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# Theoretical and experimental investigations on homologation of ethanol to butanol using a ruthenium-based catalyst

Tesi di laurea sperimentale

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A mia madre Grazia,
la cui comprensione
è stata fondamentale.

## Abstract (Italiano)

Il meccanismo di reazione del processo di omologazione del bioetanolo a butanolo e ad alcoli superiori mediante la reazione di Guerbet è stato investigato con metodi computazionali e sperimentali. La reazione, di tipo tandem, prevede un catalizzatore organometallico a base di rutenio e di un co-catalizzatore basico. A causa di problemi legati alla selettività del processo, durante la reazione si formano diversi prodotti secondari e si ha forte competizione tra la reazione principale e vari processi parassiti. In questo lavoro, è stato caratterizzato il ciclo catalitico completo, comprendente anche le reazioni parassite principali, utilizzando metodi computazionali basati sulla teoria del funzionale di densità (DFT) ed esperimenti a conferma dei risultati teorici ottenuti. A causa della complessità del meccanismo di reazione, sono state condotte simulazioni cinetiche sulla base dei risultati DFT, confermando la distribuzione sperimentale dei prodotti e fornendo approfondimenti sui fattori che governano il meccanismo di reazione.

## Abstract (English)

The mechanism of homologation of bioethanol to butanol and higher alcohols *via* the Guerbet reaction was computationally and experimentally investigated. The catalytic pathway involves a ruthenium-based complex and a base co-catalyst which work simultaneously. Due to selectivity issues, secondary products were formed and high competition between main pathway and side reactions was recorded. Herein, the overall catalytic mechanism for all the processes involved in was investigated, also considering the principal side reactions, using density functional theory (DFT) methods and experiments to confirm theoretical outcomes. Due to the complexity of the reaction network, kinetic simulations were established from DFT results, confirming experimental products distribution and giving insights into the factors governing the reaction mechanism.

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## List of abbreviations

DFT — Density Functional Theory

BO — Born-Oppenheimer

HF — Hartree-Fock

XC — Exchange-correlation

LDA — Local Density Approximation

LSDA — Local Spin-Density Approximation

GGA — Generalized Gradient Approximation

FES — Free Energy Surface

TS — Transition State

TST — Transition State Theory

TOF — Turnover frequency

TDTS — Turnover frequency determining transition state

NHC — N-heterocyclic carbene

GC — Gas Chromatography

NMR — Nuclear magnetic resonance

ESI-MS — Electrospray ionization mass spectrometry

IR — Infrared

ODE — Ordinary differential equations

# 1. Introduction

## 1.1 The Guerbet reaction

Future depletion of fossil fuels and environmental issues are hot-topics in chemical research and in political agendas. As widely reported, our society will need more and more energy to provide essential services and industrial production. Nevertheless, fossil fuels, which are our main source of energy, are about to run out and have proven dangerous for the environment. In this perspective, the need to develop sustainable and renewable fuels is central to the scientific community. [1]

One of the most important promising biofuels is bioethanol, which is a widely available, renewable and sustainable feedstock obtained from industrial wastes and non-food biomasses. Even though it can be used in many current engines, it is not a good fuel and a truly eligible alternative to gasoline. A better alternative to bioethanol is butanol and higher alcohols, which chemical-physical characteristics are closer to gasoline and more suitable for engines. [2]

Butanol can be obtained from bioethanol by means of the Guerbet reaction, [3] a process which enables catalytic upgrading of ethanol to higher alcohols, according to an apparently simple mechanism: i) a catalyst dehydrogenates a molecule of bioethanol to acetaldehyde, ii) an acid or base species co-catalyses an aldol condensation leading to an α,β-aldehyde, iii) which is reduced to a saturated alcohol (Figure 1.1).

Even though this process has been known for more than a century [3] and the catalytic pathway proposed by Veibel and Nielsen in 1966 is still accepted by the scientific community, [4] the interest in this reaction is still high as reported by Wass et al. [5]
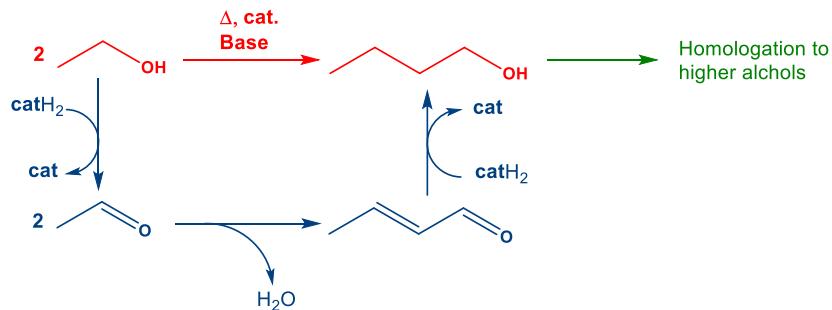


**Figure 1.1** Guerbet reaction as proposed by Veibel and Nielsen. [4]

Indeed, the Guerbet reaction has got many strengths on paper – such as the possibility to avoid direct adjunct of molecular hydrogen for reductions, being ethanol itself an internal $H_2$-storage, and the usage of the main reagent as a solvent – but also some limitations. For example, experimental yields and selectivity on alcohols are not high, since it is difficult to control aldol condensation, [6-12] and many other side reactions occur during the catalysis (Figure 1.2). This turns into separation issues and limitations to industrial applications.
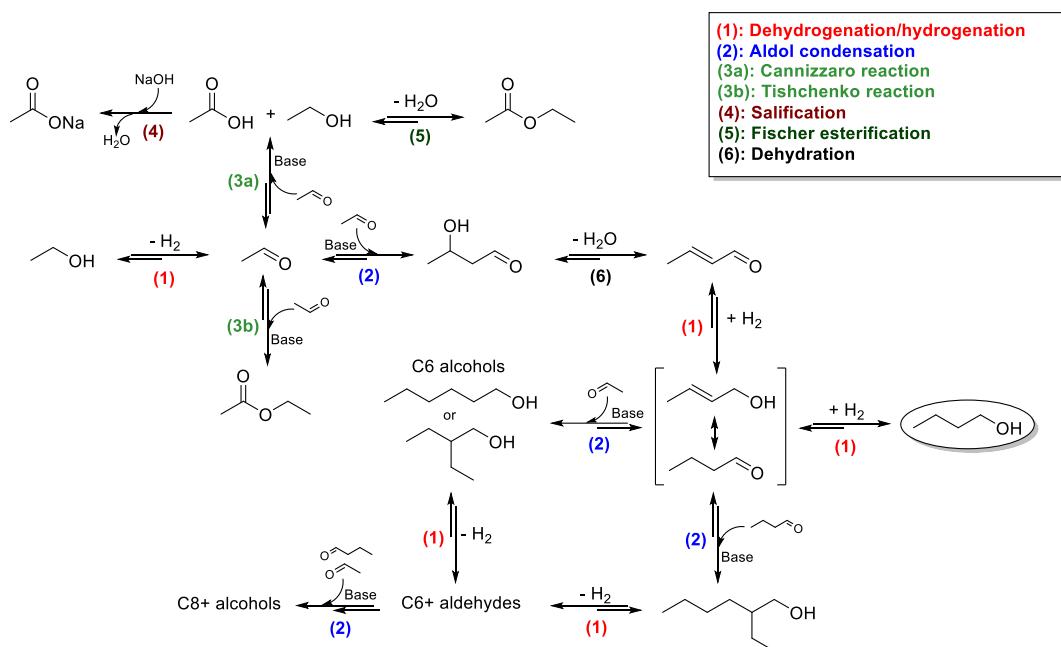


**Figure 1.2** Side reactions associated to the Guerbet process, as reported in reference [40].

However, research is ongoing to find new and better catalysts. Most performing processes to date are homogenous, thanks to higher selectivity and milder conditions than for heterogeneous ones. [5] In particular, dehydrogenation/hydrogenation pathways are catalysed by an organometallic complex and aldol condensation is co-catalysed by an acid or base system. Homogeneous catalysts active for the Guerbet reaction are mainly bifunctional systems based on iridium, ruthenium or manganese. [13, 14] Especially ruthenium and iridium-based complexes have shown high selectivity, as reported by Wass [14] and Jones [15].

However, as highlighted by Wass et al. in a recent review, "there are [still] unanswered questions regarding mechanism that could unlock possibilities for rational catalyst design". [5]

## 1.2 Theoretical background

Computational chemistry has providing insights and accurate predictions in many scientific fields for decades, thanks to the development of more powerful methods gathered to also an incredible increasing computer power. In particular, within the framework of Quantum Chemistry, density functional theory (DFT) and DFT-based methods are extremely popular, as they allow studying large chemical systems with hundreds of particles, otherwise inaccessible with other (eventually more accurate) methodologies, such as post-Hartree-Fock methods. Since the aim of this work is to apply standard DFT methodologies, the detailed description of the various computational methods in Quantum Chemistry will not be considered, [17, 18] and just the fundamental concepts will be briefly reviewed here.

### 1.2.1 Wavefunction theory and Hartree-Fock method

The energy of a multi-electrons system in Born-Oppenheimer (BO) [19] non-relativistic approximation is given by the sum between the nuclear-nuclear repulsion energy, $V_{nn}$, and the electron energy, E, computed by solving the time-independent Schrödinger equation (1.1),

$$\hat{H}\Psi = E\Psi \qquad (1.1)$$

Where, $\Psi = \Psi(r_1, r_2, \ldots, r_N)$ is the N-electrons wavefunction which quantum-mechanically describes the entire system, and $\hat{H}$ is the Hamiltonian operator which enables to obtain electron energy from the wavefunction. Its formulation comprehends three mathematical operators which correspond to specific energy terms,

$$\hat{H} = \hat{T} + \hat{V}_{ne} + \hat{V}_{ee} \qquad (1.2)$$

Where, $\hat{T}$ is the kinetic energy operator, $\hat{V}_{ne}$ is the nuclear-electron operator and $\hat{V}_{ee}$ is the electron-electron repulsion one. The Hamiltonian (1.2) could be also written in a more explicit way as

$$\hat{H} = \sum_{i=1}^{N} \frac{1}{2} \nabla_i^2 - \sum_{i=1}^{N} \sum_{\alpha} \frac{Z_\alpha}{r_{i\alpha}} + \sum_{i<j}^{N} \frac{1}{r_{ij}} \qquad (1.3)$$

$$E[\Psi] = \frac{\langle \Psi | \widehat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_0 \qquad (1.4)$$

Note that the kinetic energy operator refers only to electrons, since within the BO approximation the nuclei are considered fixed (i.e. the Schrödinger equation is solved for a given set of atomic coordinates) and thus the kinetic energy of the nuclei is zero. Energy calculation (1.4) could be done according to different *ab initio* theories, where the Hamiltonian and/or the electronic wavefunction can be defined in specific ways. All of them have been widely used in many computational applications of Quantum Chemistry. The basic formalism for *ab initio* methods is given by the Hartree-Fock (HF) theory. [20, 21]

The HF theory recurs to a mono-determinant representation of the electronic wavefunction and a Hamiltonian formalisation (1.5) such as

$$\widehat{H}_{HF} = \widehat{T} + \widehat{V}_{ne} + \widehat{J} - \widehat{K} \qquad (1.5)$$

where the electron-electron interaction is described with a $(\widehat{J} - \widehat{K})$ term, which takes in account the Coulomb interaction as mean-field approximation, $\widehat{J}$, and the exchange energy term, $\widehat{K}$, which shapes interactions between electrons with parallel spins. [22]

Even though the HF theory could be good enough to describe molecular systems, it suffers some big limitations, i.e. the electron correlation energy is not considered (if not just within a "limited" mean-field approximation), leading to a systematic error in computing the ground state energy ($E_0$).

## 1.2.2 Density Functional Theory

A different approach to solve a N-electrons problem is studying the system in terms of the electron density, $\rho$, instead of wavefunction formalism. DFT has been developed since 1920s by Thomas and Fermi, [23-25] but even though many contributions have advanced the theory for decades, [26, 27] the decisive input was made by Hohenberg, Kohn and Sham in 1960s. Hohenberg and Kohn proposed two theorems, [28] which state that:

**Theorem 1**: "The external potential $V_{ext}(\mathbf{r})$ is (to within a constant) a unique functional of $\rho(\mathbf{r})$; since, in turn $V_{ext}(\mathbf{r})$ fixes $\widehat{H}$ we see that the full many particles ground state is a unique functional of $\rho(\mathbf{r})$". [28]

The first theorem, as written by the authors in 1964, states that all the ground state properties of a system can be determined only by knowing its electron density, i.e. each physical property can be expressed as a functional of the electron density.

**Theorem 2**: The total energy functional $E[\rho]$ satisfies the variational principle (1.6).

$$E_0 \leq E[\varrho] = \int \rho(\mathbf{r})V_{ne}d\mathbf{r} + F[\rho] \qquad (1.6)$$

where $F[\rho]$ contains the kinetic energy and both the classical and non-classical electron-electron interactions and it can be written as,

$$F[\varrho] = T[\varrho] + V_{ee}[\varrho] \qquad (1.7)$$

Therefore, since the exact functional form of $F[\rho]$ is unknown, its approximation highly influences the ground state energy estimation.

For this huge practical limit, a primary approximated solution was elegantly proposed by Kohn and Sham, [29] who defined $F[\rho]$ in separated terms as

$$F[\varrho] = T_s[\varrho] + J[\varrho] + E_{xc}[\varrho] \qquad (1.8)$$

where $J[\rho]$ is the Coulomb term and $T_s[\rho]$ describes the kinetic energy defined as

$$T_s[\varrho] = -\frac{1}{2}\sum_i^N \langle\phi_i|\nabla^2|\phi_i\rangle \qquad (1.9)$$

with $\phi_i$ the eigenfunctions of density matrix in HF formalism. [18]

Furthermore, as it is clear from (1.8), the Kohn-Sham approach explicitly move the problem of exact form of $F[\rho]$ into that of an exchange-correlation (XC) functional, $E_{xc}[\rho]$, which will determine the accuracy of energy calculations. Since the exact form of $E_{xc}[\rho]$ is unknown, many approximations have been proposed since the publication of the DFT Kohn-Sham formalism. The Local Density Approximation (LDA), proposed by Kohn and Sham themselves, states that the exchange-correlation energy in a point can be computed by knowing the exchange energy of an electron gas with the same electron density at that point. This approximation assumes that the electron density does change slowly and it is treatable as an electron gas. [29, 30]

Since in many chemical systems the electron density is not as uniform as assumed by the LDA, new approaches were needed and subsequently proposed. Particularly relevant is the Generalized Gradient Approximation (GGA), [31] which also takes into account the derivative of local density.

Even though the class of functionals built by LDA and GGA have been largely used for long, with reasonably good performance, the level of accuracy required to make direct comparison between computational results and experimental evidences pushed the development of new types of XC functionals. To date, the most popular DFT XC-functional in computational chemistry is the B3LYP, which belongs to a class of functionals known as hybrid XC-functionals. It is built from the gradient-corrected B88 exchange functional by Becke and the LYP gradient-corrected correlation functional by Lee Yang and Parr, which define the BLYP functional by Colle-Salvetti. This was further corrected with a contribution from the HF exchange potential, [32-34] reading as

$$E_{xc}^{B3LYP} = (1-a)E_{xc}^{LSDA} + aE_{xc}^{HF} + bE_{xc}^{B88} + E_c^{LYP} + (1-c)E_c^{VWN} \qquad (1.10)$$

with a = 0.20, b = 0.72 and c = 0.81.

DFT calculations based on hybrid functionals, such as B3LYP or similar, provide a good compromise between computational cost and accuracy, yielding reliable energies and physico-chemical observables, becoming increasingly popular and largely used in computational chemistry. Nowadays, Quantum Chemistry software involving DFT methodologies are able to predict and to model experimental data in an incredible and unprecedent way.

### 1.2.3 Transition State Theory and kinetic methods

Computational methods based on DFT, as discussed above, offer the possibility of carrying out investigations at a reasonable computational cost, allowing characterization of free energy surfaces (FESs) of molecular systems. Thus, DFT computations are suitable to obtain insights into catalytic mechanisms by characterizing stationary points along the FESs that characterize the reaction pathways. Moreover, thanks to computational kinetic simulations, it is accessible to estimate the time-evolving products distribution, if the reaction FESs are known.

Indeed, according to the Transition State Theory (TST), developed in the 1930s, the rate constant of an elementary step is proportional to the height of the energy barrier between the transition state (TS) and the relative reagent(s).

In TST, an elementary step is, thus, modelled as a quasi-equilibrium process (Figure 1.3) and the statistical probability that reactant(s) overcome a TS barrier can be expressed in terms of Boltzmann distribution.

$$A + B \rightleftharpoons [AB]^{\ddagger} \longrightarrow C$$
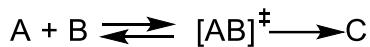
**Figure 1.3** Quasi equilibrium model in TST for an elementary step.

This turns into the Eyring equation (1.11), which directly links the free energy of a TS and the rate constant of the related elementary step.

$$k = \frac{k_b T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \qquad (1.11)$$

For simple reaction pathways, it is possible to use approximation, i.e. assuming the rate determining step is the one related to the highest energy barrier and the intermediates concentration is close to zero since they are consumed as quickly as they are formed. Even though this assumption is good enough for simple reactions, many chemical transformations require a more dept study. For example, if a reaction mechanism involves more than one catalyst and/or some side reactions occur and/or many TSs are close in energy to the highest one, it is difficult to predict the kinetics and the final products distribution. Therefore, in those complex cases it is necessary to use the so-called kinetic networks, which take in account all elementary steps in order to best evaluate the effect of variation of intermediates concentration. Several examples of kinetic simulations have been reported in literature for heterogeneous, [35] but not for homogeneous catalysis, where theoretical kinetic applications are still uncommon. Nevertheless, some successful examples have shown the power of this method. [36-38] In particular, Kalek and Himo demonstrated that gathering DFT calculations and kinetic networks for studying homogeneous catalysis leads to unprecedent accurate reproduction of experimental data – also for complex pathways involving more than only one catalyst and tens of elementary steps – and gives the possibility to gain insight into hidden reasons of selectivity distribution. [36]

## 1.3 Computational studies on the Guerbet reaction

Despite the scientific interest into the Guerbet reaction, only one computational work on the catalytic pathway characterization for a homogeneous organometallic complex was found in literature. [39] Pathak et al. [39] proposed a mechanism for the upgrading of ethanol to 1-buthanol and 1-hexanol catalysed by a Mn-based homogeneous catalyst (Figure 1.4).
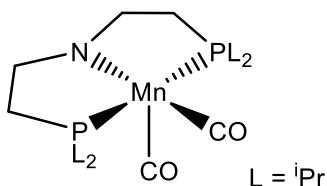


**Figure 1.4** Active catalyst studied by Pathak et al.

The authors showed the important role played by the organometallic complex, which efficiently promotes hydrogen transfer pathways, being an effective bifunctional catalyst. In fact, the metal centre seems to be acid and it can bind a hydride species, whilst the N-ligand is easily protonated. Moreover, thanks to the presence of a co-catalysing base, i.e. sodium ethoxide, the aldol condensation is favoured and it runs in parallel to dehydrogenation/hydrogenation pathways. Therefore, bifunctional catalysts seem to be highly performing in hydrogen transferring during the Guerbet reaction. In this context, a greater interest is growing toward cyclopentadienone-ruthenium complexes, both as ionic species in presence of an imidazolium salt [40] and as neutral systems with a N-heterocyclic carbene ligand (NHC) (Figure 1.5), as it has been widely studied by the Mazzoni group.

Ruthenium systems containing a cyclopentadienone ligand have previously demonstrated to be active in $H_2$-transfert processes thanks to a cooperation between the metal-centre and the ligand itself, which easily promotes redox pathways. [41]
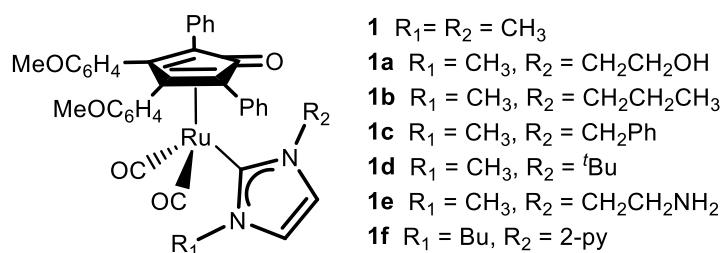


**Figure 1.5** Ruthenium(0) complexes with N-heterocyclic carbene ligands.

Moreover, a proper carbene choice provides electronic and steric modulations which could enhance catalytic performances. [42, 43] Therefore, the combination of these two ligands have given rise to new class of catalysts for $H_2$-transfer processes.

In particular, **1** has proven to be active in the Guerbet reaction if 0.002 eq. of pre-catalyst are added in presence of 0.20 eq. of sodium ethoxide to ethanol, under inert atmosphere, autogenous pressure and at 423.15 K. Indeed, after 4 hours 49.4 % conversion of ethanol, 32.2 % yield in 1-butanol, 11.3 % yield in $C_{6-10}$ chain long valuable alcohols and 5.9 % of carbon-loss are recorded, reaching high selectivity (i.e. 65.2 %) in 1-butanol. Hence, **1** is an eligible system to be computationally studied in order to try answering some of the questions on the mechanism that Wass et al. highlighted. [5]

## 2. Aim

Starting from the state-of-the-art described above, the aim of this work is to hypothesize and verify by reactivity experiments and DFT calculations the catalytic mechanism for the Guerbet reaction using the ruthenium based homogeneous catalyst **1** (Figure 2.1a) in presence of sodium ethoxide as co-catalyst. A particular interest has been devoted to the role played by the carbene ligand in the catalytic pathway, also attempting to explain why species **24** (Figure 2.1b) is not active for the Guerbet reaction at the same experimental conditions of **1**.

To this aim a synergic experimental and computational approach was used. Starting from experimental clues a mechanistic hypothesis was formulated and then investigated theoretically. Subsequently, specific tests such as *in situ* NMR, $^{13}$CO enriched and NOESY-1D experiments were designed to confirm the theoretical results. All intermediates and transition states were computationally characterized and advanced kinetic models were built to interpret experimental data.
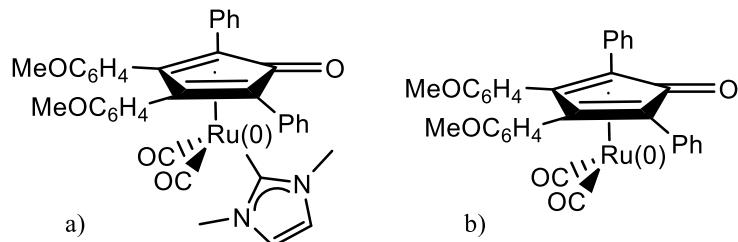


**Figure 2.1** Structures of a) complex **1** and of b) catalyst **24**.

# 3. Results and discussion

## 3.1 The Guerbet reaction: primary experimental evidence

The Guerbet reaction could be carried out using different transition metal-based catalysts, including ruthenium-based ones.

It was already observed that if the reaction is performed using **1** in presence of sodium ethoxide as co-catalyst at 423.15 K under inert atmosphere and in autogenous pressure (see section 6.6), a substantial conversion of ethanol and a high yield in 1-butanol – and in $C_{4-10}$ chain long valuable alcohols in general – is reached after 4 hours. [44] Nevertheless, by carrying out the catalysis at different reaction times, products distribution features a peculiar trend: after 60 minutes the reaction rate slows down (Figure 3.1) until reaching a plateau, indicating that an equilibrium involving sodium ethoxide was hit or the catalyst was partially deactivated. The explanation of this trend is a key point to understand the reaction mechanism and to suggest improvements for better catalytic performances.
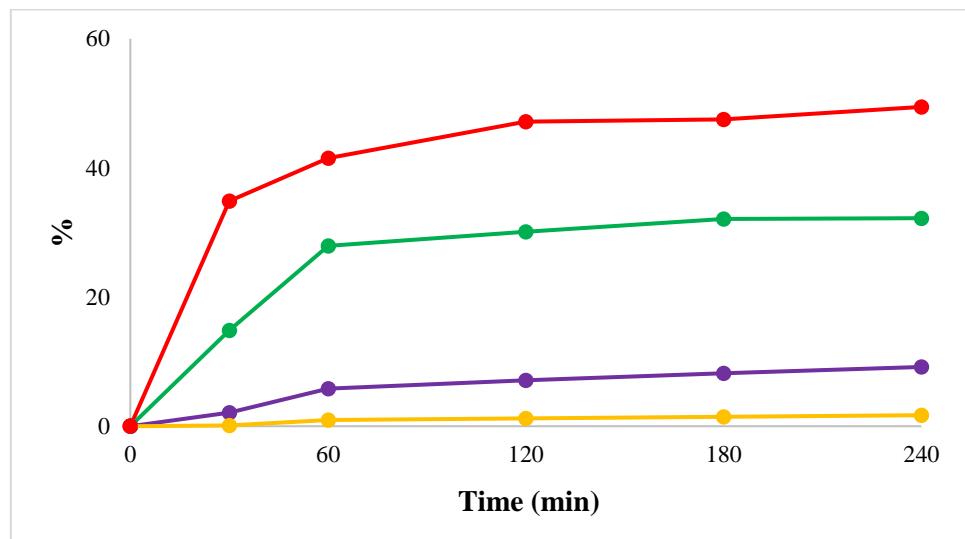


**Figure 3.1** Experimental products distribution. Conversion of ethanol (red), yield of butanol (green), of $C_6$ alcohols (violet) and of $C_8$ alcohols (yellow) are reported in presence of 0.002 eq. of **1** and 0.20 eq. of sodium ethoxide.

Moreover, by looking at shapes of products yield and their derivatives at the start of the process, it is clear that 1-butanol is the main and direct product $\left( \lim_{t \to 0} \frac{dY_{BuOH}}{dt} > 0 \right)$, whilst $C_{6+}$ chain long alcohols are likely formed starting from 1-butanol itself, as secondary products.

## 3.2 The catalytic cycle

As first assumption, to simplify the reaction route, it was considered that the catalyst only homologates ethanol to 1-butanol, without taking in account any subsequent (and side) reactions. Thus, it was assumed that the catalyst selectively converts ethanol to 1-butanol, approximating the total yield in $C_{4-10}$ chain long alcohols to that of 1-butanol. In fact, as it will be demonstrated below, homologation of 1-butanol to higher alcohols crosses the synthesis of 1-butanol itself, making difficult a linear representation of the pathway.

Therefore, a first and simplified catalytic cycle has been proposed for the overall transformation (Figure 3.2) and consisting of four main steps: i) the catalyst is activated through a carbon monoxide dissociation, ii) the ethanol is dehydrogenated and a molecule of acetaldehyde is formed, and iii) thanks to an off-cycle organic pathway catalysed by sodium ethoxide, two molecules of acetaldehyde are coupled to get (*E/Z*)-crotonaldehyde, iv) which is reduced twice to 1-butanol. The proposed mechanism, thus, shows the tandem nature of the reaction, where the main catalyst is active both in dehydrogenation and in hydrogenation and works with a base co-catalyst.
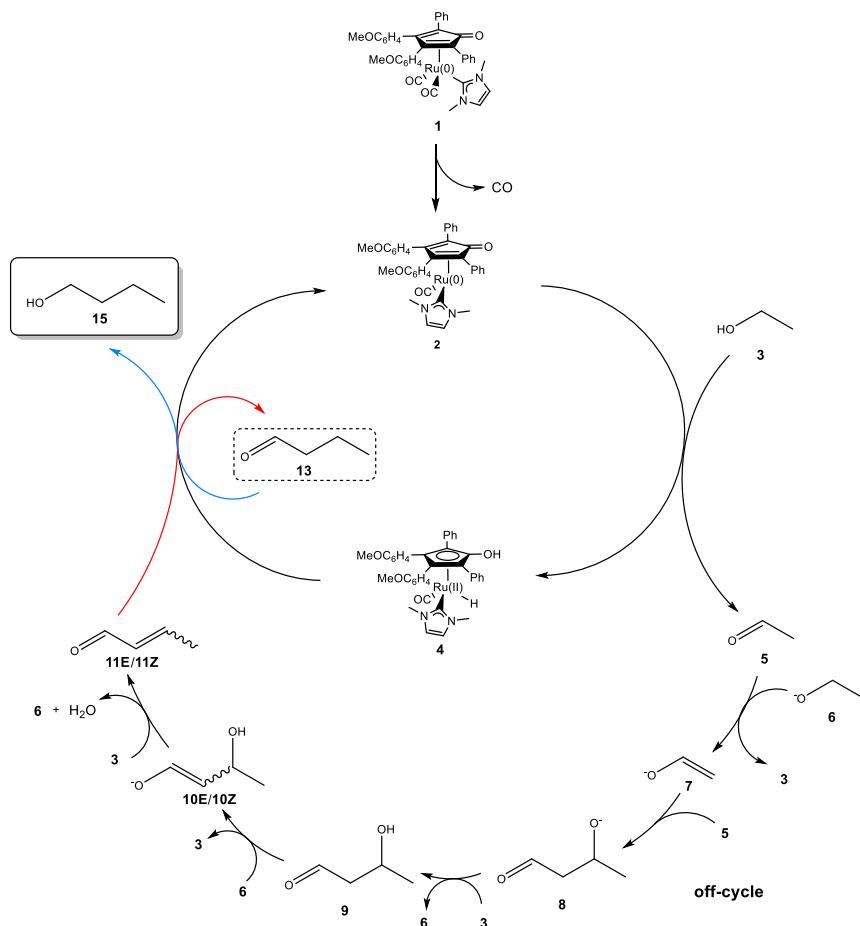


**Figure 3.2** Simplified catalytic scheme proposed for homologation of ethanol (**3**) to 1-butanol (**15**).

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### 3.2.1 Activation of the catalyst

The first step to consider is the activation of the catalyst. According to the mechanism scheme proposed, the pre-catalyst (**1**) should thermally loose a terminal CO bonded to the ruthenium centre. Thus, the so-obtained 16 electrons intermediate should represent the real catalyst, namely the species prone to dehydrogenate a molecule of ethanol.

However, it is important to underline that two ligand dissociations are possible in **1**: i) carbon monoxide dissociation or ii) carbene dissociation which likely yields an ionic species, close to some already reported in literature. [40] For both these two steps, DFT computations suggested barrier-less processes, i.e. no transition states were found and the energetic costs of activation are equal to the free energy differences between products and reagent(s).

By comparing the computed free energies associated to the two ligand dissociations, the CO one appears to be the favoured pathway, as shown in Figure 3.3.
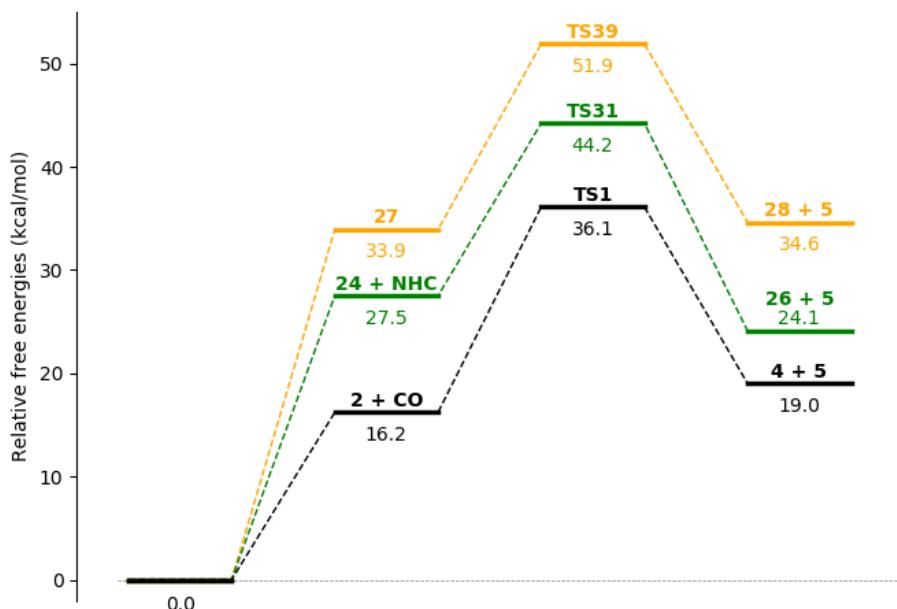


**Figure 3.3** Free energy profile showing three possible activation and dehydrogenation mechanisms. The CO dissociation (black pathway) seems to be favoured rather than spontaneous or $Na^+$-driven NHC dissociations, respectively in green and in yellow. The dehydrogenation transition states were evaluated to check the energy trend was respected after activation step.

This step is associated to a 16.2 kcal/mol free energy barrier, easily accessible at 423.15 K, much lower than that of carbene dissociation, equal to 27.5 kcal/mol. In order to definitely exclude carbene dissociation as a possible activation pathway of **1**, the influence of the sodium cation was considered.

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In fact, a study on carbenes stabilization by sodium cation was previously reported in literature for a Fe system, [45] suggesting that the presence of sodium could promote the carbene loss. The Guerbet reaction with **1** was then carried out in presence of a 20% excess (with respect to sodium ethoxide) of 15-crown-5 ether, which coordinates sodium and potassium cations, [46] and it was recorded that the reaction rate sensibly slows down. Since the added ether is a liquid that affect the overall volume, the standard Guerbet reaction was repeated but in the presence of toluene to match the volume of the reaction with the 15-crown-5 ether. As reported in Table 3.1 the dissolution effect by toluene is not enough to slow down the reaction rate as much as the presence of the 15-crown-5 ether does, confirming the real effect of the ether.

**Table 3.1** Products distribution for three different tests. All the reactions were carried out for 4 hours at 423.15 K, under inert atmosphere, in autogenous pressure and adding 0.002 eq. of catalyst (**1**) and 0.2 eq. of co-catalyst (**6**).

| Entry | Test | conv. EtOH[a] | yield BuOH[a] | yield $C_6$[a] | yield $C_8$[a] | yield $C_{10}$[a] | C-loss[a] |
|---|---|---|---|---|---|---|---|
| 1 | standard Guerbet | 49.4 | 32.2 | 9.2 | 1.7 | 0.4 | 5.9 |
| 2 | with 15-crown-ether[b] | 15.5 | 10.4 | 4.2 | 1.1 | 0.4 | -0.6 |
| 3 | with toluene[b] | 40.9 | 32.0 | 5.7 | 0.7 | 0.1 | 2.5 |

[a]In percentage (**%**). [b]V = 0.420 mL.

This suggests that the cation plays a central role in the catalysis. Nevertheless, DFT calculations showed that this mechanism is energetically more expensive (33.9 kcal/mol) than the others discussed above. Thus, the hypothesis that sodium affects carbene loss is not supported by DFT simulations, indicating that another role for the cation should be considered, as discussed below. The CO dissociation was also experimentally confirmed thanks to different tests. At the end of the catalysis, having assumed a part of the dissociated carbon monoxide left off the solution, the gases in reactor's headspace were analysed *via* GC (see section 6.2 for experimental) and presence of CO was detected. Since it was not possible to quantify it and, thus, to distinguish if it was a degradation product or not, it was also carried out a [13]CO isotopic labelling experiment. To check how much movable are the terminal carbon monoxides in reaction-type conditions, the catalyst (0.0042 eq.) was dissolved in ethanol in a Schlenk-bomb under a pressurized [13]CO atmosphere and in presence of sodium ethoxide (0.021 eq.). Then, the mixture was stirred for an hour at 423.15 K giving the possibility to not labelled CO to be replaced by [13]CO (Figure 3.4).
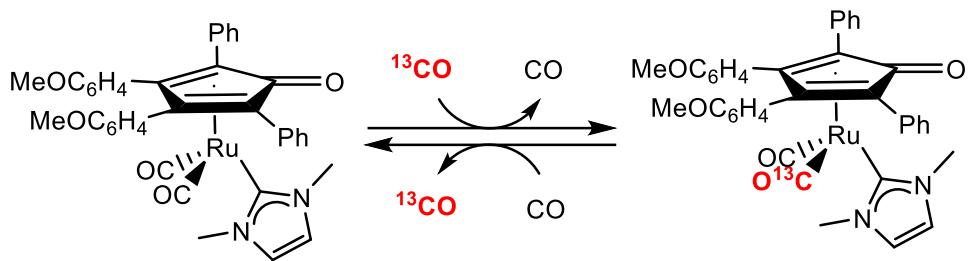
**Figure 3.4** Hypothesized dynamic equilibrium for terminal carbon monoxides.

$^{13}$C-NMR (Figure 3.5) analysis confirmed a substantial isotopic enrichment and theoretical outcome about carbon monoxide dissociation.
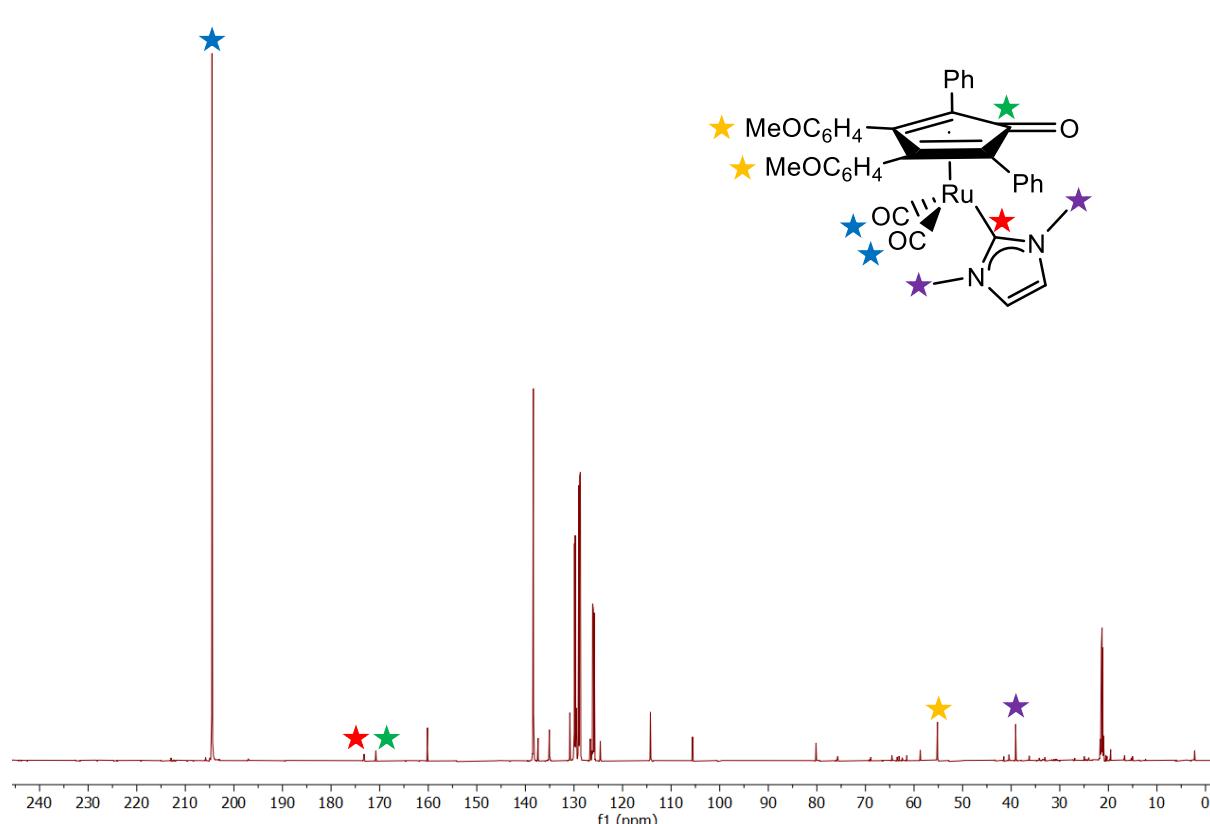


**Figure 3.5** Experimental $^{13}$C-NMR spectrum, showing a very intense peak at 203.99 ppm (blue star), respect to other characteristic signals of the catalyst **1**, confirming an isotopic labelling of a carbon monoxide ligand.

## 3.2.2 Ethanol dehydrogenation

Ethanol, to be homologated to 1-butanol and higher alcohols, needs to be dehydrogenated *via* a hydrogen-transfer process. The catalyst (**1**) must be activated by ligand loss, as mentioned above, which is a barrier-less process for all three possible activation pathways already

discussed (see Figure 3.3). The FES for the ethanol dehydrogenation step following ligand dissociation was computed, indicating 8.1 kcal/mol difference in energy between the TS associated with loss of CO and carbene, i.e. **TS1** and **TS31**, respectively. This implies that at 423.15 K a rate ratio ($k_{TS1}/k_{TS29}$) of ca. 15000 is obtained, which means that dehydrogenation following CO dissociation is at least 15000 times more likely rather than the mechanism involving carbene loss.

The activated catalyst (**2**) formed upon CO loss, got a vacant site on the metal centre, which allows the system to accept an electron-donor ligand (i.e. a hydride), whilst the cyclopentadienone's carbonyl could be easily protonated, thanks to an outer-sphere mechanism. [47] Due to ligands' nature and their actual dispositions, **2** is highly asymmetric and, thus, the respective dehydrogenation TS is asymmetric too. This turns into two possible configurations in which ethanol could be bonded to the catalyst for concerted process. Indeed, ethanol could interact transferring to ruthenium two different prochiral hydrogens on its -$CH_2$- (Figure 3.6), resulting in two non-degenerate TS configurations.
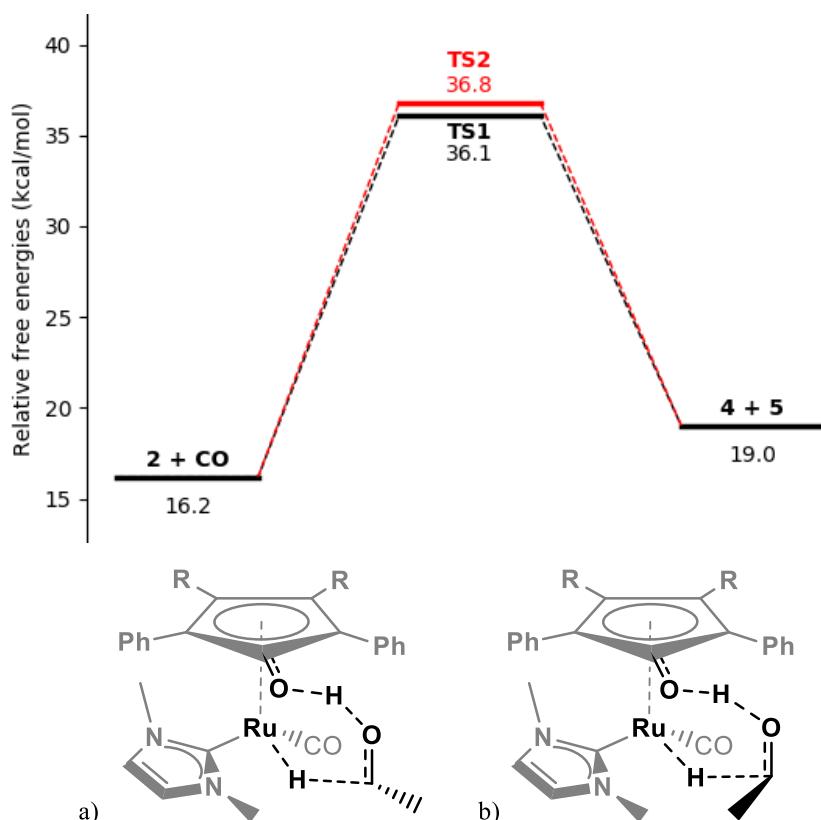


**Figure 3.6** In the dehydrogenation transition state, ethanol could arrange its a) pro-R proton (**TS2**) or b) the pro-S one (**TS1**). In a) the NCH···O distance is 0.14 Å longer than in b).

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Even though the TS for which ethanol gives its pro-R hydrogen is the less geometrically hindered one (**TS2**), calculations showed it is not the lowest one in energy. Whereas, when ethanol's methyl is put next to the carbene, a weak H-bond NCH···O (2.28 Å) lowers the TS by 0.7 kcal/mol. CH···O are interactions largely diffused in biological systems and strong enough to steady a preferential pathway in catalysis. [48]

Therefore, the carbene results taking part in the pathway not only as a sigma-donor ligand to ruthenium, but also as a configurational driver. This point could become central for a systematic study to modulate the carbene's N-substituents and improving the catalytic performances by lowering **TS1**. Moreover, this outcome highlights that this complex could be eligible for chiral dehydrogenation/hydrogenation processes.

In order to experimentally prove the mechanism of this step, and to verify further the activation of **1** through CO dissociation, the catalytic Guerbet reaction was carried out in deuterated ethanol into a J-Young valve equipped NMR tube in milder condition (at 353.15 K for 2 days and then at 363.15 K for 4 days and with a lower amount of catalysts – **1** 0.007 eq. and **6** 0.010 eq.) to slow down the reaction rate and make easier *in situ* NMR studies on the reaction mixture (see sections 6.1 and 6.6 for experimental details). The formation of two hydrides with chemical shifts at -9.84 ppm and -11.32 ppm was recorded during the reaction (Figure 3.7). Furthermore, several NOESY-1D experiments were performed to check if at least one of these hydrides was next to carbene's methyl groups, eventually confirming the presence of hypothesized intermediate **4** but, unfortunately, it was not possible due to experimental limits. Indeed, the entity of the NOE effect depends on the molecular tumbling rate. Molecular tumbling, in turn, depends on many parameters including viscosity of solution, temperature and molecular weight of sampling molecule(s). For instance, as the molecular weight increases, the NOE effect crosses a zero-NOE-point in correspondence to which there is not any spectroscopic outcome and no signals are recorded. The zero-NOE-effect is not very important for middle-sized systems studied in standard conditions, whilst becomes central for molecules bigger than 600 u.m.a., such as metal-based catalysts and bio-molecules.

