.00018800
H	2.45260500	-1.74360700	-0.88141200
H	2.45277800	-1.74324600	0.88171500

Int1-^{t}Bu_6

C	-4.57125500	0.87596000	-0.76253100
C	-4.84306300	-0.10942900	0.19061700
C	-3.82415500	-0.58400700	1.02255900
C	-2.52502300	-0.11362900	0.87961800
C	-2.23860800	0.86994300	-0.08628700
C	-3.28351200	1.38749300	-0.87639600
H	-5.85290600	-0.49485900	0.29773800
H	-4.04229800	-1.33112200	1.77945200
H	-1.73779400	-0.47897100	1.52657800
C	1.31913900	2.26240900	0.09426100
H	-3.07021600	2.17711000	-1.59162700
H	-5.36478400	1.25772200	-1.39734700
C	-0.94799500	1.52298300	-0.22378800
H	-1.05051900	2.57089100	-0.47914500
N	0.27706600	1.11040000	-0.04360000
C	1.88448200	2.57737000	-1.29458400
C	2.40191200	1.86626200	1.10993400
C	0.65143400	3.53071000	0.66395300
H	1.07808100	2.88000500	-1.97193300
H	2.40025800	1.71973200	-1.72432300
H	2.59109700	3.41002200	-1.21205100
H	3.08936400	2.71277600	1.20026600
H	2.97754000	0.99665900	0.80526700
H	1.96001400	1.67175900	2.09013800
H	1.44912500	4.21824500	0.95807200
H	0.05316700	3.30807900	1.55385300
H	0.03188600	4.06575100	-0.06103600
B	0.70289300	-0.41829800	-0.04180100
Br	2.51114100	-0.76148200	-0.92370000
Br	-0.56790600	-1.57642300	-1.12121600
Br	0.79659200	-1.05871000	1.88594900

TS1-^{t}Bu_6

C	-3.46310300	4.18942900	-0.12965100
C	-2.14549500	4.61624700	0.07484300
C	-1.14437200	3.70006800	0.41677000
C	-1.43669800	2.34958900	0.51254500
C	-2.75835000	1.90194700	0.29403000
C	-3.77604900	2.84642900	0.01097600
H	-1.90213200	5.67104100	-0.01250000
H	-0.12802200	4.03436900	0.59361300
H	-0.66842300	1.65170300	0.81179400
C	-3.27100300	-1.78604300	1.16663300
H	-4.79916000	2.50381600	-0.11365200
H	-4.23900500	4.90674600	-0.37569500
C	-3.19620600	0.55102900	0.47074400
H	-4.23551900	0.48109700	0.76106900
N	-2.56811700	-0.61724300	0.38914100
C	-2.20693800	-2.46356600	2.04278600
C	-3.95942500	-2.72908900	0.17501700
C	-4.34335900	-1.24495300	2.12733000
H	-1.79345200	-1.75010600	2.76172900
H	-1.39329100	-2.89955600	1.47064600
H	-2.69744900	-3.26657900	2.60130900
H	-4.50770100	-3.48869300	0.74077000
H	-3.25998200	-3.23718200	-0.48517000
H	-4.67991700	-2.17324600	-0.43487600
H	-4.65353600	-2.08425700	2.75518400
H	-5.24216800	-0.88272100	1.61930100
H	-3.95511600	-0.46191200	2.78739200
B	-1.42194700	-0.86631600	-0.55132000
Br	-0.92555700	0.41954600	-1.87640500
Br	-0.79596100	-2.63241100	-0.97625900
Br	3.88343600	0.03474100	1.45716800
B	2.27314200	0.11352000	0.24895800
Br	2.45455700	-1.12285900	-1.31653200
Br	0.63559400	-0.48721100	1.40089200
Br	1.95026600	2.00229900	-0.39358300

Int2-^{t}Bu_6

C	-2.56539800	4.18810100	1.06707700
C	-1.88638600	4.39378100	-0.13811900
C	-1.25384200	3.32814700	-0.78847900
C	-1.32571700	2.05053000	-0.25596900
C	-2.02855000	1.82815400	0.94462000
C	-2.61611200	2.91537000	1.62270700
H	-1.82645400	5.39309900	-0.55871500
H	-0.68021200	3.49810500	-1.69351200
H	-0.75961000	1.25582400	-0.72639000
C	-2.18297100	-1.94677500	1.76286500
H	-3.12562300	2.74544500	2.56650800
H	-3.03743000	5.02153900	1.57697300
C	-2.14656900	0.53215300	1.56212500
H	-2.28262500	0.52145500	2.63690700
N	-2.14380800	-0.62616300	0.95815400
C	-0.74508900	-2.45561100	1.89742300
C	-3.06849100	-2.92854300	0.98502500
C	-2.79476500	-1.70482600	3.14357300
H	-0.11886000	-1.72289400	2.41039700