In this specific case, given the high molecular weight of the pre-catalyst (**1**), the same NOE spectra were recorded at 273.15 K, 298.15 K and 348.15 K to check the best temperature for NOE enhancement. At room temperature, the zero NOE point was very close because no outcome was recorded despite experiment has been carried out for several hours; whereas at 273.15 K a part of the sample began to precipitate. At 348.15 K, NOE signals were recorded even though at the actual conditions the hydrides, which were characterized with a standard ^{1}H-NMR spectroscopy at room temperature, began to degrade (Figure 3.8 and 3.9). An alternative

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way to avoid the zero-NOE-point would have been to change the solvent, thus acting on viscosity: it was impossible due to the characteristic conditions of the experiment, i.e. if the J-Young valve equipped NMR tube was opened, the autogenous pressure would have changed. The NOE effect, which is transient in time, could also be optimized by selecting an accurate mixing time: a good choice of this parameter can be done by knowing the experimental T1 decay time. Therefore, an inversion recovery experiment was carried out at 298 K, but due to the low concentration of the species of interest, it was not possible to obtain any accurate T1 value.
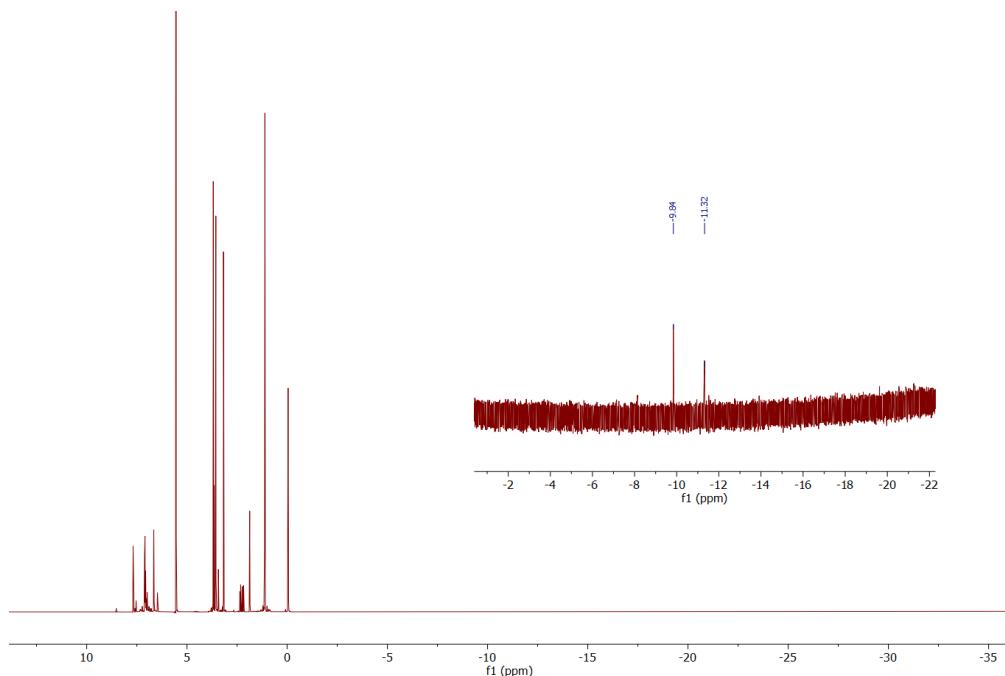


**Figure 3.7** $^1$H-NMR spectra of reaction mixture. Two hydrides are recorded at -9.84 ppm and -11.32 ppm.
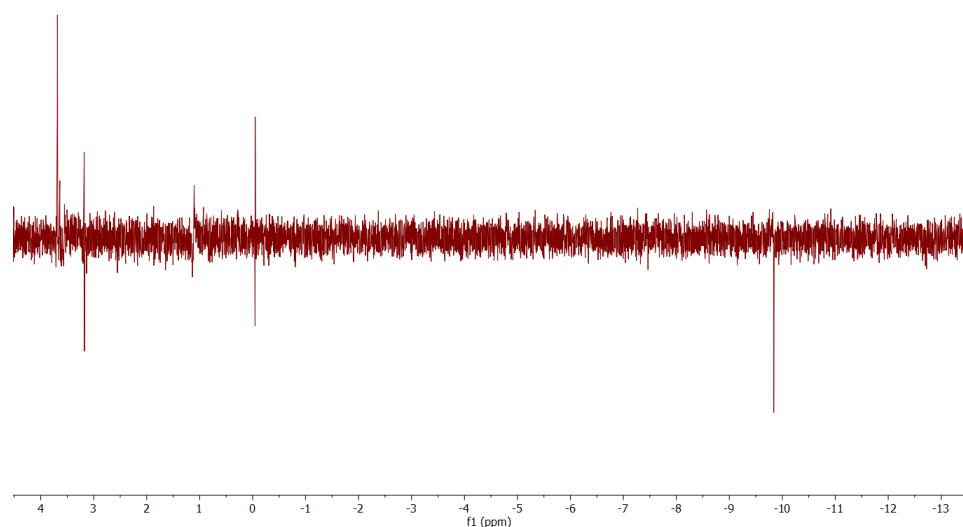


**Figure 3.8** 1D-NOESY NMR spectrum at 298.15 K. The quality of signals is low and the noise makes difficult any interpretation of the spectrum: many (or maybe all of them) are meaningless due to positive/negative spikes, and any interpretation would be misleading.
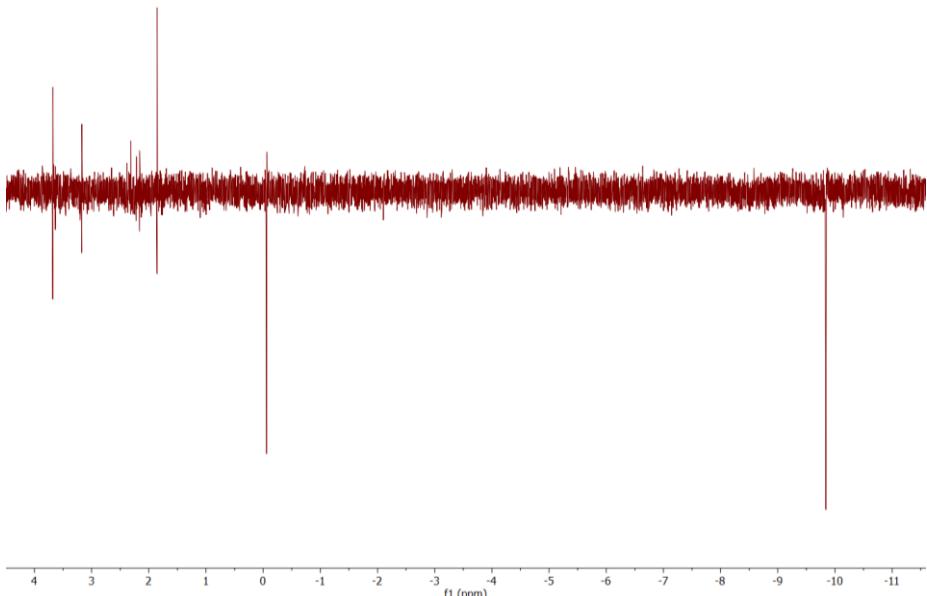
**Figure 3.9** 1D-NOESY NMR spectrum at 323.15 K. The quality of signals is still low and the noise makes difficult any interpretation of the spectrum. Anyway, new weak signals are displayed into the 1.8-2.3 ppm spectral window. They would have been meaningful, but the sample degraded after the current analysis.

Anyway, supposing those hydrides correspond to structure **4** and its twin structure **4b** (Figure 3.10) in which the reduced ketone is deprotonated and the proton is replaced by a sodium ion, theoretical NMR simulations were performed. DFT calculations showed a $\Delta\delta_{th} = 1.12$ ppm between hydridic peaks which is close to the experimental value, $\Delta\delta_{exp} = 1.48$ ppm, supporting the current hypothesis.
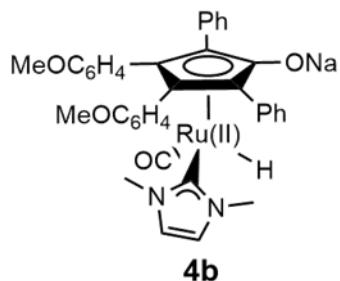


**Figure 3.10** Structure of **4b**.

Another indirect confirmation went from an already known **4**-type species to which is associated a -9.55 ppm $^1$H-NMR peak (RuH) in toluene-d$^8$. The structure got two carbonyls bonded to ruthenium and no carbenes are present. Because of the lack of steric hindrance made by the carbene, the **4**-type system seems to be always in resonance with a dimeric species with a bridging hydride [-17.82 ppm (RuHRu)]. [49] This suggests that if one of the hydrides experimentally recorded in the sample was carbene-less, a bridging hydride would have been observed.

### 3.2.3 C-C coupling process

The C-C coupling aldol condensation is an off-cycle process, catalysed by a base (i.e. sodium ethoxide), which plays an important role since it enables to get an unsaturated $C_4$ aldehyde, which will be transformed in 1-butanol after a double hydrogenation performed by **4**.

A molecule of acetaldehyde (**5**), one of the products from the previous step, is firstly deprotonated by a molecule of base (**TS3** = 14.4 kcal/mol) to form an enolate (**7**) which reacts with another molecule of **5** to form sodium 4-oxobutan-2-olate (**8**), following a barrier-less process. To allow the system to eliminate a molecule of water and, thus, to be transformed in crotonaldehyde, **8** is protonated to 3-hydroxybutanal (**9**). Then, a molecule of sodium ethoxide accomplishes a deprotonation, which results in formation of two different possible alkenes: depending on which configuration the organic substrate takes in the transition state (**TS4E**/**TS4Z**), **10E** or **10Z** are formed. Each **10**-type system, regardless of its configuration, is transformed into (*E*/*Z*)-crotonaldehyde (**11E**/**11Z**) for involvement of a molecule of ethanol, which actually drives the water elimination process (Figure 3.11).
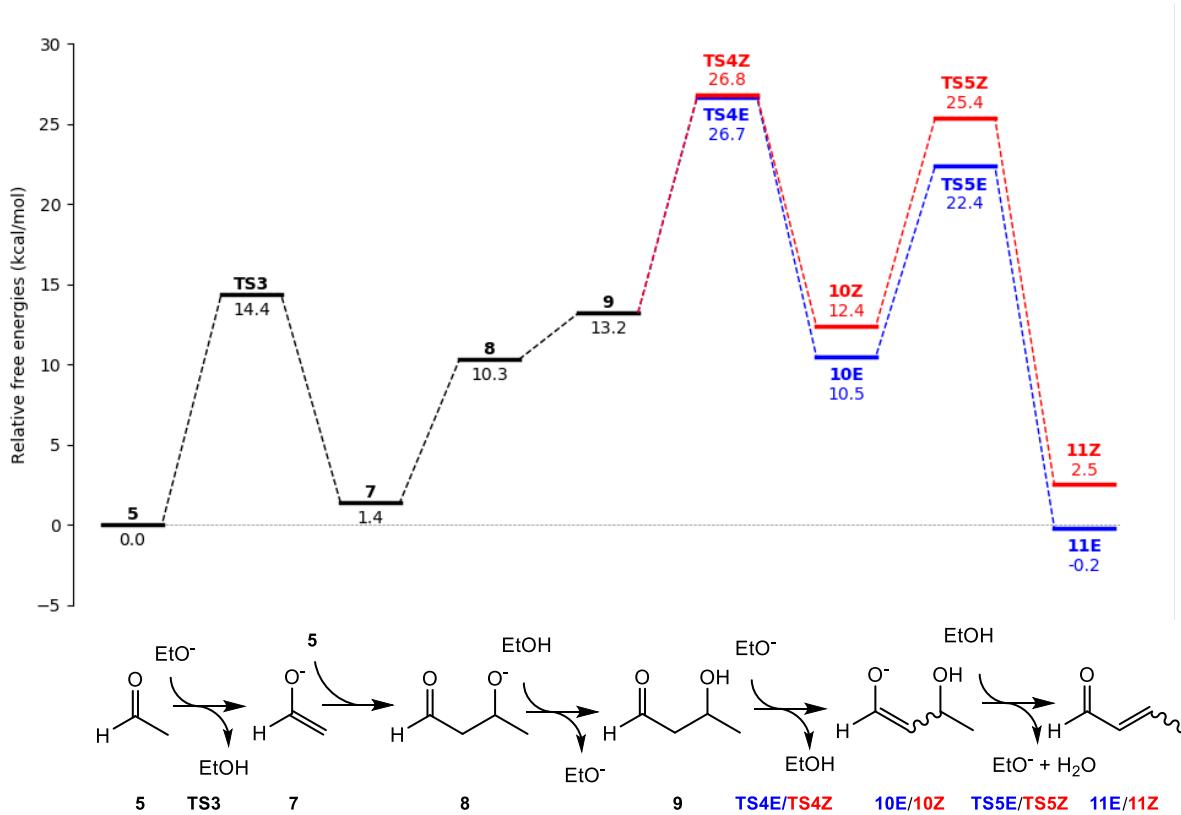


**Figure 3.11** Free energy profile for base-catalysed C-C coupling. In black are reported the initial four steps, whilst in blue and in red are drawn the two pathways that **9** may follow. Each of them is associated to an *E* or a *Z* configuration of the organic substrate, respectively. The reference was set to 0.0 kcal/mol to best appreciate the energy differences.

According to the computed free energy profile (Figure 3.11), the difference in energy between the two configurations in the turnover frequency (TOF) determining TS (TDTS) steps is no larger than 0.1 kcal/mol (**TS4E/TS4Z**) and the system seems to indifferently lead to both the products. Anyway, by considering the total free energy difference for each configuration (2·**5** → **11E/11Z** + **H$_2$O**), the thermodynamics is in favour of product **11E**, since it is slightly exergonic, instead of **11Z**. This implies two different backwards kinetic rates, in favour of accumulation of the thermodynamic product (*E*)-crotonaldehyde, which is confirmed to be a leading intermediate, i.e. thanks to a $\Delta G$ = -0.2 kcal/mol with respect to the initial reactants, the C-C aldol condensation step pulls the reactants towards 1-butanol.

Even though **11Z** should not be the main product of this step, its formation is not negligible and both the configurations of crotonaldehyde will be taken in account in further steps.
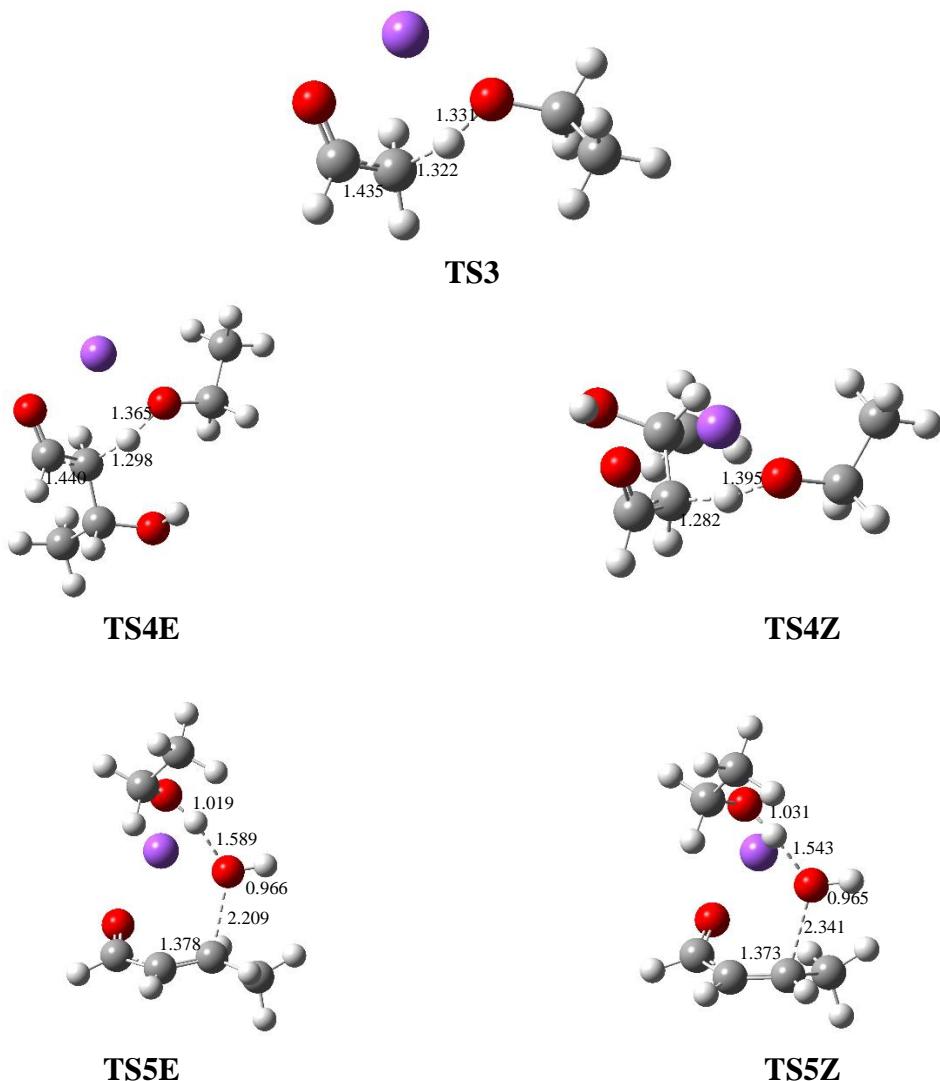


**Figure 3.12** Optimized TSs for C-C coupling mechanism (violet Na; red O; grey C; white H). Distances are reported in Å.

### 3.2.4 Hydrogenation: a complex pathway

As described above, the crotonaldehyde (**11**) is an important intermediate of the Guerbet reaction, which is converted to 1-butanol after a double hydrogenation done by two molecules of **4**. However, the hydrogenation pathway is not as simple as it could appears: indeed, either the C=O or the C=C double bond could be the first bond to be reduced in the hydrogenation pathway. Moreover, since **11** can assume two different configurations, both of them have to be considered for each hydrogenation step.

Furthermore, due to the asymmetry of **4,** each double bond of both configurations of **11** could interact with two different pro-chiral faces (i.e. the Re face or the Si one). Then, once the first unsaturation is reduced, the other double bond should be hydrogenated by another molecule of **4** to get 1-butanol (**15**). In case of the first step, if the product is the crotyl alcohol (**12E**/**12Z**) four more TSs and configurations have to be considered, otherwise if the product is butanal (**13**) only two TSs have to be considered, thanks to the lack of a C=C racemic unsaturation. To summarize, to best investigate the mechanism, 16 possible pathways were considered (Figure 3.13). All transition state geometries and energies are reported in the "Appendix" and in Table 3.10, respectively, but only the most stable TSs will be described in detail below, for clarity.
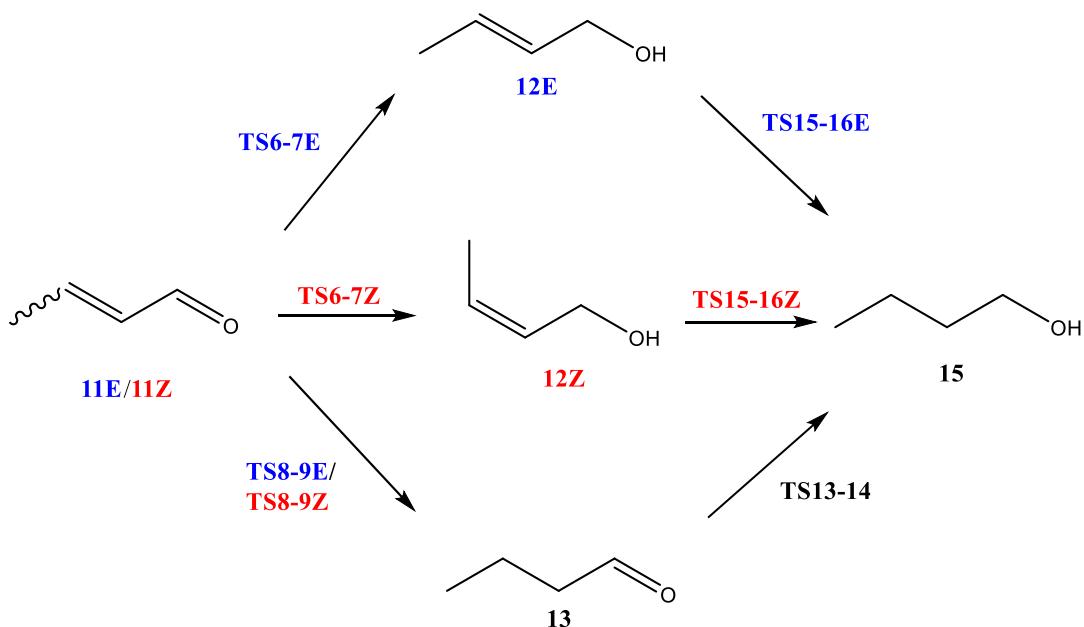


**Figure 3.13** 16 different hydrogenation pathways are possible.

DFT calculations showed that free energy barriers for the first hydrogenation elementary reactions (**TS8E** = 21.5 kcal/mol; **TS8Z** = 20.8 kcal/mol) are similar to the second step one (**TS13** = 16.4 kcal/mol) if the C=C bond is the first unsaturation to be reduced and **13** is the main intermediate.

On the contrary, if the C=O bond is the first one reduced (**TS6E** = 18.9 kcal/mol; **TS7Z** = 17.8 kcal/mol), the second hydrogenation elementary steps result to be more than 10 kcal/mol higher in energy (**TS15E** = 32.0 kcal/mol; **TS16Z** = 31.1 kcal/mol) than the first step TSs.

Taking in account also the thermodynamics of all the hydrogenation steps, it results butanal (**13**) as the thermodynamic intermediate, whereas (*E*/*Z*)-crotyl aldehyde (**12E**/**12Z**) are the kinetic ones. However, considering the second hydrogenation step, **13** should overcome a sensibly lower energy barrier (to be transformed into 1-butanol) than **12**.

Since thermodynamics and kinetics are in contrast and the stoichiometry of the process involves a single molecule of **11E**/**11Z** and two molecules of **4** (synthetized from ethanol dehydrogenation), it would be misleading to define one preferred pathway without any kinetic network simulation. Therefore, final considerations on the best mechanism are postponed to section 3.3.

Considering the geometry of TSs, the hydrogen transfer displacements are quite different depending on the nature of each bond. In case of the reduction of the carbonyl (**TS6E**/**TS7Z** and **TS13**), the mechanism is similar to that observed for the dehydrogenation of ethanol, and it involves a concerted movement for each H atom, as it occurs for hydrogenation of crotyl alcohol (**TS15E** and **TS16Z**). On the other hand, the C=C hydrogenations that lead to **13** (**TS8E**/**TS8Z**) involve different TS geometries: for *E* configuration the TS (**TS8E**) mostly resembles a hydride transfer with the proton already transferred, while for *Z* configuration the two H atoms transfers occur simultaneously in **TS8Z**. This different behaviour is likely to be addressed to a different electron density distribution on the α,β-unsaturated systems.
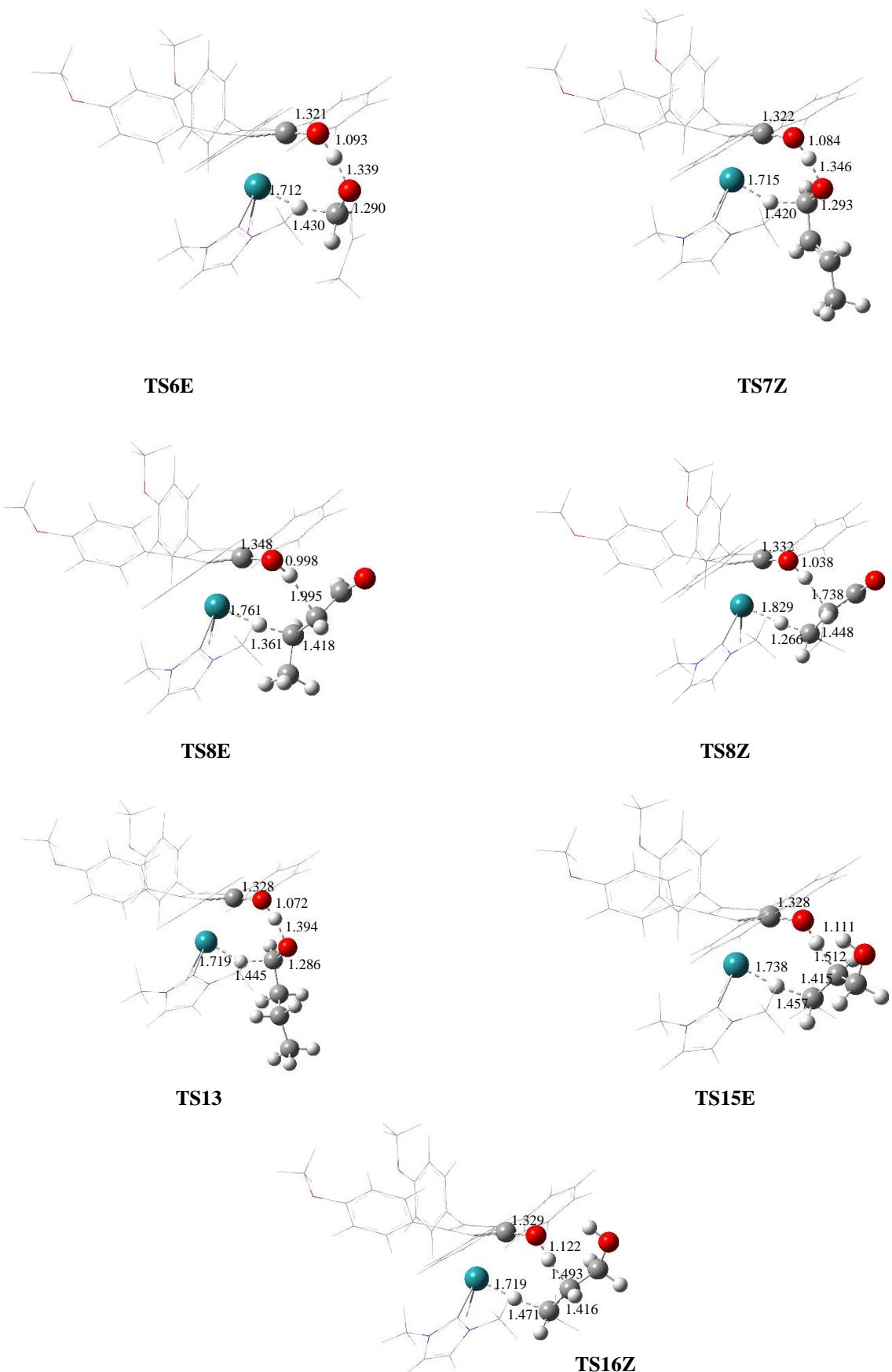
**Figure 3.14.** Optimized TSs for hydrogenation mechanism. Ligands and cyclopentadienone's substituents are shown in a simplified fashion (green Ru; red O; blue N; grey C; white H). Distances are reported in Å.

If **13** is considered as an intermediate in the hydrogenation cycle, its keto-enol tautomerism could be of interest, since it leads to two possible enolates, **14E** and **14Z**. In turn, these species would be then hydrogenated to 1-butanol.

Therefore, for each configuration of **14** three possible pathways were considered (Figures 3.15 and 3.16): $H_\beta$ transfer can be assisted by a proton shuttle, either water (**TS11E**/**TS11Z**) or ethanol (**TS10E**/**TS10Z**), or not



**Figure 3.15** Keto-enol tautomerism process involving **13**. Three possible transition states are considered for each configuration.

(**TS12E**/**TS12Z**). DFT calculations showed that the ethanol-driven proton shuttles lower the TSs' energies more than 18.0 kcal/mol with respect to unassisted hydrogen transfer. Anyway, the free energy barriers are too high (ca. 50 kcal/mol) to consider this mechanism as plausible.
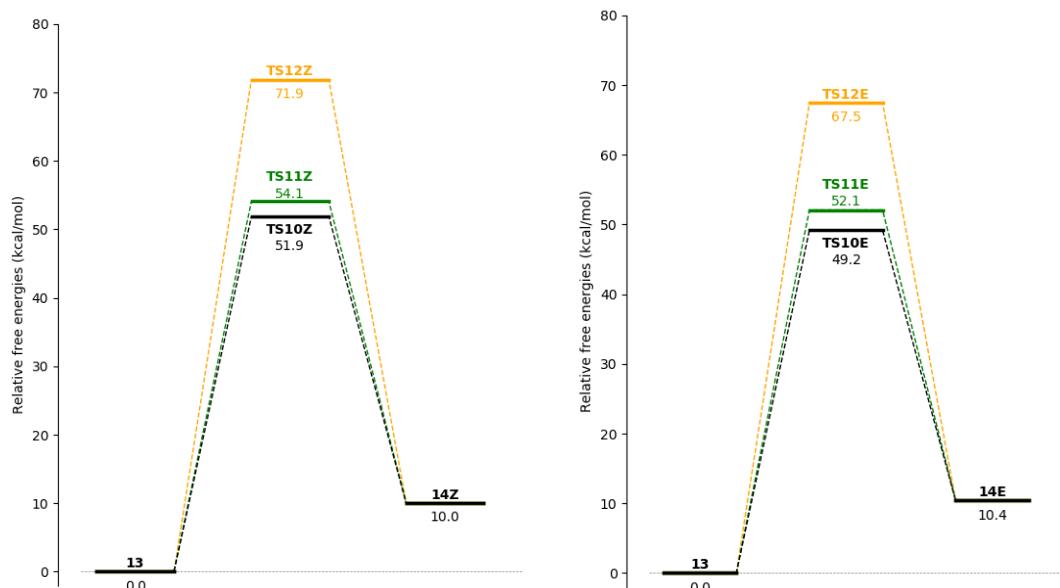


**Figure 3.16** Free energy surfaces of keto-enol tautomerism pathways for **13**. In black and in green the catalysed proton shuttle pathways process by ethanol and water, respectively. In orange, the energy profile for unassisted tautomerism.

### 3.2.5 Hydrogen-loss: a side reaction

During the catalytic reaction, it was experimentally observed the development of a great amount of gas and, thus, an increase in autogenous pressure in function of time, following a trend similar to the conversion of ethanol and the yield in alcohols (Figure 3.1). GC analyses on headspace gases after 4 hours confirmed that the main gaseous product is molecular hydrogen, which is accumulated during the whole reaction, except for a constant amount of inert gas which is added before the reaction starts (see sections 6.2 and 6.6 for experimental details). Assuming the composition of headspace gases remains constant during the catalysis, it is possible to estimate the yield of $H_2$ as a function of time (Table 3.2).

**Table 3.2** Main products distribution versus experimental and expected yield of molecular hydrogen.

| t (min) | conv. **3**[a, b] | yield alcohols[a, b, c] | yield $H_2$ [a, b] | theor. yield $H_2$[a, d] |
|---------|-------------------|--------------------------|----------------------|----------------------------|
| 0 | 0.0 | 0.0 | N/A | 0.0 |
| 30 | 34.9 | 17.0 | N/A | 17.3 |
| 60 | 41.5 | 34.8 | N/A | 25.2 |
| 120 | 47.2 | 38.7 | N/A | 28.5 |
| 180 | 47.5 | 41.9 | N/A | 28.9 |
| 240 | 49.4 | 43.5 | 27.8 | 29.6 |

[a]In percentage (%). [b]Experimental values. [c]Alcohols yield corresponds to the sum of $C_4$-$C_{10}$ saturated alcohols. [d]Theoretical yield computed assuming all the pressure is to address to $H_2$ development, but for 1 atm.

Molecular hydrogen production is essentially a side reaction, since it is likely formed from **4**, which loses a molecule of the gas instead of running the last step of the Guerbet reaction, namely a hydrogen transfer to reduce the aldehyde.

In analogy to the keto-enol tautomerism of **13**, three possible pathways can be considered for the $H_2$-loss mechanism: i) an unassisted process, according to which the proton/hydride coupling is intramolecular, or a proton shuttle assisted mechanism involving a molecule of ii) water or iii) ethanol. [49] Outcome showed the first hypothesis is unlikely, since the corresponding TS energy barrier is 36.3 kcal/mol. This is due to the long distance between the two H atoms in structure **4**, giving rise to a tense TS geometry (**TS22**), see Figure Figure 3.17. On the contrary, proton shuttle increases the reaction rate by lowering the free energy of corresponding TSs: water or ethanol, thanks to their own -OH sites, can accept and donate a proton at the same time, catalysing the proton/hydride coupling. As for keto-enol tautomerism

of **13**, proton shuttle better works if assisted by a molecule of ethanol (**TS20** = 20.6 kcal/mol), likely thanks to higher acidity of its proton, rather than water (**TS21** = 24.3 kcal/mol). Given the experimentally measured high impact of this side reaction, it is important to underline that **TS20** and **TS6-9E**/**TS6-9Z** are very close in energy, indicating strong competition between hydrogenation of crotonaldehyde and hydrogen loss of **4**.
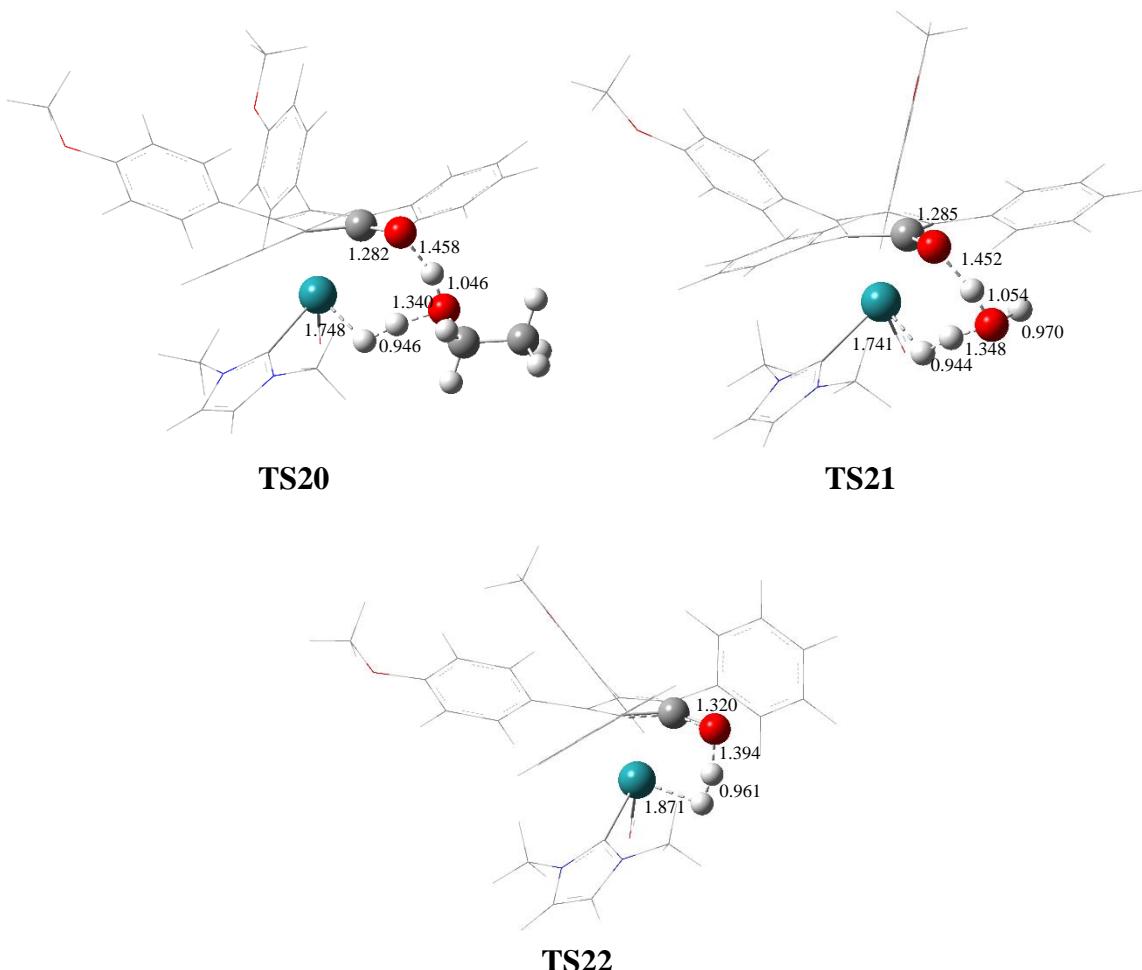


**Figure 3.17**. Optimized TSs for hydrogen-loss mechanism. Ligands and cyclopentadienone's substituents are shown in a simplified fashion (green Ru; red O; blue N; grey C; white H). Distances are reported in Å.

### 3.2.6 1-butanol and higher alcohols homologation

After the main catalytic pathway was computed and the behaviour of the catalyst in the cycle was deeply understood, it was also considered the homologation of 1-butanol (**15**) to 1-hexanol (**22**). As suggested by experimental data (Figure 3.1), $C_6$ chain long alcohols are – after **15** –

the main products. So, to better appreciate the selectivity of the catalyst with respect to **15**, it has been computed a new catalytic cycle (Figures 3.20 and 3.21), also considering homologation to higher alcohols. Even though experimental data showed 1-hexanol is not the unique $C_6$ product, but a mixture of $C_6$ chain long alcohols is produced during the reaction, the model was simplified assuming that only 1-hexanol was formed. In fact, $C_6$ yields can be grouped and considered as an upper limit for 1-hexanol yield.

Comparing the already discussed pathway for ethanol with that for 1-butanol, the most noteworthy differences recorded are in the off-cycle aldolic condensation pathway (Figure 3.18). There is no longer involvement of two molecules of acetaldehyde (**5**) as reactants, but only a molecule of **5** and one of **13**. Moreover, the actual C-C coupling step (i.e., **5** + **7** ➔ **15**) is not barrier-less (**TS17** = 13.4 kcal/mol) as it is for ethanol, and the TDTS for *E* configuration crosses in energy the *Z*'s one (**TS19E** > **TS18Z**). Since the difference between TDTSs is sizeable (2.6 kcal/mol), it is now possible to distinguish **19Z** as the kinetic product of C-C coupling pathway, whilst **19E** is the thermodynamic product.
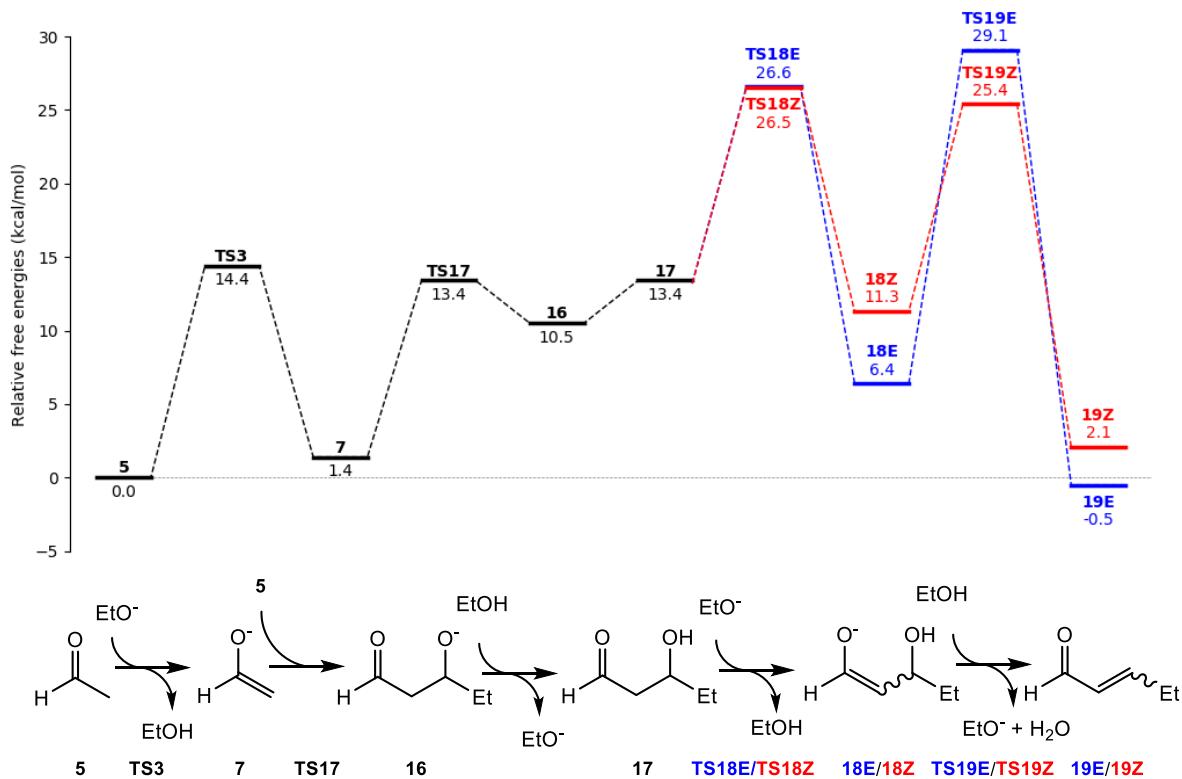


**Figure 3.18** Free energy profile for base-catalysed ethanol aldolic condensation of butanal. In black are reported the initial four steps, whilst in blue and in red are drawn the two pathways **17** may follow, each of them is associated to an *E* or a *Z* configuration of the organic substrate, respectively. The reference was set to 0.0 kcal/mol to best appreciate the energy differences.

As for dehydrogenation pathways, the behaviour of (*E*/*Z*)-hex-2-enal (**19E**/**19Z**) is similar to (*E*/*Z*)-crotonaldehyde (**11E**/**11Z**) and the most likely intermediate seems to be **21** (Figure 3.19 and Table 3.4). TSs, as expected, are close in energy and in geometry to those discussed in section 3.2.4, confirming the hypothesis that the carbon-chain length does not affect TSs energy differences. It implies that alcohol distribution is likely dependent only by their own alcoholic precursor's concentration in the reaction environment and not by catalyst-driven selectivity.
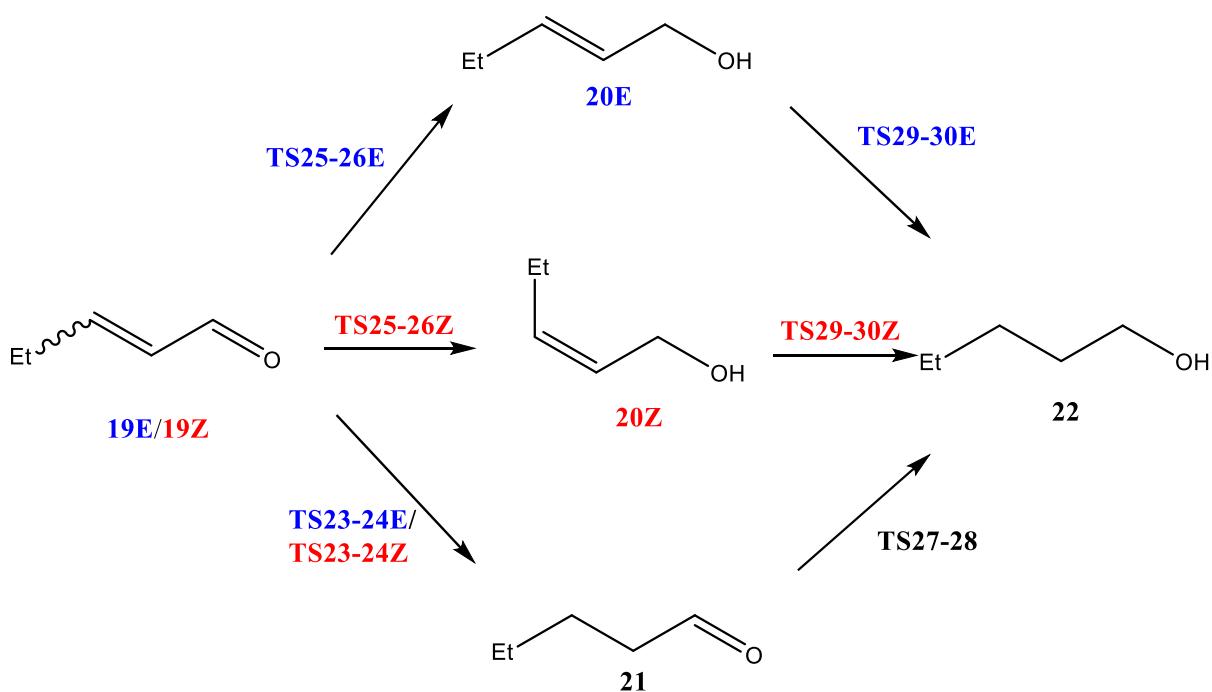


**Figure 3.19** Various (16) possible hydrogenation pathways for **19**.
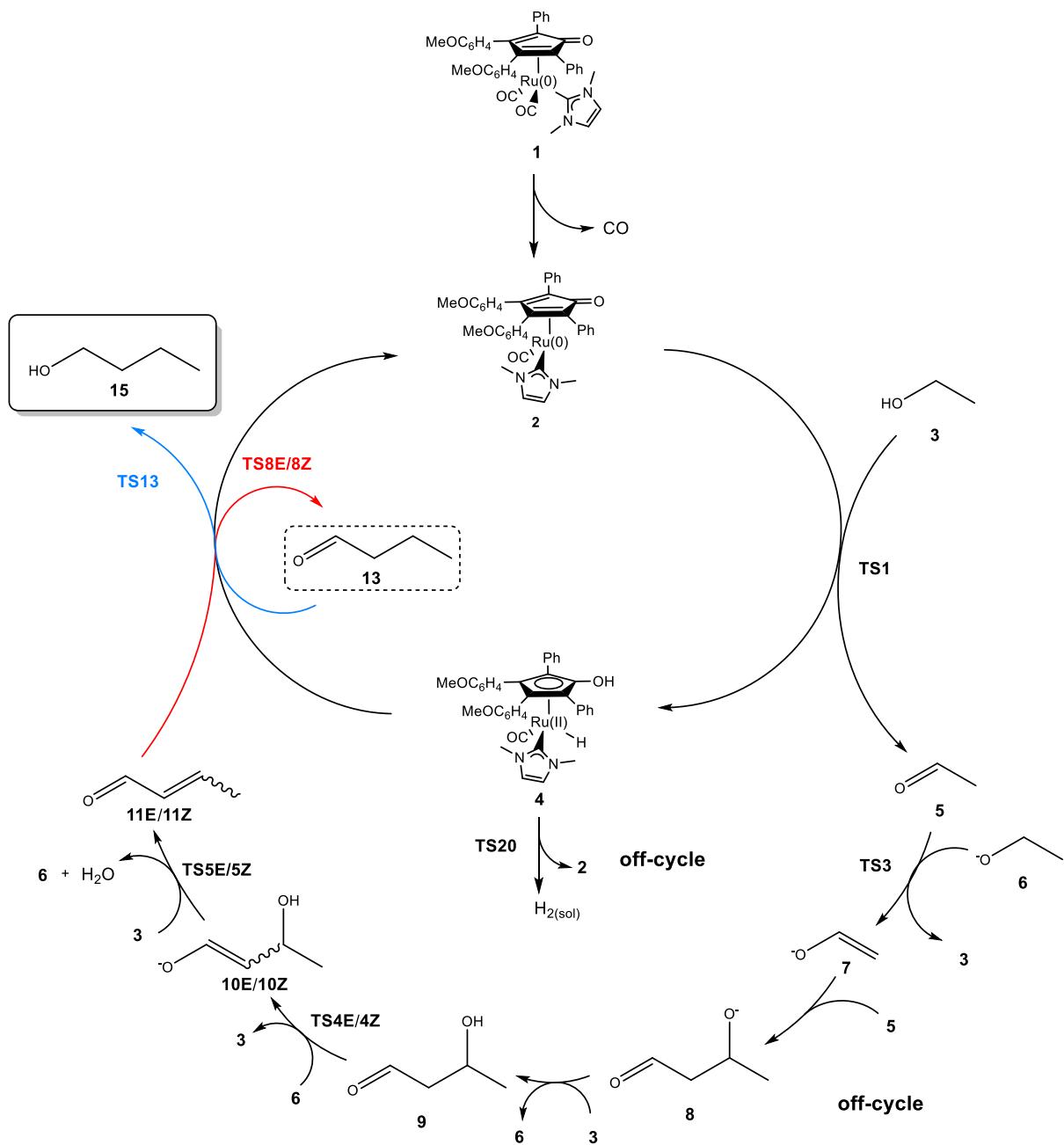
**Figure 3.20** Complete catalytic scheme proposed for homologation of ethanol (**3**) to 1-butanol (**15**).
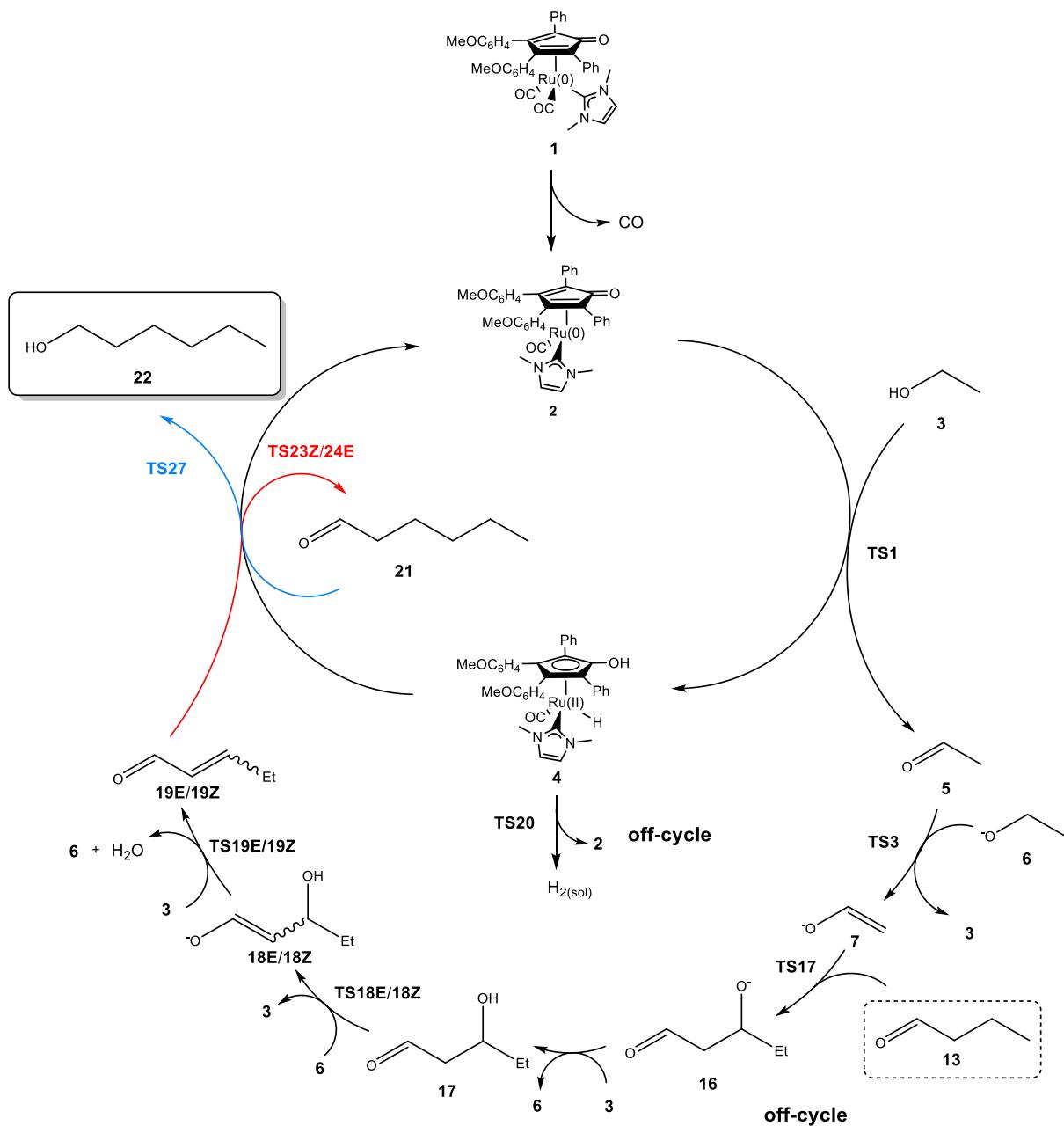
**Figure 3.21** Complete catalytic scheme proposed for homologation of 1-butanol (**15**) to 1-hexanol (**22**).

## 3.3 Kinetic models

DFT calculations discussed above have shown the complexity of the Guerbet reaction pathways, involving **2** as main catalyst that cooperates with a base as co-catalyst (**6**). Sodium ethoxide co-catalyses a partially overlapped off-cycle process, which leads to two different configurational intermediates. Each product coming from the off-cycle pathway is then involved in a complex hydrogen transfer mechanism to get 1-butanol (**15**), the main product. Moreover, one of the hydrogen transfer intermediates is **13**, which is also the starting reagent for a consecutive homologation reaction, which leads to 1-hexanol (**22**), a secondary alcoholic product. In parallel to the main pathway, an off-cycle side reaction also takes place, i.e. the hydrogen loss catalysed by ethanol as a proton shuttle, which is both the solvent and the starting reactant. This side reaction lowers the concentration of intermediate **4** but increases the turnover of **2**.

In such a complex mechanism, it is not possible to easily determinate theoretical selectivity without considering relative rates of all the processes involved in. Since the reactions described above are interconnected by sharing some intermediates, a way to best evaluate products distribution is building a kinetic network, which considers the dependence of intermediates' concentration by estimating the rate constants of each elementary step.

For all the kinetic networks discussed below, elementary steps were considered as equilibria and forward and backward rate constants were computed using the Eyring equation (1.11) and transition states barriers height at 423.15 K,

$$k = \frac{k_b T}{h} e^{-\frac{\Delta G^{\ddagger}}{RT}} \qquad (1.11)$$

For the spontaneous steps ($\Delta G^{\ddagger}$ = 0.0 kcal/mol), the rate constant was assumed to be equal to the pre-exponential constant (3.1) of the Eyring equation at 423.15 K,

$$k = \frac{k_b T}{h} = 8.81 \cdot 10^{12} \text{ L/(mol} \cdot \text{s)} \qquad (3.1)$$

The first kinetic network considered involved all the elementary steps discussed in section 3.2 (Table 3.4) and showed that the preferential reaction pathway involves **13** and **21** as main dehydrogenation intermediates, thus first the C=C unsaturation of **11** and **19** and then the C=O carbonyl of **13** and **21** are reduced (see section 3.2.4). Therefore, the model was simplified

considering only two steps for dehydrogenation, as reported in Figures 3.20 and 3.21. Kinetic simulation was performed to predict products distribution after 4 hours, entering real concentrations of reactants (i.e. [**2**] = 0.03440 mol/L; [**3**] = 17.12 mol/L; [**6**] = 3.424 mol/L). The remarkable agreement between theoretical and experimental data (**Model 1**, Table 3.3) suggests that the theoretical model is in keeping with the experiments. In fact, the exponential nature of equation (1.11) implies that a 1.9 kcal/mol error in estimating the energy of a step turns into a ca. 10-fold deviation of the overall rate constant, with deep consequences on products distribution. Therefore, a 10-points in percentage deviation from experiments has to be considered as a small error for theoretical simulations.

Because it is a good strategy to work with not-redundant kinetic networks, **Model 1** was further simplified by assuming that the overall rate constant of the C-C coupling off-cycle process was only affected by the highest TS in the process (**Model 2**, see Figures 3.23 and 3.24). Theoretical outcomes do not show any substantial difference between the two network models, confirming these simplifications are not affecting the quality of the model (see Table 3.3).

**Table 3.3** Comparison between experimental and theoretical concentrations after 4 hours at 423.15K, according to different kinetic models.

|  | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield H$_2$[a] |
|---|---|---|---|---|
| Experimental | 49.4 | 32.2 | 9.2 | 27.8 |
| Model 1 | 57.4 | 22.3 | 7.6 | 11.2 |
| Model 2[b] | 57.3 | 22.3 | 7.5 | 11.0 |
| Model 3 | 55.6 | 32.1 | 4.7 | 32.2 |
| Model 4a[b] | 47.3 | 23.8 | 10.2 | 27.8 |
| Model 4b[b] | 55.0 | 30.4 | 9.8 | 28.5 |

[a]In percentage (%). [b]All the values reported are computed respect to [**3**]$_0$ = 17.12 mol/L, even though the effective concentration putted in the simulation is higher (i.e. [**3**] + [**6**]).

Even though experimental data are well reproduced by the models discussed above, it is important to remark two shortcomings in the theoretical models.

First of all, the real concentration of ethanol is likely underestimated in the previously discussed models (**Model 1** and **Model 2**) because sodium ethoxide (**6**), thanks to the formation of a substantial amount of water during reaction (see section 3.2.3), is likely to be involved in fast equilibrium with ethanol (pKa = 15.9). Moreover, in **Model 2**, it has been considered a 17.12 mol/L concentration of ethanol since 0.5 mL of this liquid were experimentally added to the reactor, without considering the presence of a 20% of sodium ethoxide.

Secondly, molecular hydrogen is the only product for which simulated distribution is not close to the experiments, with concentration increasing up to a maximum and then decreasing as a typical reaction intermediate, instead of raising steadily until reaching a plateau as typical of products. In fact, the $H_2$-loss step happens in solution following a reversible process, it means that molecular hydrogen – once is formed – is dissolved in a condensed phase, but according to Henry's law it should be also involved in fast liquid/gas equilibrium (3.2), which was not included in the model.

$$K = \frac{[H_{2(gas)}]}{[H_{2(sol.)}]} = \frac{k_1}{k_2} \qquad (3.2)$$

These two faults in theoretical networks are easy to solve, since it is possible to assume new conditions or add new reaction steps, in order to better simulate experimental data. Therefore, two new models were computed, taking in account different approaches.

The first way to solve the problem is adding two new steps to **Model 1**. In this case, explicit $H_{2(sol)}$/$H_{2(gas)}$ and **3**/**6** equilibria were added to the model. Given the complexity of real solvent and its deeply variable composition, it is not possible to know the effective value of the equilibrium constants, so they should be guessed, proceeding by trial and error. The values which best fit experimental data are pKa = 8.10 for acid/base equilibrium and 0.909/0.091 gas/solution ratio, with associated $k_1 = 0.10$ s$^{-1}$ and $k_2 = 0.01$ s$^{-1}$. Despite the fitted pKa of ethanol is significantly lower than expected one (equal to ca. 15.9), it still represents a plausible value because it still indicates that the **3**/**6** equilibrium is in favour of **3** while the concentration of **6** is higher than expected, in line with the fact that **6** is necessary to catalyse the C-C coupling step. Moreover, also the prediction that the gas/solution ratio is in favour of gas phase is plausible because $H_2$ is a small and volatile molecule, and the reaction happens at 423.15 K. In addition, the viscosity of the solvent rapidly increases during the reaction, therefore it is likely that molecular hydrogen is more dissolved than expected. Also the rate constants are consistent, because the equilibrium is expected to be fast (it is reached in 60 s at least).

Once these corrections are added to **Model 1**, the model well reproduced experimental data, showing a good fit for both the yields and the ethanol conversion after 4 hours (**Model 3**, Table 3.3) and the shape of concentrations as a function of time (Figure 3.22). In particular, comparing experimental and theoretical data, it is clear the relationship between acid/base equilibrium and the trend of alcohols' yields. Theoretical simulations indicate that the concentration of sodium ethoxide dramatically decreases after 15 minutes, due to high-rate formation of water.

This implies that the overall reaction rate is slowed down because of the lack of a sufficient amount of co-catalyst **6**. This outcome would explain the singular behaviour experimentally observed: the conflict between C-C coupling and acid/base equilibria should be one of the main problems to solve in order to improve the reaction yield and to boost the total rate.
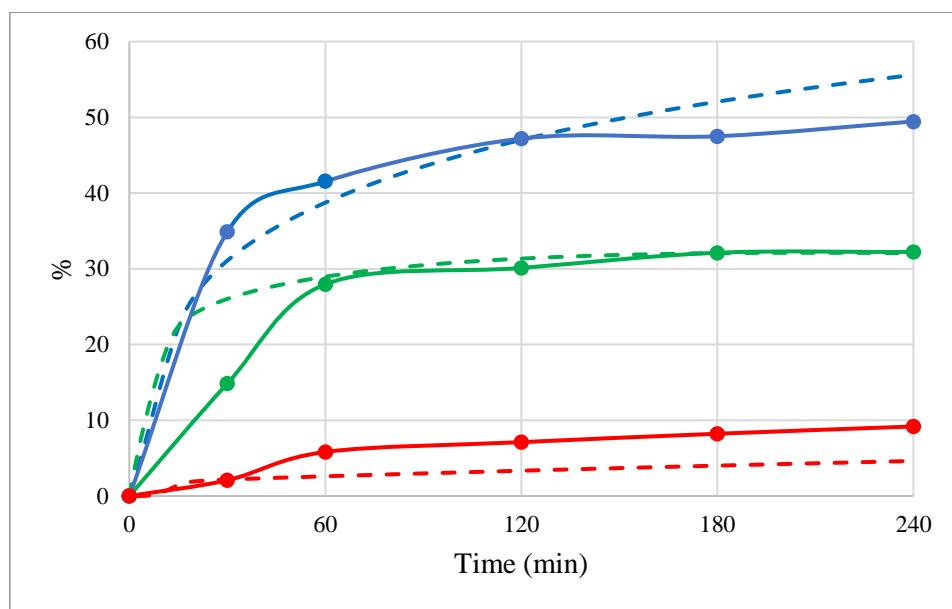


**Figure 3.22** Comparison between experimental data (solid lines) and simulated products distribution (dashed line). Conversion of ethanol (blue), yield of butanol (green) and hexanol (red) are reported. The shape of each distribution well suits experimental data, since a plateau is reached after an initial high rate region.

Also the simplified kinetic network implemented in **Model 2** can be refined in order to take into account the corrections required for the **3**/**6** and the $H_{2(sol)}/H_{2(gas)}$ equilibria (Figures 3.23 and 3.24). Since in **Model 2** sodium ethoxide, which is virtually catalytic, is not explicitly present it was assumed that the concentration of ethanol is 20.54 mol/L (1.2 eq.) instead of 17.12 (1 eq.). This approximation could seem rough-hewn, but it could be good enough for **Model 2** as it is clear that the acid/base equilibrium is in favour of ethanol and that quasi total amount of sodium ethoxide is converted in a short time after enough water is formed.

Still, in this case, the $H_{2(sol)}/H_{2(gas)}$ equilibrium will be considered explicitly. Since the boundary conditions are slightly different from **Model 3**, a new gas/solution ratio was guessed, i.e. 0.813/0.187. After these new corrections, the simulation shows a good reproduction of molecular hydrogen's distribution, ethanol conversion and hexanol yield, while the yield of butanol is not satisfactory (**Model 4a**, Table 3.3). As already discussed, theoretical calculations are affected by numerical errors great enough to deeply change products distribution in kinetic

simulations. Thus, it is common to carry out adjustments, which consist in changing as less parameters as possible to find and check numerical errors. [50]

If it is true that

$$-\frac{d}{dt}[\mathbf{3}] \propto \frac{d}{dt}[\mathbf{15}] \propto \frac{d}{dt}[\mathbf{11E}] \qquad (3.3)$$

and that

$$\frac{d}{dt}[\mathbf{11E}] \propto \frac{1}{k_{2(\mathbf{TS4E}\text{ backwark})}} \qquad (3.4)$$

only by changing the backward value of **TS4E**, the yield of butanol and the conversion of ethanol will raise. Indeed, after lowering the value of $\Delta G_{(2\cdot\mathbf{5} \rightarrow \mathbf{11E})}$ from -0.2 kcal/mol to -0.7 kcal/mol, the experimental data are much better reproduced (**Model 4b**, Table 3.3). For clarity, the estimated numerical error in the DFT computations performed here is documented to be ca. 5 kcal/mol, [51] so 10-fold greater than the correction done, confirming the reliability of the computed mechanism.

In summary, a complete kinetic network model was successfully built starting from theoretical mechanistic outcomes discussed in section 3.2, confirming the plausibility of proposed pathway. Further approximations leaded to a simplified pathway (Figures 3.23 and 3.24), but due to models' limitations (i.e. two equilibria were not taken in account, $H_{2(\text{sol.})}/H_{2(\text{gas})}$ and **3**/**6**), minor (rather legitimate) adjustments provided two new models (**Model 3** and **Model 4b**) that better reproduce experiments. Both final models, even though different assumption were taken, would be useful for further insights into the reaction mechanism.

**Table 3.4** Full list of the elementary steps which were taken in account for the kinetic simulation. Starting from this list, several kinetic models have been created. The simplified ones approximated the organic pathways as a single step. In that case, the **TS5E/TS5Z TS18Z/TS19E** are referred to different reagents, i.e. their values are different from those reported in this table.

| Entry | Reaction | TS | $\Delta G^{\ddagger}_{forward}$[a] | $\Delta G$[a] | $\Delta G^{\ddagger}_{backward}$[a] | $k_{forward}$[b] | $k_{backward}$[b] |
|---|---|---|---|---|---|---|---|
| 1 | **1 ⇌ 2 + CO** | N/A | 16,2 | 16,2 | 0,0 | 3,64E+04 | 8,81E+12 |
| 2 | **2 + 3 ⇌ 5 + 4** | **TS1** | 19,8 | 2,8 | 17,1 | 4,95E+02 | 1,32E+04 |
| 3 | **5 + 6 ⇌ 3 + 7** | **TS3** | 14,4 | 1,4 | 12,9 | 3,33E+05 | 1,83E+06 |
| 4 | **7 + 5 ⇌ 8** | N/A | 8,8 | 8,8 | 0,0 | 2,39E+08 | 8,81E+12 |
| 5 | **8 + 3 ⇌ 6 + 9** | N/A | 3,0 | 3,0 | 0,0 | 2,60E+11 | 8,81E+12 |
| 6 | **9 + 6 ⇌ 10E + 3** | **TS4E** | 13,5 | -2,8 | 16,3 | 9,45E+05 | 3,46E+04 |
| 7 | **9 + 6 ⇌ 10Z + 3** | **TS4Z** | 13,6 | -0,8 | 14,4 | 8,33E+05 | 3,26E+05 |
| 8 | **10E + 3 ⇌ 6 + $H_2O$ + 11E** | **TS5E** | 11,9 | -10,7 | 22,6 | 5,99E+06 | 1,86E+01 |
| 9 | **10Z + 3 ⇌ 6 + $H_2O$ + 11Z** | **TS5Z** | 12,9 | -9,9 | 22,9 | 1,88E+06 | 1,38E+01 |
| 10 | **4 + 11E ⇌ 2 + 12E** | **TS6E** | 18,9 | 1,7 | 17,2 | 1,60E+03 | 1,19E+04 |
| 11 | **4 + 11E ⇌ 2 + 13** | **TS8E** | 21,5 | -11,1 | 32,6 | 7,28E+01 | 1,35E-04 |
| 12 | **4 + 11Z ⇌ 2 + 12Z** | **TS7Z** | 17,8 | 0,2 | 17,6 | 5,73E+03 | 7,45E+03 |
| 13 | **4 + 11Z ⇌ 2 + 13** | **TS8Z** | 20,8 | -13,8 | 34,6 | 1,56E+02 | 1,14E-05 |
| 14 | **12E + 4 ⇌ 2 + 15** | **TS15E** | 32,0 | -15,6 | 47,6 | 2,64E-04 | 2,32E-12 |
| 15 | **12Z + 4 ⇌ 2 + 15** | **TS16Z** | 31,1 | -16,8 | 47,9 | 7,66E-04 | 1,53E-12 |
| 16 | **13 + 4 ⇌ 2 + 15** | **TS13** | 16,4 | -2,8 | 19,2 | 2,91E+04 | 1,03E+03 |
| 17 | **13 + 7 ⇌ 16** | **TS17** | 12,0 | 9,1 | 3,0 | 5,51E+06 | 2,62E+11 |
| 18 | **16 + 3 ⇌ 17 + 6** | N/A | 2,9 | 2,9 | 0,0 | 2,68E+11 | 8,81E+12 |
| 19 | **17 + 6 ⇌ 18E + 3** | **TS18E** | 13,2 | -7,0 | 20,2 | 1,35E+06 | 3,10E+02 |
| 20 | **17 + 6 ⇌ 18Z + 3** | **TS18Z** | 13,1 | -2,1 | 15,2 | 1,49E+06 | 1,25E+05 |
| 21 | **18E + 3 ⇌ 19E + 6 + $H_2O$** | **TS19E** | 22,7 | -6,9 | 29,6 | 1,68E+01 | 4,46E-03 |
| 22 | **18Z + 3 ⇌ 19Z + 6 + $H_2O$** | **TS19Z** | 14,0 | -9,2 | 23,3 | 5,00E+05 | 8,35E+00 |
| 23 | **19E + 4 ⇌ 2 + 20E** | **TS25E** | 18,6 | 1,7 | 17,0 | 2,15E+03 | 1,54E+04 |
| 24 | **19Z + 4 ⇌ 2 + 20Z** | **TS25Z** | 17,8 | 0,2 | 17,6 | 5,77E+03 | 7,47E+03 |
| 25 | **20E + 4 ⇌ 2 + 22** | **TS29E** | 30,8 | -15,8 | 46,7 | 1,05E-03 | 7,03E-12 |
| 26 | **20Z + 4 ⇌ 2 + 22** | **TS30Z** | 30,9 | -17,0 | 47,9 | 1,02E-03 | 1,65E-12 |
| 27 | **19E + 4 ⇌ 2 + 21** | **TS24E** | 21,2 | -11,4 | 32,7 | 9,77E+01 | 1,20E-04 |
| 28 | **19Z + 4 ⇌ 2 + 21** | **TS23Z** | 20,1 | -14,1 | 34,2 | 3,56E+02 | 1,90E-05 |
| 29 | **21 + 4 ⇌ 2 + 22** | **TS27** | 16,0 | -2,7 | 18,8 | 4,59E+04 | 1,80E+03 |
| 30 | **4 ⇌ 2 + H2** | **TS20** | 20,6 | -1,3 | 21,8 | 2,06E+02 | 4,60E+01 |

[a]All the energies are reported in kcal/mol. [b]The rate constants are given in $s^{-1} \cdot mol^n \cdot L^{-n}$, where $n$ is (total order of the reaction-1).
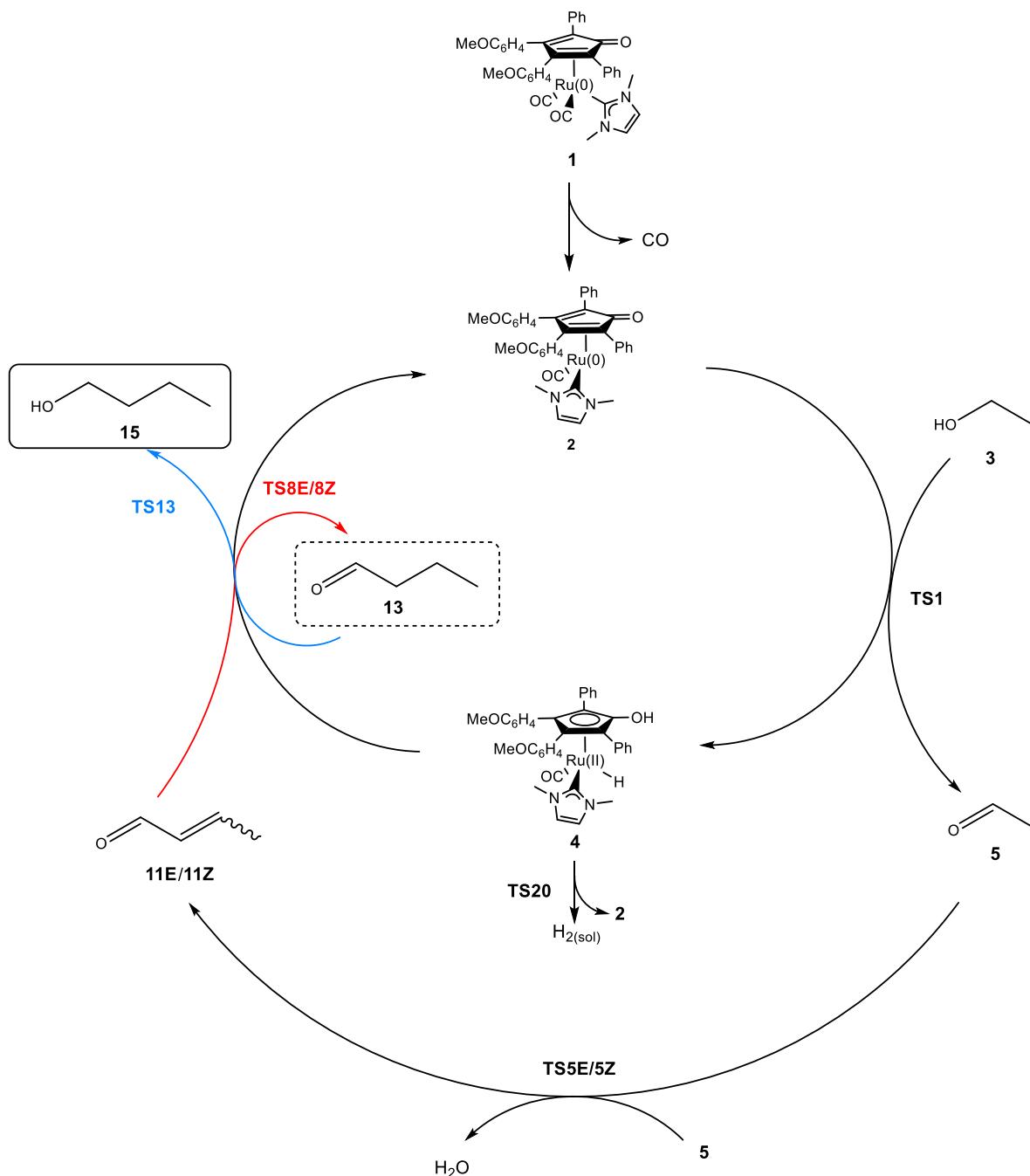
**Figure 3.23** Simplified catalytic scheme proposed for homologation of ethanol (**3**) to 1-butanol (**15**).
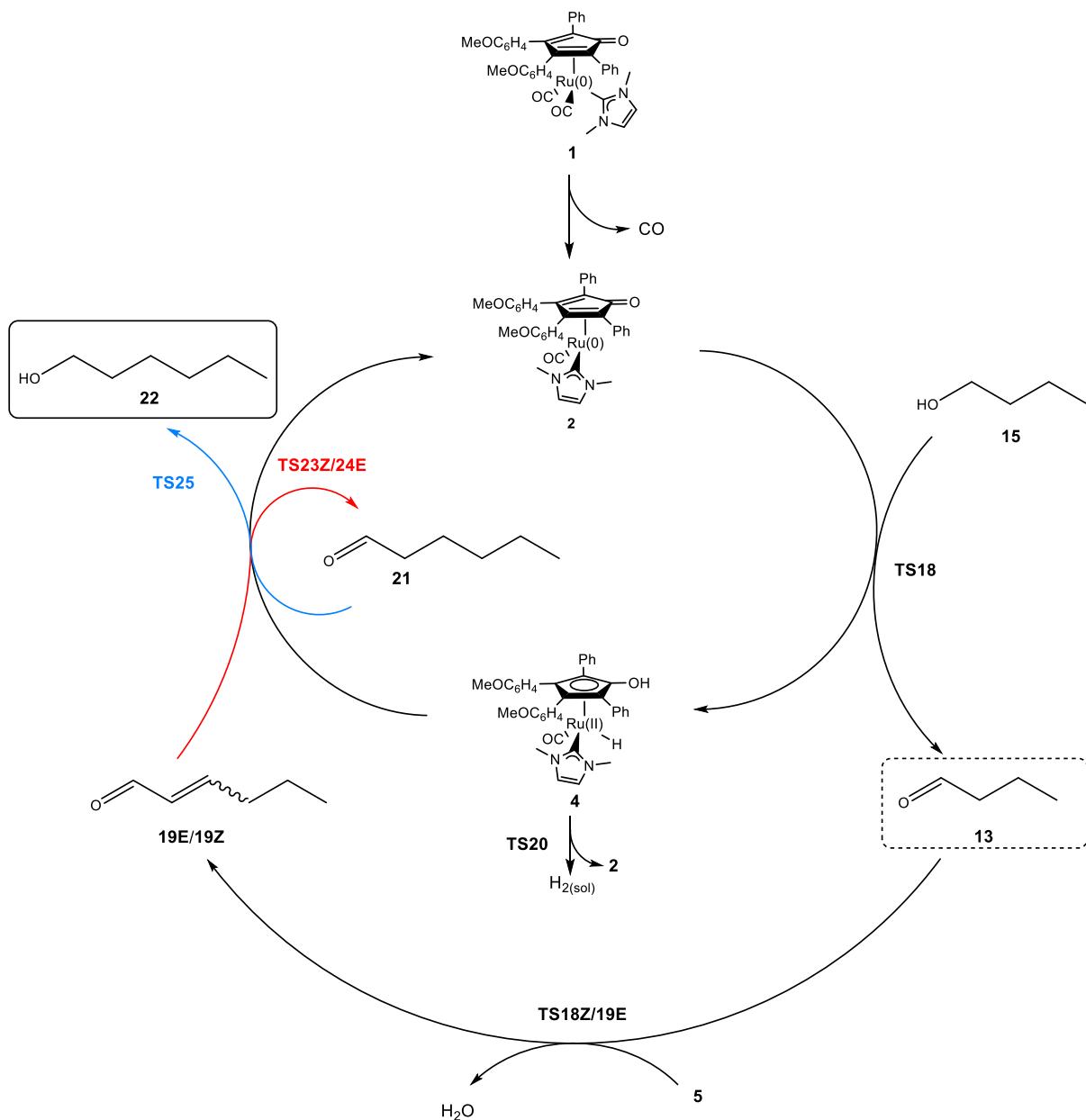
**Figure 3.24** Simplified catalytic scheme proposed for homologation of 1-butanol (**15**) to 1-hexanol (**22**).

## 3.4 Sensitivity analysis of external and internal factors

With reliable kinetic networks in hand, they can be used to get insights into the influence of internal and external parameters on reaction rate, such as energy barriers, reactants concentrations, reaction time and temperature. This should turn into a deeper comprehension of the mechanism and into the opportunity to optimize reaction conditions: theoretical models allow to simulate and predict data, otherwise difficult to be collected experimentally, indeed. In the following section, both **Model 3** and **Model 4b** will be considered for a sensitivity analysis of reaction parameters.

By running simulation for a longer time than 4 hours (Table 3.5), it is interesting to highlight that the selectivity in **22** rises compared to **3**, as expected. Indeed, 1-hexanol is a secondary product which is formed starting from **13**, implying that it is needed a substantial concentration in 1-butanol and in butanal to get high yield of 1-hexanol. On the other hand, it is expected the total amount of molecular hydrogen decreases after a maximum. This is not in contrast with the molecular hydrogen plateau expected at shorter reaction time (as mentioned above), since a dynamic equilibrium is always present and once the concentration of ethanol decreases, i.e. at long reaction time, a competition between **3** and $H_2$ as proton/hydride source it is likely.

As for temperature (Table 3.6), simulations show that if the reaction is performed at higher temperature than experimental one, the reaction rate is boosted and the selectivity is deeply changed, i.e. 1-hexanol seems to be the only one alcoholic product according to **Model 3**, whereas in **Model 4b** its concentration is ca. 10-fold greater than in standard conditions. On the contrary, if temperature is lowered the total reaction rate is close to zero: no actual conversion is recorded in both models.

**Table 3.5** Effect of increasing reaction time on the conversion[d] and the products distribution[d].

| | Model 3[b] | | | | Model 4b[c] | | | |
|---|---|---|---|---|---|---|---|---|
| $t$ (h) | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| 4 | 55.6 | 32.1 | 4.7 | 32.2 | 55.0 | 30.4 | 9.8 | 28.5 |
| 5 | 58.3 | 33.8 | 5.2 | 31.7 | 59.6 | 32.6 | 12.6 | 27.2 |
| 8 | 63.6 | 37.5 | 6.7 | 30.0 | 68.9 | 36.1 | 19.9 | 23.5 |
| 24 | 74.6 | 44.6 | 11.9 | 24.8 | 87.4 | 35.2 | 40.3 | 16.7 |

[a]In percentage (**%**). [b]Initial concentrations in the model are the experimental ones. [c]Initial concentration of ethanol is equal to the sum of experimental [**3**] and [**6**]. It is assumed ethoxide is converted to ethanol during the reaction. [d]Values computed respect to $[3]_0 = 17.12$ mol/L.

**Table 3.6** Effect of increasing or decreasing temperature on the conversion[e] and the products distribution[e].

| T (K) | Model 3[b] | | | | Model 4b[c] | | | |
|---|---|---|---|---|---|---|---|---|
| | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| 373.15[d] | 2.7 | 6.7 | N/A | 4.5 | N/A | N/A | N/A | N/A |
| 423.15 | 55.6 | 32.1 | 4.7 | 32.2 | 55.0 | 30.4 | 9.8 | 28.5 |
| 473.15[d] | 89.4 | N/A | 61.6 | 20.5 | 99.8 | 21.9 | 60.3 | 14.2 |

[a]In percentage (**%**). [b]Initial concentrations are the experimental ones. [c]Initial concentration of ethanol is equal to the sum of experimental [**3**] and [**6**]. It is assumed ethoxide is converted to ethanol during the reaction. [d]Thermal correction were not computed again, only the temperature value was modified in the Eyring equation (a). [e]Values computed respect to $[3]_0 = 17.12$ mol/L.

In addition to time and temperature, another important parameter which should be easily modified (while time and resource consuming) in experiments is concentration. Reactants and catalysts concentrations deeply influence products distribution and total reaction rate. In Table 3.7 are reported the effects on final products distribution of increasing or decreasing some species concentration. What is most interesting is that if catalyst concentration is raised by 20% a slight improvement in 1-butanol concentration is predicted, same as if the concentration of sodium ethoxide increases (by directly raising its concentration or by lowering the ethanol one). These outcomes remark again the importance of **6** in the whole pathway, since its concentration – despite the presence of the acid base equilibrium involving **3** and **6** – should be as much high as possible to maintain a good reaction rate.

**Table 3.7** Effect of increasing or decreasing species concentration on conversion and products distribution.

| | Model 3[b] | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | raised by 20% | | | | lowered by 20% | | | |
| Species | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| **1** | 56.3 | 32.7 | 4.7 | 31.9 | 54.7 | 31.6 | 4.5 | 32.2 |
| **3** | 52.7 | 30.7 | 4.0 | 29.1 | 59.4 | 34.2 | 5.6 | 36.2 |
| **6** | 59.1 | 35.9 | 6.3 | 33.0 | 51.6 | 27.9 | 3.2 | 31.0 |

| | Model 4b[c] | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | raised by 20% | | | | lowered by 20% | | | |
| Species | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| **1** | 56.9 | 31.4 | 10.9 | 28.0 | 52.6 | 29.2 | 8.6 | 29.1 |
| **3** | 54.5 | 30.2 | 9.5 | 25.9 | 55.3 | 30.7 | 10.2 | 32.2 |
| **6** | N/A | N/A | N/A | N/A | N/A | N/A | N/A | N/A |

[a]In percentage (%). [b]Initial concentrations in the model are the experimental ones. [c]Initial concentration of ethanol is equal to the sum of experimental [**3**] and [**6**]. It is assumed ethoxide is converted to ethanol during the reaction.

The role played by **3**/**6** equilibrium could also help rationalizing data reported in Table 3.1. In fact, it was observed that if an excess of 15-crow-5 ether is added, the reaction rate slows down (see section 3.2.1). In view of the kinetic results, it would be possible that the presence of a coordinating ether deeply modifies the acid/base equilibrium in favour of **3**, reducing the concentration of the co-catalyst and, thus, the reaction rate. This provides a new potential role of the sodium cation in the Guerbet reaction, different from that of affecting the carbene loss equilibria, as mentioned above.

Kinetic networks give also the chance to alter the energetics of single steps, in order to identify which TSs are mostly responsible for experimental selectivity and reaction rate (Table 3.8). For example, by lowering by 1.9 kcal/mol the energy barrier of carbon monoxide dissociation $\Delta G_{(1 \rightarrow 2 + CO)}$, the reaction rate is boosted (**Model 3**: conv. **5**, 61.6%; yield **15**, 38.3%; yield **22**, 6.0%; yield $H_2$, 27.9%. **Model 4b**: conv. **5**, 77.1%; yield **15**, 37.6%; yield **22**, 27.6%; yield $H_2$, 20.5%). This outcome suggests the importance of the step described in section 3.2.1, underling that if a cheaper activation was possible for **1**, the total reaction rate would be improved. Computations also show the essential role played by hydrogenation and hydrogen loss. If each of these steps was optimized, the Guerbet's performances would be noticeably improved.

**Table 3.8** Effect of increasing or decreasing the energy of some transition state on the conversion[e] and the products distribution[e].

| | **Model 3**[b] | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | raised by 1.9 kcal/mol | | | | lowered by 1.9 kcal/mol | | | |
| Modified TS | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| TS1 | 53.5 | 29.2 | 6.3 | 31.6 | 32.5 | 4.5 | 32.1 | 55.4 |
| TS8E-Z/13[d] | 43.4 | 11.0 | 2.7 | 47.9 | 59.1 | 39.8 | 5.7 | 24.7 |
| TS20 | 40.1 | 37.2 | 5.0 | 14.7 | 55.2 | 32.1 | 3.4 | 33.6 |
| | **Model 4b**[c] | | | | | | | |
| | raised by 1.9 kcal/mol | | | | lowered by 1.9 kcal/mol | | | |
| Modified TS | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] | conv. **3**[a] | yield **15**[a] | yield **22**[a] | yield $H_2$[a] |
| TS1 | 52.0 | 28.9 | 9.2 | 28.2 | 55.4 | 30.7 | 9.9 | 28.6 |
| TS8E-Z/13[d] | 27.0 | 5.6 | 2.9 | 37.4 | 89.0 | 67.7 | 8.8 | 18.7 |
| TS20 | 35.5 | 31.4 | 6.6 | 15.6 | 54.0 | 31.0 | 10.3 | 26.9 |

[a]In percentage (%). [b]Initial concentrations in the model are the experimental ones. [c]Initial concentration of ethanol is equal to the sum of experimental [**3**] and [**6**]. It is assumed ethoxide is converted to ethanol during the reaction. [d]All transition states were modified at the same time. [e]Values computed respect to [**3**]$_0$ = 17.12 mol/L.

Hence, sensitivity analyses on **Model 3** and **Model 4b** show important dependences of conversion and yields on reaction time, temperature, substantial concentration of sodium ethoxide and hydrogenation energy barriers.

## 3.5 The Shvo's-type catalyst and the Guerbet reaction

The role played by the carbene ligand in the mechanism is not trivial, since if the homologation of ethanol was carried out using the Shvo's-type complex **23**, instead of **1**, as pre-catalyst (see section 6.8), the reaction is not observed. **23** could be seen as a dimeric form of **24**, which is known to be active in many redox reactions, as already reported in literature for similar systems. [41] Since Shvo's-type catalysts are active in many reactions it is interesting to understand why its precursor **24** is not able to catalyse the Guerbet reaction. In order to understand that, another complete catalytic cycle for homologation of ethanol to 1-butanol was computed and kinetic simulations carried out, assuming the mechanism virtually followed by **24** was the same as that of **2** (Figure 3.33).

Formation of **24** is easier than **2** because it does not involve any ligand dissociation, but it consists in a "monomerization" of **23**. This dissociation process, as expected from experimental data, is not high in energy (7.1 kcal/mol) and it is easily accessible at 423.15 K.

After this step, the active catalyst seems to be able to dehydrogenate a molecule of ethanol, with an associated TS (**TS31**) and energy barrier 12.2 kcal/mol lower than that computed for **1** (i.e. **TS1**). The overall thermodynamics of the process is also in favour of **24**-driven catalysis, since this reaction is exergonic and it leads to acetaldehyde (Figure 3.25), in contrast with what happens using **2** (Figure 3.3).

Furthermore, it is interesting to underline that the symmetry of **24**'s active site does not impose any chiral issue and only one TS is possible.
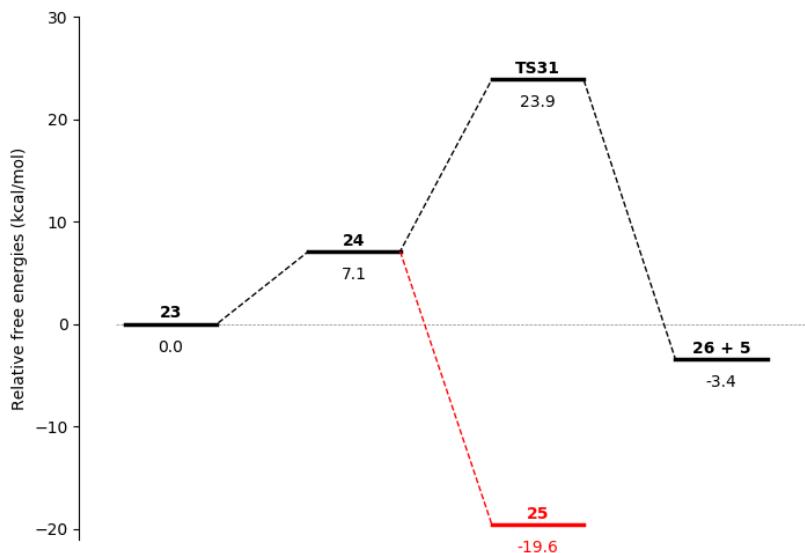
**Figure 3.25** Free energy surfaces of activation and dehydrogenation pathway for **23** (black route). In red it is reported a side reaction, which involves **24** and a molecule of **6**. **25** seems to be very stable.

Once acetaldehyde is formed it should be involved in the off-cycle organic pathway catalysed by sodium ethoxide and already discussed in section 3.2.3. Since this mechanism is not affected by the nature of dehydrogenating/hydrogenation catalyst, it is shared by both **1** and **23** cycles. Then, the formed (*E/Z*)-crotonaldehyde is involved in a double hydrogenation process. Thanks to the lack of carbene bound to metal centre and the degeneracy of its carbonyl ligands, **26** got a higher symmetry than **4**. It means that the total number of configurations the organic substrates could assume when interacting with **26** is limited to 4 (Figure 3.26).
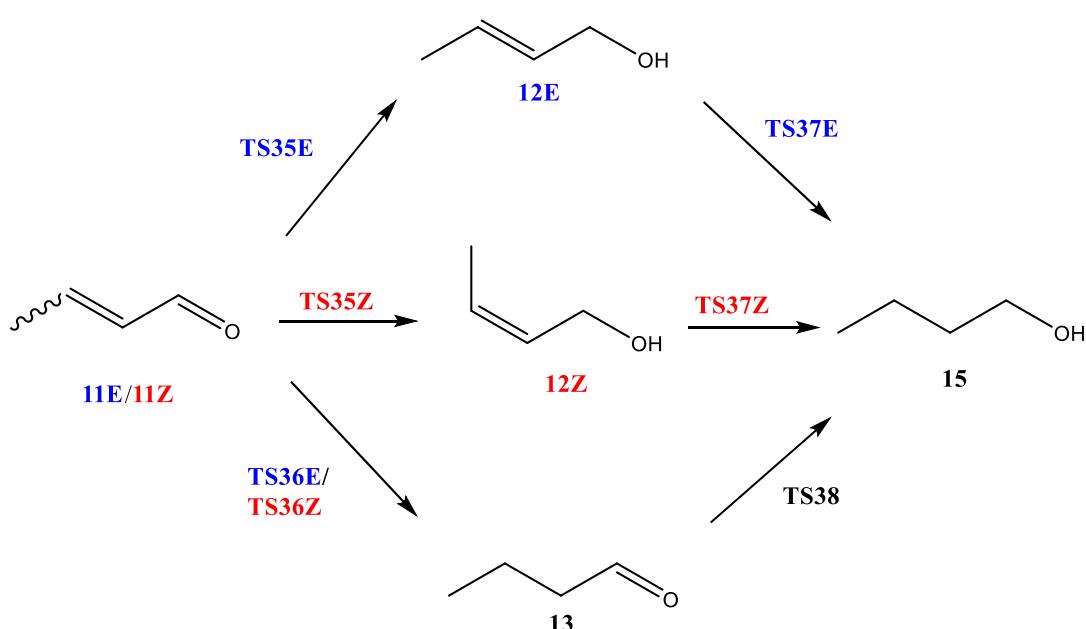


**Figure 3.26** Only 6 different hydrogenation transition states are possible for **11**, if **23** is used as pre-catalyst.