H	-0.28479400	-2.65626200	0.93055100
H	-0.76178800	-3.38427500	2.47703200
H	-3.13485700	-3.85912600	1.55488900
H	-2.65042900	-3.18365300	0.00679000
H	-4.08096200	-2.53505500	0.85173000
H	-2.93485500	-2.68281200	3.61230000
H	-3.77347400	-1.21824400	3.07691600
H	-2.14020800	-1.12478200	3.80040800
B	-2.19929800	-0.74014100	-0.52914500
Br	-3.79798600	-0.14236100	-1.37222300
Br	-0.79963400	-1.51534900	-1.50323700
Br	1.75260500	0.85990200	-1.71856400
B	2.44946600	0.05209700	0.02167900
Br	4.33146200	0.71083600	0.35566800
Br	1.25104900	0.64432600	1.56386900
Br	2.43482800	-1.97015000	-0.11150200

TS2-^{t}Bu_6

C	-1.69442500	3.70863900	1.11785200
C	-1.72968500	3.73528600	-0.28552000
C	-1.38081800	2.60766100	-1.01643800
C	-1.05154900	1.41569400	-0.34316600
C	-1.04433400	1.40535800	1.08313900
C	-1.34739600	2.54866200	1.81453500
H	-1.99967700	4.65430900	-0.79517600
H	-1.33734700	2.64064400	-2.10010200
H	-0.40057000	0.70261600	-0.85646000
C	-1.75195800	-2.27669100	1.24576100
H	-1.37954100	2.51931100	2.89846200
H	-1.96247300	4.60116900	1.67444600
C	-1.06544600	0.07467800	1.64918900
H	-0.72885900	-0.15491600	2.64849600
N	-1.66009400	-0.80272300	0.89151100
C	-0.73704300	-3.03587500	0.37688700
C	-3.18748500	-2.74488200	0.98033000
C	-1.40828200	-2.47682000	2.72427500
H	0.26526300	-2.62753400	0.51499500
H	-0.99437100	-2.97811600	-0.68032600
H	-0.74361700	-4.08615200	0.68487200
H	-3.25742400	-3.80395000	1.24440600
H	-3.46148800	-2.64506700	-0.07240600
H	-3.90628900	-2.18683000	1.58727100
H	-1.56323600	-3.53245300	2.96248600
H	-2.05547000	-1.88358300	3.37910400
H	-0.36057800	-2.24394700	2.93558800
B	-2.35574500	-0.15071600	-0.32086800
Br	-2.25408900	-1.01231900	-2.06141500
Br	-4.11056600	0.61052100	0.13606100
Br	1.38502100	-0.79537100	-1.52839000
B	2.56406300	0.02462800	-0.08323800
Br	2.30849700	2.03089300	-0.05504600
Br	1.97952100	-0.72989300	1.73506000
Br	4.48748000	-0.46086800	-0.40703600

Int3-^{t}Bu_6

C	-1.06624400	3.73340600	1.11611700
C	-1.26885200	3.73746000	-0.27432900
C	-1.26889400	2.54611000	-0.97886500
C	-1.09715400	1.31006100	-0.28998600
C	-0.90674900	1.35560500	1.13969500
C	-0.88278000	2.54492700	1.83975000
H	-1.39986100	4.68212000	-0.79074700
H	-1.36007000	2.53840600	-2.06050900
H	-0.35450900	0.65469900	-0.80145000
C	-1.90196600	-2.23845100	1.22641400
H	-0.78098700	2.56272600	2.91939000
H	-1.06640100	4.67792300	1.65129400
C	-1.04814700	0.02800400	1.70225800
H	-0.73044900	-0.24305500	2.69725500
N	-1.70170300	-0.77581500	0.91587100
C	-0.90637400	-3.03044900	0.35982200
C	-3.35314500	-2.61394000	0.90606900
C	-1.61021100	-2.50669000	2.70612700
H	0.11512500	-2.69299000	0.54673400
H	-1.12465100	-2.91133300	-0.70094800
H	-0.98960600	-4.08934000	0.62428500
H	-3.48838800	-3.67740500	1.12354300
H	-3.58898400	-2.44972300	-0.14694800
H	-4.05388800	-2.03879200	1.51734600
H	-1.84118200	-3.55537300	2.91027400
H	-2.23146700	-1.88814300	3.36294100
H	-0.55489700	-2.35249000	2.95229200
B	-2.26657200	0.01874800	-0.31987400
Br	-2.30429600	-0.90602300	-2.06959000
Br	-4.07280800	0.76783300	0.16973600
Br	1.27447800	-0.79613900	-1.51276200
B	2.52760300	-0.04307000	-0.08437100
Br	2.30923000	1.96664800	-0.01073700
Br	1.97117300	-0.83585700	1.71933500
Br	4.41994000	-0.56392400	-0.49349800