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Subsequent kinetic analyses will confirm the order of reduction for (*E/Z*)-crotonaldehyde's unsaturation is the same described in section 3.3 for **4**. Indeed, the C=C bond is the first being reduced, following two (*E/Z*) pathways (**TS36E** = 25.2 kcal/mol and **TS36Z** = 24.7 kcal/mol) and then another molecule of **26** reduces the aldehydic group to get 1-butanol from crotyl aldehyde (**TS38** = 18.4 kcal/mol), as shown in Figures 3.27-3.29.
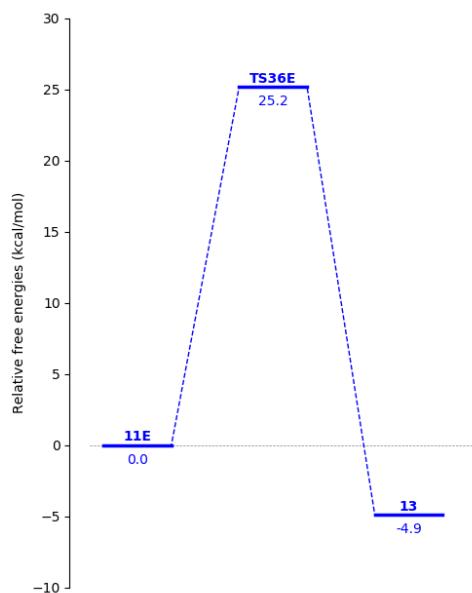


**Figure 3.27** Free energy surface of elementary step of C=C dehydrogenation of *E*-crotonaldehyde.
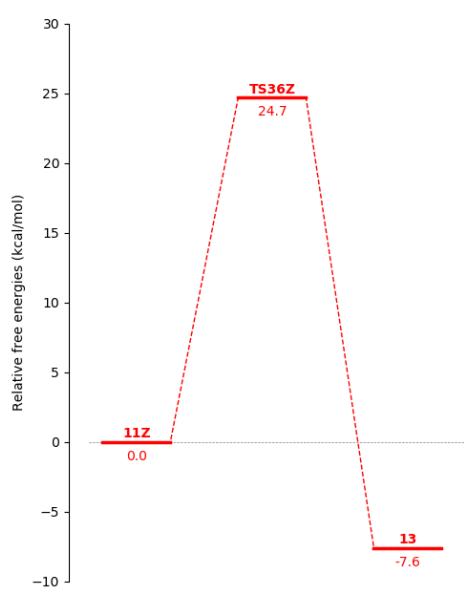


**Figure 3.28** Free energy surface of elementary step of C=C dehydrogenation of *E*-crotonaldehyde.
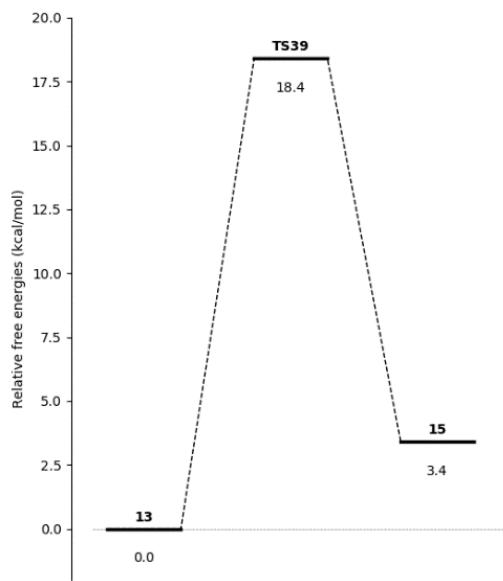


**Figure 3.29** Free energy surface of elementary step of C=O dehydrogenation of crotyl aldehyde.

As for **2**, in case the C=C bond is reduced after the C=O one (**TS35E** = 21.1 kcal/mol and **TS35Z** = 19.2 kcal/mol), the overall rate of the catalysis is slowed down (**TS37E** = 30.0 kcal/mol and **TS37Z** = 30.7 kcal/mol).

Even though it was not recorded high pressure at the end of experimental tests, it was assumed that if the total rate of the catalysis was comparable to the one discussed in section 3.1, similar $H_2$-loss mechanism should be considered. Even in this case, three different pathways were taken in account: i) a spontaneous proton/hydride coupling or proton shuttle played by a molecule of ii) water or iii) ethanol (Figure 3.30).

As already observed for **4**, hypothesis iii) is the best one and, moreover, **TS32**-**34** seem to be lower than **TS20**-**22**.
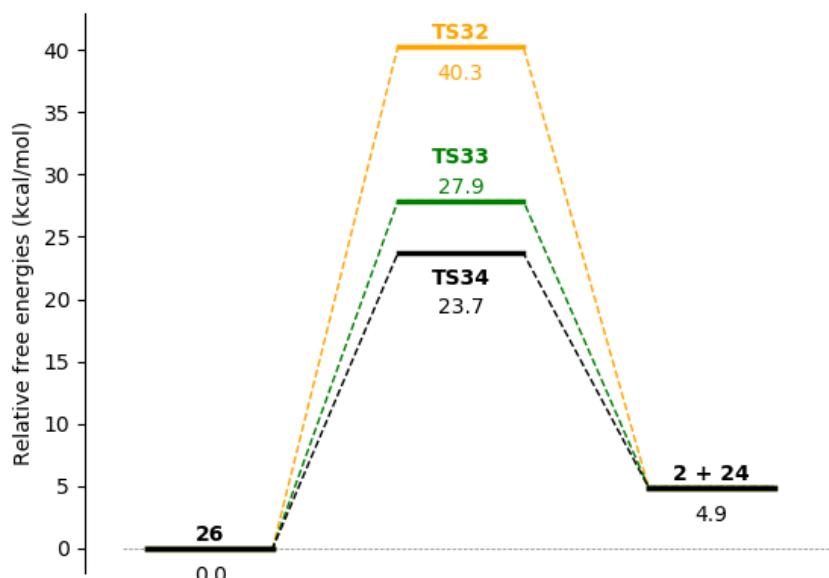


**Figure 3.30** Free energy surfaces of $H_2$-loss processes catalysed proton shuttle played by ethanol (black pathway), by water (green pathway) or spontaneous (yellow pathway). Even though **26** is -3.4 kcal/mol high in energy respect to **23** (see Figure 3.25, the reference was set to 0.0 kcal/mol to better compare this step with the hydrogenation's elementary steps).

Therefore, all TSs computed starting from **23** seemed to be lower in energy than ones computed in section 3.2. Rough kinetic network simulation was performed for the new computed cycle without adding any corrections on solution/gas or acid/base equilibria. Outcomes show the reaction should go faster than expected and faster than what recorded using **1**, i.e. conversion of ethanol is set to be 98.8% and yield of butanol is 86.0%.

This outcome is deeply in contrast with experimental data, mirroring a fault in the model and suggesting that an inactive form of the catalyst should be present in real reaction mixture and

which was not considered in the theoretical mechanism, yet. Moreover, the inactive form of **24** should be unstable for **2**, because on contrary also **2** should be deactivated.

By knowing that ruthenium has high affinity for oxygen, it was found a stable neutral complex (**25**) between **24** and **6**, very low in energy. **25** is 19.6 kcal/mol more stable than to the starting dimer (Figure 3.25), which definitely increases the total cost of dehydrogenation from 23.9 kcal/mol (directly from **23**) to 43.5 kcal/mol (while considering formation of **25**). Because of FES's shape, it is clear that **24** is more likely converted to **25** than to **26**. This turns into a substantial lowering of reaction rate, as shown by a further kinetic simulation which demonstrated how the presence of **25** in the cycle prevents any conversion of ethanol (Table 3.9). This outcome is drastic, but it is not the aim of this work to exactly reproduce this second mechanism. Anyway, this calculation suggests why **23** should not be active for the Guerbet and it is also clear that if **25** was not as stable as computed, **24** could be a better catalyst of **2**.

**Table 3.9** Full list of the elementary steps which were taken in account for the kinetic simulations.

| Entry | Reaction | TS | $\Delta G^{\ddagger}_{forward}{}^{a}$ | $\Delta G^{a}$ | $\Delta G^{\ddagger}_{backward}{}^{a}$ | $k_{forward}{}^{b}$ | $k_{backward}{}^{b}$ |
|---|---|---|---|---|---|---|---|
| 1 | **23 ⇋ 24 + 24** | N/A | 7,1 | 7,1 | 0,0 | 1,83E+09 | 8,81E+12 |
| 2 | **24 + 6 ⇋ 25** | N/A | 0,0 | -19,6 | 19,6 | 8,81E+12 | 6,70E+02 |
| 3 | **24 + 3 ⇋ 5 + 26** | TS31 | 16,8 | -3,4 | 20,2 | 1,94E+04 | 3,37E+02 |
| 4 | **5 + 5 ⇋ 11E** + $H_2O$ | TS5E | 26,7 | -0,2 | 26,9 | 1,37E-01 | 1,08E-01 |
| 5 | **5 + 5 ⇋ 11Z** + $H_2O$ | TS5Z | 26,8 | 2,5 | 24,3 | 1,21E-01 | 2,39E+00 |
| 6 | **26 + 11E ⇋ 2 + 13** | TS36E | 25,2 | -4,9 | 30,2 | 8,01E-01 | 2,27E-03 |
| 7 | **26 + 11Z ⇋ 2 + 13** | TS36Z | 24,7 | -7,6 | 32,3 | 1,58E+00 | 1,77E-04 |
| 8 | **13 + 26 ⇋ 2 + 15** | TS38 | 18,4 | 3,4 | 15,0 | 2,79E+03 | 1,51E+05 |
| 9 | **26 + 11E ⇋ 2 + 12E** | TS35E | 21,1 | 7,9 | 13,2 | 1,18E+02 | 1,34E+06 |
| 10 | **26 + 11Z ⇋ 2 + 12Z** | TS35Z | 19,2 | 6,4 | 12,8 | 1,10E+03 | 2,19E+06 |
| 11 | **26 + 11E ⇋ 2 + 15** | TS37E | 30,0 | -9,4 | 39,5 | 2,73E-03 | 3,67E-08 |
| 12 | **26 + 11Z ⇋ 2 + 15** | TS37Z | 30,7 | -10,7 | 41,3 | 1,27E-03 | 3,87E-09 |
| 13 | **26 ⇋ 2 + $H_2$** | TS34 | 23,7 | 4,9 | 18,8 | 5,04E+00 | 1,72E+03 |

[a]All the energies are reported in kcal/mol. [b]The rate constants are given in $s^{-1} \cdot mol^{n} \cdot L^{-n}$, where $n$ is (total order of the reaction-1).

To check this theoretical hypothesis, two tests were carried out. First, a **25**-type structure was computationally optimized adding a carbene ligand instead of a carbon monoxide (**2b**). The so-optimized molecule seems to be stable, but higher in energy than **2** (+ 4.0 kcal/mol). Thus, the presence of a carbene is enough to destabilize the inactive catalyst, thanks to its sigma-donor nature and steric hindrance. Furthermore, a synthesis of **25** was attempted in ethanol in presence of **24** and a large excess of **6**, i.e. 200 eq. (see section 6.10 for experimental details). At the end of the reaction, IR analysis (Figure 3.31) showed the characteristic bands of **23** in $CH_2Cl_2$

($\nu_{C\equiv O}$ = 2019 cm$^{-1}$, 1965 cm$^{-1}$) and the presence of two unknown red-shifted signals (2003 cm$^{-1}$, 1944 cm$^{-1}$). This outcome is in line with formation of **25**, since ethoxide is an electron-donor species that should increase electron density on ruthenium and, thus, back-bonding on carbon monoxides. Moreover, these experimental assumptions are supported by theoretical IR spectra computed *via* DFT which showed a red-shift from **23** to **25** (Figure 3.32).
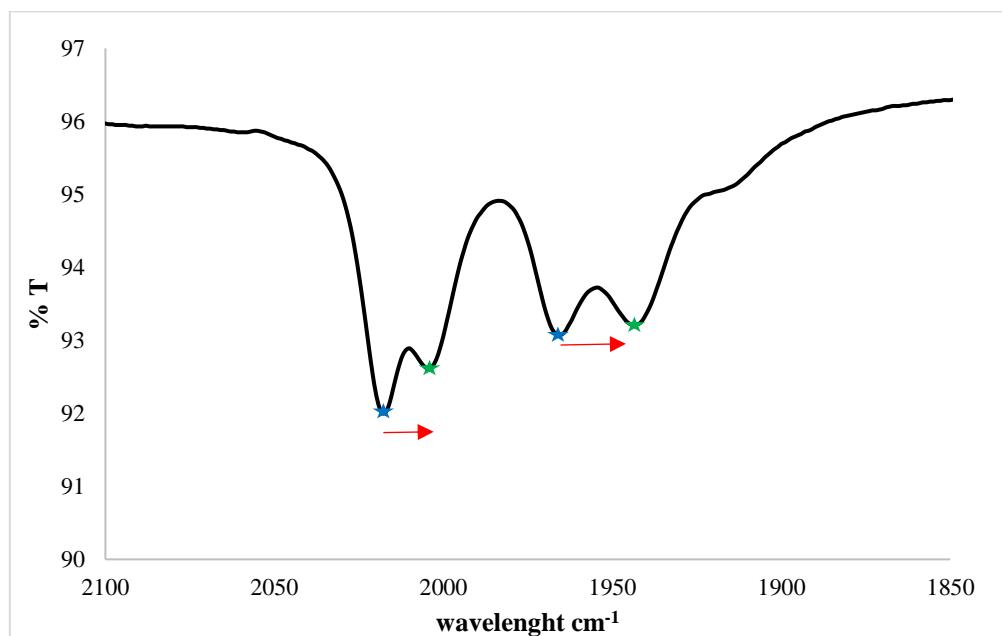


**Figure 3.31** Experimental IR spectrum of a solution of **23** (blue stars) and, likely, **25** (green stars). Red arrows show a red shift for **23**. The spectrum was recorded in CH$_2$Cl$_2$.
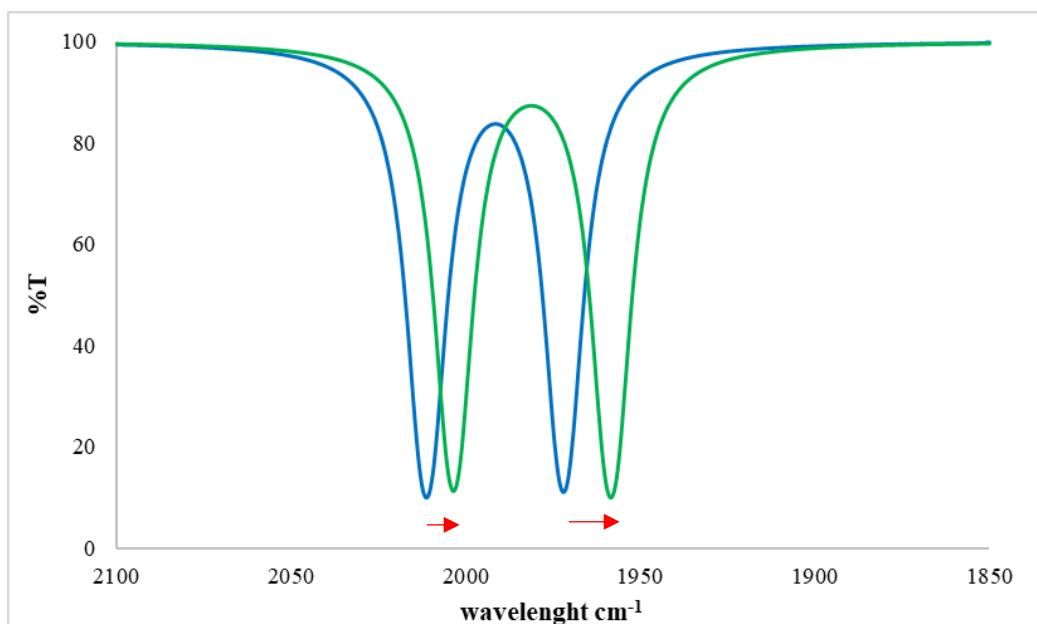


**Figure 3.32** Theoretical IR spectra of **23** (in blue) and **25** (in green). Red arrows show a red shift for **23**. The spectrum was computed in gas-phase.
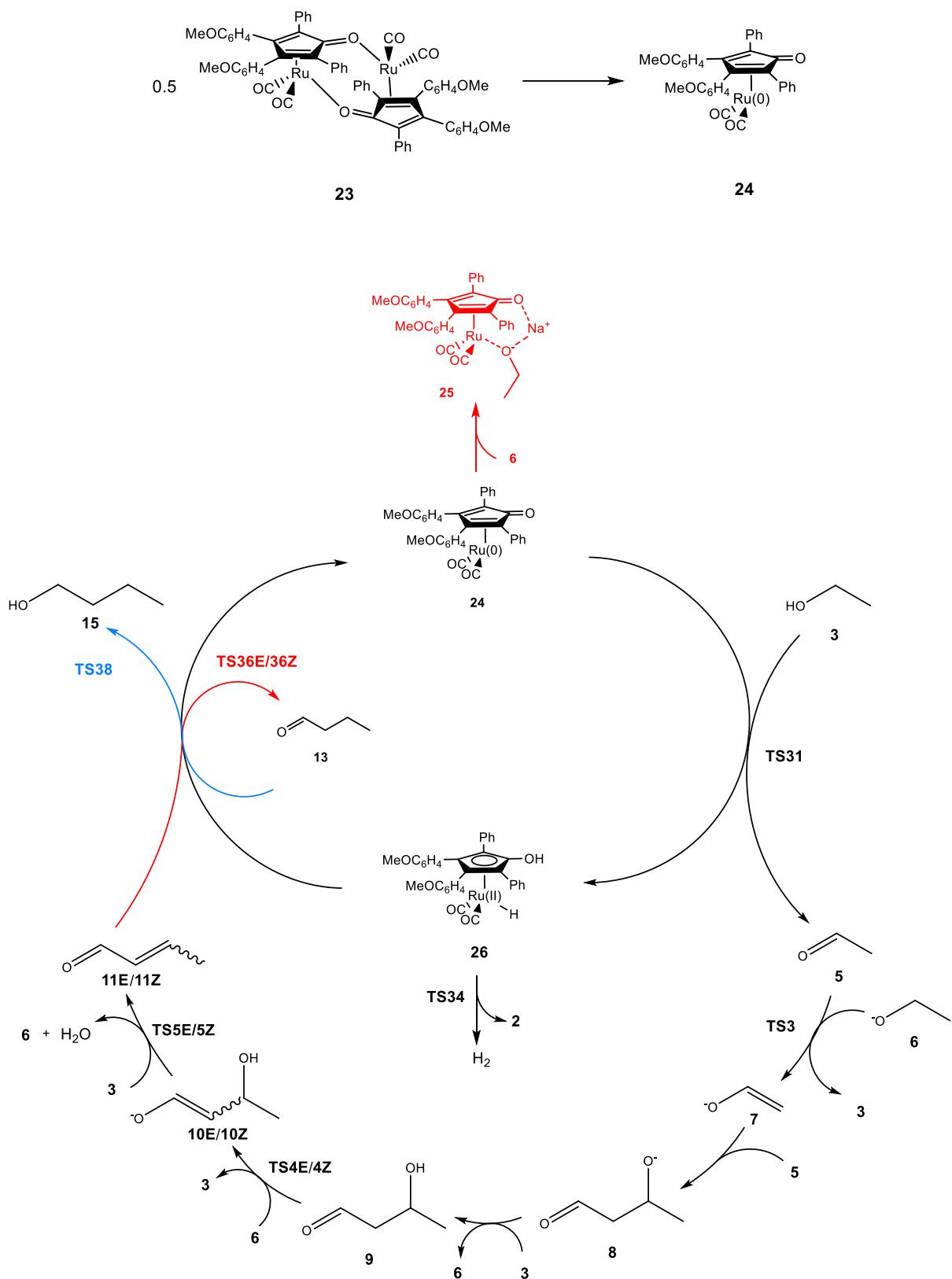
**Figure 3.33** Catalytic scheme proposed for homologation of ethanol (**3**) to 1-butanol (**15**) using **23**.

**Table 3.10** Energies and energy corrections of all the stationary points. All the energies are reported in atomic units (1 Hartree = 627.51 kcal/mol).

| Stationary point | B3LYP / 6-31G(d.p) (optimization) | B3LYP / 6-31G(d.p) Gibbs free energy at 423.15 K | B3LYP / 6-311+G(2d. 2p) (single point)[a] | Total Gibbs free energy |
|---|---|---|---|---|
| 1 | -2046.888392 | -2046.412114 | -2047.594197 | -2047.117919 |
| 2 | -1933.524450 | -1933.055881 | -1934.184533 | -1933.715965 |
| 2b | -2250.358216 | -2249.829352 | -2251.102649 | -2250.573785 |
| CO | -113.309453 | -113.333225 | -113.352314 | -113.376086 |
| 3 | -155.046675 | -155.005182 | -155.109719 | -155.068226 |
| TS1 | -2088.563269 | -2088.024671 | -2089.291162 | -2088.752565 |
| TS2 | -2088.561283 | -2088.022585 | -2089.290039 | -2088.751341 |
| 4 | -1934.728844 | -1934.241552 | -1935.389189 | -1934.901898 |
| 4b | -2096.483685 | -2096.011117 | -2097.175773 | -2096.703206 |
| 5 | -153.835728 | -153.818115 | -153.895510 | -153.877896 |
| 6 | -316.748774 | -316.725611 | -316.861418 | -316.838255 |
| TS3 | -470.614605 | -470.550423 | -470.757432 | -470.693250 |
| 7 | -315.541588 | -315.538256 | -315.648977 | -315.645645 |
| 8 | -469.413905 | -469.359590 | -469.563764 | -469.509449 |
| 9 | -307.687506 | -307.616836 | -307.805367 | -307.734697 |
| TS4E | -624.461820 | -624.345476 | -624.667792 | -624.551448 |
| TS4Z | -624.461460 | -624.344548 | -624.668190 | -624.551278 |
| 10E | -469.392786 | -469.339632 | -469.562311 | -469.509157 |
| 10Z | -469.411450 | -469.353827 | -469.563606 | -469.505983 |
| TS5E | -624.479218 | -624.363249 | -624.674321 | -624.558350 |
| TS5Z | -624.473306 | -624.357435 | -624.669497 | -624.553630 |
| H₂O | -76.419737 | -76.425308 | -76.468654 | -76.474225 |
| 11E | -231.242908 | -231.197507 | -231.327298 | -231.281897 |
| 11Z | -231.238570 | -231.193101 | -231.323038 | -231.277569 |
| TS6E | -2165.964657 | -2165.400236 | -2166.718157 | -2166.153736 |
| TS6Z | -2165.961399 | -2165.397105 | -2166.714725 | -2166.150430 |
| TS7E | -2165.961247 | -2165.397821 | -2166.717151 | -2166.153725 |
| TS7Z | -2165.958006 | -2165.394096 | -2166.715031 | -2166.151122 |
| TS8E | -2165.945981 | -2165.380450 | -2166.715131 | -2166.149599 |
| TS8Z | -2165.943714 | -2165.376632 | -2166.713374 | -2166.146292 |
| TS9E | -2165.947203 | -2165.381216 | -2166.714090 | -2166.148103 |
| TS9Z | -2165.943231 | -2165.377224 | -2166.711644 | -2166.145637 |
| TS10E | -387.466972 | -387.335931 | -387.606452 | -387.475411 |
| TS10Z | -387.462364 | -387.329907 | -387.603562 | -387.471105 |
| TS11E | -308.839967 | -308.756622 | -308.960055 | -308.876710 |
| TS11Z | -308.837386 | -308.752726 | -308.958148 | -308.873488 |
| TS12E | -232.358362 | -232.296791 | -232.439513 | -232.377941 |
| TS12Z | -232.353283 | -232.290223 | -232.433942 | -232.370883 |
| 12E | -232.443321 | -232.376321 | -232.532134 | -232.465134 |
| 12Z | -232.440723 | -232.374042 | -232.529832 | -232.463152 |
| 13 | -232.468334 | -232.401736 | -232.552113 | -232.485515 |
| TS13 | -2167.194153 | -2166.605244 | -2167.950156 | -2167.361246 |

Table 3.10 continued

| Stationary point | B3LYP / 6-31G(d,p) (optimization) | B3LYP / 6-31G(d,p) Gibbs free energy at 423.15 K | B3LYP / 6-311+G(2d, 2p) (single point)[a] | Total Gibbs free energy |
|---|---|---|---|---|
| TS14 | -2167.191572 | -2166.602761 | -2167.948170 | -2167.359359 |
| TS15E | -2167.139268 | -2166.553049 | -2167.902270 | -2167.316051 |
| TS15Z | -2167.135879 | -2166.550175 | -2167.899214 | -2167.313509 |
| TS16E | -2167.138211 | -2166.552028 | -2167.901978 | -2167.315795 |
| TS16Z | -2167.138051 | -2166.551584 | -2167.901962 | -2167.315495 |
| 14E | -232.452550 | -232.384248 | -232.537287 | -232.468985 |
| 14Z | -232.451954 | -232.384226 | -232.537330 | -232.469602 |
| 15 | -233.679474 | -233.588959 | -233.766439 | -233.675923 |
| TS17 | -548.036988 | -547.938268 | -548.210739 | -548.112020 |
| 16 | -548.045587 | -547.942255 | -548.220064 | -548.116730 |
| 17 | -386.319296 | -386.199376 | -386.461943 | -386.342020 |
| TS18E | -703.095079 | -702.929422 | -703.324905 | -703.159250 |
| TS18Z | -703.094695 | -702.928430 | -703.325649 | -703.159384 |
| 18E | -548.019352 | -547.919242 | -548.223386 | -548.123276 |
| 18Z | -548.045417 | -547.938952 | -548.221836 | -548.115371 |
| TS19E | -703.101450 | -702.933676 | -703.323116 | -703.155342 |
| TS19Z | -703.105487 | -702.939761 | -703.326964 | -703.161239 |
| 19E | -309.875846 | -309.781290 | -309.984611 | -309.890056 |
| 19Z | -309.871495 | -309.776894 | -309.980455 | -309.885855 |
| TS20 | -2089.757846 | -2089.206821 | -2090.488349 | -2089.937325 |
| TS21 | -2011.137952 | -2010.632558 | -2011.842815 | -2011.337421 |
| TS22 | -1934.661556 | -1934.177518 | -1935.328049 | -1934.844011 |
| TS23E | -2244.575677 | -2243.960171 | -2245.371775 | -2244.756269 |
| TS23Z | -2244.572868 | -2245.370904 | -2243.957648 | -2244.755683 |
| TS24E | -2244.574484 | -2243.959158 | -2245.373479 | -2244.758153 |
| TS24Z | -2244.574680 | -2243.958450 | -2245.371842 | -2244.755612 |
| TS25E | -2244.596212 | -2243.982757 | -2245.375749 | -2244.762294 |
| TS25Z | -2244.592905 | -2243.979859 | -2245.372461 | -2244.759415 |
| TS26E | -2244.589864 | -2243.975460 | -2245.372760 | -2244.758356 |
| TS26Z | -2244.587374 | -2243.974251 | -2245.371646 | -2244.758523 |
| 20E | -311.076276 | -310.960129 | -311.189497 | -311.073350 |
| 20Z | -311.073606 | -310.957809 | -311.187237 | -311.071440 |
| 21 | -311.101496 | -310.985853 | -311.209873 | -311.094230 |
| TS27 | -2245.825803 | -2245.187944 | -2246.608429 | -2245.970569 |
| TS28 | -2245.823262 | -2245.185830 | -2246.606433 | -2245.969001 |
| TS29E | -2245.767634 | -2245.132790 | -2246.559446 | -2245.924603 |
| TS29Z | -2245.765358 | -2245.130414 | -2246.558543 | -2245.923599 |
| TS30E | -2245.767137 | -2245.132160 | -2246.561089 | -2245.926113 |
| TS30Z | -2245.768776 | -2245.132486 | -2246.560461 | -2245.924171 |
| 22 | -312.312536 | -312.172986 | -312.424049 | -312.284500 |
| 23 | -3484.074925 | -3483.318259 | -3485.269957 | -3484.513291 |
| 24 | -1742.015557 | -1741.655806 | -1742.605034 | -1742.245283 |
| 25 | -2058.857075 | -2058.440175 | -2059.531658 | -2059.114758 |
| TS31 | -1897.057825 | -1896.632521 | -1897.712099 | -1897.286795 |

Table 3.10 continued

| Stationary point | B3LYP / 6-31G(d,p) (optimization) | B3LYP / 6-31G(d,p) Gibbs free energy at 423.15 K | B3LYP / 6-311+G(2d, 2p) (single point)[a] | Total Gibbs free energy |
|---|---|---|---|---|
| **26** | -1743.231014 | -1742.850960 | -1743.821094 | -1743.441041 |
| **TS32** | -1743.155420 | -1742.783709 | -1743.748500 | -1743.376789 |
| **TS33** | -1819.633847 | -1819.237520 | -1820.267146 | -1819.870818 |
| **TS34** | -1898.258978 | -1897.816441 | -1898.914031 | -1898.471494 |
| **TS35E** | -1974.461127 | -1974.009756 | -1975.140756 | -1974.689385 |
| **TS35Z** | -1974.458594 | -1974.006795 | -1975.139856 | -1974.688056 |
| **TS36E** | -1974.445356 | -1973.992325 | -1975.135731 | -1974.682700 |
| **TS36Z** | -1974.441805 | -1973.991329 | -1975.129757 | -1974.679281 |
| **TS37E** | -1975.641573 | -1975.170443 | -1976.329453 | -1975.858323 |
| **TS37Z** | -1975.639855 | -1975.167932 | -1976.327234 | -1975.855311 |
| **TS38** | -1975.691192 | -1975.216700 | -1976.371739 | -1975.897247 |
| **Dimethyl NHC** | -304.803848 | -304.725551 | -304.907169 | -304.828873 |
| **27** | -2209.043366 | -2208.585713 | -2209.785710 | -2209.328058 |
| **TS39** | -2364.088642 | -2363.562176 | -2364.894092 | -2364.367627 |
| **28** | -2210.246672 | -2209.771465 | -2210.992505 | -2210.517298 |
| **H$_2$** | -1.178539 | -1.186315 | -1.180168 | -1.187943 |

[a]The calculations were done adding solvation (C-PCM) and dispersion (Grimme-D3) corrections.

## 4. Conclusions

The Guerbet reaction catalysed by homogeneous ruthenium-based catalyst **1** and sodium ethoxide co-catalyst was experimentally and theoretically investigated. A plausible mechanism was proposed and characterized for all the pathways throughout the overall cycle, i.e. ruthenium-driven dehydrogenation and hydrogenation, C-C couplings and hydrogen loss. All intermediates and transition states were computationally characterized.

The theoretical outcomes did demonstrate the CO-loss activation mechanism, which was previously widely discussed only on the basis of experimental data. Moreover, DFT calculations highlighted the substantial impact of this step in terms of energy cost.

Because of the complexity of crossing reaction pathways in the mechanism and the presence of side and secondary products, it was not possible to use approximation, as described in section 1.2.3. Thus, advanced kinetic networks were built to directly compare DFT results and experimental data. Kinetic simulations accurately reproduced experiments, demonstrating the accuracy and usefulness of using DFT-based investigations also for large systems. Moreover, they supplied important information on the role and weaknesses of the co-catalyst. Thanks to the theoretical outcomes it was also possible to get insights into the role played by the carbene ligand, which is both steric and electronic, and without which the catalyst would be deactivated. Sensitivity analysis gave insights into important dependences of conversion and yields on internal and external factors.

In conclusion, the reported results represent the primary step towards more in-depth investigations that could bring to the design of new catalytic systems in the future, overcoming co-catalyst limitations and optimizing steric and electronics effects of ruthenium ligands, in order to avoid catalyst deactivation and promote optimal ligand dissociation.

## 5. Computational methods

All density functional theory (DFT) computations were carried out using the Gaussian16 package [52] and the B3LYP functional [32-34] as implemented in the software.

For geometry optimizations the full structures of reagents and the catalyst were used, without any geometrical simplification. In order to find the conformer with the lowest energy, a conformational analysis (Figure 5.1) was performed on each stationary point[1]. Geometry optimizations were carried out using 6-31G(d,p) basis set for Na, H, C, N and O [53] and the LANL2Z basis set with pseudopotential for Ru. [54] The nature of each stationary point, as minimum (no imaginary frequency) or as transition state (one imaginary frequency), was confirmed by computing analytical frequencies at the same level of theory. IR frequencies reported in this work have been rescaled using a 0.961 scaling factor. [55]
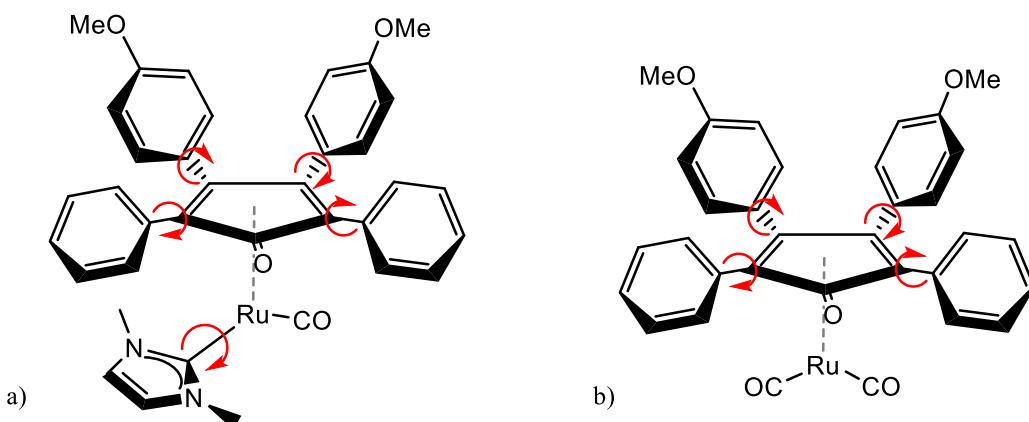


**Figure 5.2** Structures of a) species **2** and b) species **24**. Spinning bonds are highlighted by red arrows. Even though many conformers seem to be possible (i.e. 16 for **2** and 8 for **24**), only few of them are stable due to high steric hindrance of upper side ligands.

To obtain more accurate energies, the reported Gibbs free energies have been computed from single-point calculations on optimized structures with a larger basis set – i.e. 6-311+G(2d,2p) – for all atoms but for ruthenium, corrected for zero-point and thermal effects at 423.15 K from

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[1] Since the large amount of computed structures, to avoid a chaotic nomenclature, it was chosen to call each configuration with a different number. If a specific catalyst configuration could interact with a substrate with two geometric isomers, a capital letter (i.e. E/Z) was added to the unique catalyst configuration number. For example, **TS8E** corresponds to transition state number 8, where the organic substrate got an E configuration.

Because of multiple conformers are characterized for each stationary point, only the most stable one was reported, without adding any label.

Gibbs free energy computation, Grimme-D3 corrections for dispersions and solvation effects. [56] Solvation effects were performed using the conductor like polarizable continuum model (C-PCM) for ethanol, [57, 58] assuming it was a good approximation of the more complex real-solvent, which is composed of 80% in ethanol and 20% in sodium ethoxide. Nevertheless, it is important to underline that the role of the solvent in this reaction is central, being ethanol and sodium ethoxide the main reagent and the co-catalyst, respectively. Moreover, the presence of a substantial amount of base modifies the basicity of the whole solution, virtually altering some reactive steps (e.g. proton-shuttling). [59, 60] All the energies and the energy corrections of all the stationary point are collected in Table 3.10.

NMR shielding tensors were computed using the Gauge-Independent Atomic Orbital (GIAO) method [61-65] on minima as a single point using a 6-311+G(2d,p) basis set for all the elements but for Ru, for which was used the LANL2DZ basis set, and adding solvation corrections.

All the kinetic simulations reported in this work were performed using the LSODA algorithm [67] for ordinary differential equations (ODEs), implemented in COPASI software (version 4.30, built 240). [68]

All free-energy-difference graphs were drawn with homemade Python3 code. [69]

## 6. Experimental

Due to the lability of most of the reagents and the products discussed above, all the reactions described in this work were carried out under inert atmosphere ($N_2$ or Ar) and using Schlenk glassware. Tetrahydrofuran (THF), dichloromethane ($CH_2Cl_2$) and acetonitrile ($CH_3CN$) were dried, distilled and stored under inert atmosphere before being used. Whereas, as for ethanol (EtOH), diethyl ether ($Et_2O$), toluene, 15-crown-5-ether (98%, Alfa Aesar), ethanol-$d^6$ (99.50% D, Sigma Aldrich), chloroform-d (99.80% D, VWR Chemicals), toluene-$d^8$ (99.50% D, Eurisotop) and acetone-$d^6$ (99.80% D, VWR Chemicals), no further purifications were needed. Carbon isotopic labelling was done by adding a slight overpressure of $^{13}CO$ (≥99% atom $^{13}C$, Sigma Aldrich) to reactors, instead of using molecular nitrogen or argon.

Pressure measures were carried out using a 50 mL or 200 mL gas burette filled with distilled water, at room temperature and no later than 30 minutes after the end of each reaction to avoid any leakage of gas.

Infrared (IR) spectra were recorded into 2300 cm$^{-1}$ – 1800 cm$^{-1}$ spectral window at room temperature using a Perkin-Elmer Spectrum 2000 FT-IR spectrometer at a 1 cm$^{-1}$ resolution and using 0.1 mm thick $CaF_2$ IR-cells.

Electron Spray Ionization Mass Spectrometry (ESI-MS) analyses were performed injecting samples dissolved in methanol (HPLC quality) in a Waters Micromass ZQ 4000 instrument, using a 3.54 kV ESI positive ion probe's capillary and a 2.56 kV ESI negative ion probe's capillary with a 10-20 or 60-100 V ion reception cone. Direct infusion with a 20 µL/min rate of the solution and 200 L/h rate of the nebulizing gas were set.

### 6.1 Nuclear Magnetic Resonance spectroscopy

Nuclear Magnetic Resonance (NMR) spectra were recorded using Varian Mercury Plus VX 400 ($^1$H, 399.9 MHz; $^{13}C$, 100.6 MHz) and Varian Inova 600 ($^1$H, 599.7 MHz; $^{13}C$, 150.8 MHz), equipped with a Triple Resonance Indirect Detection Probe $^1$H{$^{13}C/^{15}N$}. NOESY and Inversion Recovery experiments were carried out using Varian pulse sequences and chemical shifts were internally referred to non-deuterated residual solvent peaks.

For NOESY experiments, selective *rsnob*-type pulses (pulse width = 20 Hz – 150 Hz) were used: the narrowest pulse to improve selectivity in studying each signal, and the widest one to magnify the NOE effect efficiency (only for signals distant from others).

All the spectra were recorded at 298.15 K, except for NOESY-1D ones, which were recorded at 273.15, 298.15 and 348.15 K.

## 6.2 Gas chromatography

Gas Chromatography (GC) analyses were carried out both to study product distribution in liquid phase and to detect the presence of carbon monoxide (CO) in the headspace of reactor and to quantify the amount of molecular hydrogen ($H_2$) produced during a reaction.

GC analyses for product distribution in the liquid phase were carried out using an Agilent Technologies 7890A Gas Chromatograph equipped with an Agilent 19091J-433 HP-5 (5% phenyl)-methylpolysiloxane (30 m x 0.320 mm, thickness 0.25 μm) capillary column with Helium (He) as carrier gas (column flow 0.909 mL/min, total flow 40.25 mL). Samples to inject were prepared acting a 1:10 dilution in diethyl ether, then 150 μL of tetrahydrofuran were added as internal standard. The so obtained solution was filtered using PFTE syringe filters (< 0.45 μm) to avoid solid injection into the chromatograph. 1 μL was sampled and injected. The injector was maintained in split mode (40:1) at 230 °C. Starting oven temperature was 30 °C (11 min), then the oven heated to 270 °C with 30 °C/min rate (kept 5 min). [40]

GC analyses of the gas phase were performed using an Agilent Technologies 7890A Gas Chromatograph equipped with a TCD detector. 0.04 mL of gas were sampled and manually injected. $H_2$ was quantified through an Agilent 19095P-MS0S (30 m x 0.530 mm, thickness 50 μm) capillary column with $N_2$ as carrier gas (column flow 3.0 mL/min). The injector was maintained in split mode (5:1) at 150 °C. Oven temperature was kept constant at 50 °C for the whole time.

To detect the presence of CO the instrument was equipped with an Agilent 7514 (27.5 m x 0.530 mm, thickness 25 μm) capillary column with $H_2$ as carrier gas (column flow 6.0 mL/min). The injector was maintained at 150 °C, whilst the oven temperature was kept constant at 50 °C for the whole time.

GC-MS analyses were performed using an Agilent Technologies 6890N gas-chromatograph coupled with an Agilent Technologies 5973 Inert mass spectrometer, equipped with an HP-5MS (30 m x 250 μm x 0.25 μm) capillary column with He as carrier gas (column flow 1.0

mL/min). The 0.4 mL injection was made maintaining a 50:1 split ratio. The starting oven temperature was 40 °C (held for 11 min), then the oven heated to 250 °C (held for 10 min) with a 10 °C/min rate.

## 6.3 Synthesis of 1,3-dimethylimidazolium iodide
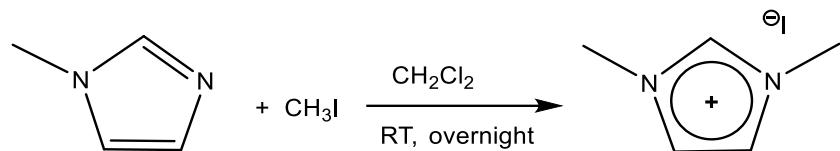


1-methylimidazole 0.485 mL (6.09 mmol) was dissolved in $CH_2Cl_2$ 15 mL. Then, $CH_3I$ 1.14 mL (6.09 mmol) was added in excess. The mixture was stirred overnight at room temperature. At the end of the reaction, a white solid is obtained by drying the reaction mixture. [70]

^{1}H-NMR (300.1 MHz, CDCl$_3$): δ 10.02 (s, 1H, NCHN), 7.39 (s, 2H, CH$_{im}$), 4.09 (s, 6H, NCH$_3$).
^{1}H-NMR (300.1 MHz, CD$_3$CN) δ 8.72 (s, 1H, NCHN), 7.38 (s, 2H, CH$_{im}$), 3.84 (s, 6H, NC$H_3$).

ESI-MS (m/z) (+) = 97 [M]$^+$; 321 [2M+I]$^+$, (-) = 127 [I]$^-$

## 6.4 Synthesis of dicarbonyl(η$^4$-3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone)-rutemium dimer (23)
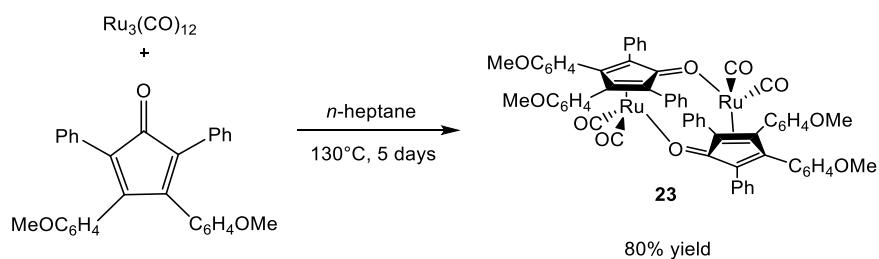


3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone 1.04 g (2.35 mmol) and Ru$_3$(CO)$_{12}$ 0.50 g (0.78 mmol) were dissolved in *n*-heptane 120 mL and stirred at 403.15 K for 5 days under inert atmosphere. Hence, **23** was filtered and dried as a yellow solid.

$^1$H-NMR (399.9 MHz, CDCl$_3$): δ 7.10-6.40 (m, 36H, CH$_{aryl}$), 3.60 (s, 12H, -OCH$_3$);

$^{13}$C-NMR (100.6 MHz, CDCl$_3$): δ 206.91 (CO), 169.65 (C=O), 158.53 (-COCH$_3$), 132.70 (CH$_{aryl}$), 130.96 (Cq$_{aryl}$), 130.58 (CH$_{aryl}$), 126.27 (CH$_{aryl}$), 122.67 (Cq$_{aryl}$), 113.32 (-CH$_{aryl}$), 112.54 (CH$_{aryl}$), 97.78 (C$_{2,5}$ Cp), 87.76 (C$_{3,4}$ Cp), 54.90 (-OCH$_3$).

IR (CH$_2$Cl$_2$, cm$^{-1}$): 2018, 1967 ($\nu_{CO}$); 1610, 1519 ($\nu_{C=C}$).

## 6.5 Synthesis of dicarbonyl(η$^4$-3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone)(1,3-dimethylimidazol-2-ylidene)ruthenium (2)
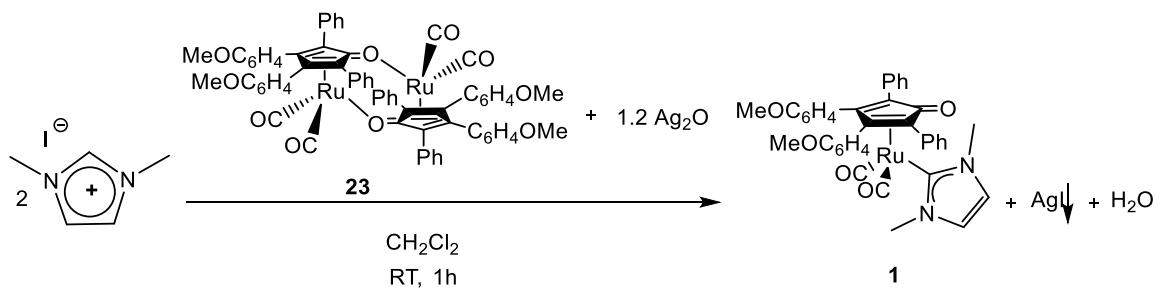


1,3-dimethylimidazolium iodide 0.074 g (0.332 mmol, 2 eq.) and Ag$_2$O 0.092 g (0.398 mmol, 1.2eq.) and dicarbonyl(η$^4$-3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone)-rutemium dimer 0.200 g (0.166 mmol, 1 eq.) were dissolved in CH$_2$Cl$_2$ 15 mL into a 100 mL Schlenk flask under inert atmosphere and protected from light. The solution was stirred at room temperature for 1 hour and the formation of the complex was verified via IR spectroscopy. Then, the mixture was filtered upon a celite pad in order to remove Ag salts and carbene residuals. The solid product is obtained by removing CH$_2$Cl$_2$ in vacuum. [43]

$^1$H-NMR (599.7 MHz, CDCl$_3$): δ 7.79 (m, 4H, CH$_{aryl}$), 7.17-7.04 (m, 10H, CH$_{aryl}$), 6.76 (s, 2H, CH$_{NHC}$), 6.65 (m, 4H, CH$_{aryl}$), 3.71 (s, 6H, -OCH$_3$), 3.09 (s, 6H, -NCH$_3$).
$^1$H-NMR (599.7 MHz, toluene-d$^8$): δ 8.29 (dd, 4H, CH$_{aryl}$), 7.31 (d, 4H, CH$_{aryl}$), 7.06 (t, 4H, CH$_{aryl}$), 6.93 (dt, 2H, CH$_{aryl}$), 6.49 (d, 4H, CH$_{aryl}$), 5.84 (s, 2H, CH$_{NHC}$), 3.07 (s, 6H, -OCH$_3$), 2.84 (s, 6H, -NCH$_3$).

$^{13}$C-NMR (150.8 MHz, CDCl$_3$): δ 202.47 (CO), 172.72 (C$_{carb.}$), 169.33 (C=O, Cp), 158.54 (-COCH$_3$), 135.43 (C$_{q.aryl}$), 133.62 (CH$_{aryl}$), 129.16 (CH$_{aryl}$), 127.43 (CH$_{aryl}$), 125.27 (C$_{q.aryl}$), 124.90 (CH$_{aryl}$), 123.62 (CH$_{NHC}$), 112.93 (CH$_{aryl}$), 103.85 (C$_{2,5, Cp}$), 78.46 (C$_{3,4, Cp}$), 55.00 (-OCH$_3$), 38.23 (-NCH$_3$).

$^{13}$C-NMR (150.8 MHz, toluene-d$^8$): δ 204.21 (CO), 173.71 (C$_{carb.}$), 171.14 (C=O, Cp), 159.63 (-COCH$_3$), 134.58 (C$_{q.aryl}$), 130.25 (CH$_{aryl}$), 123.63 (CH$_{NHC}$), 113.75 (CH$_{aryl}$), 105.22 (C$_{2,5, Cp}$), 79.00 (C$_{3,4, Cp}$), 54.62 (-OCH$_3$), 38.52 (-NCH$_3$). Some signals expected in the 130.00 ppm - 124.00 ppm spectral window for CH$_{aryl}$ and Cq$_{aryl}$ are not visible since they are covered by residual signals of toluene-d$^8$.

IR (CH$_2$Cl$_2$, cm$^{-1}$): 2004, 1945 ($\nu_{CO}$); 1586 cm$^{-1}$ ($\nu_{C=O}$); 1601, 1518 ($\nu_{C=C}$).

IR (Computationally simulated in gas, spectral window 2100 - 1800 cm$^{-1}$): 1992, 1948 ($\nu_{C=O}$).

ESI-MS (m/z) (+): 721 [M + Na]$^+$

## 6.6 Guerbet reaction 2-catalyzed

**2** 11.95 mg (0.0171 mmol, 0.002 eq.), sodium ethoxide 116.3 mg (1.712 mmol, 0.200 eq.) and ethanol 0.5 mL (8.56 mmol, 1 eq.) were introduced into a Schlenk-bomb reactor under inert atmosphere. The reaction mixture was stirred at 423.15 K for up to 4 hours. After 4 hours, the reactor was cooled down with a water-ice bath. Then, the autogenous pressure was measured with a gas burette and investigations of the headspace were carried out using GC and GC-MS. The gas phase was sampled from a septum installed in the connection between the Schlenk bomb and the gas burette. Liquid products distribution was studied via GC, ESI-MS, IR, $^1$H-NMR and $^{13}$C-NMR spectroscopy.

The reaction was also performed under different conditions into a J-Young valve equipped NMR tube in order to study (**2**)-type intermediates *in situ* during the catalytic route. In this case, **1** 8.38 mg (0.0120 mmol, 0.007 eq.), sodium ethoxide 17.0 mg (1.715 mmol, 0.01 eq.) and ethanol-d$^6$ 1.0 mL (1.715 mmol, 1 eq.) were mixed and held at 353.15 K for 48 hours, then heated to 363.15 K for 4 additional days.

## 6.7 Guerbet reaction - Isotopic labelling

**2** 25.0 mg (0.0358 mmol, 0.0042 eq.), sodium ethoxide 12.2 mg (0.179 mmol, 0.021 eq.) were dissolved in EtOH 0.5 mL (8.56 mmol, 1 eq.) under inert atmosphere ($N_2$) in a Schlenk-bomb reactor. Then, $N_2$-atmosphere was replaced with a $^{13}CO$ enriched pressurized atmosphere. The as-is solution was stirred at 423.15 K for 1 hour, then it was cooled down with a water-ice bath. The obtained mixture was dried with a high-vacuum pump for more than 1 hour to reduce the amount of higher alcohols. Then, the resulting yellow powder was dissolved in toluene-$d^8$ 0.5 mL and the solution was filtered. The sample was studied using IR, $^1H$-NMR and $^{13}C$-NMR spectroscopy.

## 6.8 Guerbet reaction *via* 24

Dicarbonyl($\eta$4-3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone) ruthenium dimer precursor (**23**) 9.550 mg (0.00855 mmol, 0.001 eq.), sodium ethoxide 116.3 mg (1.712 mmol, 0.200 eq.) and ethanol 0.5 mL (8.56 mmol, 1 eq.) were added to a Schlenk-bomb reactor under inert atmosphere (Ar). The reaction mixture was stirred at 423.15 K for up to 4 hours. After 4 hours, the reactor was cooled down with a water-ice bath. Liquid product distribution was studied via GC analyses.

The reaction was performed also adding only 0.9550 mg (0.00171 mmol, 0.0002 eq.) of the catalyst, in the same conditions described above.

## 6.9 Guerbet reaction with 15-crown-5-ether

**2** 11.95 mg (0.0171 mmol, 0.002 eq.), sodium ethoxide 116.3 mg (1.712 mmol, 0.200 eq.) and ethanol 0.5 mL (8.56 mmol, 1 eq.) were introduced into a Schlenk-bomb reactor under inert atmosphere. Then, 15-crown-5 ether 420 μL (2.05 mmol, 0.24 eq.) was added dropwise under stirring. The solution from yellow turned into red. After 15 minutes, the reaction mixture was stirred at 423.15 K for up to 4 hours. As the reaction was heated up, it rapidly became black. After 1 hour it was dark red and as the reaction went ahead it became lighter and lighter. At the end of the reaction, the Schlenk-bomb was cooled down with a water-ice bath.

The autogenous pressure was measured with a gas burette. Liquid products distribution was studied via GC, $^1$H-NMR and $^{13}$C-NMR spectroscopy.

The experiment was also repeated by adding toluene instead of the same amount of 15-crown-ether.

**6.10 Attempted synthesis of 25**



Dicarbonyl(η4-3,4-bis(4-methoxyphenyl)-2,5-diphenylcyclopenta-2,4-dienone)       ruthenium dimer precursor (**23**) 19.1 mg (1 eq., 0.0171 mmol), sodium ethoxide 232.6 mg (200 eq., 3.424 mmol) and ethanol 1.5 mL (25.68 mmol) were added to a 50 mL flask under inert atmosphere (N$_2$). The reaction mixture was stirred at reflux for 30 minutes.

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# Appendix - Cartesian coordinates of stationary points

**1**

| Ru | -1.05829700 | -0.30633500 | -1.01205600 |
|----|-------------|-------------|-------------|
| N | -3.87754600 | -1.67306500 | -0.56014300 |
| N | -4.17146900 | 0.34558100 | -1.23763300 |
| O | -0.62800200 | -2.57220300 | -3.02587500 |
| O | -0.94797600 | 1.81396200 | -3.21713900 |
| O | -2.20258000 | -0.76883000 | 2.29909600 |
| O | 4.11377000 | 4.99886000 | -0.34147500 |
| O | 6.03276800 | -2.37930300 | -0.80933000 |
| C | -0.79945300 | -1.69914700 | -2.28450600 |
| C | -1.03516600 | 1.00980800 | -2.38605100 |
| C | -1.25987500 | -0.46908600 | 1.55068600 |
| C | -0.93596900 | 0.87632200 | 0.97215800 |
| C | 0.37991200 | 0.78906900 | 0.37076300 |
| C | 0.75485700 | -0.60087500 | 0.28557300 |
| C | -0.29768600 | -1.39493900 | 0.90273300 |
| C | -1.67006500 | 2.12133500 | 1.30402400 |
| C | -2.53095800 | 2.16441500 | 2.41812700 |
| H | -2.66479700 | 1.26503300 | 3.00570600 |
| C | -3.21535900 | 3.33568400 | 2.74722000 |
| H | -3.87226300 | 3.34081400 | 3.61317200 |
| C | -3.06315100 | 4.49085600 | 1.98044100 |
| H | -3.59670100 | 5.40070400 | 2.24115400 |
| C | -2.21683200 | 4.46195700 | 0.86892700 |
| H | -2.08761800 | 5.35093300 | 0.25718000 |
| C | -1.53230700 | 3.29537100 | 0.53406900 |
| H | -0.88370900 | 3.29521100 | -0.33496000 |
| C | -0.18777100 | -2.83719500 | 1.22979000 |
| C | -0.65365600 | -3.31621600 | 2.46990200 |
| H | -1.12970600 | -2.62319900 | 3.15264300 |

| C | -0.52940900 | -4.66462800 | 2.80836200 |
| H | -0.89671100 | -5.00776700 | 3.77205800 |
| C | 0.06047300 | -5.56762400 | 1.92349400 |
| H | 0.15423300 | -6.61711700 | 2.18841500 |
| C | 0.52742700 | -5.10646900 | 0.69029100 |
| H | 0.98840800 | -5.79619400 | -0.01157600 |
| C | 0.40504400 | -3.76127100 | 0.34801200 |
| H | 0.77424700 | -3.42572500 | -0.61433700 |
| C | 1.32230600 | 1.91678200 | 0.14455300 |
| C | 1.65116100 | 2.73502300 | 1.23410400 |
| H | 1.17397900 | 2.56054100 | 2.19346000 |
| C | 2.57834100 | 3.77187000 | 1.12034000 |
| H | 2.80302200 | 4.37795200 | 1.98989400 |
| C | 3.19897800 | 4.01258600 | -0.11090200 |
| C | 2.87938000 | 3.20548200 | -1.21191400 |
| H | 3.36430600 | 3.40722300 | -2.16134700 |
| C | 1.95835700 | 2.17444800 | -1.08168400 |
| H | 1.71928200 | 1.56714900 | -1.94666100 |
| C | 4.47047900 | 5.84772100 | 0.73726700 |
| H | 5.20202200 | 6.55210500 | 0.33803300 |
| H | 4.92551900 | 5.28539100 | 1.56300000 |
| H | 3.60495300 | 6.40474800 | 1.11900400 |
| C | 2.13005500 | -1.08155900 | -0.02502900 |
| C | 2.64947700 | -1.17248700 | -1.32652100 |
| H | 2.01757600 | -0.91082500 | -2.16899800 |
| C | 3.94929600 | -1.60594200 | -1.55643300 |
| H | 4.34747000 | -1.67937300 | -2.56318400 |
| C | 4.77396100 | -1.96481900 | -0.48138300 |
| C | 4.27464400 | -1.88641900 | 0.82399500 |
| H | 4.88596100 | -2.16144000 | 1.67526800 |
| C | 2.96586200 | -1.45049000 | 1.03685400 |
| H | 2.58742800 | -1.40050800 | 2.05356500 |
| C | 6.90635900 | -2.76333400 | 0.23968600 |
| H | 7.84244200 | -3.05592300 | -0.23877600 |

| | | | |
|---|---|---|---|
| H | 6.50993400 | -3.61560600 | 0.80683300 |
| H | 7.09992000 | -1.93318000 | 0.93148100 |
| C | -3.19043800 | -0.56308900 | -0.95386600 |
| C | -5.24507800 | -1.45897700 | -0.58845900 |
| H | -5.95118800 | -2.21810200 | -0.29311400 |
| C | -5.43149000 | -0.18889900 | -1.01963600 |
| H | -6.33302000 | 0.37749400 | -1.18870800 |
| C | -3.29043100 | -2.90657800 | -0.04047100 |
| H | -4.04243200 | -3.69579200 | -0.09783300 |
| H | -2.98041700 | -2.75526100 | 0.99429100 |
| H | -2.42698900 | -3.19191900 | -0.63799700 |
| C | -3.97602900 | 1.71054100 | -1.71855900 |
| H | -4.92297300 | 2.24400300 | -1.62128700 |
| H | -3.67161900 | 1.71598600 | -2.76722700 |
| H | -3.22773100 | 2.21851700 | -1.11219900 |

**2**

| | | | |
|---|---|---|---|
| Ru | 0.50308000 | -1.19924700 | 0.83902100 |
| N | 3.48553200 | -1.62148700 | 1.51617700 |
| N | 2.70531000 | -0.10936800 | 2.83608700 |
| O | -1.11865600 | -1.66806200 | 3.37182000 |
| O | 0.99167900 | -2.80273800 | -1.98936600 |
| O | 0.49576700 | 6.02236800 | 0.00349500 |
| O | -6.13322200 | 1.93765800 | 0.79503600 |
| C | -0.46865700 | -1.52199200 | 2.41435300 |
| C | 0.47167900 | -1.78085300 | -1.51785000 |
| C | 1.12702700 | -0.47380500 | -1.26325500 |
| C | 0.15921100 | 0.40440600 | -0.67496400 |
| C | -1.09546700 | -0.34525700 | -0.47508400 |
| C | -0.88614200 | -1.68831600 | -0.89181000 |
| C | 2.50292300 | -0.15978900 | -1.71111400 |
| C | 3.02145100 | -0.78355000 | -2.86240200 |

A3

| | | | |
|---|---|---|---|
| H | 2.40970400 | -1.50540200 | -3.38930100 |
| C | 4.31367600 | -0.50282700 | -3.30813300 |
| H | 4.68898400 | -0.99764200 | -4.19995700 |
| C | 5.12021400 | 0.40492600 | -2.62037100 |
| H | 6.12553800 | 0.62285600 | -2.97018500 |
| C | 4.62030700 | 1.02915000 | -1.47445600 |
| H | 5.23737600 | 1.73556400 | -0.92528200 |
| C | 3.33198600 | 0.74819700 | -1.02399400 |
| H | 2.96150100 | 1.23237400 | -0.12752200 |
| C | -1.86413600 | -2.79194800 | -1.01095500 |
| C | -1.47017600 | -4.11269700 | -0.73276900 |
| H | -0.45434500 | -4.30053500 | -0.40597100 |
| C | -2.36517200 | -5.17012500 | -0.88342800 |
| H | -2.04187400 | -6.18272900 | -0.65798700 |
| C | -3.66874000 | -4.93353300 | -1.32500000 |
| H | -4.36605700 | -5.75856700 | -1.44151100 |
| C | -4.06614400 | -3.62926200 | -1.62308600 |
| H | -5.07408600 | -3.43393000 | -1.97897500 |
| C | -3.17300200 | -2.56886200 | -1.47145400 |
| H | -3.49081600 | -1.56198300 | -1.71796100 |
| C | 0.28112900 | 1.87142100 | -0.49940600 |
| C | 0.76642800 | 2.67211700 | -1.54178400 |
| H | 1.08421700 | 2.20621000 | -2.46869000 |
| C | 0.85228100 | 4.06119500 | -1.41997600 |
| H | 1.23326900 | 4.64174900 | -2.25175200 |
| C | 0.44903600 | 4.67901600 | -0.23090600 |
| C | -0.04757500 | 3.89254700 | 0.82072700 |
| H | -0.36605400 | 4.38807200 | 1.73227400 |
| C | -0.13354600 | 2.51453100 | 0.68258300 |
| H | -0.52766700 | 1.91475700 | 1.49594800 |
| C | 0.98528000 | 6.86667200 | -1.02637300 |
| H | 0.93629800 | 7.88294900 | -0.63225400 |
| H | 0.36839500 | 6.80124700 | -1.93192600 |
| H | 2.02539200 | 6.62973900 | -1.28502500 |

A4

| | | | |
|---|---|---|---|
| C | -2.39335100 | 0.28003200 | -0.10523000 |
| C | -3.21634300 | -0.21785900 | 0.92194000 |
| H | -2.88663000 | -1.06396000 | 1.51184100 |
| C | -4.44954900 | 0.35506300 | 1.19726500 |
| H | -5.07855300 | -0.02748500 | 1.99438500 |
| C | -4.90929300 | 1.44608800 | 0.44437800 |
| C | -4.11297600 | 1.95038300 | -0.58917200 |
| H | -4.44063700 | 2.78875100 | -1.19234000 |
| C | -2.87088700 | 1.36692000 | -0.85047100 |
| H | -2.26635200 | 1.76927800 | -1.65674200 |
| C | -6.64636600 | 3.04054600 | 0.06612600 |
| H | -7.61855600 | 3.26772400 | 0.50653800 |
| H | -6.78020200 | 2.79824100 | -0.99622900 |
| H | -5.99692900 | 3.92148700 | 0.15214800 |
| C | 2.33728800 | -0.94496800 | 1.81995900 |
| C | 4.53825100 | -1.21294400 | 2.31982300 |
| H | 5.52621400 | -1.63652400 | 2.23395500 |
| C | 4.04972900 | -0.25549900 | 3.14623000 |
| H | 4.53148900 | 0.32941900 | 3.91349600 |
| C | 3.61334000 | -2.67350000 | 0.50926100 |
| H | 4.49993900 | -2.48514200 | -0.10009800 |
| H | 2.74111900 | -2.67388900 | -0.14383800 |
| H | 3.70144600 | -3.65060300 | 0.99398500 |
| C | 1.82229600 | 0.85548700 | 3.48303200 |
| H | 1.61620200 | 1.69744200 | 2.81802100 |
| H | 2.30890000 | 1.21880600 | 4.39026800 |
| H | 0.88077800 | 0.37407100 | 3.74663200 |

**2b**

| | | | |
|---|---|---|---|
| Ru | 0.94247600 | -0.68046200 | 0.70064400 |
| N | 3.50640500 | 0.92607800 | 1.39660200 |
| N | 1.99204700 | 1.38509600 | 2.85606000 |
| O | -0.21456100 | -1.95099000 | 3.19073600 |

A5

| O | 1.65791900 | -1.49438300 | -2.58226400 |
| O | -2.85254700 | 5.79327400 | 0.08770000 |
| O | -6.46117500 | -0.88464900 | 1.12819500 |
| C | 0.26479500 | -1.45286700 | 2.24754000 |
| C | 0.83681900 | -0.88235100 | -1.82619600 |
| C | 0.89815000 | 0.50031500 | -1.36638200 |
| C | -0.28326500 | 0.76385200 | -0.54682200 |
| C | -1.00081800 | -0.48462200 | -0.38740700 |
| C | -0.27012400 | -1.52025500 | -1.07948400 |
| C | 1.86773500 | 1.50434400 | -1.85230500 |
| C | 2.59051700 | 1.28738700 | -3.04383500 |
| H | 2.43187600 | 0.36433600 | -3.58689900 |
| C | 3.50932700 | 2.22897200 | -3.50843200 |
| H | 4.05101900 | 2.03295200 | -4.43045000 |
| C | 3.73453900 | 3.41374400 | -2.80536100 |
| H | 4.45017400 | 4.14536200 | -3.17040700 |
| C | 3.02406100 | 3.64520500 | -1.62456500 |
| H | 3.18467700 | 4.56165900 | -1.06227300 |
| C | 2.10695400 | 2.70712900 | -1.15484700 |
| H | 1.57420400 | 2.90387600 | -0.23201200 |
| C | -0.67103600 | -2.93354900 | -1.25620900 |
| C | -0.45701200 | -3.58859600 | -2.49036600 |
| H | -0.01603800 | -3.03035200 | -3.30861400 |
| C | -0.81143800 | -4.93085500 | -2.66591100 |
| H | -0.64233700 | -5.40493800 | -3.62946900 |
| C | -1.39940400 | -5.64981300 | -1.62533900 |
| H | -1.68015600 | -6.68987900 | -1.76401000 |
| C | -1.62693600 | -5.01233200 | -0.40105300 |
| H | -2.08482200 | -5.55817900 | 0.41930600 |
| C | -1.26126600 | -3.68154400 | -0.21497900 |
| H | -1.42625700 | -3.21122600 | 0.74753700 |
| C | -0.91619400 | 2.09686100 | -0.35609100 |
| C | -1.13035000 | 2.91454100 | -1.47578700 |
| H | -0.78668600 | 2.57953000 | -2.44923900 |

A6

| | | | |
|---|---|---|---|
| C | -1.77004300 | 4.15118800 | -1.37678500 |
| H | -1.91037200 | 4.74644100 | -2.27142700 |
| C | -2.21947200 | 4.60106700 | -0.13024100 |
| C | -2.02142300 | 3.79709000 | 0.99984200 |
| H | -2.37953600 | 4.15510200 | 1.95996300 |
| C | -1.38079200 | 2.56950800 | 0.88206400 |
| H | -1.23737600 | 1.96230900 | 1.76640200 |
| C | -3.08119700 | 6.64033900 | -1.02541800 |
| H | -3.59128700 | 7.52264600 | -0.63484300 |
| H | -3.71981800 | 6.15960900 | -1.77812700 |
| H | -2.14137000 | 6.94936700 | -1.50173400 |
| C | -2.41974900 | -0.60872500 | 0.05034100 |
| C | -2.86415800 | -0.45316100 | 1.37328600 |
| H | -2.14292500 | -0.27652100 | 2.16185100 |
| C | -4.21111800 | -0.55013300 | 1.70064900 |
| H | -4.54880900 | -0.43651300 | 2.72572800 |
| C | -5.16397400 | -0.80700300 | 0.70611900 |
| C | -4.74471200 | -0.97056100 | -0.61901700 |
| H | -5.45562400 | -1.17314600 | -1.41134800 |
| C | -3.38736400 | -0.87202400 | -0.92929000 |
| H | -3.07420600 | -1.00072700 | -1.96119400 |
| C | -7.46403800 | -1.14746000 | 0.16148400 |
| H | -8.41030900 | -1.16682700 | 0.70483000 |
| H | -7.31128500 | -2.11747600 | -0.32971900 |
| H | -7.50548600 | -0.36262300 | -0.60516600 |
| C | 2.22023000 | 0.61075100 | 1.74577600 |
| C | 4.04741000 | 1.87306800 | 2.25077000 |
| H | 5.04796200 | 2.25411300 | 2.12178400 |
| C | 3.09850400 | 2.15996400 | 3.17234200 |
| H | 3.10783000 | 2.83169500 | 4.01604900 |
| C | 4.26412700 | 0.36899800 | 0.27413200 |
| H | 4.27804600 | 1.07232700 | -0.55998600 |
| H | 3.79547600 | -0.57129000 | -0.01831500 |
| H | 5.28684300 | 0.17803000 | 0.61143200 |

| | | | |
|---|---|---|---|
| C | 0.79553400 | 1.38085000 | 3.68502600 |
| H | -0.00707200 | 0.89776800 | 3.13601400 |
| H | 0.51003900 | 2.40931900 | 3.92074400 |
| H | 0.97162300 | 0.83131400 | 4.61494400 |
| O | 2.57415800 | -2.15356200 | 0.56417600 |
| C | 3.22815000 | -2.61025600 | 1.71397000 |
| H | 2.51220600 | -2.96095600 | 2.47791000 |
| H | 3.81239000 | -1.80308100 | 2.19466900 |
| C | 4.18483000 | -3.75952800 | 1.38012900 |
| H | 4.72222700 | -4.10591400 | 2.27100400 |
| H | 4.92666900 | -3.44252000 | 0.63703700 |
| H | 3.63401500 | -4.61959800 | 0.97431200 |
| Na | 2.13556800 | -3.19442200 | -1.26815500 |

**CO**

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | -0.65024200 |
| O | 0.00000000 | 0.00000000 | 0.48768200 |

**3**

| | | | |
|---|---|---|---|
| C | -1.21572700 | -0.23959800 | -0.02160000 |
| C | 0.08470000 | 0.55550300 | 0.04676800 |
| H | -1.28184100 | -0.95911600 | 0.80375100 |
| O | 1.24028200 | -0.26046300 | -0.10950500 |
| H | 1.25168500 | -0.89077300 | 0.62286200 |
| H | -2.08547400 | 0.42296800 | 0.04727300 |
| H | -1.27536200 | -0.79567400 | -0.96183700 |
| H | 0.12710000 | 1.28016200 | -0.77287000 |
| H | 0.12779600 | 1.13070300 | 0.98585400 |

**TS1**

| | | | |
|---|---|---|---|
| Ru | 0.81268900 | -0.87641000 | 0.79566900 |
| N | 3.80638000 | -0.19955200 | 1.26540400 |
| N | 2.59577700 | 0.83488800 | 2.71583500 |
| O | -0.36802000 | -1.62624800 | 3.48070400 |
| O | 1.59193800 | -1.92174500 | -2.23778100 |
| O | -1.67293800 | 6.19303500 | 0.12235000 |
| O | -6.55129800 | 0.25847600 | 1.00771100 |
| C | 0.09746200 | -1.31990100 | 2.45365700 |
| C | 0.75842500 | -1.12618300 | -1.57624900 |
| C | 1.00155500 | 0.25544200 | -1.28642700 |
| C | -0.14922800 | 0.76493900 | -0.55295000 |
| C | -1.07719700 | -0.33624600 | -0.38224700 |
| C | -0.51561400 | -1.51615400 | -0.98690500 |
| C | 2.17454100 | 1.02815200 | -1.75782500 |
| C | 2.78429300 | 0.71009000 | -2.98566000 |
| H | 2.40267500 | -0.12110400 | -3.56582900 |
| C | 3.88331700 | 1.43582000 | -3.44716900 |
| H | 4.33793800 | 1.16904200 | -4.39736700 |
| C | 4.39647300 | 2.49643700 | -2.69908100 |
| H | 5.25217400 | 3.06016400 | -3.06010500 |
| C | 3.79655700 | 2.82671300 | -1.48101400 |
| H | 4.18437100 | 3.65057800 | -0.88793300 |
| C | 2.70010700 | 2.10312300 | -1.01646700 |
| H | 2.24689000 | 2.36648600 | -0.06768000 |
| C | -1.17536000 | -2.82686100 | -1.18227700 |
| C | -1.01242300 | -3.51968900 | -2.39609800 |
| H | -0.37019200 | -3.10160500 | -3.16273700 |
| C | -1.65643900 | -4.73732500 | -2.61517600 |
| H | -1.51449300 | -5.25420600 | -3.56029700 |
| C | -2.47710600 | -5.28992100 | -1.63127200 |
| H | -2.97734100 | -6.23881900 | -1.80311100 |
| C | -2.64329800 | -4.61505300 | -0.41968200 |

A9

| | | | |
|---|---|---|---|
| H | -3.27349600 | -5.03734900 | 0.35817000 |
| C | -1.99699800 | -3.40116500 | -0.19476700 |
| H | -2.12517900 | -2.89309200 | 0.75449300 |
| C | -0.50760200 | 2.19239400 | -0.36777600 |
| C | -0.38139800 | 3.09393900 | -1.43480100 |
| H | 0.01497200 | 2.74479900 | -2.38252600 |
| C | -0.75467100 | 4.43446100 | -1.31725500 |
| H | -0.63644100 | 5.09169000 | -2.17070100 |
| C | -1.27931800 | 4.90548900 | -0.10883300 |
| C | -1.42662700 | 4.01787200 | 0.96653300 |
| H | -1.84209100 | 4.39337000 | 1.89617800 |
| C | -1.04652300 | 2.68912800 | 0.83371400 |
| H | -1.17733800 | 2.01534600 | 1.67275900 |
| C | -1.55445700 | 7.12871400 | -0.93638100 |
| H | -1.92013300 | 8.07860500 | -0.54284400 |
| H | -2.16288600 | 6.84026100 | -1.80345900 |
| H | -0.51149000 | 7.24944100 | -1.25746800 |
| C | -2.50625700 | -0.19215700 | 0.01929400 |
| C | -2.95790700 | -0.12749700 | 1.34741800 |
| H | -2.24654100 | -0.21119200 | 2.16090600 |
| C | -4.30713400 | 0.02220500 | 1.64435000 |
| H | -4.65382900 | 0.06603300 | 2.67171500 |
| C | -5.25226800 | 0.11320600 | 0.61353000 |
| C | -4.82467200 | 0.04788700 | -0.71745800 |
| H | -5.53059000 | 0.11149500 | -1.53700300 |
| C | -3.46560100 | -0.10437000 | -0.99777400 |
| H | -3.14597100 | -0.15786800 | -2.03443500 |
| C | -7.54993500 | 0.34552700 | 0.00458100 |
| H | -8.49917200 | 0.45315900 | 0.53198700 |
| H | -7.58291000 | -0.55997700 | -0.61518300 |
| H | -7.39820800 | 1.21747400 | -0.64497000 |
| C | 2.50609000 | -0.03711300 | 1.66201500 |
| C | 4.66983200 | 0.55556000 | 2.04324500 |
| H | 5.73440400 | 0.56462400 | 1.87238600 |

A10

| C | 3.91077300 | 1.20242500 | 2.95905300 |
|---|---|---|---|
| H | 4.18196200 | 1.87829800 | 3.75424200 |
| C | 4.28571700 | -0.98327400 | 0.12661900 |
| H | 4.48849300 | -0.32528000 | -0.72124000 |
| H | 3.55011700 | -1.72735700 | -0.16879700 |
| H | 5.20579500 | -1.49608100 | 0.41857500 |
| C | 1.47380400 | 1.33875200 | 3.50103400 |
| H | 1.82581800 | 2.17808600 | 4.10380400 |
| H | 1.07616500 | 0.56503900 | 4.16050200 |
| H | 0.68489000 | 1.68296200 | 2.83360700 |
| C | 2.68695500 | -4.20379900 | 1.59096400 |
| C | 1.88973700 | -3.70234000 | 0.39620600 |
| H | 2.14823500 | -4.04047900 | 2.52821900 |
| H | 3.66598200 | -3.72093600 | 1.63914700 |
| H | 2.84842800 | -5.28126400 | 1.46145900 |
| H | 1.66755200 | -2.34862100 | 0.87142500 |
| H | 0.82265200 | -3.97658800 | 0.42349500 |
| O | 2.47372600 | -3.65583700 | -0.74347500 |
| H | 1.88249200 | -2.76725300 | -1.66757600 |

**TS2**

| Ru | 0.73395700 | -0.97423200 | 0.82095200 |
|---|---|---|---|
| N | 3.75736200 | -0.49342600 | 1.38561900 |
| N | 2.56599700 | 0.58103000 | 2.82282600 |
| O | -0.56957900 | -1.68997000 | 3.45677400 |
| O | 1.39400800 | -2.15255900 | -2.18562200 |
| O | -0.91040800 | 6.33223300 | 0.00664100 |
| O | -6.43896000 | 1.06860600 | 0.97139900 |
| C | -0.05349100 | -1.39551500 | 2.45088600 |
| C | 0.65617700 | -1.25156500 | -1.53832100 |
| C | 1.06406000 | 0.09646400 | -1.26994000 |
| C | -0.02728900 | 0.75200800 | -0.56360700 |

A11

| | | | |
|---|---|---|---|
| C | -1.07763900 | -0.22737700 | -0.38096300 |
| C | -0.66019500 | -1.47736400 | -0.96519900 |
| C | 2.32560400 | 0.71555600 | -1.74080700 |
| C | 2.91532300 | 0.29545500 | -2.94736300 |
| H | 2.45002000 | -0.50135700 | -3.51423300 |
| C | 4.09986800 | 0.87463100 | -3.40419700 |
| H | 4.53675600 | 0.52991100 | -4.33745500 |
| C | 4.72081600 | 1.88843800 | -2.67319800 |
| H | 5.64285000 | 2.33831800 | -3.03073800 |
| C | 4.14147200 | 2.32094100 | -1.47713300 |
| H | 4.61174000 | 3.11100900 | -0.89779800 |
| C | 2.96002700 | 1.74296600 | -1.01705000 |
| H | 2.52495800 | 2.08425000 | -0.08478600 |
| C | -1.48702400 | -2.68764900 | -1.17407200 |
| C | -1.37916600 | -3.41170200 | -2.37586800 |
| H | -0.65589100 | -3.09888300 | -3.11989000 |
| C | -2.18031800 | -4.52914000 | -2.61083000 |
| H | -2.07673900 | -5.07320900 | -3.54565300 |
| C | -3.10865500 | -4.94692800 | -1.65667000 |
| H | -3.73161300 | -5.81764100 | -1.84093100 |
| C | -3.22403900 | -4.23840400 | -0.45837800 |
| H | -3.93681700 | -4.55679400 | 0.29733600 |
| C | -2.42067900 | -3.12582800 | -0.21711500 |
| H | -2.50920500 | -2.59585200 | 0.72421000 |
| C | -0.21698500 | 2.21468600 | -0.40385000 |
| C | 0.03758100 | 3.07818000 | -1.47948900 |
| H | 0.41002600 | 2.67004300 | -2.41315800 |
| C | -0.17680800 | 4.45507500 | -1.38830600 |
| H | 0.03645900 | 5.08012300 | -2.24746100 |
| C | -0.66751800 | 5.00376100 | -0.19860700 |
| C | -0.94323000 | 4.15648200 | 0.88408000 |
| H | -1.33236500 | 4.59279800 | 1.79843100 |
| C | -0.72094900 | 2.79025900 | 0.77745200 |
| H | -0.95347900 | 2.15034700 | 1.62090400 |

| | | | |
|---|---|---|---|
| C | -0.65834200 | 7.23066100 | -1.06100800 |
| H | -0.91690200 | 8.22324500 | -0.68847000 |
| H | -1.27768300 | 7.00289500 | -1.93835500 |
| H | 0.39833200 | 7.22170000 | -1.35898600 |
| C | -2.47963200 | 0.10042900 | 0.00920100 |
| C | -2.93775700 | 0.18184100 | 1.33415300 |
| H | -2.25571700 | -0.02494800 | 2.15096800 |
| C | -4.25817700 | 0.50517700 | 1.62245100 |
| H | -4.61102800 | 0.56210600 | 2.64708200 |
| C | -5.16636100 | 0.75951500 | 0.58571400 |
| C | -4.73170800 | 0.68122000 | -0.74227400 |
| H | -5.40988300 | 0.86904500 | -1.56617900 |
| C | -3.40207100 | 0.35369300 | -1.01398600 |
| H | -3.07706200 | 0.29257300 | -2.04856600 |
| C | -7.40099800 | 1.32639500 | -0.03821300 |
| H | -8.33427700 | 1.54578500 | 0.48296900 |
| H | -7.54867000 | 0.45561100 | -0.69015800 |
| H | -7.12118100 | 2.19067400 | -0.65460000 |
| C | 2.45614300 | -0.25808700 | 1.74372000 |
| C | 4.63970200 | 0.18270500 | 2.21374200 |
| H | 5.70799000 | 0.12637800 | 2.07848400 |
| C | 3.89236900 | 0.85517300 | 3.12021700 |
| H | 4.17825700 | 1.49476600 | 3.93992400 |
| C | 4.23890400 | -1.29030500 | 0.25671300 |
| H | 4.70148900 | -0.63405200 | -0.48388800 |
| H | 3.42298700 | -1.83413300 | -0.21067300 |
| H | 4.97659500 | -2.01195800 | 0.61842600 |
| C | 1.45388700 | 1.13804500 | 3.58552500 |
| H | 1.83402800 | 1.95639500 | 4.20002200 |
| H | 1.00196500 | 0.38308300 | 4.23182900 |
| H | 0.69972400 | 1.52408300 | 2.90164400 |
| C | 1.97444900 | -3.82105000 | 0.57564800 |
| H | 1.47363900 | -2.49538500 | 0.92032500 |
| O | 2.33012700 | -3.83815600 | -0.64941500 |

A13

| | | | |
|---|---|---|---|
| H | 1.67410300 | -2.96058100 | -1.58865300 |
| H | 2.78129700 | -3.71767800 | 1.32754000 |
| C | 0.81389000 | -4.68089300 | 1.04782900 |
| H | 1.13612400 | -5.72879000 | 0.99404100 |
| H | -0.05634800 | -4.55849100 | 0.40096300 |
| H | 0.53892700 | -4.45133800 | 2.08098500 |

**4**

| | | | |
|---|---|---|---|
| Ru | 0.55049800 | -1.31439400 | 0.94074900 |
| N | 3.54439700 | -1.77602600 | 1.43169300 |
| N | 2.85076300 | -0.17399800 | 2.69361500 |
| O | -0.69104000 | -1.49037500 | 3.68213500 |
| O | 0.97624400 | -2.73199000 | -2.09231400 |
| O | 0.43330000 | 6.11300600 | -0.01833800 |
| O | -6.16535800 | 1.90509600 | 0.90127200 |
| C | -0.20790300 | -1.40601200 | 2.61918600 |
| C | 0.42208100 | -1.66814700 | -1.43728800 |
| C | 1.08186400 | -0.42374300 | -1.24748600 |
| C | 0.12417300 | 0.47199000 | -0.60324900 |
| C | -1.07601300 | -0.28150800 | -0.35606600 |
| C | -0.88848500 | -1.63117700 | -0.85811500 |
| C | 2.44333800 | -0.09743200 | -1.73594900 |
| C | 2.90171800 | -0.61831900 | -2.96006100 |
| H | 2.25673200 | -1.27482600 | -3.53268400 |
| C | 4.17463500 | -0.30717200 | -3.44040600 |
| H | 4.50459900 | -0.72317800 | -4.38853100 |
| C | 5.01688400 | 0.53551900 | -2.71462100 |
| H | 6.00702200 | 0.77862800 | -3.08992100 |
| C | 4.57304200 | 1.06416300 | -1.49975000 |
| H | 5.21846400 | 1.72160000 | -0.92350400 |
| C | 3.30452100 | 0.75160600 | -1.01608300 |
| H | 2.97190000 | 1.16424200 | -0.07069700 |

| | | | |
|---|---|---|---|
| C | -1.90306000 | -2.69371300 | -1.05604500 |
| C | -2.15795900 | -3.16290600 | -2.35897900 |
| H | -1.61882400 | -2.72674900 | -3.19571300 |
| C | -3.10562800 | -4.16157700 | -2.59142100 |
| H | -3.28499600 | -4.50716900 | -3.60586000 |
| C | -3.82770100 | -4.70247600 | -1.52770600 |
| H | -4.56855400 | -5.47660300 | -1.70612100 |
| C | -3.58724700 | -4.24385300 | -0.22984200 |
| H | -4.13870700 | -4.66481500 | 0.60623600 |
| C | -2.62918300 | -3.25959000 | 0.00542900 |
| H | -2.41893600 | -2.93403600 | 1.01788500 |
| C | 0.24650100 | 1.94077400 | -0.45479800 |
| C | 0.75232500 | 2.73229100 | -1.49633900 |
| H | 1.08557800 | 2.25728800 | -2.41306200 |
| C | 0.83815700 | 4.12357500 | -1.39362800 |
| H | 1.24054900 | 4.68985200 | -2.22553400 |
| C | 0.39683700 | 4.76237600 | -0.23072000 |
| C | -0.12973000 | 3.99196900 | 0.81665500 |
| H | -0.47616700 | 4.49999400 | 1.71107200 |
| C | -0.19932600 | 2.61045700 | 0.70312100 |
| H | -0.61435000 | 2.02965200 | 1.52051300 |
| C | 0.94917800 | 6.93617200 | -1.04992100 |
| H | 0.88795700 | 7.96093900 | -0.67939900 |
| H | 0.35888400 | 6.85135600 | -1.97192700 |
| H | 1.99686100 | 6.69721200 | -1.27611600 |
| C | -2.39815200 | 0.30054100 | 0.00934800 |
| C | -3.06968600 | 0.03233200 | 1.21395600 |
| H | -2.60156300 | -0.59880600 | 1.96015300 |
| C | -4.31921100 | 0.57905600 | 1.48093200 |
| H | -4.83281000 | 0.37357200 | 2.41459100 |
| C | -4.93970800 | 1.41693300 | 0.54481000 |
| C | -4.28832100 | 1.70035800 | -0.66082700 |
| H | -4.74009700 | 2.34674900 | -1.40402800 |
| C | -3.03400400 | 1.14183600 | -0.91352400 |

| H | -2.53665800 | 1.37036800 | -1.85143400 |
|---|---|---|---|
| C | -6.83324900 | 2.76323800 | -0.00775900 |
| H | -7.77743500 | 3.03279900 | 0.46863800 |
| H | -7.04230600 | 2.26181600 | -0.96194200 |
| H | -6.25590300 | 3.67624600 | -0.20438500 |
| C | 2.41595500 | -1.07216900 | 1.75557600 |
| C | 4.64262400 | -1.32918300 | 2.14991100 |
| H | 5.62459200 | -1.75650800 | 2.02526800 |
| C | 4.20698700 | -0.32285000 | 2.94613200 |
| H | 4.73307200 | 0.29786500 | 3.65362600 |
| C | 3.59790900 | -2.89370300 | 0.49355900 |
| H | 3.07410600 | -2.64392400 | -0.42793100 |
| H | 3.13267700 | -3.77913600 | 0.93403400 |
| H | 4.64574900 | -3.10196600 | 0.26814800 |
| C | 2.01195200 | 0.82306400 | 3.35153100 |
| H | 2.66084600 | 1.54077300 | 3.85739900 |
| H | 1.35160100 | 0.35430100 | 4.08416300 |
| H | 1.40790200 | 1.34353100 | 2.60832800 |
| H | 0.88725900 | -2.85792400 | 1.17614900 |
| H | 0.41105100 | -3.50184300 | -1.92696000 |

**4b**

| Ru | 0.43009900 | -1.32938000 | 0.89934500 |
|---|---|---|---|
| N | 3.40965300 | -1.47981200 | 1.72721500 |
| N | 2.39004900 | -0.08539100 | 3.01127900 |
| O | -1.15272500 | -1.83578300 | 3.42906700 |
| O | 0.57888200 | -2.73855500 | -2.21879900 |
| O | 1.17956100 | 6.07314800 | -0.34800500 |
| O | -5.71576100 | 2.86205500 | 0.88629400 |
| C | -0.53241200 | -1.62918300 | 2.45853200 |
| C | 0.25273400 | -1.67267100 | -1.58637700 |
| C | 1.10100500 | -0.53731500 | -1.23673500 |

| | | | |
|---|---|---|---|
| C | 0.26998400 | 0.46844300 | -0.56885700 |
| C | -1.02796400 | -0.10410700 | -0.34827000 |
| C | -1.03363900 | -1.45238700 | -0.89464700 |
| C | 2.49329700 | -0.36509500 | -1.70564300 |
| C | 2.95819800 | -1.06361600 | -2.83921400 |
| H | 2.27924200 | -1.73562500 | -3.34928200 |
| C | 4.27212000 | -0.91505300 | -3.28552500 |
| H | 4.60112900 | -1.46608300 | -4.16311500 |
| C | 5.15906800 | -0.06647000 | -2.62142500 |
| H | 6.18090600 | 0.04873800 | -2.97267300 |
| C | 4.71281700 | 0.63512500 | -1.49812300 |
| H | 5.38834400 | 1.30211000 | -0.96818700 |
| C | 3.40324700 | 0.48759400 | -1.04609200 |
| H | 3.07881700 | 1.03465100 | -0.16842700 |
| C | -2.20671500 | -2.34933900 | -1.03179600 |
| C | -2.37583900 | -3.12769600 | -2.19971000 |
| H | -1.63759200 | -3.04871700 | -2.98966300 |
| C | -3.46790500 | -3.99018000 | -2.33909500 |
| H | -3.57398600 | -4.57120300 | -3.25173400 |
| C | -4.42543200 | -4.09135900 | -1.32980800 |
| H | -5.27658300 | -4.75684200 | -1.44196400 |
| C | -4.27618100 | -3.32187500 | -0.17115900 |
| H | -5.01295100 | -3.38861500 | 0.62479100 |
| C | -3.18242700 | -2.47326400 | -0.01882400 |
| H | -3.07315800 | -1.90118500 | 0.89519700 |
| C | 0.55311400 | 1.92387600 | -0.49162600 |
| C | 1.03685500 | 2.59981400 | -1.62204900 |
| H | 1.24386300 | 2.03863000 | -2.52723200 |
| C | 1.26117100 | 3.97815300 | -1.62054100 |
| H | 1.63734000 | 4.45241600 | -2.51949400 |
| C | 0.99440100 | 4.72288000 | -0.46694000 |
| C | 0.49982700 | 4.06987400 | 0.67036300 |
| H | 0.28914000 | 4.66013600 | 1.55668100 |
| C | 0.28664700 | 2.69756600 | 0.65257800 |