TS3-^{t}Bu_6

C	0.01197100	3.58827800	1.15306000
C	-0.44175200	3.71008100	-0.16617500
C	-1.09487200	2.65080000	-0.79817000
C	-1.25756100	1.43232900	-0.11361200
C	-0.80701900	1.35236700	1.23892500
C	-0.15939800	2.40019300	1.87454900
H	-0.28265000	4.64145200	-0.70019400
H	-1.43908300	2.74582100	-1.82394000
H	-0.12710600	0.67031600	-0.74493200
C	-2.12810900	-2.13966800	1.20080900
H	0.19856600	2.30896000	2.89468000
H	0.51905200	4.42600900	1.62098000
C	-1.12427500	0.03758700	1.75999100
H	-0.81679500	-0.31091800	2.73551900
N	-1.83883500	-0.68564500	0.94844700
C	-1.12552400	-2.94377900	0.35153900
C	-3.57283700	-2.44619200	0.79179900
C	-1.93004600	-2.48032400	2.68172000
H	-0.09912400	-2.67944800	0.62019300
H	-1.27167000	-2.75282300	-0.71194700
H	-1.27813700	-4.01029000	0.54476400
H	-3.75368300	-3.51422900	0.94569900
H	-3.74845500	-2.21613300	-0.26023500
H	-4.28326700	-1.87803600	1.39757100
H	-2.24587300	-3.51554200	2.83699700
H	-2.53741300	-1.83832700	3.32898600
H	-0.88170900	-2.41267900	2.98999300
B	-2.30553300	0.20994900	-0.28545300
Br	-2.34887400	-0.68010900	-2.08345100
Br	-4.16906600	0.91169800	0.17082100
Br	2.87196800	1.81676000	0.09187400
B	2.56435900	-0.13665000	-0.01184600
Br	1.94805100	-0.91944200	1.72595300
Br	0.93610200	-0.42475100	-1.39366500
Br	4.05900800	-1.16704700	-0.81648600

33a-^{t}Bu

C	-4.07168700	1.28402700	0.05091500
C	-3.98695100	-0.11245600	0.16185500
C	-2.75010300	-0.76936700	0.16358600
C	-1.58281200	-0.02186800	0.05861100
C	-1.68607000	1.38026900	-0.05006200
C	-2.91362000	2.05170100	-0.05758500
H	-4.90185900	-0.69262500	0.24723400
H	-2.70793300	-1.85194000	0.24705500
C	2.04613900	1.47966000	-0.07070900
H	-2.96153700	3.13352200	-0.14495400
H	-5.04465700	1.76596300	0.05008000
C	-0.35944500	1.94371800	-0.13653200
H	-0.15696300	3.00788400	-0.19594400
N	0.59961300	1.06133800	-0.11662100
C	2.28697700	2.62898900	-1.06011600
C	2.95853500	0.30669700	-0.44520000
C	2.33339000	1.93174100	1.37124100
H	1.77675700	3.55275200	-0.77115100
H	1.96514500	2.34782700	-2.06846700

H	3.35905600	2.84591700	-1.09027000
H	3.99573100	0.63427700	-0.32351800
H	2.81020000	-0.00223900	-1.48160100
H	2.79104000	-0.55581600	0.20185000
H	3.38578300	2.21847800	1.46569700
H	2.12221800	1.11964400	2.07173900
H	1.71421500	2.79474900	1.63955100
B	-0.03945600	-0.38988600	0.00134400
Br	0.36781100	-1.49350800	-1.65839000
Br	0.60952300	-1.31840600	1.68828500

HBr

Br	0.00000000	0.00000000	0.03999300
H	0.00000000	0.00000000	-1.39975400

Int4-L3_6

C	3.18938600	-1.18876200	-0.20811000
C	3.85973100	0.00066500	-0.45842700
C	3.18916600	1.18996400	-0.20818100
C	1.84200900	1.18506600	0.13375800
N	1.13905400	0.00041800	0.13309800
C	1.84226000	-1.18415100	0.13391000
H	4.90371400	0.00075300	-0.75436500
H	3.70701100	2.14217100	-0.23410800
C	1.24074000	2.47025700	0.63595200
C	1.24125200	-2.46946900	0.63625700
H	3.70742200	-2.14086600	-0.23399500
H	2.01271700	2.96410200	1.23590200
H	0.36989500	2.29672100	1.26612100
H	0.95804700	3.14671100	-0.17235900
H	0.95903800	-3.14625100	-0.17190900
H	0.37027700	-2.29600300	1.26629600
H	2.01325700	-2.96279900	1.23661500
B	-0.46274800	0.00002700	0.00819100
Br	-1.14776200	-1.58670500	-1.06217100
Br	-1.21971200	-0.00074900	1.88331300
Br	-1.14933400	1.58662500	-1.06119300

TS4-L3_6

H	-1.31604600	0.10778500	-2.62123200
H	0.17357900	1.05961800	-2.72423000
B	-2.08452900	-0.37542800	-0.07124900
Br	-1.80958900	-1.37092500	1.53240700
Br	-3.22968600	-1.13294700	-1.40336600
Br	3.41116600	-1.42670400	0.56356400
Br	1.10285700	0.71538700	1.61450600
Br	0.48518200	-1.34965500	-0.93575000
Br	2.58381900	1.19531100	-1.29941600
B	1.92208600	-0.19416500	0.01704000
H	-3.92861800	0.70584800	1.49817900
H	-1.37903500	1.77784600	-3.18547400
C	-0.47314500	2.93450800	-0.90273600
C	-0.69859500	3.63703800	0.26881000
C	-1.60450500	3.12317200	1.19045600
C	-2.16216900	1.87270000	1.00431800
N	-1.80141700	1.11976700	-0.10206000
C	-1.05542700	1.69081500	-1.11499300
H	-0.22584000	4.59907600	0.43614800
H	-1.89676400	3.69079200	2.06621500
C	-3.21931900	1.39566800	1.95964300
C	-0.89089200	1.09220900	-2.48132400
H	0.15218800	3.34108600	-1.68703900
H	-3.77552800	2.27308300	2.30037100
H	-2.78867300	0.91143600	2.83941500

Int5-L3_6

H	0.90149100	-1.70112900	-0.72674100
H	1.18110800	-2.05912900	0.97010600
B	2.01721300	0.56862100	0.10603500
Br	1.29549500	0.83722700	1.81253900
Br	1.33650400	1.36712200	-1.44394800
Br	-1.83352700	1.77784100	0.25078100
Br	-4.29497900	-0.41313300	-0.16083100
Br	-1.56410900	-1.28603700	1.50630700
Br	-1.43170400	-0.82001900	-1.78210000
B	-2.28825700	-0.17313600	-0.04288800
H	4.19453400	2.18902000	-0.82262100
H	1.56747600	-3.27337900	-0.26069600
C	4.08235300	-2.54410100	-0.27938700
C	5.36930900	-2.01794500	-0.31767200
C	5.55808200	-0.64257200	-0.20091700
C	4.46566600	0.19729600	-0.05900500
N	3.20934900	-0.35296100	-0.03088300
C	2.98938500	-1.70275400	-0.12771100
H	6.22389800	-2.67638000	-0.43322900
H	6.54982200	-0.20717700	-0.21979900
C	4.59574000	1.68353600	0.06287400
C	1.58759300	-2.20543600	-0.03581300
H	3.90590300	-3.60982900	-0.36059200
H	5.64789600	1.95432400	0.16341700
H	4.06007700	2.06377800	0.94021800

Int6-L3_6

C	-5.10096600	-1.01322700	-2.18926800
C	-6.41137900	-0.64582700	-1.87329900
C	-6.65411500	0.49796900	-1.10701100
C	-5.58758200	1.26476400	-0.65391900
C	-4.26131500	0.85966300	-0.90803500
C	-4.02708800	-0.27354800	-1.70595600
H	-7.24378000	-1.23808800	-2.24160900
H	-7.67214900	0.79896100	-0.88060800
H	-5.76969500	2.16891200	-0.08002500
C	-1.17145000	2.84217200	0.16021400
H	-3.01260000	-0.54051500	-1.97131700
H	-4.91198400	-1.88158400	-2.81260100
C	-3.21867200	1.74179400	-0.39638800
H	-3.51411200	2.78410400	-0.43544000
N	-2.02941800	1.51990300	0.08305100
C	-1.15429600	3.41888700	-1.26758900
C	0.28298900	2.63082700	0.58480300
C	-1.83788600	3.78488000	1.16880400
H	-2.14087200	3.73525800	-1.61770100
H	-0.75948800	2.66643000	-1.95569600
H	-0.50006100	4.29465300	-1.29084400
H	0.78925900	3.58596800	0.41286200
H	0.80157900	1.87919500	-0.00765700
H	0.38434600	2.38658700	1.63809900
H	-1.24158300	4.70090700	1.22405000
H	-1.85941600	3.33528000	2.16588700
H	-2.85580200	4.07672400	0.89354500
C	-3.68644600	-3.07608100	0.50221700
C	-4.80385800	-2.59942700	1.17129800
C	-4.71756900	-1.35281200	1.77270400
C	-3.59259100	-0.55832700	1.59534800
N	-2.58446700	-0.96693000	0.74871200
C	-2.56239900	-2.27631400	0.32392000
H	-5.69155900	-3.21303400	1.28329400
H	-5.51031800	-0.98067800	2.41151400
C	-3.50335000	0.70555900	2.40912600
C	-1.33554500	-2.92103900	-0.25523500
H	-3.65366900	-4.09127700	0.12470500
H	-3.93227900	0.48880200	3.39164000
H	-4.09022300	1.52147400	1.97717200
H	-2.47899400	1.03923200	2.55393100
H	-1.40418900	-3.99156500	-0.04360400
H	-0.41924600	-2.53322000	0.19054200
H	-1.26240000	-2.79669900	-1.33716100
B	-1.43238100	0.07625500	0.34219600
Br	-0.16316100	-0.13974800	1.88610500
Br	-0.48606700	-0.21813900	-1.42144500
Br	2.89731000	0.91357100	-1.74748000
Br	3.30788000	0.90235100	1.53710800
Br	5.47173100	-0.70172900	-0.40698100
Br	2.39835700	-1.88900900	-0.02815500
B	3.51153700	-0.19655800	-0.15741100