A17

| | | | |
|---|---|---|---|
| H | -0.10131300 | 2.21249400 | 1.53985400 |
| C | 1.67178800 | 6.77944100 | -1.47343500 |
| H | 1.74345200 | 7.82483500 | -1.16786300 |
| H | 0.99190800 | 6.70177900 | -2.33217800 |
| H | 2.66599300 | 6.42366600 | -1.77481300 |
| C | -2.25559900 | 0.66629300 | 0.00508500 |
| C | -2.67479800 | 0.92524200 | 1.32026900 |
| H | -2.09517100 | 0.53300900 | 2.14894200 |
| C | -3.82736300 | 1.65692500 | 1.58254500 |
| H | -4.15005300 | 1.85158400 | 2.60035600 |
| C | -4.60237600 | 2.15530700 | 0.52700200 |
| C | -4.20762100 | 1.90523400 | -0.79217300 |
| H | -4.78654000 | 2.27535800 | -1.63013400 |
| C | -3.04752200 | 1.16747800 | -1.03638000 |
| H | -2.75043400 | 0.98016300 | -2.06431000 |
| C | -6.53441800 | 3.38831900 | -0.14419200 |
| H | -7.35312400 | 3.90876800 | 0.35578400 |
| H | -6.94803600 | 2.59486100 | -0.78055500 |
| H | -5.98680800 | 4.10112700 | -0.77466800 |
| C | 2.17258700 | -0.93506100 | 1.95601200 |
| C | 4.35579300 | -0.98381600 | 2.61084900 |
| H | 5.38964800 | -1.28822500 | 2.57554600 |
| C | 3.71576200 | -0.10770500 | 3.42033000 |
| H | 4.07846400 | 0.50270700 | 4.23207100 |
| C | 3.72580000 | -2.50755700 | 0.74039100 |
| H | 4.78364900 | -2.42615500 | 0.48236200 |
| H | 3.13028000 | -2.35668600 | -0.15559200 |
| H | 3.52261600 | -3.50185000 | 1.15047100 |
| C | 1.38578100 | 0.73749500 | 3.66998900 |
| H | 1.74487600 | 1.76704700 | 3.74903800 |
| H | 1.16767200 | 0.34980800 | 4.66980200 |
| H | 0.47879600 | 0.71216000 | 3.07161000 |
| H | 0.97679700 | -2.88592800 | 1.04690100 |
| Na | -0.08107700 | -4.00132300 | -0.53349900 |

A18

**5**

| | | | |
|---|---|---|---|
| C | -1.17015400 | -0.14917000 | 0.00006100 |
| H | -1.71129900 | 0.21778000 | -0.88074500 |
| H | -1.71313700 | 0.22032600 | 0.87847600 |
| H | -1.15321500 | -1.24022700 | 0.00157700 |
| C | 0.23353600 | 0.40007100 | 0.00006000 |
| H | 0.29967200 | 1.51236200 | 0.00006400 |
| O | 1.23721100 | -0.27695600 | -0.00001200 |

**6**

| | | | |
|---|---|---|---|
| C | 1.89255900 | -0.61696200 | -0.00012600 |
| H | 2.96475000 | -0.37819600 | 0.00721200 |
| H | 1.67992100 | -1.22005100 | -0.89142800 |
| H | 1.67036200 | -1.23136700 | 0.88109900 |
| C | 1.01489000 | 0.64563400 | 0.00328100 |
| H | 1.32401000 | 1.26082300 | -0.87238800 |
| H | 1.31361000 | 1.24910400 | 0.89066400 |
| O | -0.32571900 | 0.36137400 | -0.00699700 |
| Na | -2.16287300 | -0.24939400 | 0.00198900 |

**TS3**

| | | | |
|---|---|---|---|
| C | 3.02663800 | 0.26431600 | -0.69250500 |
| H | 4.04608500 | 0.55197900 | -0.40697500 |
| H | 2.61663500 | 1.04734300 | -1.33932500 |
| H | 3.08219900 | -0.66012900 | -1.27837200 |
| C | 2.13559200 | 0.06342700 | 0.53603500 |
| H | 2.12582800 | 1.00228400 | 1.12158900 |
| H | 2.60184700 | -0.69438600 | 1.19127300 |
| O | 0.83275900 | -0.31307600 | 0.19350400 |

A19

| Na | -0.79483400 | -1.61985500 | 0.12398900 |
| C | -1.10043800 | 1.43773300 | 0.50257300 |
| H | -1.28484900 | 1.17953100 | 1.54948500 |
| H | -0.92422600 | 2.50324700 | 0.35716800 |
| H | -0.02629300 | 0.70052900 | 0.27888400 |
| C | -2.04087300 | 0.85556300 | -0.41109600 |
| H | -2.30197900 | 1.44597000 | -1.31323300 |
| O | -2.49745700 | -0.30994800 | -0.33530700 |

**7**

| C | 0.89444100 | 0.40157400 | -0.18836600 |
| H | 1.61693300 | 0.80411400 | -0.92714000 |
| C | 1.02089600 | -0.94522100 | 0.11783500 |
| H | 0.57752200 | -1.33137000 | 1.03975200 |
| H | 1.82771500 | -1.53124400 | -0.30759700 |
| O | -0.01584700 | 1.20611700 | 0.23632200 |
| Na | -1.39885600 | -0.39350400 | -0.11567300 |

**8**

| C | 2.54186900 | -0.10758700 | 0.20821600 |
| H | 3.10709900 | -0.89182200 | -0.30449800 |
| H | 3.09186200 | 0.83724700 | 0.11727500 |
| H | 2.47381600 | -0.38096800 | 1.26741300 |
| C | 1.12940800 | -0.04236100 | -0.40998400 |
| C | 0.36280600 | 1.18869000 | 0.38220100 |
| H | 0.97106800 | 2.09632900 | 0.32597900 |
| H | 0.27976900 | 0.84615200 | 1.41879300 |
| C | -0.96124600 | 1.41135300 | -0.21059900 |
| H | -1.03689100 | 2.20079200 | -0.98555900 |
| O | -1.96565700 | 0.72576200 | 0.02009300 |
| O | 0.46204100 | -1.19696400 | -0.32774300 |

| H  | 1.24737500  | 0.33939200  | -1.45262300 |
|----|-------------|-------------|-------------|
| Na | -1.50383600 | -1.45255200 | 0.20503800  |

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| C | 2.20691500  | -0.35836300 | 0.10374400  |
|---|-------------|-------------|-------------|
| H | 2.88328300  | 0.40871200  | 0.48947400  |
| H | 2.41476900  | -1.30052200 | 0.62086400  |
| H | 2.41610100  | -0.49000500 | -0.96287000 |
| C | 0.76196000  | 0.07730800  | 0.30910600  |
| C | -0.23477600 | -0.96725400 | -0.22027900 |
| H | -0.10042900 | -1.94270200 | 0.26866500  |
| H | -0.06071500 | -1.14384600 | -1.29328100 |
| C | -1.68072800 | -0.56481900 | -0.06887400 |
| H | -2.42573100 | -1.36047300 | -0.28862300 |
| O | -2.05778600 | 0.54443100  | 0.25909500  |
| O | 0.59356700  | 1.31842800  | -0.36038100 |
| H | 0.57624500  | 0.19873500  | 1.38961700  |
| H | -0.30999900 | 1.60601100  | -0.15574000 |

**TS4E**

| C | 3.28427000  | -0.63754000 | 0.69740400  |
|---|-------------|-------------|-------------|
| H | 4.04663700  | -1.33931500 | 0.34642200  |
| H | 3.73730200  | 0.35379400  | 0.79774100  |
| H | 2.94668500  | -0.96644900 | 1.68584300  |
| C | 2.10609700  | -0.59797800 | -0.27179500 |
| C | 0.98096700  | 0.33195600  | 0.17074700  |
| H | -0.17676800 | -0.01485000 | -0.30365200 |
| H | 0.74605200  | 0.24760500  | 1.23918100  |
| C | 1.01766800  | 1.69981000  | -0.27714300 |
| H | 1.71800700  | 1.93739000  | -1.10553300 |

| O  | 0.24557500  | 2.60909300  | 0.10346700  |
|----|-------------|-------------|-------------|
| O  | 1.65309800  | -1.95274900 | -0.38967300 |
| H  | 2.47558500  | -0.24887500 | -1.25318600 |
| H  | 0.88110500  | -1.94698600 | -0.97108000 |
| O  | -1.50707900 | -0.16613000 | -0.56922700 |
| C  | -1.94133300 | -1.47344300 | -0.32164600 |
| H  | -2.24519900 | -1.97484200 | -1.25897100 |
| H  | -1.11625700 | -2.08161600 | 0.09618800  |
| C  | -3.11796500 | -1.53127900 | 0.65645300  |
| H  | -3.44777600 | -2.56159300 | 0.83631800  |
| H  | -3.97308900 | -0.96878000 | 0.26082900  |
| H  | -2.83366800 | -1.09397700 | 1.62179400  |
| Na | -1.80632700 | 1.81705600  | 0.08431400  |

**TS4Z**

| C | 1.15270900  | 2.48685200  | 0.00163600  |
|---|-------------|-------------|-------------|
| H | 1.34336900  | 3.05885500  | -0.91051100 |
| H | 0.15817900  | 2.74315400  | 0.37901900  |
| H | 1.89721300  | 2.77733400  | 0.74990400  |
| C | 1.25165800  | 0.99382100  | -0.28049300 |
| C | 0.95983600  | 0.16424100  | 0.98584700  |
| H | -0.29581500 | -0.07648400 | 0.89279400  |
| H | 1.18277600  | 0.67475500  | 1.92570500  |
| C | 1.41004700  | -1.19770800 | 0.97453500  |
| H | 1.61341800  | -1.68016200 | 1.94968000  |
| O | 1.48193700  | -1.90940600 | -0.06073300 |
| O | 2.55274200  | 0.75505300  | -0.82018800 |
| H | 0.49202700  | 0.74658600  | -1.04325600 |
| H | 2.61168200  | -0.20121600 | -0.96280200 |
| O | -1.52766900 | -0.51443000 | 0.40534200  |
| C | -2.59385800 | 0.34414500  | 0.68320400  |
| H | -3.35084100 | -0.15361700 | 1.31691100  |

| | | | |
|---|---|---|---|
| H | -2.24689600 | 1.21810000 | 1.26689900 |
| C | -3.28302300 | 0.85754000 | -0.58451200 |
| H | -4.10773400 | 1.54195400 | -0.35092100 |
| H | -3.69415900 | 0.02088000 | -1.16370800 |
| H | -2.56461900 | 1.38946000 | -1.21886400 |
| Na | -0.58899000 | -1.87297100 | -0.88250200 |

**10E**

| | | | |
|---|---|---|---|
| C | 2.45069000 | -0.60289400 | -0.75457400 |
| H | 3.46750800 | -0.47667900 | -0.37097200 |
| H | 2.29599300 | -1.65416600 | -1.01305300 |
| H | 2.35699600 | -0.00365500 | -1.66708000 |
| C | 1.42430100 | -0.15013800 | 0.28136400 |
| C | 0.00723700 | -0.24635900 | -0.19774100 |
| H | -0.16190300 | -0.01476400 | -1.25766600 |
| C | -1.00726900 | -0.87120200 | 0.51146000 |
| H | -0.71130600 | -1.31800700 | 1.48269500 |
| O | -2.25268000 | -0.94174300 | 0.18974500 |
| O | 1.81036600 | 1.20359400 | 0.63209700 |
| H | 1.52695300 | -0.78639900 | 1.17760000 |
| H | 1.13751700 | 1.50686700 | 1.25587600 |
| Na | -2.14754500 | 1.07959600 | -0.47501700 |

**10Z**

| | | | |
|---|---|---|---|
| C | 2.38045900 | 0.14596700 | 0.30259700 |
| H | 2.99641800 | -0.71337800 | 0.58799500 |
| H | 2.97610900 | 0.80555700 | -0.33762200 |
| H | 2.11207400 | 0.70614200 | 1.20422700 |
| C | 1.11517400 | -0.31103500 | -0.43313200 |
| C | 0.21521900 | 0.84420300 | -0.83527400 |

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| H | 0.55205400 | 1.46997200 | -1.65747300 |
|---|---|---|---|
| C | -0.79616100 | 1.31218600 | -0.02590600 |
| H | -1.26858500 | 2.26768100 | -0.32057300 |
| O | -1.30244300 | 0.69646400 | 1.01176800 |
| O | 0.39028300 | -1.26095000 | 0.40500800 |
| H | 1.42495500 | -0.88794200 | -1.31481200 |
| H | -0.04930400 | -0.67275100 | 1.06864400 |
| Na | -1.72132600 | -0.94612100 | -0.41948200 |

**TS5E**

| C | 2.17154900 | 2.39033700 | 0.03975100 |
|---|---|---|---|
| H | 1.84952600 | 2.90181200 | -0.86827100 |
| H | 1.59973700 | 2.78257400 | 0.88439800 |
| H | 3.22950800 | 2.63691000 | 0.20569400 |
| C | 2.01746100 | 0.90424300 | -0.07336800 |
| C | 2.03683900 | 0.08094700 | 1.03100200 |
| H | -1.42526800 | 0.32658800 | -0.55209600 |
| H | 2.03402300 | 0.50957900 | 2.03047000 |
| C | 2.06065400 | -1.34098500 | 0.92948400 |
| H | 2.29901700 | -1.88752900 | 1.86322500 |
| O | 1.82229900 | -2.01539500 | -0.09916900 |
| O | -0.01205800 | 0.93860100 | -0.94545000 |
| H | 2.26484000 | 0.45669900 | -1.02976900 |
| H | -0.02433100 | 1.59055000 | -1.65789600 |
| O | -2.05862300 | -0.46204000 | -0.43169800 |
| C | -2.86731600 | -0.28958700 | 0.72250600 |
| H | -3.30780100 | -1.26599700 | 0.95789500 |
| H | -2.25031000 | 0.00342200 | 1.58685700 |
| C | -3.97385100 | 0.73835900 | 0.50402700 |
| H | -4.60678300 | 0.82683200 | 1.39454300 |
| H | -4.60441500 | 0.44730700 | -0.34178000 |
| H | -3.55034000 | 1.72539300 | 0.28975000 |

| Na | -0.01748800 | -1.24030400 | -1.07935400 |

**TS5Z**

| C  | 2.68124200  | 1.40595800  | -0.37738900 |
| H  | 2.20744600  | 2.22010300  | -0.92633500 |
| H  | 3.65952900  | 1.76581400  | -0.02683100 |
| H  | 2.85630800  | 0.56232900  | -1.04518600 |
| C  | 1.86944900  | 1.02397400  | 0.82596500  |
| C  | 1.78113100  | -0.23561300 | 1.36612300  |
| H  | -1.46724900 | 0.59787700  | -0.32656200 |
| H  | 1.47455200  | -0.33477200 | 2.40490100  |
| C  | 1.98708800  | -1.47297000 | 0.66926400  |
| H  | 2.14605000  | -2.36038000 | 1.31371100  |
| O  | 1.94609100  | -1.64729700 | -0.56690300 |
| O  | -0.16082800 | 1.41647200  | -0.27102600 |
| H  | 1.61132400  | 1.84853800  | 1.48309500  |
| H  | -0.23407900 | 2.31629500  | -0.61258300 |
| O  | -2.02320000 | -0.22679400 | -0.59701800 |
| C  | -2.94002400 | -0.58479800 | 0.42266400  |
| H  | -3.26846000 | -1.61283300 | 0.22401100  |
| H  | -2.44358800 | -0.59017600 | 1.40673100  |
| C  | -4.15147200 | 0.34340000  | 0.46322500  |
| H  | -4.86311200 | 0.02640600  | 1.23451300  |
| H  | -4.66514700 | 0.34311800  | -0.50324500 |
| H  | -3.84536900 | 1.37118000  | 0.68562800  |
| Na | 0.12461900  | -0.48838700 | -1.27739900 |

**H₂O**

| H | 0.000000000 | 0.759279000 | -0.47674800 |
| O | 0.000000000 | 0.000000000 | 0.119187000 |

H          0.000000000   -0.759279000   -0.47674800

**11E**

| C | 1.40534400 | 0.33374200 | 0.00003500 |
|---|---|---|---|
| H | 1.36360700 | 1.44773900 | 0.00008700 |
| O | 2.47150900 | -0.25313600 | -0.00006500 |
| C | 0.09201800 | -0.32479200 | 0.00008800 |
| H | 0.08820500 | -1.41265700 | 0.00002600 |
| C | -1.04304600 | 0.39088700 | 0.00003000 |
| H | -0.96034300 | 1.47960000 | -0.00017100 |
| C | -2.43034900 | -0.16587900 | -0.00004500 |
| H | -2.98794000 | 0.18292800 | -0.87825300 |
| H | -2.98778600 | 0.18247000 | 0.87848300 |
| H | -2.43161400 | -1.25873900 | -0.00030100 |

**11Z**

| C | 1.11931100 | -0.36693400 | -0.00009800 |
|---|---|---|---|
| H | 0.68833300 | -1.38976500 | -0.00033300 |
| O | 2.32826600 | -0.20977700 | 0.00008700 |
| C | 0.16479300 | 0.75087400 | -0.00001000 |
| H | 0.62659500 | 1.73532100 | 0.00005300 |
| C | -1.17628700 | 0.64071900 | -0.00005900 |
| H | -1.74875900 | 1.56846600 | -0.00004000 |
| C | -2.01186400 | -0.60443000 | 0.00004400 |
| H | -2.66996100 | -0.61542500 | -0.87753800 |
| H | -2.66914100 | -0.61569900 | 0.87826500 |
| H | -1.42891300 | -1.52605800 | -0.00036300 |

**TS6E**

| Ru | -1.10200300 | -0.15161000 | 0.60155100 |
|---|---|---|---|
| N | -2.37703100 | -2.93619700 | 1.15474900 |
| N | -0.98636500 | -2.44281300 | 2.72382900 |
| O | -1.30078900 | 1.45179600 | 3.15922700 |
| O | -2.13307400 | -0.23186700 | -2.52605200 |
| O | 6.01356900 | -2.63503900 | 0.63072000 |
| O | 4.37912000 | 4.88120500 | 1.10382800 |
| C | -1.21469800 | 0.81085000 | 2.18572100 |
| C | -1.04979200 | -0.04691900 | -1.77274000 |
| C | -0.15356500 | -1.08850200 | -1.36456500 |
| C | 0.90253000 | -0.47391700 | -0.57402300 |
| C | 0.60839300 | 0.94071800 | -0.48058200 |
| C | -0.60639000 | 1.21617100 | -1.20618600 |
| C | -0.24834400 | -2.50696900 | -1.78313600 |
| C | -0.78446900 | -2.84198700 | -3.04024000 |
| H | -1.14822600 | -2.05343900 | -3.68735000 |
| C | -0.87386400 | -4.17361800 | -3.44781400 |
| H | -1.29495700 | -4.40609900 | -4.42215500 |
| C | -0.42665100 | -5.20085800 | -2.61559400 |
| H | -0.49685500 | -6.23697700 | -2.93484300 |
| C | 0.11562200 | -4.88164400 | -1.36766900 |
| H | 0.47026900 | -5.67021100 | -0.70933700 |
| C | 0.20398400 | -3.55311100 | -0.95687000 |
| H | 0.62158900 | -3.31983900 | 0.01582700 |
| C | -1.17977100 | 2.54371100 | -1.52414000 |
| C | -1.74042400 | 2.77989200 | -2.79299100 |
| H | -1.78006700 | 1.97150500 | -3.51377200 |
| C | -2.25651400 | 4.03300600 | -3.12428700 |
| H | -2.68732800 | 4.18959600 | -4.10945800 |
| C | -2.21919300 | 5.07923800 | -2.20171700 |
| H | -2.62105200 | 6.05471900 | -2.46098600 |
| C | -1.66420200 | 4.85774700 | -0.93889000 |

| | | | |
|---|---|---|---|
| H | -1.63394100 | 5.66119700 | -0.20794300 |
| C | -1.15599300 | 3.60528700 | -0.60149500 |
| H | -0.74664400 | 3.44349700 | 0.38879100 |
| C | 2.21919100 | -1.07473600 | -0.24959700 |
| C | 2.92491400 | -1.79276600 | -1.22634700 |
| H | 2.48169200 | -1.93499200 | -2.20636100 |
| C | 4.18912900 | -2.33156500 | -0.97805000 |
| H | 4.69292700 | -2.87941900 | -1.76569300 |
| C | 4.78668000 | -2.15137800 | 0.27402500 |
| C | 4.10487900 | -1.42438800 | 1.26025800 |
| H | 4.58248100 | -1.28401700 | 2.22465800 |
| C | 2.84691900 | -0.89897000 | 0.99785100 |
| H | 2.34120200 | -0.32946300 | 1.76912600 |
| C | 6.74916400 | -3.36867800 | -0.33415200 |
| H | 7.68367300 | -3.65481700 | 0.15136800 |
| H | 6.97529300 | -2.76154900 | -1.22043500 |
| H | 6.21524100 | -4.27459600 | -0.64991600 |
| C | 1.58136700 | 1.97851600 | -0.03172200 |
| C | 1.76474400 | 2.37070100 | 1.30420500 |
| H | 1.15587800 | 1.92408200 | 2.08206600 |
| C | 2.70115300 | 3.33731800 | 1.65057800 |
| H | 2.83701500 | 3.64249600 | 2.68307500 |
| C | 3.48883100 | 3.94449000 | 0.66305500 |
| C | 3.32072000 | 3.57074400 | -0.67505400 |
| H | 3.91177900 | 4.02360600 | -1.46220000 |
| C | 2.37418500 | 2.59912600 | -1.00546400 |
| H | 2.24996000 | 2.31974900 | -2.04769100 |
| C | 5.19499400 | 5.53318300 | 0.14449400 |
| H | 5.81924600 | 6.23196200 | 0.70380900 |
| H | 4.59542500 | 6.09135100 | -0.58632900 |
| H | 5.83952300 | 4.82329600 | -0.39019000 |
| C | -1.52098900 | -1.94703100 | 1.56204500 |
| C | -2.36538300 | -4.00862800 | 2.03304900 |
| H | -2.96909700 | -4.88724700 | 1.87093800 |

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| C | -1.49483800 | -3.69801400 | 3.02216700 |
|---|---|---|---|
| H | -1.19477700 | -4.24695900 | 3.90045300 |
| C | -3.18303500 | -2.96325400 | -0.06603500 |
| H | -2.78589300 | -3.71462200 | -0.75226600 |
| H | -3.17553800 | -1.99373100 | -0.55675000 |
| H | -4.21510200 | -3.21449700 | 0.19405200 |
| C | 0.00123500 | -1.76970000 | 3.56064200 |
| H | 0.40988700 | -2.49816100 | 4.26363800 |
| H | -0.44982700 | -0.94645400 | 4.11801700 |
| H | 0.80580800 | -1.38297600 | 2.93686500 |
| C | -4.12344000 | 0.34404900 | 0.01980800 |
| H | -2.78082900 | 0.05974200 | 0.51333200 |
| O | -4.19942300 | -0.03602800 | -1.19565400 |
| H | -3.02072000 | -0.00494400 | -2.02774000 |
| H | -4.54045100 | -0.33639100 | 0.78264100 |
| C | -4.23028100 | 1.79283300 | 0.34258100 |
| H | -3.98469800 | 2.44964000 | -0.48743000 |
| C | -4.63436800 | 2.31971800 | 1.50864200 |
| H | -4.70208000 | 3.40610800 | 1.56393400 |
| C | -4.99351500 | 1.59798500 | 2.77590300 |
| H | -5.97892200 | 1.91671600 | 3.13773200 |
| H | -4.27126000 | 1.84199200 | 3.56478000 |
| H | -5.00744200 | 0.51161000 | 2.66493400 |

**TS6Z**

| Ru | 0.93007900 | -0.27216000 | 0.72066100 |
|---|---|---|---|
| N | 3.13859500 | 1.86181900 | 1.18020600 |
| N | 1.60348300 | 2.08032100 | 2.67477300 |
| O | 0.40878600 | -1.59159100 | 3.39723300 |
| O | 2.03980900 | -0.74094300 | -2.34810300 |
| O | -4.87352500 | 4.48326400 | 0.28728300 |
| O | -5.94534800 | -3.12151900 | 1.11724100 |

| | | | |
|---|---|---|---|
| C | 0.61246100 | -1.06444500 | 2.37464900 |
| C | 0.94113200 | -0.49453300 | -1.65771900 |
| C | 0.44637900 | 0.81229900 | -1.33000600 |
| C | -0.77699200 | 0.64412100 | -0.55836600 |
| C | -0.99707500 | -0.78218200 | -0.39623500 |
| C | 0.07243000 | -1.49355700 | -1.04273200 |
| C | 1.03989200 | 2.08504900 | -1.80253100 |
| C | 1.69719600 | 2.14088600 | -3.04567900 |
| H | 1.78462000 | 1.23840200 | -3.63803100 |
| C | 2.25494800 | 3.33417400 | -3.50657100 |
| H | 2.75944800 | 3.35050800 | -4.46885700 |
| C | 2.16705700 | 4.49896200 | -2.74273600 |
| H | 2.60201600 | 5.42694300 | -3.10335100 |
| C | 1.51153000 | 4.45893400 | -1.50927600 |
| H | 1.43402400 | 5.35784200 | -0.90353700 |
| C | 0.95518800 | 3.26869600 | -1.04522900 |
| H | 0.45416700 | 3.25055000 | -0.08423000 |
| C | 0.18363200 | -2.95453400 | -1.25249700 |
| C | 0.63730800 | -3.45265300 | -2.48778300 |
| H | 0.93922000 | -2.75586300 | -3.26121100 |
| C | 0.71314300 | -4.82600100 | -2.71883200 |
| H | 1.06744000 | -5.18719400 | -3.68037900 |
| C | 0.33837500 | -5.73160600 | -1.72563900 |
| H | 0.39933100 | -6.80100500 | -1.90682900 |
| C | -0.10815700 | -5.25036400 | -0.49277700 |
| H | -0.39554200 | -5.94433200 | 0.29227500 |
| C | -0.18027700 | -3.87900100 | -0.25614800 |
| H | -0.51697000 | -3.51783800 | 0.70918100 |
| C | -1.81706000 | 1.67620100 | -0.32821000 |
| C | -2.20133700 | 2.53231200 | -1.37069800 |
| H | -1.70418800 | 2.45687500 | -2.33205100 |
| C | -3.21225700 | 3.48240500 | -1.21140700 |
| H | -3.47204700 | 4.12136100 | -2.04719100 |
| C | -3.87580900 | 3.59086100 | 0.01552000 |

| | | | |
|---|---|---|---|
| C | -3.51651500 | 2.73548200 | 1.06690800 |
| H | -4.04416500 | 2.82382900 | 2.01115600 |
| C | -2.50689800 | 1.79867800 | 0.89251500 |
| H | -2.25104100 | 1.13875700 | 1.71351900 |
| C | -5.28218500 | 5.36458500 | -0.74564700 |
| H | -6.07751300 | 5.97960900 | -0.32131800 |
| H | -5.67363900 | 4.81877900 | -1.61399700 |
| H | -4.46058500 | 6.01454400 | -1.07418100 |
| C | -2.28201500 | -1.40224700 | 0.03813900 |
| C | -2.65572100 | -1.60874800 | 1.37587800 |
| H | -1.97461800 | -1.33165500 | 2.17221400 |
| C | -3.87847900 | -2.18220700 | 1.70310300 |
| H | -4.16219500 | -2.34604600 | 2.73763300 |
| C | -4.77115900 | -2.56835500 | 0.69405500 |
| C | -4.41758300 | -2.37481200 | -0.64615900 |
| H | -5.08373800 | -2.66603000 | -1.44955400 |
| C | -3.18447000 | -1.79909600 | -0.95713100 |
| H | -2.91915300 | -1.65769200 | -2.00084400 |
| C | -6.88107400 | -3.53860300 | 0.13658000 |
| H | -7.73165700 | -3.94663800 | 0.68502200 |
| H | -6.46565800 | -4.31788300 | -0.51554200 |
| H | -7.22165000 | -2.69869100 | -0.48292000 |
| C | 1.95482200 | 1.31417500 | 1.59394100 |
| C | 3.50339400 | 2.93631100 | 1.97552900 |
| H | 4.40422800 | 3.50105400 | 1.79623800 |
| C | 2.54143800 | 3.07232900 | 2.91869700 |
| H | 2.44085600 | 3.77214200 | 3.73284500 |
| C | 3.93198400 | 1.46472700 | 0.01748600 |
| H | 3.78923100 | 2.18381700 | -0.79239500 |
| H | 3.64080000 | 0.47666000 | -0.32813000 |
| H | 4.98596100 | 1.43695700 | 0.30412000 |
| C | 0.40489800 | 1.90517100 | 3.48798300 |
| H | 0.27665200 | 2.79475300 | 4.10765600 |
| H | 0.49154000 | 1.02821100 | 4.13250800 |

A31

| | | | |
|---|---|---|---|
| H | -0.46337600 | 1.79160100 | 2.84044800 |
| C | 4.25531000 | -2.09444400 | 1.38605700 |
| C | 3.32963300 | -2.08267000 | 0.21645600 |
| H | 3.75850500 | -2.34654200 | 2.32203800 |
| H | 2.45573200 | -1.08058300 | 0.71551500 |
| H | 2.56914400 | -2.87850500 | 0.28282300 |
| O | 3.74284500 | -1.75117000 | -0.96377200 |
| H | 2.77934000 | -1.31684300 | -1.78582100 |
| C | 5.58333400 | -1.89462900 | 1.40172600 |
| H | 6.07378700 | -2.00324400 | 2.37044700 |
| C | 6.49686400 | -1.56946000 | 0.25599200 |
| H | 7.31862700 | -2.29581000 | 0.20993100 |
| H | 6.96741300 | -0.58775800 | 0.40746000 |
| H | 5.96338400 | -1.56057900 | -0.69288400 |

**TS7E**

| | | | |
|---|---|---|---|
| Ru | -0.76287100 | -0.78826900 | 0.64959300 |
| N | -0.09952900 | -3.75924900 | 1.31612700 |
| N | 0.71718000 | -2.46972700 | 2.83542800 |
| O | -1.87130700 | 0.47458800 | 3.16873100 |
| O | -1.60878900 | -1.52290300 | -2.43903900 |
| O | 6.45105900 | 1.37835600 | 0.49564200 |
| O | 0.73462200 | 6.50497800 | 0.97799900 |
| C | -1.42662700 | -0.02676400 | 2.21265500 |
| C | -0.82565700 | -0.72909000 | -1.72872300 |
| C | 0.51760900 | -1.04083100 | -1.32345900 |
| C | 1.02284600 | 0.09206200 | -0.56355700 |
| C | -0.04296400 | 1.07128500 | -0.47864200 |
| C | -1.19771400 | 0.56752900 | -1.17571700 |
| C | 1.26643500 | -2.25500700 | -1.72453800 |
| C | 0.99619500 | -2.88148700 | -2.95534800 |

A32

| | | | |
|---|---|---|---|
| H | 0.21772900 | -2.48007700 | -3.59220500 |
| C | 1.69796900 | -4.02245300 | -3.34631400 |
| H | 1.46776800 | -4.48927000 | -4.30016800 |
| C | 2.68781300 | -4.56257900 | -2.52388000 |
| H | 3.23327200 | -5.45077800 | -2.83046400 |
| C | 2.97136000 | -3.94625800 | -1.30197900 |
| H | 3.74041800 | -4.35369700 | -0.65110900 |
| C | 2.27049100 | -2.80842800 | -0.90728100 |
| H | 2.49614100 | -2.34511900 | 0.04632800 |
| C | -2.44923200 | 1.29700500 | -1.48171400 |
| C | -3.07767900 | 1.12194100 | -2.72867700 |
| H | -2.65497200 | 0.42317100 | -3.44089600 |
| C | -4.24265200 | 1.82116900 | -3.04599000 |
| H | -4.71125500 | 1.66609600 | -4.01398600 |
| C | -4.80324100 | 2.71383100 | -2.13160400 |
| H | -5.70992300 | 3.25812600 | -2.38049500 |
| C | -4.18830300 | 2.89715700 | -0.89029500 |
| H | -4.61543900 | 3.58551600 | -0.16609400 |
| C | -3.02952400 | 2.19443200 | -0.56677000 |
| H | -2.57594400 | 2.33175500 | 0.40779200 |
| C | 2.44735200 | 0.38811900 | -0.27364700 |
| C | 3.41791200 | 0.20384900 | -1.26951600 |
| H | 3.12122700 | -0.19265900 | -2.23480400 |
| C | 4.76191000 | 0.51828700 | -1.05837900 |
| H | 5.47355300 | 0.35658000 | -1.85943800 |
| C | 5.16710200 | 1.04018400 | 0.17485500 |
| C | 4.21065900 | 1.24598700 | 1.17926600 |
| H | 4.53575700 | 1.65985300 | 2.12840100 |
| C | 2.87897500 | 0.92525100 | 0.95323600 |
| H | 2.15262000 | 1.10456100 | 1.73731800 |
| C | 7.45580200 | 1.19810600 | -0.48856100 |
| H | 8.39034800 | 1.52582700 | -0.03020100 |
| H | 7.26167500 | 1.80427000 | -1.38302800 |
| H | 7.54986100 | 0.14526000 | -0.78530600 |

A33

| | | | |
|---|---|---|---|
| C | 0.14592700 | 2.49110700 | -0.06272900 |
| C | 0.10636100 | 2.94147200 | 1.26683900 |
| H | -0.09896700 | 2.23726100 | 2.06511500 |
| C | 0.30515700 | 4.28034700 | 1.58146200 |
| H | 0.26811900 | 4.62679400 | 2.60919100 |
| C | 0.55246900 | 5.21570800 | 0.56741400 |
| C | 0.59313700 | 4.78912700 | -0.76485800 |
| H | 0.77861100 | 5.48792700 | -1.57189200 |
| C | 0.38949900 | 3.44060900 | -1.06328000 |
| H | 0.41946500 | 3.12196600 | -2.10119400 |
| C | 0.97876100 | 7.49395400 | -0.00870700 |
| H | 1.08995600 | 8.43662700 | 0.52961100 |
| H | 0.14210300 | 7.57867100 | -0.71435800 |
| H | 1.89982200 | 7.28909500 | -0.56985300 |
| C | -0.00992500 | -2.43963200 | 1.67275400 |
| C | 0.55570100 | -4.57481500 | 2.22549100 |
| H | 0.60087200 | -5.64533300 | 2.10436000 |
| C | 1.06627600 | -3.76585100 | 3.18329300 |
| H | 1.63784200 | -3.99002700 | 4.06975600 |
| C | -0.73755700 | -4.31570600 | 0.12257100 |
| H | 0.02480400 | -4.72464500 | -0.54424600 |
| H | -1.30302700 | -3.55391100 | -0.40724000 |
| H | -1.42494200 | -5.11094100 | 0.42433700 |
| C | 1.09397300 | -1.30896800 | 3.63460000 |
| H | 1.86595400 | -1.61502300 | 4.34328600 |
| H | 0.23729200 | -0.91437500 | 4.18453700 |
| H | 1.49235300 | -0.53180000 | 2.98450200 |
| C | -3.45577400 | -2.21504900 | 0.11698600 |
| H | -2.24896200 | -1.64177600 | 0.58635900 |
| O | -3.27710100 | -2.63250300 | -1.09353600 |
| H | -2.44521600 | -1.93630300 | -1.88200900 |
| H | -3.43937600 | -2.98578100 | 0.90923900 |
| C | -4.42849600 | -1.12014700 | 0.38148200 |
| H | -4.54448900 | -0.38675900 | -0.41272400 |

| | | | |
|---|---|---|---|
| C | -5.15584500 | -1.04955900 | 1.50257800 |
| H | -5.00938100 | -1.81280000 | 2.26978400 |
| C | -6.17870900 | 0.00536100 | 1.80169900 |
| H | -5.93155700 | 0.53634600 | 2.72980600 |
| H | -7.17331500 | -0.43555100 | 1.94835700 |
| H | -6.24266000 | 0.73994000 | 0.99420800 |

**TS7Z**

| | | | |
|---|---|---|---|
| Ru | -0.96590500 | -0.25094900 | -0.63314600 |
| N | -3.13821700 | 1.93420500 | -1.02100500 |
| N | -1.66333700 | 2.09694100 | -2.58205400 |
| O | -0.60725900 | -1.61318600 | -3.31477800 |
| O | -1.94633600 | -0.63652500 | 2.49235900 |
| O | 4.99042700 | 4.33540800 | -0.53979700 |
| O | 5.80359000 | -3.30175800 | -1.28893100 |
| C | -0.74702500 | -1.07008700 | -2.28962100 |
| C | -0.87436500 | -0.43425100 | 1.74750600 |
| C | -0.35714900 | 0.85169800 | 1.37543800 |
| C | 0.82457600 | 0.63540200 | 0.55239300 |
| C | 0.99550400 | -0.79886200 | 0.40472300 |
| C | -0.06338900 | -1.46814500 | 1.11137100 |
| C | -0.89160500 | 2.14882700 | 1.85208200 |
| C | -1.48951800 | 2.24371400 | 3.12262700 |
| H | -1.57666200 | 1.35331900 | 3.73304200 |
| C | -1.99018800 | 3.46030300 | 3.58817000 |
| H | -2.44946300 | 3.50670300 | 4.57189300 |
| C | -1.90309800 | 4.60997400 | 2.80167100 |
| H | -2.29354100 | 5.55613500 | 3.16598900 |
| C | -1.30649100 | 4.53103200 | 1.54052100 |
| H | -1.23057200 | 5.41767000 | 0.91675800 |
| C | -0.80725100 | 3.31751700 | 1.07178400 |
| H | -0.35168100 | 3.26954500 | 0.08940400 |

| | | | |
|---|---|---|---|
| C | -0.20560900 | -2.92159000 | 1.35240900 |
| C | -0.62111300 | -3.38526200 | 2.61433100 |
| H | -0.87163300 | -2.66679700 | 3.38623300 |
| C | -0.72507200 | -4.75164800 | 2.87384200 |
| H | -1.04897300 | -5.08571800 | 3.85570500 |
| C | -0.41707700 | -5.68482000 | 1.88321900 |
| H | -0.49987500 | -6.74874300 | 2.08666200 |
| C | -0.00920100 | -5.23794200 | 0.62433800 |
| H | 0.22618400 | -5.95334200 | -0.15881500 |
| C | 0.09075700 | -3.87348900 | 0.35939100 |
| H | 0.39704600 | -3.53948500 | -0.62561100 |
| C | 1.88302900 | 1.63192300 | 0.25859400 |
| C | 2.33667400 | 2.49465200 | 1.26720900 |
| H | 1.87951000 | 2.45117500 | 2.25012300 |
| C | 3.36685700 | 3.41126300 | 1.04689300 |
| H | 3.68077100 | 4.05701400 | 1.85853800 |
| C | 3.97986800 | 3.47790600 | -0.20895400 |
| C | 3.55108900 | 2.61482800 | -1.22749700 |
| H | 4.04006100 | 2.67036400 | -2.19479100 |
| C | 2.52311100 | 1.71177600 | -0.99245900 |
| H | 2.21308600 | 1.04497900 | -1.78893400 |
| C | 5.46789400 | 5.22255900 | 0.45797000 |
| H | 6.26144700 | 5.80653400 | -0.01120000 |
| H | 5.88057100 | 4.68106400 | 1.31918100 |
| H | 4.67991800 | 5.90189600 | 0.80871300 |
| C | 2.24176000 | -1.46234400 | -0.07606700 |
| C | 2.54205500 | -1.71369500 | -1.42458400 |
| H | 1.82843700 | -1.44025000 | -2.19326500 |
| C | 3.73264900 | -2.32637300 | -1.79648000 |
| H | 3.95969300 | -2.52449700 | -2.83898000 |
| C | 4.66582900 | -2.70807100 | -0.82303000 |
| C | 4.38542800 | -2.47009600 | 0.52727900 |
| H | 5.08434900 | -2.75652400 | 1.30412500 |
| C | 3.18384900 | -1.85512200 | 0.88339400 |

A36

| | | | |
|---|---|---|---|
| H | 2.97541700 | -1.67893900 | 1.93470800 |
| C | 6.77768200 | -3.71580000 | -0.34509300 |
| H | 7.58943000 | -4.15962800 | -0.92377800 |
| H | 6.37755000 | -4.46666400 | 0.34861200 |
| H | 7.16913600 | -2.86844600 | 0.23283600 |
| C | -1.98791900 | 1.35126500 | -1.47880200 |
| C | -3.50818600 | 3.01028000 | -1.81179600 |
| H | -4.38504700 | 3.60097900 | -1.60022700 |
| C | -2.58446800 | 3.11119000 | -2.79675500 |
| H | -2.50083900 | 3.79966000 | -3.62241300 |
| C | -3.88571900 | 1.57483600 | 0.18400900 |
| H | -3.65813800 | 2.27992800 | 0.98674400 |
| H | -3.63214000 | 0.56968000 | 0.51022900 |
| H | -4.95354500 | 1.60904200 | -0.04406800 |
| C | -0.50304400 | 1.88397600 | -3.44058400 |
| H | -0.38062100 | 2.76224900 | -4.07734700 |
| H | -0.63500200 | 1.00077100 | -4.06863800 |
| H | 0.38809000 | 1.75933200 | -2.82688500 |
| C | -4.38924600 | -1.98870400 | -1.07981700 |
| C | -3.37950200 | -1.99499800 | 0.01690100 |
| H | -4.02557200 | -2.28603400 | -2.06280600 |
| H | -2.50526900 | -1.01725000 | -0.55244100 |
| H | -2.64144900 | -2.80824600 | -0.07063000 |
| O | -3.73488900 | -1.62495500 | 1.20193900 |
| H | -2.72692900 | -1.19996700 | 1.97421400 |
| C | -5.67732300 | -1.68447300 | -0.87976200 |
| H | -5.97691000 | -1.41257700 | 0.13126900 |
| C | -6.74359900 | -1.71294200 | -1.93281600 |
| H | -7.22432900 | -0.73107000 | -2.03563000 |
| H | -7.54078800 | -2.41968500 | -1.66842900 |
| H | -6.34399000 | -1.99957300 | -2.91026200 |

**TS8E**

| Ru | -0.96116900 | -0.04205800 | 0.88279000 |
|---|---|---|---|
| N | -2.58243300 | -2.65518300 | 1.31908400 |
| N | -1.02762500 | -2.51671400 | 2.80221700 |
| O | -0.55740700 | 1.30020000 | 3.56587100 |
| O | -2.40381300 | 0.27311800 | -2.04108400 |
| O | 5.65666100 | -3.45292000 | -0.19582400 |
| O | 5.15356200 | 4.20910300 | 1.00213500 |
| C | -0.71232800 | 0.75835100 | 2.54204400 |
| C | -1.19329000 | 0.26002100 | -1.44902700 |
| C | -0.41063300 | -0.92006700 | -1.25565800 |
| C | 0.81293600 | -0.51956700 | -0.57641800 |
| C | 0.73562700 | 0.90788900 | -0.34379900 |
| C | -0.51100800 | 1.39951400 | -0.87196700 |
| C | -0.74467200 | -2.26693800 | -1.77431800 |
| C | -1.45483100 | -2.40582700 | -2.98068200 |
| H | -1.76914800 | -1.51969700 | -3.51912800 |
| C | -1.77311200 | -3.66886300 | -3.48158100 |
| H | -2.32524900 | -3.74986100 | -4.41373900 |
| C | -1.38466700 | -4.82017100 | -2.79502900 |
| H | -1.63265200 | -5.80275600 | -3.18643200 |
| C | -0.66875700 | -4.69623000 | -1.60099200 |
| H | -0.35626300 | -5.58412900 | -1.05810200 |
| C | -0.35201600 | -3.43645600 | -1.09704300 |
| H | 0.19897400 | -3.35250600 | -0.16740700 |
| C | -0.93471800 | 2.81055200 | -1.01303700 |
| C | -1.48749200 | 3.25261100 | -2.22801000 |
| H | -1.63331700 | 2.54557800 | -3.03760100 |
| C | -1.86428100 | 4.58513100 | -2.39765700 |
| H | -2.30165300 | 4.90126500 | -3.33993900 |
| C | -1.69032200 | 5.50227300 | -1.36120100 |
| H | -1.98763300 | 6.53873000 | -1.49199500 |
| C | -1.13985300 | 5.07560300 | -0.14954000 |

| | | | |
|---|---|---|---|
| H | -1.00600200 | 5.78024300 | 0.66648600 |
| C | -0.76998500 | 3.74392700 | 0.02561300 |
| H | -0.35706400 | 3.41813300 | 0.97408800 |
| C | 2.05714100 | -1.31914200 | -0.47092300 |
| C | 2.55114600 | -2.00358000 | -1.59087900 |
| H | 1.99629800 | -1.97053600 | -2.52285400 |
| C | 3.74402300 | -2.72803600 | -1.54560100 |
| H | 4.08441100 | -3.24068500 | -2.43752600 |
| C | 4.48229300 | -2.77545400 | -0.35794300 |
| C | 4.01152600 | -2.08827400 | 0.77026500 |
| H | 4.59684200 | -2.12797500 | 1.68329400 |
| C | 2.82148800 | -1.37613500 | 0.70919600 |
| H | 2.47635800 | -0.84442400 | 1.58873200 |
| C | 6.18374500 | -4.15506200 | -1.30965700 |
| H | 7.11191300 | -4.61431100 | -0.96569900 |
| H | 6.40445000 | -3.48055100 | -2.14712200 |
| H | 5.49945800 | -4.94088600 | -1.65542000 |
| C | 1.88312100 | 1.77676300 | 0.04416200 |
| C | 2.30910800 | 1.98465300 | 1.36586700 |
| H | 1.77131200 | 1.51672000 | 2.18235900 |
| C | 3.39844000 | 2.79796100 | 1.65286700 |
| H | 3.72220700 | 2.96207100 | 2.67550200 |
| C | 4.09956900 | 3.43200000 | 0.61798900 |
| C | 3.68955900 | 3.24150400 | -0.70662900 |
| H | 4.20793500 | 3.72087200 | -1.52847100 |
| C | 2.59211600 | 2.42239500 | -0.97705800 |
| H | 2.28065700 | 2.28550100 | -2.00854500 |
| C | 5.89092100 | 4.88416300 | -0.00419700 |
| H | 6.67196400 | 5.44079900 | 0.51616400 |
| H | 5.26159800 | 5.58632000 | -0.56622300 |
| H | 6.35706800 | 4.18091700 | -0.70652700 |
| C | -1.56326900 | -1.83906000 | 1.73731900 |
| C | -2.67185700 | -3.79727000 | 2.09979700 |
| H | -3.40958900 | -4.56184000 | 1.91545600 |