Int7-L3_6

H	0.29005700	2.38418200	-0.33464900

H	0.95890300	2.41206700	-1.96155300
B	1.84454200	-0.00702600	0.07366100
Br	0.89297900	0.12623700	1.85173400
Br	0.46158700	-0.17523300	-1.37140800
Br	-5.04163000	0.04544300	0.56226900
Br	-3.00295100	-0.10586300	-2.05476000
Br	-2.18924100	-1.62830900	0.78250500
Br	-2.16822700	1.69504700	0.60599600
B	-3.09072900	0.00071400	-0.02466200
C	4.71400800	-2.15416200	-1.35948400
C	4.63576900	-3.32672200	-0.62067200
C	3.53091300	-3.50821800	0.19523900
C	2.58055300	-2.50234100	0.35072700
N	2.77994700	-1.27729500	-0.24198500
C	3.77490700	-1.14538000	-1.19159200
H	5.38375100	-4.10535100	-0.72892900
H	3.36521000	-4.44803500	0.70875500
C	1.32708000	-2.83792100	1.10196900
C	3.86287800	0.04051000	-2.11552600
H	5.49599300	-2.00738700	-2.09531200
H	1.22675300	-3.92627100	1.10601900
H	0.44510100	-2.40566300	0.62646800
H	1.34854200	-2.49606600	2.13829100
H	4.33721700	-0.29730000	-3.04017200
H	4.48021300	0.84876400	-1.71423800
H	2.87725400	0.43084000	-2.36465400
C	3.38466400	3.53889900	-0.42200000
C	4.63208300	3.39963300	0.16203100
C	4.89869500	2.22648600	0.85331100
C	3.97795200	1.18729100	0.87280100
N	2.79902900	1.28865200	0.15625800
C	2.45581900	2.50058600	-0.39743000
H	5.35858400	4.20495600	0.12682000
H	5.82184800	2.10143200	1.40711800
C	4.31690200	-0.00301600	1.73234100
C	1.09226600	2.79634500	-0.94784200
H	3.09351000	4.46827400	-0.89616400
H	4.98632300	0.34282700	2.52320600
H	4.84703600	-0.78424000	1.18102800
H	3.43404100	-0.43221300	2.20175600
H	0.98275600	3.88302200	-0.98370600

Int1-^{i}Pr_6

C	4.55674900	0.76443800	0.79271000
C	4.77367900	-0.28376000	-0.10671100
C	3.73097400	-0.74851100	-0.91387100
C	2.45854700	-0.20179400	-0.79876800
C	2.22837300	0.84448100	0.11494800
C	3.29759800	1.34714600	0.88085200
H	5.76200500	-0.72606200	-0.19255500
H	3.90942100	-1.54405800	-1.63062500
H	1.65449900	-0.54657500	-1.43702100
C	-1.28757400	2.22880200	-0.17126200
H	3.12517000	2.18161100	1.55488900
H	5.37115000	1.13653500	1.40645500
C	0.96321300	1.54886700	0.20769800
H	1.06935600	2.61826600	0.37713300
N	-0.25885400	1.13194400	0.05376900
C	-0.89907000	3.08807300	-1.37178900
H	-2.20152100	1.69679600	-0.42206500
C	-1.52286100	3.01370100	1.11438700
H	-0.02304200	3.71552600	-1.17706000
H	-0.69784600	2.45170300	-2.23936600
H	-1.73705000	3.74925200	-1.61560500
Br	0.34955000	-1.65474100	1.02658600
Br	-2.62513300	-0.38904100	0.95769500
Br	-1.02229700	-0.81963000	-1.92644800
H	-2.32927300	3.73608600	0.95110700
H	-1.81986100	2.33689200	1.92005900
H	-0.63076800	3.56896200	1.42381100
B	-0.80244700	-0.33756100	0.03822300

Int2-^{i}Pr_6

C	-3.07100100	3.97632600	0.78622900
C	-2.42775300	4.15291500	-0.44332200
C	-1.66902500	3.11966200	-1.00709700
C	-1.57979500	1.89626900	-0.36403500
C	-2.25064300	1.69787000	0.86106700
C	-2.96303000	2.76235100	1.45251500
H	-2.49344600	5.10995700	-0.95210300
H	-1.12641800	3.27926100	-1.93298400
H	-0.91445200	1.13897800	-0.76469800
C	-1.94657800	-1.94355700	1.98817500
H	-3.44660700	2.61351500	2.41338600
H	-3.63964400	4.78867700	1.22663100
C	-2.22115800	0.45319500	1.57321000
H	-2.34828600	0.49542400	2.65167800
N	-2.07710800	-0.74153500	1.05553900
C	-0.59601000	-1.91752000	2.69070600
H	-1.98849600	-2.80908400	1.32533100
C	-3.14206200	-2.00658100	2.93352300
H	-0.51031000	-1.04419700	3.34497100
H	0.23327500	-1.89791800	1.98024000
H	-0.51194000	-2.81946000	3.30619200
Br	4.16464200	1.03852200	0.02450500
Br	1.17627100	1.00240300	1.45657200
Br	2.48570100	-1.81229900	0.29439800
H	-3.10585400	-2.96187600	3.46579400
H	-4.08639300	-1.95406200	2.38224900
H	-3.12107800	-1.20949300	3.68344900
B	-2.11303700	-1.06133200	-0.39009200
Br	-3.63879400	-0.54367100	-1.40375500
Br	-0.74580400	-2.11026300	-1.12619800
Br	1.46382800	0.53062500	-1.82656600
B	2.33247600	0.18719900	-0.01154600