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| C | -1.69687500 | -3.70919500 | 3.03484000 |
| H | -1.41974700 | -4.37828200 | 3.83376800 |
| C | -3.46634400 | -2.43563800 | 0.17756300 |
| H | -3.31572200 | -3.22400800 | -0.56303200 |
| H | -3.24098700 | -1.47756100 | -0.28210200 |
| H | -4.50728700 | -2.44155300 | 0.51242600 |
| C | 0.11127300 | -2.07990600 | 3.60325000 |
| H | 0.48451500 | -2.93656400 | 4.16762600 |
| H | -0.17511300 | -1.28810400 | 4.29832900 |
| H | 0.89772900 | -1.71245600 | 2.94553400 |
| H | -2.64284200 | 0.47224000 | 0.98347400 |
| H | -3.07283400 | 0.78556000 | -1.50616700 |
| C | -3.81776700 | 1.15362800 | 1.06639900 |
| C | -4.50310800 | 1.18675300 | -0.17505900 |
| H | -5.14473900 | 0.35526400 | -0.46440400 |
| C | -4.43863700 | 0.42001300 | 2.24973000 |
| H | -3.72602800 | 0.30390400 | 3.07123300 |
| H | -4.80358900 | -0.57026300 | 1.96394600 |
| H | -5.29864600 | 0.99429200 | 2.61283200 |
| C | -4.63160100 | 2.40174600 | -0.94561900 |
| H | -4.04293500 | 3.26060000 | -0.54799900 |
| H | -3.38748600 | 2.11780900 | 1.34838500 |
| O | -5.33162300 | 2.54130800 | -1.94851600 |

**TS8Z**

| Ru | -0.93027500 | -0.19003600 | 0.90660700 |
| N | -2.10660900 | -3.00955300 | 1.49187100 |
| N | -0.55616500 | -2.57287300 | 2.92006700 |
| O | -0.64845000 | 1.29848700 | 3.53112600 |
| O | -2.45505100 | -0.10186000 | -1.99445600 |
| O | 6.05980600 | -2.65766900 | -0.29047900 |
| O | 4.55149400 | 4.85230100 | 0.83070800 |

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|---|---|---|---|
| C | -0.76969600 | 0.70399500 | 2.53337000 |
| C | -1.25722900 | 0.05252300 | -1.43232800 |
| C | -0.31810500 | -1.01035700 | -1.22035700 |
| C | 0.84518600 | -0.43573600 | -0.56510200 |
| C | 0.57715700 | 0.97617900 | -0.35387000 |
| C | -0.73143200 | 1.28316200 | -0.86503000 |
| C | -0.47172900 | -2.39885500 | -1.71455400 |
| C | -1.17971600 | -2.65438600 | -2.90315300 |
| H | -1.62571700 | -1.82907600 | -3.44492100 |
| C | -1.32979700 | -3.95741300 | -3.37957300 |
| H | -1.88397000 | -4.12892700 | -4.29815500 |
| C | -0.77249200 | -5.03282600 | -2.68649200 |
| H | -0.88949500 | -6.04644500 | -3.05940600 |
| C | -0.05809600 | -4.79179700 | -1.50954300 |
| H | 0.38493800 | -5.61904500 | -0.96159300 |
| C | 0.09056200 | -3.49228200 | -1.02934300 |
| H | 0.64188500 | -3.31863800 | -0.11227300 |
| C | -1.35722700 | 2.61815700 | -0.99837800 |
| C | -2.06490600 | 2.94592100 | -2.16883300 |
| H | -2.18227200 | 2.20221200 | -2.94876000 |
| C | -2.63060000 | 4.21114900 | -2.32982400 |
| H | -3.18241600 | 4.43699700 | -3.23742800 |
| C | -2.49710800 | 5.17505200 | -1.33055500 |
| H | -2.94076900 | 6.15861300 | -1.45542000 |
| C | -1.79616800 | 4.86195500 | -0.16289200 |
| H | -1.69144800 | 5.60202200 | 0.62557300 |
| C | -1.23603000 | 3.59739800 | 0.00459600 |
| H | -0.70630900 | 3.36125900 | 0.92070000 |
| C | 2.19193800 | -1.05161300 | -0.48248100 |
| C | 2.74765000 | -1.67169000 | -1.61100400 |
| H | 2.16930900 | -1.72719300 | -2.52741600 |
| C | 4.03129900 | -2.22050600 | -1.59355100 |
| H | 4.41714000 | -2.68917700 | -2.49110500 |
| C | 4.79888900 | -2.15283600 | -0.42549300 |

| C | 4.26541900 | -1.52720200 | 0.71062100 |
| H | 4.87378200 | -1.47540100 | 1.60780900 |
| C | 2.98660800 | -0.98832000 | 0.67654400 |
| H | 2.59447400 | -0.49987600 | 1.56106800 |
| C | 6.65141600 | -3.29198800 | -1.41292100 |
| H | 7.64290900 | -3.61356700 | -1.09019500 |
| H | 6.75465200 | -2.60258900 | -2.26084000 |
| H | 6.07483300 | -4.16919800 | -1.73421100 |
| C | 1.60695000 | 1.99573000 | -0.00452700 |
| C | 2.05985000 | 2.25556700 | 1.29893000 |
| H | 1.62840000 | 1.71716200 | 2.13471000 |
| C | 3.03852900 | 3.21057500 | 1.54499900 |
| H | 3.38197100 | 3.41477600 | 2.55388100 |
| C | 3.59849000 | 3.93873000 | 0.48623300 |
| C | 3.15883100 | 3.69806700 | -0.82064000 |
| H | 3.56828700 | 4.24718300 | -1.66010600 |
| C | 2.17320600 | 2.73676600 | -1.04998000 |
| H | 1.83651100 | 2.56251300 | -2.06777400 |
| C | 5.14206100 | 5.62699200 | -0.20065800 |
| H | 5.86162700 | 6.28419700 | 0.29013600 |
| H | 4.39676000 | 6.23745200 | -0.72669200 |
| H | 5.66830400 | 4.99768400 | -0.93009200 |
| C | -1.21208700 | -2.03242800 | 1.84461000 |
| C | -2.00660200 | -4.11431000 | 2.32335700 |
| H | -2.62556400 | -4.98775500 | 2.19375300 |
| C | -1.03337400 | -3.83926600 | 3.22334000 |
| H | -0.63835600 | -4.42299000 | 4.03942400 |
| C | -3.04839100 | -2.97346700 | 0.37571500 |
| H | -2.88621900 | -3.84318800 | -0.26463100 |
| H | -2.88624500 | -2.07587400 | -0.21328400 |
| H | -4.07504600 | -2.98000500 | 0.75257000 |
| C | 0.51426100 | -1.93073600 | 3.67560400 |
| H | 1.04959800 | -2.69846800 | 4.23750500 |
| H | 0.11614000 | -1.18746400 | 4.36957800 |

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|---|---|---|---|
| H | 1.20216600 | -1.44502900 | 2.98577900 |
| H | -2.74136000 | 0.04538000 | 1.00722500 |
| H | -3.23970700 | 0.21726400 | -1.39369300 |
| C | -3.98161200 | 0.29845700 | 1.04136000 |
| C | -4.57230500 | 0.30042100 | -0.28111500 |
| H | -4.97433400 | -0.64077200 | -0.65619000 |
| C | -4.04312500 | 1.56030400 | 1.90266200 |
| H | -3.54970900 | 1.39360800 | 2.86390800 |
| H | -5.08768400 | 1.83052700 | 2.09167500 |
| H | -3.55571900 | 2.41020700 | 1.42018000 |
| C | -5.09216500 | 1.47307100 | -0.94623200 |
| H | -4.80105200 | 2.44865800 | -0.50019500 |
| H | -4.26781900 | -0.58408600 | 1.62144800 |
| O | -5.80415100 | 1.45157700 | -1.95162900 |

**TS9E**

| | | | |
|---|---|---|---|
| Ru | 0.92771300 | -0.17609500 | 0.90919200 |
| N | 2.90946400 | 2.13662700 | 1.51813800 |
| N | 1.29230400 | 2.18570000 | 2.93818600 |
| O | 0.18308100 | -1.49860200 | 3.52559900 |
| O | 2.35092700 | -0.64047400 | -2.01892800 |
| O | -5.00866300 | 4.32177400 | -0.21660800 |
| O | -5.82703500 | -3.32911300 | 0.74700900 |
| C | 0.48630900 | -0.97331100 | 2.52645300 |
| C | 1.15518400 | -0.44274300 | -1.43660100 |
| C | 0.58000900 | 0.84580500 | -1.21130000 |
| C | -0.70800700 | 0.63453600 | -0.56762800 |
| C | -0.87485600 | -0.79190700 | -0.38063600 |
| C | 0.28462600 | -1.47028200 | -0.90319200 |
| C | 1.15013600 | 2.13369000 | -1.67161200 |
| C | 1.91179800 | 2.19215400 | -2.85291700 |
| H | 2.09203600 | 1.28501400 | -3.41698800 |

A43

| | | | |
|---|---|---|---|
| C | 2.45303700 | 3.39987200 | -3.29552400 |
| H | 3.04166700 | 3.41769600 | -4.20842500 |
| C | 2.24102300 | 4.57612100 | -2.57524700 |
| H | 2.66262600 | 5.51554500 | -2.92150000 |
| C | 1.47704900 | 4.53387800 | -1.40552600 |
| H | 1.30054500 | 5.44264600 | -0.83649000 |
| C | 0.93840200 | 3.32900300 | -0.95909900 |
| H | 0.35252300 | 3.30806500 | -0.04734800 |
| C | 0.47782900 | -2.92812800 | -1.07353700 |
| C | 1.05940800 | -3.42609700 | -2.25392400 |
| H | 1.38578800 | -2.73371300 | -3.02219900 |
| C | 1.22516600 | -4.79850900 | -2.44520300 |
| H | 1.68212100 | -5.15851100 | -3.36258200 |
| C | 0.80652300 | -5.70209300 | -1.46843800 |
| H | 0.93669400 | -6.77007600 | -1.61758700 |
| C | 0.22239100 | -5.22068100 | -0.29387200 |
| H | -0.10438300 | -5.91380800 | 0.47627100 |
| C | 0.06414300 | -3.85082500 | -0.09527100 |
| H | -0.37671400 | -3.48841700 | 0.82657100 |
| C | -1.80523200 | 1.62686100 | -0.46558500 |
| C | -2.14318500 | 2.41561800 | -1.57503300 |
| H | -1.57179800 | 2.31734400 | -2.49225100 |
| C | -3.20049300 | 3.32677100 | -1.53793900 |
| H | -3.42246800 | 3.91380300 | -2.42129500 |
| C | -3.95822900 | 3.46315100 | -0.36951500 |
| C | -3.64386600 | 2.67571100 | 0.74745600 |
| H | -4.24325300 | 2.78651200 | 1.64536200 |
| C | -2.58696200 | 1.77719800 | 0.69454900 |
| H | -2.36402200 | 1.17077800 | 1.56492500 |
| C | -5.37519400 | 5.13451000 | -1.31969200 |
| H | -6.22463400 | 5.73234700 | -0.98541900 |
| H | -5.67788900 | 4.53128600 | -2.18543000 |
| H | -4.55881500 | 5.80444800 | -1.61962200 |
| C | -2.16334400 | -1.46427500 | -0.04795900 |

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|---|---|---|---|
| C | -2.66711000 | -1.61734900 | 1.25389700 |
| H | -2.09007400 | -1.25890700 | 2.09843600 |
| C | -3.88662600 | -2.24131400 | 1.48643500 |
| H | -4.27087500 | -2.36400900 | 2.49381600 |
| C | -4.64492500 | -2.73362000 | 0.41531400 |
| C | -4.15997900 | -2.59460700 | -0.89027000 |
| H | -4.72032200 | -2.96763000 | -1.73927200 |
| C | -2.93199200 | -1.96691100 | -1.10588700 |
| H | -2.56423100 | -1.86833500 | -2.12310300 |
| C | -6.62992200 | -3.85418800 | -0.29794600 |
| H | -7.51188700 | -4.27930000 | 0.18374600 |
| H | -6.10725500 | -4.64344100 | -0.85368900 |
| H | -6.94515300 | -3.07132100 | -0.99994200 |
| C | 1.76072400 | 1.47396000 | 1.86337600 |
| C | 3.14273700 | 3.21946600 | 2.35145300 |
| H | 3.99692300 | 3.86569300 | 2.22672100 |
| C | 2.12791600 | 3.24893900 | 3.24689200 |
| H | 1.92423400 | 3.92216300 | 4.06422700 |
| C | 3.79616900 | 1.82175600 | 0.40179200 |
| H | 3.85058200 | 2.67568100 | -0.27695900 |
| H | 3.40555100 | 0.96815400 | -0.14434900 |
| H | 4.79556800 | 1.58633400 | 0.77719400 |
| C | 0.06917100 | 1.90289000 | 3.68182700 |
| H | -0.20361800 | 2.79475400 | 4.24919800 |
| H | 0.20899600 | 1.06671500 | 4.36988900 |
| H | -0.73140600 | 1.66317000 | 2.98386900 |
| H | 2.50734700 | -0.95918900 | 1.02152000 |
| H | 2.91893300 | -1.27578700 | -1.49283800 |
| C | 3.66243200 | -1.72197000 | 1.05004600 |
| C | 4.11530400 | -2.08552200 | -0.24353400 |
| C | 3.22691500 | -2.82853300 | 2.00017500 |
| H | 2.49991400 | -3.49091100 | 1.52249000 |
| H | 2.78386300 | -2.43117800 | 2.91612100 |
| H | 4.10301200 | -3.42997500 | 2.26930300 |

A45

| | | | |
|---|---|---|---|
| H | 4.26864400 | -0.95049800 | 1.53326900 |
| H | 3.78390900 | -3.02784100 | -0.67903700 |
| C | 5.22289700 | -1.42113700 | -0.88584500 |
| H | 5.60077800 | -0.52600500 | -0.32928000 |
| O | 5.76300800 | -1.76042600 | -1.93602700 |

**TS9Z**

| | | | |
|---|---|---|---|
| Ru | 0.88654400 | -0.22858800 | 0.88744300 |
| N | 2.97170000 | 2.00385700 | 1.46497500 |
| N | 1.37028600 | 2.13832500 | 2.89720500 |
| O | 0.13868300 | -1.55205100 | 3.51193200 |
| O | 2.27170300 | -0.81753500 | -2.02263500 |
| O | -4.82869700 | 4.50316100 | -0.22754900 |
| O | -5.99540300 | -3.06113400 | 0.82931700 |
| C | 0.44053500 | -1.02221800 | 2.51658800 |
| C | 1.10259700 | -0.54746600 | -1.45696200 |
| C | 0.59253700 | 0.77429800 | -1.22409000 |
| C | -0.69172800 | 0.63342900 | -0.55822700 |
| C | -0.93260100 | -0.78829200 | -0.36267800 |
| C | 0.18228300 | -1.52365900 | -0.88915700 |
| C | 1.21722300 | 2.02800700 | -1.70716700 |
| C | 1.97908200 | 2.03075700 | -2.88997400 |
| H | 2.12065500 | 1.10507100 | -3.43434700 |
| C | 2.57163100 | 3.20521300 | -3.35555500 |
| H | 3.15920600 | 3.17998600 | -4.26894900 |
| C | 2.41309800 | 4.40300700 | -2.65718100 |
| H | 2.87518200 | 5.31627900 | -3.02125700 |
| C | 1.65073800 | 4.41604400 | -1.48577800 |
| H | 1.51601800 | 5.34193300 | -0.93313300 |
| C | 1.06044100 | 3.24447200 | -1.01638900 |
| H | 0.47717100 | 3.26693300 | -0.10300800 |
| C | 0.30691900 | -2.99181100 | -1.03305500 |

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|---|---|---|---|
| C | 0.82667400 | -3.53551300 | -2.22174800 |
| H | 1.16402200 | -2.87090000 | -3.00930300 |
| C | 0.92344700 | -4.91684500 | -2.39105600 |
| H | 1.33256500 | -5.31476600 | -3.31528900 |
| C | 0.50032500 | -5.78208700 | -1.38149000 |
| H | 0.57864700 | -6.85741400 | -1.51332000 |
| C | -0.01854500 | -5.25408000 | -0.19677700 |
| H | -0.34563400 | -5.91760200 | 0.59882400 |
| C | -0.11086600 | -3.87499000 | -0.02160200 |
| H | -0.50240500 | -3.47597800 | 0.90756300 |
| C | -1.74424400 | 1.67391900 | -0.46068100 |
| C | -2.05619900 | 2.46060400 | -1.57898200 |
| H | -1.49514900 | 2.32673100 | -2.49798000 |
| C | -3.07471800 | 3.41493600 | -1.54758100 |
| H | -3.27852000 | 3.99862800 | -2.43745300 |
| C | -3.81703800 | 3.59927600 | -0.37570700 |
| C | -3.52804700 | 2.81438600 | 0.75004200 |
| H | -4.11606800 | 2.96219800 | 1.65008800 |
| C | -2.51103800 | 1.87087700 | 0.70206600 |
| H | -2.30901400 | 1.26539400 | 1.57801800 |
| C | -5.16925800 | 5.31624800 | -1.33908200 |
| H | -5.98997100 | 5.95376500 | -1.00655200 |
| H | -5.50396500 | 4.71481600 | -2.19413000 |
| H | -4.32758500 | 5.94687400 | -1.65369500 |
| C | -2.24992700 | -1.39069400 | -0.01114300 |
| C | -2.75040900 | -1.50484600 | 1.29575400 |
| H | -2.14951400 | -1.16790200 | 2.13236000 |
| C | -3.99759300 | -2.06471600 | 1.54346700 |
| H | -4.37952800 | -2.15837200 | 2.55482100 |
| C | -4.78785600 | -2.52921400 | 0.48301000 |
| C | -4.30643500 | -2.42810500 | -0.82740800 |
| H | -4.89088800 | -2.78176900 | -1.66836200 |
| C | -3.05033600 | -1.86517000 | -1.05849000 |
| H | -2.68561700 | -1.79649300 | -2.07925000 |

A47

| | | | |
|---|---|---|---|
| C | -6.83138100 | -3.55715400 | -0.20410600 |
| H | -7.72950800 | -3.93272200 | 0.28868400 |
| H | -6.35254700 | -4.37729000 | -0.75449300 |
| H | -7.11279000 | -2.76717900 | -0.91243300 |
| C | 1.79713100 | 1.39859100 | 1.82554800 |
| C | 3.26053600 | 3.08198400 | 2.28655100 |
| H | 4.14294100 | 3.68662100 | 2.15033500 |
| C | 2.25508100 | 3.16566300 | 3.18950700 |
| H | 2.08882300 | 3.85461300 | 4.00218000 |
| C | 3.83823400 | 1.63537600 | 0.34821100 |
| H | 3.89640400 | 2.46248900 | -0.36239100 |
| H | 3.43075700 | 0.76718800 | -0.16191400 |
| H | 4.83823600 | 1.39893500 | 0.72021900 |
| C | 0.14754200 | 1.90708800 | 3.65887700 |
| H | -0.06879700 | 2.80237600 | 4.24473200 |
| H | 0.25812900 | 1.05461700 | 4.33222800 |
| H | -0.67708300 | 1.71908600 | 2.97331200 |
| H | 2.51386300 | -1.12378800 | 0.94775100 |
| H | 2.90638400 | -1.42341700 | -1.43053300 |
| C | 3.35819700 | -2.03132100 | 0.93910000 |
| C | 3.91435500 | -2.25077500 | -0.39217700 |
| C | 4.26921900 | -1.63486900 | 2.10549800 |
| H | 4.98765500 | -2.43846000 | 2.29946300 |
| H | 3.67948300 | -1.46954500 | 3.01288800 |
| H | 4.84010300 | -0.72570100 | 1.90501100 |
| H | 2.71376500 | -2.86336300 | 1.23012800 |
| H | 3.59554300 | -3.15262000 | -0.91489600 |
| C | 5.16710700 | -1.70137000 | -0.84915100 |
| H | 5.57857500 | -0.86975200 | -0.22567200 |
| O | 5.78100700 | -2.05378600 | -1.85580400 |

**TS10E**

| C | 1.09191600 | 1.63028600 | -0.06177500 |
|---|---|---|---|
| H | 1.97675700 | 2.05934400 | -0.56149700 |
| C | 2.05474200 | -2.03446200 | -0.17387800 |
| H | 1.47719500 | -2.49512200 | 0.63609700 |
| H | 2.97227100 | -2.61958800 | -0.29789700 |
| H | 1.46681100 | -2.12675000 | -1.09359500 |
| O | 0.04679200 | 2.36565200 | -0.02448500 |
| C | 2.36510800 | -0.56371000 | 0.13613100 |
| H | 2.95342000 | -0.14252500 | -0.68973100 |
| H | 3.01555400 | -0.52183700 | 1.02237700 |
| C | 1.12066200 | 0.28065200 | 0.34326800 |
| H | 0.57810800 | 0.07656200 | 1.27271700 |
| H | -0.90371300 | 1.47766200 | -0.21587400 |
| O | -1.31051300 | 0.46378800 | -0.53552800 |
| H | -0.19856900 | 0.06547500 | -0.34736200 |
| C | -2.23351700 | -0.09819300 | 0.41074400 |
| H | -3.06952500 | 0.60247700 | 0.51053400 |
| H | -1.75528000 | -0.18621900 | 1.39696900 |
| C | -2.71427100 | -1.45360600 | -0.07907700 |
| H | -3.44506400 | -1.87286700 | 0.61998700 |
| H | -1.88046900 | -2.15742500 | -0.16384800 |
| H | -3.18556000 | -1.36050700 | -1.06125200 |

**TS10Z**

| C | -1.06316100 | 1.58211800 | 0.11843100 |
|---|---|---|---|
| H | -1.51336700 | 2.50709900 | 0.51522200 |
| O | -0.18283700 | 1.72088100 | -0.80342200 |
| C | -1.33132600 | 0.35999100 | 0.76169900 |
| H | 0.79123100 | 0.94421800 | -0.31212500 |
| O | 1.26996900 | 0.36761800 | 0.52590700 |

| | | | |
|---|---|---|---|
| H | 0.18482800 | 0.25595500 | 0.96541600 |
| C | 1.94376600 | -0.84855900 | 0.15301900 |
| H | 1.39012400 | -1.35790100 | -0.64423400 |
| H | 1.94317100 | -1.50017700 | 1.03322300 |
| C | 3.36348300 | -0.53005100 | -0.28574000 |
| H | 3.89590700 | -1.45278200 | -0.53887000 |
| H | 3.90829900 | -0.02171800 | 0.51427300 |
| H | 3.36429700 | 0.11680600 | -1.16834200 |
| H | -2.00464200 | 0.43361100 | 1.61573700 |
| C | -1.46249600 | -0.94085800 | -0.03496600 |
| H | -1.02663000 | -1.78758200 | 0.51290100 |
| H | -0.89429900 | -0.84598500 | -0.96738600 |
| C | -2.92360200 | -1.27581800 | -0.36991100 |
| H | -2.99824500 | -2.21848300 | -0.92406800 |
| H | -3.37475900 | -0.48561800 | -0.97845800 |
| H | -3.52295400 | -1.37637500 | 0.54163900 |

**TS11E**

| | | | |
|---|---|---|---|
| C | 0.84767300 | -1.06955700 | -0.12063200 |
| H | 0.62813000 | -1.94341000 | -0.75530500 |
| C | -2.56435500 | 0.59265900 | -0.12113800 |
| H | -2.57865900 | 1.18499500 | 0.80105300 |
| H | -3.59639100 | 0.29946400 | -0.34057900 |
| H | -2.21803700 | 1.24669300 | -0.92858500 |
| O | 2.08176000 | -0.76018700 | 0.00806300 |
| C | -1.65363900 | -0.63386500 | 0.02364200 |
| H | -1.67613800 | -1.20711100 | -0.91240300 |
| H | -2.07457700 | -1.29602600 | 0.79445600 |
| C | -0.21596500 | -0.27362000 | 0.35418500 |
| H | -0.06541700 | 0.12251700 | 1.36378400 |
| H | 2.03423200 | 0.52003600 | 0.02991200 |
| O | 1.54275200 | 1.55420500 | -0.17876600 |

| H | 0.49844000 | 0.93567400 | -0.12862500 |
| H | 1.57004500 | 2.09132100 | 0.62557000 |

**TS11Z**

| C | -0.67554800 | -1.17432700 | 0.27645900 |
| H | -0.85942400 | -2.11479100 | 0.81815300 |
| O | -1.44285400 | -0.93288200 | -0.72240300 |
| C | 0.22490300 | -0.22837500 | 0.80398100 |
| H | -1.70558800 | 0.30936800 | -0.53398200 |
| O | -1.77201600 | 1.27339200 | 0.11635300 |
| H | -0.89559300 | 0.74388000 | 0.76192600 |
| H | 0.68964700 | -0.52063400 | 1.74524900 |
| C | 1.13460100 | 0.60084800 | -0.11239300 |
| H | 1.24767700 | 1.62326300 | 0.27461900 |
| H | 0.66494000 | 0.68930100 | -1.09919200 |
| C | 2.52908900 | -0.01966200 | -0.27327600 |
| H | 3.16726800 | 0.60053300 | -0.91269100 |
| H | 2.46338000 | -1.01634400 | -0.72098200 |
| H | 3.02768100 | -0.12240100 | 0.69659000 |
| H | -1.35929500 | 2.01284600 | -0.34992500 |

**TS12E**

| C | -1.43155600 | 0.47365900 | -0.01837600 |
| H | -1.73442300 | 1.50917100 | -0.20813000 |
| C | 2.29581500 | -0.43753700 | -0.13161000 |
| H | 2.41793700 | -0.99890600 | 0.80152800 |
| H | 3.25285700 | 0.04313300 | -0.35863100 |
| H | 2.07624500 | -1.15949000 | -0.92427700 |
| O | -2.30054700 | -0.46510000 | -0.15677700 |
| C | 1.16967700 | 0.59773000 | -0.00731800 |

| | | | |
|---|---|---|---|
| H | 1.09006000 | 1.15483500 | -0.94897800 |
| H | 1.44917800 | 1.33373500 | 0.76197000 |
| C | -0.16292000 | -0.05168900 | 0.31326300 |
| H | -0.20399700 | -0.55599400 | 1.28593200 |
| H | -1.16957300 | -1.09866500 | -0.09095600 |

**TS12Z**

| | | | |
|---|---|---|---|
| C | 1.26535200 | 0.60025800 | -0.11327400 |
| H | 1.57342900 | 1.57645400 | -0.50370100 |
| C | -2.09703100 | 0.22071400 | -0.40663400 |
| H | -2.49713200 | 0.94548800 | 0.31089500 |
| H | -2.92366600 | -0.42544900 | -0.72460000 |
| H | -1.74743500 | 0.77814300 | -1.28209300 |
| O | 1.99762100 | -0.42667400 | -0.38227600 |
| C | -0.96158100 | -0.60461600 | 0.21638500 |
| H | -0.58265100 | -1.32429100 | -0.51847900 |
| H | -1.36282600 | -1.19915100 | 1.04536000 |
| C | 0.20113800 | 0.25780700 | 0.75412200 |
| H | -0.14343200 | 1.03155000 | 1.44501200 |
| H | 1.25547400 | -0.81432800 | 0.58222100 |

**12E**

| | | | |
|---|---|---|---|
| C | 1.32956200 | 0.46653200 | 0.24151200 |
| H | 1.27427200 | 1.39292400 | -0.35240600 |
| C | -0.02771100 | -0.16144500 | 0.33179600 |
| H | -0.06867000 | -1.11288400 | 0.86201500 |
| C | -1.14171400 | 0.37171000 | -0.17340400 |
| H | -1.06982400 | 1.31819700 | -0.71198100 |
| C | -2.51498600 | -0.22299500 | -0.06322400 |
| H | -2.94809800 | -0.40229700 | -1.05530700 |

| H | -3.20166900 | 0.45502300 | 0.45951200 |
|---|---|---|---|
| H | -2.49971800 | -1.17356900 | 0.47793500 |
| O | 2.23093400 | -0.47795300 | -0.33869500 |
| H | 3.12498000 | -0.12524100 | -0.24319300 |
| H | 1.67034100 | 0.74865400 | 1.25290200 |

**12Z**

| C | 1.03058700 | -0.33882500 | 0.39994000 |
|---|---|---|---|
| H | 1.31106000 | -0.33316100 | 1.46810300 |
| H | 0.59671900 | -1.32679700 | 0.18825300 |
| C | 0.03853900 | 0.75803800 | 0.14881000 |
| H | 0.47908700 | 1.75370100 | 0.15763500 |
| C | -1.27674800 | 0.63831100 | -0.05886000 |
| H | -1.84278900 | 1.55860100 | -0.20235200 |
| C | -2.09576800 | -0.62032000 | -0.11236900 |
| H | -2.81198700 | -0.65642100 | 0.71870100 |
| H | -1.48886700 | -1.52753700 | -0.06509300 |
| H | -2.68756000 | -0.65668100 | -1.03509000 |
| O | 2.17557900 | -0.08926700 | -0.41674800 |
| H | 2.86004900 | -0.72079600 | -0.16129700 |

**13**

| C | -1.46348700 | 0.23629800 | 0.27150800 |
|---|---|---|---|
| H | -1.50602300 | 1.14837900 | 0.91328500 |
| O | -2.44034400 | -0.12908100 | -0.34405300 |
| C | -0.11895400 | -0.45278200 | 0.25180500 |
| H | -0.17941300 | -1.31332600 | -0.42176800 |
| C | 1.02085900 | 0.50286600 | -0.14782600 |
| H | 1.00030700 | 1.38525300 | 0.50534100 |
| C | 2.39951000 | -0.15897600 | -0.07309400 |

| H | 2.61923600 | -0.50229800 | 0.94393700 |
| H | 3.18875100 | 0.53945400 | -0.36809100 |
| H | 2.45791900 | -1.02837700 | -0.73661800 |
| H | 0.84166600 | 0.86983600 | -1.16591600 |
| H | 0.07273800 | -0.83070900 | 1.26789500 |

**TS13**

| Ru | -0.98125700 | -0.26377000 | -0.60203500 |
| N | -3.15574300 | 1.93177500 | -0.88684900 |
| N | -1.76738500 | 2.07677000 | -2.52758900 |
| O | -0.63482400 | -1.60393600 | -3.29490600 |
| O | -1.91129200 | -0.62367500 | 2.53702800 |
| O | 4.93494700 | 4.38002800 | -0.66356800 |
| O | 5.81731100 | -3.23936000 | -1.35583300 |
| C | -0.76800300 | -1.06573000 | -2.26649900 |
| C | -0.84385100 | -0.42292200 | 1.77267600 |
| C | -0.33712100 | 0.86217300 | 1.39168300 |
| C | 0.82887100 | 0.64875700 | 0.54514700 |
| C | 1.01164300 | -0.78321800 | 0.41092300 |
| C | -0.02752900 | -1.45577700 | 1.14455300 |
| C | -0.85573800 | 2.16025300 | 1.88169800 |
| C | -1.41878500 | 2.25513600 | 3.16805100 |
| H | -1.49419500 | 1.36373600 | 3.77871500 |
| C | -1.90059400 | 3.47310900 | 3.64935500 |
| H | -2.33321700 | 3.51997200 | 4.64502600 |
| C | -1.82886200 | 4.62377200 | 2.86255900 |
| H | -2.20492000 | 5.57105300 | 3.23884900 |
| C | -1.26625400 | 4.54472900 | 1.58589100 |
| H | -1.20253000 | 5.43237200 | 0.96225500 |
| C | -0.78513500 | 3.32988800 | 1.10175900 |
| H | -0.35545500 | 3.28163200 | 0.10781400 |
| C | -0.13913200 | -2.90671400 | 1.41331300 |

A54

| | | | |
|---|---|---|---|
| C | -0.54703000 | -3.35492600 | 2.68338200 |
| H | -0.81514100 | -2.62737200 | 3.44072300 |
| C | -0.62052100 | -4.71800700 | 2.96965900 |
| H | -0.93865000 | -5.03984000 | 3.95747000 |
| C | -0.28900600 | -5.66330800 | 1.99834200 |
| H | -0.34775300 | -6.72460800 | 2.22274500 |
| C | 0.11136300 | -5.23213000 | 0.73151800 |
| H | 0.36473000 | -5.95725900 | -0.03691600 |
| C | 0.18094900 | -3.87136000 | 0.43974500 |
| H | 0.48181500 | -3.55019400 | -0.55114100 |
| C | 1.87265800 | 1.65260000 | 0.22210800 |
| C | 2.36365200 | 2.50301600 | 1.22350800 |
| H | 1.94619400 | 2.44429100 | 2.22328500 |
| C | 3.38052100 | 3.42718000 | 0.97457800 |
| H | 3.72460700 | 4.06319400 | 1.78166500 |
| C | 3.94181600 | 3.51367000 | -0.30405300 |
| C | 3.47511800 | 2.66320600 | -1.31639700 |
| H | 3.92400300 | 2.73452600 | -2.30192200 |
| C | 2.46047200 | 1.75289500 | -1.05248700 |
| H | 2.11961400 | 1.09658200 | -1.84519000 |
| C | 5.44919300 | 5.25534600 | 0.32630700 |
| H | 6.22088700 | 5.84913100 | -0.16642400 |
| H | 5.89849900 | 4.70382200 | 1.16246400 |
| H | 4.67359300 | 5.92644000 | 0.71812700 |
| C | 2.25585300 | -1.43676400 | -0.08785900 |
| C | 2.54393200 | -1.67246500 | -1.44190000 |
| H | 1.82036200 | -1.39701300 | -2.20041700 |
| C | 3.73467200 | -2.27327100 | -1.83216300 |
| H | 3.95221000 | -2.45944100 | -2.87888400 |
| C | 4.68057400 | -2.65805600 | -0.87228200 |
| C | 4.41265700 | -2.43535400 | 0.48317500 |
| H | 5.12165100 | -2.72445500 | 1.24983600 |
| C | 3.21068800 | -1.83231800 | 0.85783700 |
| H | 3.01203300 | -1.66810300 | 1.91295700 |

| | | | |
|---|---|---|---|
| C | 6.80445700 | -3.65522900 | -0.42644800 |
| H | 7.61312600 | -4.08754200 | -1.01800600 |
| H | 6.41726000 | -4.41560300 | 0.26424200 |
| H | 7.19593100 | -2.81056600 | 0.15537800 |
| C | -2.03744900 | 1.33584600 | -1.40627700 |
| C | -3.55818400 | 3.01010900 | -1.65898500 |
| H | -4.41591000 | 3.61016200 | -1.40052000 |
| C | -2.68948900 | 3.09950800 | -2.69357100 |
| H | -2.64465400 | 3.78548400 | -3.52430100 |
| C | -3.84236100 | 1.58054400 | 0.35678500 |
| H | -3.57429200 | 2.28940000 | 1.14258400 |
| H | -3.57500400 | 0.57512600 | 0.67146200 |
| H | -4.92037200 | 1.61424900 | 0.18233700 |
| C | -0.65810400 | 1.85468400 | -3.44898300 |
| H | -0.54831300 | 2.74202100 | -4.07535400 |
| H | -0.84096200 | 0.98629500 | -4.08493800 |
| H | 0.25955800 | 1.69929200 | -2.88358100 |
| C | -4.27833200 | -2.37425400 | -1.01452300 |
| C | -3.27311300 | -2.11098400 | 0.10463700 |
| H | -4.76999600 | -3.32022000 | -0.73705600 |
| H | -2.50053300 | -1.06534200 | -0.52604700 |
| H | -2.45610200 | -2.84890600 | 0.11391800 |
| O | -3.70136500 | -1.67516700 | 1.23581300 |
| H | -2.67180400 | -1.19423700 | 2.04361600 |
| C | -5.34197100 | -1.29509100 | -1.21950600 |
| H | -5.79681400 | -1.06551400 | -0.24986000 |
| C | -6.42122700 | -1.70981100 | -2.22469500 |
| H | -7.16575500 | -0.91804600 | -2.36034400 |
| H | -6.95135800 | -2.60877900 | -1.88972200 |
| H | -5.98838500 | -1.93013600 | -3.20751500 |
| H | -4.85283000 | -0.37623800 | -1.56619400 |
| H | -3.72995000 | -2.56880900 | -1.94416900 |

**TS14**

| | | | |
|---|---|---|---|
| Ru | -0.80812700 | -0.74225200 | 0.63598700 |
| N | -0.33333600 | -3.76633400 | 1.24102200 |
| N | 0.54004900 | -2.56326000 | 2.79896100 |
| O | -1.69228200 | 0.60681900 | 3.19306100 |
| O | -1.63253300 | -1.39885100 | -2.50715100 |
| O | 6.52642300 | 1.00713600 | 0.58370400 |
| O | 1.10596100 | 6.46792100 | 0.97327400 |
| C | -1.34745200 | 0.06293900 | 2.21736800 |
| C | -0.82439500 | -0.66054200 | -1.74954000 |
| C | 0.49083100 | -1.04919500 | -1.33479300 |
| C | 1.04617900 | 0.04545700 | -0.55217100 |
| C | 0.03771000 | 1.08218800 | -0.47695200 |
| C | -1.13498000 | 0.64671400 | -1.19174100 |
| C | 1.18197900 | -2.29556300 | -1.74102700 |
| C | 0.90602500 | -2.88744700 | -2.98748100 |
| H | 0.16444200 | -2.43573400 | -3.63456200 |
| C | 1.55626800 | -4.05704300 | -3.38298800 |
| H | 1.32306900 | -4.49618100 | -4.34914700 |
| C | 2.49884900 | -4.66059300 | -2.54927700 |
| H | 3.00399100 | -5.57115000 | -2.85928800 |
| C | 2.78807200 | -4.07890200 | -1.31185600 |
| H | 3.52126600 | -4.53566800 | -0.65247600 |
| C | 2.13903900 | -2.91221200 | -0.91298700 |
| H | 2.36907500 | -2.47466200 | 0.05162300 |
| C | -2.33563900 | 1.45153500 | -1.51259700 |
| C | -2.94140200 | 1.33861100 | -2.77755100 |
| H | -2.54397600 | 0.62867000 | -3.49338300 |
| C | -4.05036300 | 2.11703400 | -3.11034800 |
| H | -4.50219600 | 2.00975800 | -4.09268700 |
| C | -4.57680200 | 3.02723200 | -2.19344600 |
| H | -5.44046600 | 3.63238500 | -2.45423600 |
| C | -3.98560300 | 3.14828800 | -0.93331100 |

| H | -4.38748700 | 3.84946400 | -0.20702100 |
| C | -2.88236400 | 2.36742400 | -0.59449200 |
| H | -2.44396800 | 2.46018800 | 0.39256800 |
| C | 2.48196300 | 0.25672400 | -0.24195700 |
| C | 3.45034300 | 0.04493800 | -1.23448600 |
| H | 3.14143500 | -0.31031000 | -2.21201200 |
| C | 4.80744100 | 0.27974300 | -1.00492000 |
| H | 5.51656600 | 0.09959900 | -1.80426700 |
| C | 5.22902400 | 0.74756500 | 0.24446400 |
| C | 4.27605100 | 0.97939500 | 1.24635700 |
| H | 4.61440800 | 1.35043700 | 2.20847000 |
| C | 2.93095900 | 0.73727800 | 1.00176700 |
| H | 2.20888100 | 0.93458500 | 1.78546000 |
| C | 7.52876000 | 0.79814100 | -0.39728600 |
| H | 8.47543900 | 1.06312300 | 0.07646600 |
| H | 7.37547900 | 1.43658700 | -1.27709800 |
| H | 7.56875100 | -0.25032500 | -0.72057500 |
| C | 0.29954300 | 2.48982800 | -0.05945300 |
| C | 0.31519900 | 2.93755600 | 1.27138700 |
| H | 0.09582000 | 2.24328700 | 2.07413300 |
| C | 0.58570600 | 4.26451400 | 1.58315900 |
| H | 0.59093600 | 4.60904200 | 2.61216600 |
| C | 0.85202100 | 5.19015900 | 0.56512100 |
| C | 0.83858500 | 4.76624700 | -0.76860900 |
| H | 1.03678900 | 5.45775800 | -1.57888000 |
| C | 0.56288200 | 3.43013000 | -1.06407200 |
| H | 0.55086900 | 3.11377800 | -2.10301500 |
| C | 1.37207700 | 7.44715100 | -0.01748200 |
| H | 1.54199100 | 8.38172600 | 0.51960400 |
| H | 0.52278100 | 7.57403500 | -0.70137900 |
| H | 2.26769800 | 7.20016100 | -0.60234700 |
| C | -0.17196100 | -2.46260900 | 1.62987200 |
| C | 0.26160400 | -4.64006100 | 2.13746000 |
| H | 0.24560200 | -5.70813300 | 1.99030200 |

| | | | |
|---|---|---|---|
| C | 0.80723600 | -3.88556700 | 3.11952100 |
| H | 1.35343100 | -4.16341000 | 4.00676700 |
| C | -0.98065100 | -4.25978700 | 0.02532500 |
| H | -0.23076200 | -4.69911100 | -0.63633400 |
| H | -1.49262900 | -3.45678200 | -0.49725800 |
| H | -1.71803200 | -5.01982400 | 0.29833600 |
| C | 0.98145300 | -1.45085600 | 3.63297600 |
| H | 1.76937500 | -1.81040800 | 4.29767800 |
| H | 0.15895700 | -1.05388200 | 4.23141700 |
| H | 1.38046800 | -0.65944500 | 3.00136100 |
| C | -3.59120900 | -2.07637200 | 0.03212700 |
| H | -2.34977900 | -1.47313200 | 0.57629700 |
| O | -3.38557800 | -2.46766700 | -1.16545100 |
| H | -2.47529400 | -1.74985000 | -1.99434600 |
| H | -3.55679400 | -2.85347500 | 0.82108500 |
| C | -4.60858700 | -0.97041300 | 0.29870900 |
| H | -4.29582900 | -0.05272500 | -0.20836000 |
| C | -4.91723100 | -0.71172000 | 1.77513700 |
| H | -5.20898100 | -1.65564200 | 2.25682200 |
| C | -6.03133000 | 0.32340100 | 1.96664500 |
| H | -6.23226000 | 0.50076300 | 3.02829300 |
| H | -6.96670600 | -0.00638500 | 1.49968800 |
| H | -5.75640400 | 1.28188200 | 1.51274500 |
| H | -4.01408400 | -0.36879900 | 2.28946300 |
| H | -5.52219600 | -1.30667400 | -0.21428300 |

**TS15E**

| | | | |
|---|---|---|---|
| Ru | 0.87504200 | -0.31990500 | 0.95127400 |
| N | 2.87829600 | 1.90012000 | 1.82718300 |
| N | 1.19744400 | 1.86574900 | 3.17012400 |
| O | 0.10654500 | -1.84144200 | 3.44721200 |
| O | 2.29103400 | -0.95790000 | -1.96067100 |

| | | | |
|---|---|---|---|
| O | -4.51428100 | 4.80315800 | -0.36054400 |
| O | -6.16843300 | -2.68992200 | 0.66457400 |
| C | 0.41728300 | -1.24119300 | 2.49223300 |
| C | 1.13147400 | -0.60195600 | -1.42015700 |
| C | 0.70042200 | 0.74771400 | -1.16422700 |
| C | -0.62200300 | 0.67439400 | -0.56871200 |
| C | -0.94665000 | -0.72314100 | -0.38895100 |
| C | 0.14260100 | -1.52273900 | -0.89403500 |
| C | 1.40705600 | 1.97089200 | -1.60853700 |
| C | 2.19096100 | 1.95724800 | -2.77721700 |
| H | 2.27243600 | 1.04083700 | -3.34957900 |
| C | 2.86279700 | 3.10345800 | -3.20451100 |
| H | 3.46471800 | 3.06397100 | -4.10820800 |
| C | 2.75915400 | 4.29383500 | -2.48373000 |
| H | 3.28064900 | 5.18612100 | -2.81838300 |
| C | 1.97025800 | 4.32697200 | -1.33022100 |
| H | 1.87322700 | 5.24885600 | -0.76286900 |
| C | 1.30443800 | 3.18189400 | -0.89751000 |
| H | 0.70196200 | 3.21922000 | 0.00291300 |
| C | 0.17310800 | -2.99341700 | -1.06821500 |
| C | 0.70600400 | -3.54924300 | -2.24592900 |
| H | 1.12354400 | -2.89266300 | -3.00067000 |
| C | 0.71298300 | -4.92991400 | -2.44581000 |
| H | 1.13219800 | -5.33496800 | -3.36281900 |
| C | 0.18348300 | -5.78613200 | -1.47960600 |
| H | 0.18915600 | -6.86112400 | -1.63617500 |
| C | -0.34962900 | -5.24740100 | -0.30619800 |
| H | -0.76014900 | -5.90230100 | 0.45742700 |
| C | -0.35112500 | -3.86899800 | -0.09999500 |
| H | -0.75320400 | -3.46549200 | 0.82234300 |
| C | -1.61068500 | 1.77882900 | -0.50067800 |
| C | -1.82779700 | 2.59291000 | -1.62207600 |
| H | -1.24137400 | 2.42879600 | -2.52019400 |
| C | -2.78218000 | 3.61218200 | -1.62130400 |