TS2-^{i}Pr_6

C	-1.69403700	3.68409300	0.87682400
C	-1.73378000	3.60738500	-0.52399700
C	-1.41556500	2.41934000	-1.17029900
C	-1.11656300	1.27387200	-0.41216600
C	-1.11554300	1.36365800	1.01201100
C	-1.37943700	2.56864500	1.65671800
H	-1.98056500	4.49308800	-1.10013700
H	-1.36929800	2.37202500	-2.25324600
H	-0.49633600	0.49926400	-0.87217800
C	-1.94606300	-2.25586400	1.41315200
H	-1.40826000	2.62096800	2.73990700
H	-1.93299500	4.62265100	1.36695900
C	-1.17126500	0.07944300	1.67658600
H	-0.84865700	-0.09891300	2.69323200
N	-1.78069700	-0.83250000	0.97640600
B	2.49919600	0.01660900	-0.07633800
C	-2.40164800	-2.32104500	2.86852900
C	-0.65744200	-3.03009300	1.14141400
Br	2.23442300	1.98133400	-0.47696000
Br	1.93867400	-0.33150600	1.86368100
Br	4.42021800	-0.52541200	-0.31870100
H	-2.65930600	-3.35743300	3.10522300
H	-3.28621600	-1.69702200	3.03163500
H	-1.61061900	-2.00799300	3.55745800
H	-0.80238900	-4.07229500	1.44247300
H	0.17996300	-2.60622600	1.70239400
H	-0.39806300	-2.99630800	0.08227200
B	-2.45069200	-0.32020300	-0.29310800
Br	-2.28153000	-1.43666300	-1.86800300
Br	-4.20503600	0.48528400	0.03144400
Br	1.30371100	-1.09068000	-1.30265700
H	-2.74292000	-2.64545000	0.77566200

Int3-^{i}Pr_6

C	-1.21763800	3.70554200	0.90565400
C	-1.47598600	3.62883500	-0.47351000
C	-1.44425500	2.40442700	-1.11760100
C	-1.19562000	1.21363400	-0.37455700
C	-0.96293800	1.33955700	1.04986400
C	-0.95807400	2.56582400	1.68301300
H	-1.66725100	4.53937900	-1.03078500

H	-1.56786500	2.33838200	-2.19397300
H	-0.45387300	0.55225600	-0.86860000
C	-1.72806200	-2.28178400	1.20515100
H	-0.81552600	2.64752600	2.75509300
H	-1.23586900	4.67634300	1.39113000
C	-1.01411600	0.03152100	1.67491600
H	-0.61856500	-0.20996600	2.65038300
N	-1.64552600	-0.82496100	0.93230700
B	2.47784900	-0.05617100	-0.09530100
C	-3.17499400	-2.66207100	1.52460600
C	-0.73514300	-2.71937100	2.27181400
Br	2.19266400	1.85484400	-0.70411200
Br	2.16987400	-0.14626200	1.91870700
Br	4.32565200	-0.69757100	-0.53893100
H	-3.22484500	-3.74231200	1.69073700
H	-3.84777700	-2.40762400	0.70239700
H	-3.51844900	-2.15044800	2.42952900
H	-0.73628300	-3.81227800	2.31470500
H	-1.00773300	-2.34519200	3.26516800
H	0.27696000	-2.38373200	2.02644200
B	-2.32034900	-0.12226300	-0.29044700
Br	-2.39226700	-1.23485100	-1.91976800
Br	-4.12789500	0.58191800	0.24236400
Br	1.09008500	-1.26259500	-1.00043100
H	-1.44474900	-2.73395700	0.25025300

TS3-^{i}Pr_6

C	-0.08753600	3.56988000	0.86389800
C	-0.55425000	3.59095500	-0.45597100
C	-1.20799800	2.48448300	-0.99931500
C	-1.36315400	1.31967000	-0.22327200
C	-0.90330000	1.34689000	1.13377700
C	-0.24991600	2.44086500	1.67713700
H	-0.40251600	4.47913200	-1.06083200
H	-1.55662400	2.49930600	-2.02771400
H	-0.23323500	0.52352400	-0.77426300
C	-2.32919400	-2.07745600	1.32662500
H	0.11854700	2.43002000	2.69744500
H	0.42299200	4.44124900	1.26132200
C	-1.21865800	0.07607600	1.76253000
H	-0.91002200	-0.21592900	2.75831100
N	-1.94586400	-0.68483300	1.00339700
H	-3.17422000	-2.28911500	0.66765100
C	-2.77493400	-2.22000300	2.77833000
C	-1.15889200	-2.99535500	0.95691100
Br	1.94621400	-0.64379900	1.85372300
Br	0.86374800	-0.63434000	-1.28356000
Br	4.01386600	-1.21752500	-0.67481100
H	-3.17501200	-3.22741700	2.92744100
H	-3.56125200	-1.49584600	3.01485900
H	-1.94371700	-2.08536800	3.47879900
H	-1.43228400	-4.03492100	1.16232200
H	-0.26572500	-2.74002400	1.53633900
H	-0.91740800	-2.89551200	-0.10354700
B	-2.40107500	0.07727800	-0.29399000
Br	-2.40980400	-1.08140200	-1.92879300
Br	-4.29714300	0.71884500	0.10365400
Br	2.77465800	1.84030000	-0.18578300
B	2.50799500	-0.11408200	0.00581800

33a-^{i}Pr

C	4.07632600	0.93919800	-0.00797400
C	3.87443500	-0.44819300	-0.00682000
C	2.58461500	-0.99610700	-0.00452700
C	1.48300500	-0.14934500	-0.00347100
C	1.70534700	1.24821800	-0.00513100
C	2.98583400	1.80882100	-0.00718800
H	4.73706500	-1.10910200	-0.00758700
H	2.45318300	-2.07479700	-0.00354600
C	-2.00175000	1.52897400	0.00100400
H	3.12711000	2.88592900	-0.00802400
H	5.08681100	1.33653000	-0.00945500
C	0.42834100	1.93341000	-0.00347000
H	0.29518400	3.01174200	-0.00389000
N	-0.58208700	1.11716200	-0.00075500
C	-2.32196700	2.31848100	1.26959900
H	-1.78866500	3.22973100	-1.34429200
C	-2.33391400	2.28075600	-1.28748500
H	-1.77976400	3.27054200	1.29260300
H	-2.05059700	1.73484500	2.15451600
H	-3.39447200	2.53501700	1.30742400
B	-0.08928400	-0.37026000	0.00069700
Br	-0.80931800	-1.25661200	1.68160200
Br	-0.81952300	-1.26718800	-1.66969700
H	-3.40614800	2.49947700	-1.32051100
H	-2.07325000	1.66986700	-2.15701600
H	-2.55762400	0.58912700	0.01769400

Int1-Me_6

C	4.56405900	-0.93957000	0.09253600
C	4.65675000	0.39849800	-0.30056800
C	3.55260100	1.24700300	-0.17676700
C	2.34071600	0.75958200	0.29726800
C	2.23246000	-0.59078000	0.68172700
C	3.36799400	-1.42338600	0.60952300
H	5.59572800	0.78541200	-0.68570000
H	3.63530900	2.29284200	-0.45587500
H	1.49697000	1.42636800	0.41554800
C	-1.11919400	-1.60312100	2.09576200
H	3.29514500	-2.45444100	0.94379100
H	5.42563100	-1.59517800	0.01425700
C	1.05130200	-1.18722400	1.27629600
H	1.27537700	-1.95861100	2.01006700
N	-0.21967900	-0.95258400	1.11132900
Br	-2.79768400	-0.77495500	-0.34329400
H	-1.69853900	-2.38754200	1.61082600
Br	-1.09164200	1.80694400	0.80904000
H	-0.52848100	-2.01303200	2.91452900
B	-0.92814000	-0.06269300	0.01891600
Br	0.04936400	-0.06730100	-1.73948200
H	-1.80013700	-0.84437400	2.48479900

Int2-Me_6

C	-4.62875500	2.89368200	0.40528500
C	-3.71588300	3.38867100	-0.53433600
C	-2.49156600	2.74413000	-0.75073300
C	-2.18527300	1.58323900	-0.06121700
C	-3.11024900	1.05785900	0.86988800
C	-4.31923800	1.75030700	1.12542900
H	-3.94962400	4.29625200	-1.08303500
H	-1.77135400	3.15288200	-1.45191800
H	-1.21195700	1.13175900	-0.19304700
C	-1.73781600	-2.02520500	2.53897600
H	-5.00856200	1.36089100	1.86878900
H	-5.56614800	3.41091800	0.58079900
C	-2.87194100	-0.11336400	1.64808800
H	-3.38960300	-0.16442100	2.60305600
N	-2.07956700	-1.14064300	1.38927500
Br	-0.00883700	-2.63724800	0.01102100
H	-1.92762600	-3.06713100	2.28275000
Br	0.83736300	0.44962700	-1.67268300
B	2.00695200	0.54543800	-0.00511700
B	-1.55366200	-1.56790400	0.06896000
Br	-2.54640200	-1.26262900	-1.52157800
Br	3.11065300	2.23130400	-0.04474500
Br	0.80601400	0.56838700	1.65897200
Br	3.18688000	-1.09465700	0.07577500
H	-0.67942000	-1.88064900	2.76351100
H	-2.33933600	-1.73701400	3.40002900

TS2-Me_6

C	-2.86701100	3.41721400	-0.30805900
C	-3.12850700	2.78775400	-1.53572500
C	-2.49365900	1.59667400	-1.85949500
C	-1.64931000	0.97605600	-0.91596000
C	-1.41002900	1.63156600	0.33572200
C	-2.00116100	2.85379700	0.63334600
H	-3.80362300	3.25733400	-2.24317000

H	-2.63375800	1.13944400	-2.83358600
H	-0.87441000	0.29370400	-1.27067800
C	-0.86299100	-1.61260000	2.00648800
H	-1.85186100	3.32033300	1.60106200
H	-3.36710800	4.35142900	-0.07245600
C	-0.86384600	0.73936100	1.34205000
H	-0.19847400	1.01797300	2.15105100
N	-1.30454300	-0.47202300	1.19887600
B	2.46467900	0.03926700	-0.03359300
B	-2.38844100	-0.61783500	0.11760800
Br	-2.27668400	-2.20996100	-0.98389900
Br	1.81525000	1.92923500	-0.41412700
Br	2.40376700	-0.25800500	1.98310900
Br	4.33424300	-0.21970000	-0.71979000
Br	-4.17542400	-0.12435900	0.75278000
Br	1.19602800	-1.28468200	-0.92976400
H	-0.11932300	-2.15973000	1.42284800
H	-1.72453000	-2.24711400	2.21864100
H	-0.41855800	-1.25376900	2.93307000

Int3-Me_6

C	-2.61379400	3.50712700	-0.37626900
C	-2.99021500	2.83176200	-1.55166400
C	-2.51645800	1.55715100	-1.79739000
C	-1.70289300	0.89609300	-0.82755600
C	-1.33855700	1.63272800	0.36779000
C	-1.78534000	2.92172800	0.59132900
H	-3.62820600	3.33147500	-2.27226100
H	-2.74346200	1.04788700	-2.72873900
H	-0.86816500	0.31058300	-1.24674700
C	-0.93264700	-1.63672000	1.99592200
H	-1.55555600	3.44461800	1.51325200
H	-2.99570200	4.50808400	-0.19997100
C	-0.82833300	0.72231200	1.38130500
H	-0.17341300	0.97868900	2.20519900
N	-1.29978300	-0.46987700	1.20032400
B	2.44089800	0.01417400	-0.02982700
Br	-4.15738800	-0.09928800	0.78179300
Br	1.14134400	-1.24254400	-0.97459800
Br	1.80099000	1.93099500	-0.30515200
Br	2.40214800	-0.39002700	1.96456800
Br	4.29393100	-0.21729300	-0.76139500
H	-0.20402300	-2.20960000	1.41703700
B	-2.34220800	-0.51230200	0.04026400
Br	-2.29979000	-2.17241200	-1.01818700
H	-1.82792900	-2.23495100	2.17092000
H	-0.49231400	-1.32017600	2.94005500

TS3-Me_6

C	-0.23471400	3.44202800	-0.31092700
C	-0.75924600	2.96883800	-1.51998400
C	-1.41963700	1.74253900	-1.57754700
C	-1.52259700	0.95041000	-0.41481500
C	-1.01559400	1.49036900	0.81220900
C	-0.35259100	2.70498100	0.87409900
H	-0.64650800	3.56457400	-2.41994100
H	-1.81122300	1.37004400	-2.51956800
H	-0.39310100	0.05578700	-0.70451000
C	-2.59527700	-1.44422900	2.39492200
H	0.05392100	3.08073300	1.80668000
H	0.28198900	4.39610500	-0.29268300
C	-1.33214300	0.57660800	1.89672400
H	-0.99715900	0.67517700	2.92377400
N	-2.12101300	-0.38152600	1.52132000
H	-2.23013500	-2.40066000	2.01307400
Br	-4.45524400	0.54426600	0.06624100
Br	2.65048200	1.61956000	-0.86624300
Br	1.93521300	0.06380500	1.98307000
Br	0.78643000	-1.13747100	-0.88458300
Br	3.97256800	-1.36469700	-0.21456100
B	2.44337400	-0.12261800	0.05488400
B	-2.56458400	-0.21173300	0.02001200
Br	-2.53180600	-1.96143800	-0.95645100
H	-2.24301800	-1.28231800	3.41438600
H	-3.68834500	-1.44718500	2.36539300

33a-Me

C	3.97640800	-0.00105000	0.18948900
C	3.29864000	-0.00331600	1.41716700
C	1.89884700	-0.00341100	1.47564400
C	1.16641200	-0.00128000	0.29482200
C	1.86650800	0.00090400	-0.93475900
C	3.26262100	0.00112700	-1.00844500
H	3.87342300	-0.00503000	2.33935900
H	1.39476200	-0.00519100	2.43829500
C	-1.48124400	0.00416400	-2.49217300
H	3.77444200	0.00290700	-1.96658200
H	5.06210900	-0.00100800	0.17353200
C	0.91292100	0.00296200	-2.02426000
H	1.15919000	0.00496300	-3.08342000
N	-0.32105700	0.00225100	-1.61812700
Br	-1.36060200	-1.68000100	0.54372800
H	-2.08166800	0.89121300	-2.27193400
B	-0.38517900	-0.00026200	-0.04563500
Br	-1.35830700	1.67927000	0.54871500
H	-2.08181700	-0.88376200	-2.27591300
H	-1.17199900	0.00643100	-3.53870200