A60

| | | | |
|---|---|---|---|
| H | -2.91200100 | 4.21450300 | -2.51274200 |
| C | -3.55703800 | 3.83551800 | -0.47803500 |
| C | -3.36419000 | 3.02522200 | 0.64981900 |
| H | -3.97640600 | 3.20447400 | 1.52786700 |
| C | -2.40819100 | 2.01866700 | 0.63294700 |
| H | -2.27947400 | 1.39758500 | 1.51155400 |
| C | -4.75453300 | 5.64468400 | -1.47608600 |
| H | -5.54457000 | 6.33300100 | -1.17118100 |
| H | -5.09257700 | 5.07354000 | -2.35059100 |
| H | -3.86109400 | 6.22074200 | -1.75067500 |
| C | -2.30832300 | -1.24720600 | -0.08181900 |
| C | -2.82912900 | -1.37799300 | 1.21561500 |
| H | -2.21161900 | -1.11439300 | 2.06700300 |
| C | -4.11413600 | -1.86031300 | 1.43249900 |
| H | -4.51229600 | -1.96655000 | 2.43642300 |
| C | -4.92280200 | -2.22845200 | 0.34856300 |
| C | -4.42228700 | -2.11027500 | -0.95308400 |
| H | -5.02121000 | -2.39023900 | -1.81154300 |
| C | -3.12838100 | -1.62544400 | -1.15246200 |
| H | -2.74925000 | -1.54140700 | -2.16683500 |
| C | -7.02419700 | -3.08652100 | -0.39439600 |
| H | -7.95151800 | -3.41901100 | 0.07500700 |
| H | -6.59641300 | -3.91523100 | -0.97352000 |
| H | -7.24358600 | -2.25230900 | -1.07353200 |
| C | 1.70135600 | 1.23431100 | 2.05979300 |
| C | 3.09261500 | 2.90328300 | 2.76026900 |
| H | 3.96258900 | 3.53979800 | 2.72957700 |
| C | 2.03725100 | 2.87945900 | 3.60731300 |
| H | 1.80612700 | 3.48727500 | 4.46757500 |
| C | 3.82437500 | 1.63709400 | 0.74954700 |
| H | 3.98168600 | 2.54558200 | 0.16428400 |
| H | 3.41660500 | 0.86836700 | 0.09997500 |
| H | 4.77763400 | 1.29785900 | 1.16527900 |
| C | -0.05025400 | 1.53430500 | 3.84781600 |

| | | | |
|---|---|---|---|
| H | -0.40746800 | 2.42073400 | 4.37622300 |
| H | 0.09231300 | 0.71889400 | 4.56123000 |
| H | -0.78763900 | 1.23188500 | 3.10726500 |
| H | 2.41484900 | -1.12173000 | 1.02770500 |
| H | 2.93548100 | -1.53297500 | -1.26182500 |
| C | 3.59525300 | -1.97074500 | 0.93295900 |
| C | 4.01317100 | -2.15911100 | -0.40588600 |
| C | 3.10309200 | -3.16088500 | 1.73678600 |
| H | 2.36953600 | -3.74118100 | 1.17023100 |
| H | 2.64498300 | -2.85887300 | 2.68118700 |
| H | 3.95273500 | -3.81910100 | 1.95798600 |
| H | 4.18266700 | -1.25663700 | 1.51516900 |
| H | 3.82459800 | -3.14883000 | -0.82979800 |
| C | 5.23946700 | -1.44525600 | -0.94721600 |
| H | 5.43420300 | -0.54622300 | -0.33631100 |
| O | 5.18401600 | -1.12580600 | -2.33192900 |
| H | 6.12789700 | -2.08389800 | -0.84280400 |
| H | 4.34654000 | -0.66609200 | -2.48766600 |

**TS15Z**

| | | | |
|---|---|---|---|
| Ru | 0.85971200 | -0.31615200 | 0.92112000 |
| N | 2.91550500 | 1.89679500 | 1.67286000 |
| N | 1.29787300 | 1.89638500 | 3.09253200 |
| O | 0.17145500 | -1.81979600 | 3.45335800 |
| O | 2.24096100 | -0.94763200 | -1.99870400 |
| O | -4.60869000 | 4.74079500 | -0.30783600 |
| O | -6.14765900 | -2.77287800 | 0.80614300 |
| C | 0.44300600 | -1.21887300 | 2.48716300 |
| C | 1.08076600 | -0.60243700 | -1.45026300 |
| C | 0.63649000 | 0.74225800 | -1.19439600 |
| C | -0.67271400 | 0.65743700 | -0.57149200 |
| C | -0.97923100 | -0.74378300 | -0.38156600 |

| | | | |
|---|---|---|---|
| C | 0.10921600 | -1.53184400 | -0.90323200 |
| C | 1.31866100 | 1.97236200 | -1.65638300 |
| C | 2.09661900 | 1.95861400 | -2.82897200 |
| H | 2.19579800 | 1.03571200 | -3.38780200 |
| C | 2.74518800 | 3.11162400 | -3.27321400 |
| H | 3.34264900 | 3.07267800 | -4.17996600 |
| C | 2.62496700 | 4.30828300 | -2.56516300 |
| H | 3.12868600 | 5.20573700 | -2.91303300 |
| C | 1.84330000 | 4.34045900 | -1.40674100 |
| H | 1.73507700 | 5.26633200 | -0.84804600 |
| C | 1.19967800 | 3.18901300 | -0.95759200 |
| H | 0.60412200 | 3.22580900 | -0.05261300 |
| C | 0.15886200 | -3.00374100 | -1.06272600 |
| C | 0.66266100 | -3.56263300 | -2.25165200 |
| H | 1.04214800 | -2.90663000 | -3.02699700 |
| C | 0.69000200 | -4.94521200 | -2.43641500 |
| H | 1.08616600 | -5.35328600 | -3.36226400 |
| C | 0.20988700 | -5.79957100 | -1.44302000 |
| H | 0.23168300 | -6.87604100 | -1.58748600 |
| C | -0.29452500 | -5.25739600 | -0.25857900 |
| H | -0.66657900 | -5.91114000 | 0.52546200 |
| C | -0.31603700 | -3.87714400 | -0.06785500 |
| H | -0.69596100 | -3.46966700 | 0.86226800 |
| C | -1.67343700 | 1.75015100 | -0.49082000 |
| C | -1.94119900 | 2.53727700 | -1.62032400 |
| H | -1.38472800 | 2.36111600 | -2.53521100 |
| C | -2.90801400 | 3.54465800 | -1.60594800 |
| H | -3.07791400 | 4.12641700 | -2.50427800 |
| C | -3.64357200 | 3.78279500 | -0.43984400 |
| C | -3.39859000 | 3.00020600 | 0.69737900 |
| H | -3.97981100 | 3.19187100 | 1.59367800 |
| C | -2.43066100 | 2.00529600 | 0.66661600 |
| H | -2.25864300 | 1.40626800 | 1.55329100 |
| C | -4.90158900 | 5.55389300 | -1.43180400 |

A63

| | | | |
|---|---|---|---|
| H | -5.68946700 | 6.23835600 | -1.11293800 |
| H | -5.26353000 | 4.95890900 | -2.28047800 |
| H | -4.02708300 | 6.13549400 | -1.75192200 |
| C | -2.32604500 | -1.28401000 | -0.04063300 |
| C | -2.82573400 | -1.38487300 | 1.26777100 |
| H | -2.20046000 | -1.08513100 | 2.10135700 |
| C | -4.09826700 | -1.88346100 | 1.51816100 |
| H | -4.47991300 | -1.96664000 | 2.53063500 |
| C | -4.91544200 | -2.29868100 | 0.45786900 |
| C | -4.43589700 | -2.21107500 | -0.85403800 |
| H | -5.04174200 | -2.52786700 | -1.69465300 |
| C | -3.15414000 | -1.70928400 | -1.08717100 |
| H | -2.79113600 | -1.64946200 | -2.10912900 |
| C | -7.01120300 | -3.21635600 | -0.22756200 |
| H | -7.92552100 | -3.55083800 | 0.26535700 |
| H | -6.57687500 | -4.05451200 | -0.78793600 |
| H | -7.25537700 | -2.40705000 | -0.92803800 |
| C | 1.74637600 | 1.24343200 | 1.97138700 |
| C | 3.17733100 | 2.91519500 | 2.57686900 |
| H | 4.04836400 | 3.54570300 | 2.49503500 |
| C | 2.16239500 | 2.91251700 | 3.47238200 |
| H | 1.97564800 | 3.53563300 | 4.33247100 |
| C | 3.80514000 | 1.61632300 | 0.55196400 |
| H | 3.86350900 | 2.48615000 | -0.10565200 |
| H | 3.41219500 | 0.77484300 | -0.01182900 |
| H | 4.80334200 | 1.37200300 | 0.92615300 |
| C | 0.07944300 | 1.58369300 | 3.82963600 |
| H | -0.23433700 | 2.47358100 | 4.37929300 |
| H | 0.24192000 | 0.76218900 | 4.53167600 |
| H | -0.69958500 | 1.29847400 | 3.12534200 |
| H | 2.38720100 | -1.15949700 | 0.96364500 |
| H | 2.86721800 | -1.55439800 | -1.31779600 |
| C | 3.37120200 | -2.17952100 | 0.86846200 |
| C | 3.88859300 | -2.28825600 | -0.45003900 |

A64

| C | 4.22501000 | -1.74849600 | 2.05370800 |
| H | 4.94249600 | -2.54513000 | 2.28799700 |
| H | 3.60688500 | -1.57001400 | 2.93796000 |
| H | 4.80047300 | -0.84244800 | 1.85129200 |
| H | 2.67685900 | -2.97838700 | 1.12733500 |
| H | 3.61904800 | -3.19983500 | -0.98750800 |
| C | 5.19467500 | -1.66403700 | -0.89260600 |
| H | 5.40754800 | -0.75950000 | -0.29950000 |
| O | 5.23990200 | -1.37755800 | -2.28855500 |
| H | 6.03893400 | -2.34715500 | -0.72005600 |
| H | 4.44292600 | -0.87247100 | -2.50327500 |

**TS16E**

| Ru | -0.95497500 | -0.01942400 | 0.94613500 |
| N | -2.46240800 | -2.68769800 | 1.50728800 |
| N | -0.85809300 | -2.43947500 | 2.92116000 |
| O | -0.66682700 | 1.39347000 | 3.60391800 |
| O | -2.45688300 | 0.44212600 | -1.93658500 |
| O | 5.56797100 | -3.53979900 | -0.36936200 |
| O | 5.30007300 | 4.03139800 | 0.97165900 |
| C | -0.77297200 | 0.82751800 | 2.58450700 |
| C | -1.24156400 | 0.34770800 | -1.39579700 |
| C | -0.49232600 | -0.86979100 | -1.22334200 |
| C | 0.76676100 | -0.51887800 | -0.59017300 |
| C | 0.74035500 | 0.89973300 | -0.31413200 |
| C | -0.50520800 | 1.44184000 | -0.79296100 |
| C | -0.88374900 | -2.19762800 | -1.75096800 |
| C | -1.66993000 | -2.29818400 | -2.91382900 |
| H | -2.00143500 | -1.39326100 | -3.40828400 |
| C | -2.04313400 | -3.54358000 | -3.42084400 |
| H | -2.65343300 | -3.59311000 | -4.31851200 |
| C | -1.63527900 | -4.71789400 | -2.78623400 |

A65

| | | | |
|---|---|---|---|
| H | -1.92506200 | -5.68669500 | -3.18342700 |
| C | -0.84555300 | -4.63324400 | -1.63599500 |
| H | -0.51731600 | -5.53852900 | -1.13220900 |
| C | -0.47576500 | -3.39088800 | -1.12448200 |
| H | 0.12883500 | -3.33970600 | -0.22637500 |
| C | -0.86662900 | 2.87306000 | -0.91431000 |
| C | -1.25952400 | 3.37852600 | -2.16630700 |
| H | -1.30588700 | 2.70719200 | -3.01792600 |
| C | -1.58382500 | 4.72565900 | -2.32557500 |
| H | -1.89294700 | 5.09178800 | -3.30040100 |
| C | -1.51161600 | 5.59839800 | -1.23872400 |
| H | -1.76498800 | 6.64752600 | -1.36143100 |
| C | -1.11435900 | 5.11127800 | 0.00841800 |
| H | -1.05687800 | 5.78102600 | 0.86199800 |
| C | -0.80055200 | 3.76234200 | 0.17105600 |
| H | -0.51282800 | 3.38862400 | 1.14748500 |
| C | 1.99574100 | -1.34686000 | -0.52980300 |
| C | 2.42377600 | -2.06843200 | -1.65332400 |
| H | 1.82599600 | -2.04906900 | -2.55859700 |
| C | 3.60479800 | -2.81433300 | -1.64519600 |
| H | 3.89250300 | -3.35672700 | -2.53816300 |
| C | 4.39861600 | -2.84402100 | -0.49379400 |
| C | 3.99678700 | -2.11574900 | 0.63551900 |
| H | 4.62662100 | -2.13938400 | 1.51906200 |
| C | 2.81824000 | -1.38313000 | 0.61206500 |
| H | 2.52952600 | -0.81362600 | 1.48868300 |
| C | 6.02489800 | -4.28392700 | -1.48625700 |
| H | 6.95991600 | -4.75299100 | -1.17538100 |
| H | 6.21692500 | -3.63861000 | -2.35344900 |
| H | 5.30897000 | -5.06461200 | -1.77523900 |
| C | 1.93243600 | 1.71629200 | 0.05598800 |
| C | 2.22047600 | 2.14829300 | 1.36052000 |
| H | 1.55429500 | 1.88111500 | 2.17270100 |
| C | 3.34646500 | 2.91604500 | 1.63346900 |

A66

| | | | |
|---|---|---|---|
| H | 3.56620700 | 3.25042500 | 2.64224000 |
| C | 4.22349800 | 3.27688700 | 0.60186700 |
| C | 3.95535300 | 2.85691100 | -0.70598100 |
| H | 4.61403600 | 3.11936200 | -1.52533100 |
| C | 2.81998600 | 2.08624500 | -0.96262000 |
| H | 2.62296700 | 1.76475100 | -1.98129000 |
| C | 6.21639900 | 4.42901200 | -0.03470100 |
| H | 6.98473500 | 5.01610000 | 0.47112100 |
| H | 5.73427700 | 5.05067600 | -0.80041300 |
| H | 6.68632600 | 3.56415500 | -0.52107600 |
| C | -1.46243000 | -1.81627300 | 1.85851900 |
| C | -2.47195600 | -3.80844300 | 2.32373100 |
| H | -3.18192500 | -4.60919100 | 2.19094400 |
| C | -1.46611500 | -3.65069300 | 3.21588900 |
| H | -1.12953000 | -4.28268600 | 4.02221000 |
| C | -3.40264500 | -2.53599700 | 0.40172600 |
| H | -3.23683700 | -3.32058800 | -0.33937400 |
| H | -3.25001400 | -1.56892100 | -0.06901200 |
| H | -4.42650600 | -2.60038800 | 0.78034400 |
| C | 0.28315500 | -1.92479800 | 3.67012800 |
| H | 0.75306600 | -2.75578200 | 4.20008800 |
| H | -0.02773400 | -1.16537700 | 4.39107000 |
| H | 0.99925700 | -1.48613200 | 2.97736500 |
| H | -2.61974100 | 0.41984700 | 1.03103600 |
| H | -3.25352700 | 0.65093900 | -1.20222400 |
| C | -3.88761300 | 1.11859900 | 0.98285300 |
| C | -4.43300400 | 1.10782100 | -0.32037800 |
| H | -5.16772700 | 0.32865300 | -0.54023300 |
| C | -4.56469300 | 0.38343300 | 2.12751200 |
| H | -3.89310500 | 0.24320700 | 2.97922100 |
| H | -4.94095600 | -0.59366500 | 1.81373700 |
| H | -5.42895700 | 0.97110100 | 2.46228200 |
| C | -4.63755500 | 2.41085100 | -1.08240300 |
| H | -3.44827600 | 2.07130400 | 1.28505200 |

A67

| | | | |
|---|---|---|---|
| O | -4.65135100 | 2.26434300 | -2.49599500 |
| H | -3.78533100 | 1.91249900 | -2.74714700 |
| H | -5.62092900 | 2.83506300 | -0.83419600 |
| H | -3.88246900 | 3.14401700 | -0.75891500 |

**TS16Z**

| | | | |
|---|---|---|---|
| Ru | -0.93423700 | -0.13753300 | 0.96061100 |
| N | -2.10083600 | -2.94454800 | 1.64703500 |
| N | -0.51843600 | -2.45397400 | 3.02118100 |
| O | -0.75857900 | 1.38133500 | 3.56804300 |
| O | -2.50218500 | 0.09836600 | -1.92979400 |
| O | 5.91886800 | -2.94400200 | -0.43344700 |
| O | 4.81637200 | 4.58850400 | 0.85091700 |
| C | -0.82768500 | 0.77836900 | 2.56686400 |
| C | -1.28598300 | 0.15148100 | -1.39593200 |
| C | -0.40529500 | -0.97245600 | -1.19909200 |
| C | 0.81129300 | -0.46952600 | -0.58654300 |
| C | 0.62695800 | 0.94281300 | -0.33794500 |
| C | -0.67529000 | 1.33221800 | -0.81624600 |
| C | -0.65175500 | -2.34775100 | -1.69230900 |
| C | -1.43276200 | -2.56353300 | -2.84312000 |
| H | -1.86600700 | -1.71301200 | -3.35504900 |
| C | -1.67114600 | -3.85475700 | -3.31564000 |
| H | -2.28010700 | -3.99341800 | -4.20486700 |
| C | -1.13087700 | -4.96092500 | -2.65812900 |
| H | -1.31548300 | -5.96533000 | -3.02884100 |
| C | -0.34521300 | -4.76110700 | -1.51940800 |
| H | 0.08590800 | -5.61188700 | -0.99837000 |
| C | -0.10991900 | -3.47323700 | -1.04212000 |
| H | 0.49444300 | -3.33327800 | -0.15328500 |
| C | -1.20224300 | 2.70990500 | -0.94565400 |
| C | -1.75367400 | 3.12960000 | -2.16949700 |

A68

| | | | |
|---|---|---|---|
| H | -1.80135200 | 2.42927200 | -2.99670800 |
| C | -2.23211700 | 4.42990600 | -2.33193200 |
| H | -2.65969300 | 4.72870200 | -3.28484600 |
| C | -2.16027200 | 5.34248700 | -1.27838100 |
| H | -2.53298800 | 6.35501600 | -1.40416900 |
| C | -1.60711000 | 4.94158300 | -0.06013100 |
| H | -1.54692600 | 5.64218800 | 0.76814500 |
| C | -1.13813800 | 3.63911700 | 0.10700900 |
| H | -0.72675600 | 3.33249100 | 1.06219900 |
| C | 2.12615500 | -1.15459600 | -0.53857300 |
| C | 2.61416500 | -1.82600200 | -1.66896400 |
| H | 2.00404200 | -1.87277200 | -2.56499400 |
| C | 3.86955600 | -2.43793000 | -1.67952000 |
| H | 4.20162400 | -2.94580500 | -2.57736800 |
| C | 4.67870600 | -2.38040100 | -0.53979000 |
| C | 4.21577100 | -1.70110400 | 0.59631500 |
| H | 4.85685400 | -1.65630300 | 1.47091100 |
| C | 2.96366500 | -1.10188000 | 0.59112400 |
| H | 2.62734700 | -0.57025700 | 1.47405700 |
| C | 6.43793300 | -3.63416600 | -1.55783300 |
| H | 7.42307900 | -3.99809200 | -1.26121000 |
| H | 6.54561000 | -2.97212000 | -2.42697400 |
| H | 5.80747600 | -4.48856700 | -1.83720200 |
| C | 1.71977200 | 1.89845300 | 0.00518200 |
| C | 2.07522800 | 2.25421800 | 1.31610900 |
| H | 1.52868400 | 1.83134200 | 2.15144800 |
| C | 3.10783000 | 3.15027200 | 1.56569900 |
| H | 3.37786200 | 3.42719500 | 2.57966000 |
| C | 3.82077000 | 3.72099400 | 0.50275400 |
| C | 3.48150400 | 3.38236200 | -0.81212500 |
| H | 4.01212300 | 3.80819600 | -1.65544200 |
| C | 2.44084900 | 2.48120200 | -1.04471000 |
| H | 2.18564800 | 2.22684300 | -2.06944500 |
| C | 5.56386400 | 5.20102200 | -0.18672400 |

| | | | |
|---|---|---|---|
| H | 6.29222500 | 5.84694200 | 0.30637400 |
| H | 4.92685200 | 5.81051100 | -0.84089500 |
| H | 6.09564600 | 4.45918300 | -0.79682400 |
| C | -1.20332900 | -1.94943500 | 1.94423800 |
| C | -1.97279800 | -4.02220900 | 2.51048200 |
| H | -2.58716600 | -4.90413400 | 2.42280900 |
| C | -0.98045300 | -3.71231100 | 3.37727400 |
| H | -0.56189900 | -4.26714900 | 4.20180300 |
| C | -3.07412600 | -2.94511300 | 0.55974400 |
| H | -2.91309600 | -3.81727900 | -0.07759000 |
| H | -2.94512700 | -2.04849500 | -0.03850400 |
| H | -4.08930500 | -2.97051600 | 0.96750600 |
| C | 0.56162500 | -1.78015700 | 3.73317300 |
| H | 1.15716700 | -2.53252800 | 4.25436900 |
| H | 0.16942900 | -1.06235300 | 4.45738400 |
| H | 1.18909700 | -1.25451600 | 3.01596000 |
| H | -2.63745400 | 0.06491200 | 1.07181800 |
| H | -3.32785400 | 0.17043300 | -1.17425700 |
| C | -4.07593200 | 0.36558000 | 1.00609100 |
| C | -4.54353600 | 0.36528200 | -0.33005000 |
| H | -5.05433800 | -0.54199800 | -0.66136400 |
| C | -4.08356200 | 1.62536800 | 1.85414000 |
| H | -3.59186700 | 1.45915700 | 2.81522300 |
| H | -5.12148300 | 1.92866600 | 2.04436300 |
| H | -3.57968200 | 2.45794700 | 1.35790500 |
| C | -5.01966800 | 1.62481900 | -1.03915400 |
| H | -4.29495500 | -0.53787400 | 1.57517300 |
| O | -5.06145400 | 1.47305200 | -2.45305200 |
| H | -4.15627500 | 1.28072000 | -2.73694400 |
| H | -6.05169900 | 1.86473900 | -0.74545200 |
| H | -4.39903000 | 2.48556500 | -0.75227900 |

**14E**

| C | -1.21468800 | 0.33200200 | -0.20252100 |
|---|---|---|---|
| H | -1.20456800 | 1.21743400 | -0.83284600 |
| C | 2.29426000 | -0.39714400 | -0.33029100 |
| H | 2.41012300 | -1.31825000 | 0.25184300 |
| H | 3.27207500 | 0.09433000 | -0.37327100 |
| H | 2.00931600 | -0.68278000 | -1.34781200 |
| O | -2.47014900 | -0.20323400 | -0.15130500 |
| C | 1.23577500 | 0.52489300 | 0.29722400 |
| H | 1.15146000 | 1.44365600 | -0.29634800 |
| H | 1.58529800 | 0.83695200 | 1.29199500 |
| C | -0.11919900 | -0.11990800 | 0.41375700 |
| H | -0.18936900 | -1.01767700 | 1.03177600 |
| H | -2.45003800 | -0.98685500 | 0.41609300 |

**14Z**

| C | 1.37545500 | 0.52047200 | -0.13906200 |
|---|---|---|---|
| H | 2.07565400 | 1.29686100 | -0.43203300 |
| C | -2.16205500 | -0.20627900 | -0.41197600 |
| H | -2.61420800 | 0.78796700 | -0.49368400 |
| H | -2.93854000 | -0.89985500 | -0.07245300 |
| H | -1.84610100 | -0.50823900 | -1.41529800 |
| O | 1.99881900 | -0.69416600 | -0.12463200 |
| C | -0.96922300 | -0.18526500 | 0.55841300 |
| H | -0.56281000 | -1.20368200 | 0.64240800 |
| H | -1.33417500 | 0.06211200 | 1.56528600 |
| C | 0.09982700 | 0.79624200 | 0.15555700 |
| H | -0.19784000 | 1.83912300 | 0.08086500 |
| H | 1.36344500 | -1.37198100 | 0.14437700 |

**15**

| C  | -2.40034200 | -0.15146300 | -0.13318800 |
|----|-------------|-------------|-------------|
| C  | -0.96131900 | -0.33335300 | 0.35674000  |
| H  | -3.06788700 | -0.90476200 | 0.29777500  |
| H  | -2.46113000 | -0.24006700 | -1.22391900 |
| H  | -2.79362600 | 0.83516000  | 0.13880100  |
| C  | 0.00483600  | 0.70553600  | -0.22457500 |
| H  | -0.59972700 | -1.33373600 | 0.09611500  |
| H  | -0.93625200 | -0.27272200 | 1.45387900  |
| C  | 1.44826600  | 0.51795200  | 0.22566500  |
| H  | -0.31572200 | 1.71715300  | 0.05991500  |
| H  | -0.02227600 | 0.66392700  | -1.32137200 |
| O  | 1.90985700  | -0.73924200 | -0.26177900 |
| H  | 1.50112800  | 0.55901900  | 1.32668600  |
| H  | 2.06766000  | 1.34280800  | -0.16217200 |
| H  | 2.80032900  | -0.88487400 | 0.08067000  |

**TS17**

| C  | -1.61484700 | -0.66571300 | -0.19996400 |
|----|-------------|-------------|-------------|
| H  | -1.49692600 | -0.50967500 | -1.27797100 |
| H  | -2.00287800 | -1.69025900 | -0.08756000 |
| C  | -0.24732500 | -0.68636800 | 0.46526700  |
| C  | 0.56907200  | 1.35935600  | -0.50694900 |
| H  | -0.24138000 | 2.06837800  | -0.37233700 |
| H  | 0.61907900  | 0.85521100  | -1.46977400 |
| C  | 1.73500200  | 1.54081300  | 0.22876000  |
| H  | 1.66124000  | 2.23745200  | 1.08813500  |
| O  | 2.85165200  | 0.94224600  | 0.07136500  |
| O  | 0.59300900  | -1.56512100 | 0.15827500  |
| H  | -0.19211000 | -0.20191800 | 1.45382800  |
| Na | 2.65092800  | -1.13927000 | -0.23358500 |

| C  | -2.61596700 | 0.32419400  | 0.40163500  |
|----|-------------|-------------|-------------|
| H  | -2.22801700 | 1.34350800  | 0.30256200  |
| H  | -2.70472900 | 0.13434900  | 1.47992300  |
| C  | -4.00117700 | 0.23500300  | -0.24545500 |
| H  | -4.69845200 | 0.94693400  | 0.20754800  |
| H  | -4.42977500 | -0.76752000 | -0.13392000 |
| H  | -3.95208700 | 0.45478700  | -1.31788700 |

**16**

| C  | 1.54432000  | -0.59219000 | 0.08373900  |
|----|-------------|-------------|-------------|
| H  | 1.45645300  | -0.81518100 | 1.15656600  |
| H  | 1.81857000  | -1.53711100 | -0.40259300 |
| C  | 0.12928600  | -0.26315800 | -0.46264700 |
| C  | -0.40914300 | 1.05490500  | 0.36383700  |
| H  | 0.31924300  | 1.86757200  | 0.29466800  |
| H  | -0.50896400 | 0.71700400  | 1.40071200  |
| C  | -1.70401000 | 1.48400900  | -0.18093500 |
| H  | -1.68106300 | 2.27703800  | -0.95562900 |
| O  | -2.79600500 | 0.96993800  | 0.09147100  |
| O  | -0.71455000 | -1.29623200 | -0.35866400 |
| H  | 0.26768700  | 0.10447300  | -1.50892700 |
| Na | -2.67185200 | -1.25593100 | 0.25440500  |
| C  | 2.64873800  | 0.44151800  | -0.16226500 |
| H  | 2.44382800  | 1.36384300  | 0.39726500  |
| H  | 2.64951100  | 0.72439900  | -1.22440700 |
| C  | 4.04163800  | -0.06885500 | 0.22508700  |
| H  | 4.81368400  | 0.68645600  | 0.04199200  |
| H  | 4.30735800  | -0.96383900 | -0.34863800 |
| H  | 4.08353000  | -0.33642800 | 1.28718900  |

**17**

| | | | |
|---|---|---|---|
| C | -1.20006400 | 0.57591800 | 0.18883900 |
| H | -1.26975700 | 0.64206700 | 1.28305500 |
| H | -1.52933200 | 1.54786400 | -0.19773500 |
| C | 0.27267400 | 0.42716900 | -0.19799300 |
| C | 0.94240600 | -0.80316100 | 0.43658000 |
| H | 0.44791900 | -1.73988800 | 0.14497400 |
| H | 0.86147000 | -0.75156800 | 1.53384600 |
| C | 2.40873600 | -0.94023300 | 0.10962600 |
| H | 2.88069100 | -1.89647900 | 0.42469800 |
| O | 3.07676800 | -0.09145800 | -0.45041300 |
| O | 0.93002800 | 1.61701300 | 0.21630800 |
| H | 0.33823500 | 0.31740600 | -1.29443700 |
| C | -2.12829700 | -0.52649700 | -0.33516100 |
| H | -1.83861200 | -1.49900200 | 0.08417900 |
| H | -2.00906100 | -0.61632400 | -1.42357000 |
| C | -3.60100900 | -0.26204900 | -0.00537900 |
| H | -4.24553900 | -1.06011100 | -0.38735200 |
| H | -3.94072000 | 0.68167700 | -0.44597900 |
| H | -3.75842700 | -0.19559700 | 1.07693900 |
| H | 1.84209000 | 1.53863000 | -0.10484000 |

**TS18E**

| | | | |
|---|---|---|---|
| C | 2.52462700 | 0.13987300 | 0.36294000 |
| H | 2.66266500 | 1.21807300 | 0.52220000 |
| H | 2.32181200 | -0.29938800 | 1.34959700 |
| C | 1.28151500 | -0.05981600 | -0.50850000 |
| C | 0.03003400 | 0.60299100 | 0.05648000 |
| H | -1.06638000 | 0.02733200 | -0.33429700 |
| H | -0.08877100 | 0.45175500 | 1.13661700 |
| C | -0.25909400 | 1.95558900 | -0.34368100 |

| | | | |
|---|---|---|---|
| H | 0.30169000 | 2.35101900 | -1.21672200 |
| O | -1.16860700 | 2.67375000 | 0.13042100 |
| O | 1.10611100 | -1.47742500 | -0.64047900 |
| H | 1.48635100 | 0.37655100 | -1.50393900 |
| H | 0.31639500 | -1.62047600 | -1.17850400 |
| O | -2.35319800 | -0.39618500 | -0.49913000 |
| C | -2.48178300 | -1.77097000 | -0.27014300 |
| H | -2.75923600 | -2.30350900 | -1.19847900 |
| H | -1.51363600 | -2.20074100 | 0.05071400 |
| C | -3.52638300 | -2.09785500 | 0.80060300 |
| H | -3.61699400 | -3.17839100 | 0.96472600 |
| H | -4.51225900 | -1.71932200 | 0.50235800 |
| H | -3.25228500 | -1.63264800 | 1.75577600 |
| Na | -3.00222900 | 1.46516200 | 0.25149000 |
| C | 3.80419500 | -0.46949400 | -0.22149500 |
| H | 3.99664200 | -0.02540400 | -1.20827400 |
| H | 3.63767300 | -1.53776300 | -0.39317500 |
| C | 5.02730800 | -0.26516000 | 0.67713700 |
| H | 5.92639400 | -0.70817300 | 0.23611500 |
| H | 4.87827800 | -0.72752700 | 1.65969800 |
| H | 5.22920800 | 0.79976200 | 0.84266000 |

**TS18Z**

| | | | |
|---|---|---|---|
| C | 1.98957500 | -0.00723900 | 0.50401200 |
| H | 1.63157000 | 0.91628500 | 0.97793600 |
| H | 2.45926200 | -0.60906300 | 1.29400600 |
| C | 0.77836700 | -0.77886200 | -0.01709700 |
| C | -0.27888300 | -0.96916000 | 1.08794200 |
| H | -1.05932700 | 0.03426000 | 0.92298900 |
| H | 0.12180300 | -0.97825000 | 2.10430000 |
| C | -1.25332200 | -1.99863300 | 0.86737700 |
| H | -1.73220300 | -2.45248000 | 1.75600300 |

A75

| | | | |
|---|---|---|---|
| O | -1.67698000 | -2.33868800 | -0.26778700 |
| O | 1.25528600 | -2.01686400 | -0.54960800 |
| H | 0.33151200 | -0.18246200 | -0.83346300 |
| H | 0.47155600 | -2.49655300 | -0.85556500 |
| O | -1.94040600 | 0.94564300 | 0.33926000 |
| C | -1.73343300 | 2.27306800 | 0.72156300 |
| H | -2.61075400 | 2.67305800 | 1.26266000 |
| H | -0.88818800 | 2.34552300 | 1.43229700 |
| C | -1.43779200 | 3.18957000 | -0.46926600 |
| H | -1.26235500 | 4.22499700 | -0.15266400 |
| H | -2.28131300 | 3.19097500 | -1.17142600 |
| H | -0.54877900 | 2.83945600 | -1.00638800 |
| Na | -2.48330900 | -0.44656300 | -1.12730200 |
| C | 3.02402100 | 0.32453300 | -0.57698200 |
| H | 2.54725300 | 0.93605400 | -1.35612100 |
| H | 3.33554600 | -0.60590900 | -1.06288500 |
| C | 4.24590900 | 1.06458100 | -0.02528500 |
| H | 4.96704700 | 1.29193300 | -0.81731500 |
| H | 4.76357500 | 0.46410900 | 0.73148900 |
| H | 3.96034500 | 2.01238600 | 0.44596600 |

**18E**

| | | | |
|---|---|---|---|
| C | -1.74741100 | 0.25000200 | 0.63620700 |
| C | -0.68920800 | 0.18695800 | -0.21038800 |
| C | 0.69697000 | 0.57864500 | 0.18916300 |
| C | 1.75784800 | -0.47570400 | -0.14858200 |
| C | 3.18233200 | -0.08430600 | 0.26183300 |
| H | 1.72514100 | -0.65957800 | -1.23167300 |
| H | 1.47126900 | -1.41573400 | 0.34112500 |
| C | 4.22381200 | -1.14934000 | -0.09486900 |
| H | 3.20692300 | 0.10228900 | 1.34484400 |
| H | 3.43743300 | 0.86625000 | -0.21795800 |

| H  | 4.00224900  | -2.10519300 | 0.39518900  |
|----|-------------|-------------|-------------|
| H  | 5.23161800  | -0.84657600 | 0.21022100  |
| H  | 4.24689500  | -1.33385100 | -1.17543800 |
| H  | 0.71253300  | 0.74399300  | 1.28219900  |
| O  | 1.12176000  | 1.79788700  | -0.47217100 |
| O  | -2.99431400 | -0.05072100 | 0.38379400  |
| H  | -1.53755900 | 0.59290800  | 1.66639600  |
| H  | -0.84245900 | -0.14385900 | -1.23907400 |
| H  | 0.32674400  | 2.34596400  | -0.50975500 |
| Na | -4.68603700 | -0.72377000 | -0.35993100 |

**18Z**

| C  | -2.36478300 | -0.90264100 | -0.18048100 |
|----|-------------|-------------|-------------|
| C  | -1.03970300 | -1.17599300 | -0.44011700 |
| C  | 0.09040500  | -0.59467300 | 0.38496300  |
| C  | 1.40317700  | -0.43351100 | -0.38310300 |
| C  | 2.58144600  | 0.03621200  | 0.47725000  |
| H  | 1.24057000  | 0.27338400  | -1.21272400 |
| H  | 1.64353200  | -1.39793000 | -0.85051700 |
| C  | 3.87628000  | 0.20836300  | -0.32191700 |
| H  | 2.74349800  | -0.68901100 | 1.28599000  |
| H  | 2.31332200  | 0.98038600  | 0.96404400  |
| H  | 4.18074600  | -0.73164500 | -0.79666600 |
| H  | 4.70062800  | 0.53860700  | 0.31853200  |
| H  | 3.75684300  | 0.95363500  | -1.11728500 |
| H  | 0.29474900  | -1.24766000 | 1.25405600  |
| O  | -0.28130700 | 0.70846600  | 0.92150100  |
| O  | -2.81971800 | 0.06109000  | 0.57733400  |
| H  | -3.11447000 | -1.51956900 | -0.70910500 |
| H  | -0.80276400 | -2.02890800 | -1.07061900 |
| H  | -1.19822100 | 0.55437400  | 1.26478900  |
| Na | -1.65737900 | 1.39375800  | -0.77643200 |

**TS19E**

| | | | |
|---|---|---|---|
| C | -1.65501700 | -1.22282000 | 0.53278300 |
| H | -1.98596400 | -2.03363100 | 1.20120300 |
| H | -1.52873300 | -0.33901600 | 1.16987900 |
| C | -0.31078200 | -1.64543200 | 0.00015300 |
| C | 0.82769400 | -1.66022100 | 0.80467200 |
| H | 0.33187000 | 1.44930300 | -0.86084100 |
| H | 0.88869000 | -0.98673300 | 1.66087100 |
| C | 2.04339100 | -2.16070000 | 0.26882000 |
| H | 1.94303300 | -2.98392700 | -0.47283300 |
| O | 3.18469300 | -1.69332700 | 0.49498000 |
| O | 0.06690500 | -0.14268400 | -1.25215900 |
| H | -0.34013600 | -2.37480600 | -0.81005300 |
| H | -0.32824500 | -0.30172300 | -2.12048400 |
| O | 0.98126100 | 2.15866200 | -0.56602000 |
| C | 0.32494900 | 3.33899500 | -0.12436600 |
| H | 1.10773300 | 4.08213100 | 0.06315300 |
| H | -0.31175600 | 3.74018200 | -0.92682300 |
| C | -0.50253300 | 3.11646700 | 1.13799100 |
| H | -0.97515500 | 4.05008000 | 1.46274000 |
| H | 0.12866400 | 2.74936000 | 1.95382300 |
| H | -1.29445200 | 2.38103600 | 0.96093700 |
| Na | 2.17286800 | 0.27109900 | -0.40573900 |
| C | -2.74287600 | -0.96699000 | -0.51486600 |
| H | -2.82292000 | -1.84212100 | -1.17492900 |
| H | -2.42428000 | -0.12916800 | -1.14234400 |
| C | -4.11064800 | -0.67258500 | 0.10715200 |
| H | -4.86548700 | -0.48261200 | -0.66253900 |
| H | -4.06986000 | 0.21029700 | 0.75551400 |
| H | -4.46249100 | -1.51222800 | 0.71740000 |

**TS19Z**

| | | | |
|---|---|---|---|
| C | -2.38817700 | 0.10970500 | 0.39815600 |
| H | -3.19517000 | 0.66592500 | 0.90627100 |
| H | -2.26965900 | 0.59711900 | -0.57277600 |
| C | -1.17583300 | 0.32877100 | 1.26179800 |
| C | -0.41622900 | 1.47061900 | 1.31308800 |
| H | 1.71444700 | -0.93803100 | -0.23067300 |
| H | 0.18634300 | 1.65004500 | 2.20060900 |
| C | -0.27116000 | 2.44876800 | 0.27198800 |
| H | 0.15990300 | 3.41870300 | 0.59113000 |
| O | -0.52232300 | 2.29025800 | -0.94049000 |
| O | 0.22301000 | -1.21114800 | 0.08364900 |
| H | -1.10526600 | -0.33359500 | 2.12091300 |
| H | 0.00551100 | -2.14975700 | 0.12170800 |
| O | 2.47717900 | -0.47798200 | -0.74827100 |
| C | 3.52854900 | -0.10470900 | 0.12605300 |
| H | 4.14934900 | 0.63092600 | -0.40085900 |
| H | 3.12843700 | 0.39566400 | 1.02327600 |
| C | 4.38592200 | -1.29742000 | 0.54208000 |
| H | 5.21306900 | -0.98010800 | 1.18782800 |
| H | 4.80475600 | -1.79237300 | -0.33962800 |
| H | 3.78798600 | -2.03170300 | 1.09241200 |
| Na | 0.45411100 | 0.29756100 | -1.44881600 |
| C | -2.84744300 | -1.34384500 | 0.23604500 |
| H | -2.90401900 | -1.81721800 | 1.22579800 |
| H | -2.08280700 | -1.88678000 | -0.32520900 |
| C | -4.20507300 | -1.45521200 | -0.46302400 |
| H | -4.50587200 | -2.50105300 | -0.58080300 |
| H | -4.17573000 | -1.00520800 | -1.46239500 |
| H | -4.99276000 | -0.94480900 | 0.10316900 |

**19E**

| | | | |
|---|---|---|---|
| C | -2.65379400 | 0.32068700 | -0.00925000 |
| H | -2.62129200 | 1.39161200 | 0.29826900 |
| O | -3.69802500 | -0.20037400 | -0.35492000 |
| C | -1.35705200 | -0.36774300 | 0.04442300 |
| H | -1.34590800 | -1.41557400 | -0.24795600 |
| C | -0.24537700 | 0.27266400 | 0.43869800 |
| H | -0.33256300 | 1.32642100 | 0.71453600 |
| C | 1.12888400 | -0.31619500 | 0.52458600 |
| H | 1.09825000 | -1.37999400 | 0.26113300 |
| H | 1.47377100 | -0.25824500 | 1.56806100 |
| C | 2.15196600 | 0.41699000 | -0.36713300 |
| H | 2.16030000 | 1.48312500 | -0.10539900 |
| H | 1.82077400 | 0.35983500 | -1.41108700 |
| C | 3.56515200 | -0.15726300 | -0.23645300 |
| H | 4.26987900 | 0.37742700 | -0.88066700 |
| H | 3.59146100 | -1.21506200 | -0.52043600 |
| H | 3.93085400 | -0.08139100 | 0.79367700 |

**19Z**

| | | | |
|---|---|---|---|
| C | -2.13351900 | -0.54242400 | 0.05355900 |
| H | -1.46119600 | -1.36992900 | 0.36201500 |
| O | -3.31572200 | -0.75631700 | -0.15437000 |
| C | -1.52231000 | 0.78726700 | -0.08603300 |
| H | -2.21479200 | 1.56730700 | -0.39403500 |
| C | -0.22829600 | 1.08708700 | 0.13117300 |
| H | 0.07173900 | 2.12490800 | -0.02262500 |
| C | 0.89253300 | 0.17845000 | 0.54861500 |
| H | 0.54334800 | -0.84243200 | 0.72847900 |
| H | 1.29048100 | 0.54416300 | 1.50699500 |
| C | 2.04262300 | 0.15845700 | -0.47929400 |

| H | 2.37994800 | 1.18689000 | -0.66310300 |
| H | 1.65862100 | -0.21356500 | -1.43689500 |
| C | 3.22588500 | -0.69922900 | -0.02321200 |
| H | 4.02548400 | -0.69808800 | -0.77030700 |
| H | 2.92346700 | -1.73978100 | 0.13842700 |
| H | 3.64718800 | -0.32659000 | 0.91715200 |

**TS20**

| Ru | 0.97727400 | -0.43561500 | 0.98769200 |
| N | 3.15263100 | 1.64308600 | 1.74333700 |
| N | 1.43744200 | 1.96207900 | 3.00264000 |
| O | -0.07106100 | -1.71392000 | 3.53670100 |
| O | 2.23419200 | -1.42192200 | -1.97118700 |
| O | -3.72322900 | 5.20482600 | -0.62364700 |
| O | -6.31000600 | -1.89436500 | 0.77127800 |
| C | 0.34255800 | -1.20856600 | 2.57159500 |
| C | 1.19633000 | -0.90856300 | -1.42175400 |
| C | 0.95739500 | 0.50588600 | -1.16282500 |
| C | -0.34865100 | 0.63655400 | -0.52117000 |
| C | -0.86350900 | -0.69789400 | -0.30048200 |
| C | 0.11003800 | -1.65481400 | -0.76679100 |
| C | 1.81182800 | 1.60492500 | -1.66568600 |
| C | 2.65855800 | 1.39975000 | -2.77370900 |
| H | 2.68407300 | 0.42118500 | -3.23665800 |
| C | 3.47266400 | 2.42623300 | -3.25402300 |
| H | 4.11543600 | 2.23905700 | -4.11039500 |
| C | 3.46423500 | 3.68390200 | -2.64907100 |
| H | 4.09793400 | 4.48179100 | -3.02644400 |
| C | 2.62588300 | 3.90439600 | -1.55283700 |
| H | 2.60309700 | 4.87867900 | -1.07123900 |
| C | 1.81315500 | 2.88178800 | -1.06780300 |
| H | 1.17409100 | 3.07084800 | -0.21315800 |

| | | | |
|---|---|---|---|
| C | -0.08506300 | -3.11908900 | -0.88538500 |
| C | 0.29523400 | -3.78102000 | -2.06683900 |
| H | 0.77362800 | -3.21455000 | -2.85767900 |
| C | 0.07988800 | -5.15091800 | -2.21923500 |
| H | 0.38278200 | -5.64080400 | -3.14098500 |
| C | -0.52075400 | -5.88952900 | -1.19923000 |
| H | -0.68696900 | -6.95666000 | -1.31827600 |
| C | -0.89997700 | -5.24430100 | -0.01971100 |
| H | -1.36166100 | -5.80820300 | 0.78631400 |
| C | -0.68152100 | -3.87734400 | 0.13703200 |
| H | -0.96709600 | -3.39203600 | 1.06383000 |
| C | -1.19669400 | 1.85687200 | -0.52316100 |
| C | -1.35511500 | 2.57908900 | -1.71537600 |
| H | -0.81846000 | 2.26150900 | -2.60342000 |
| C | -2.18509700 | 3.69866000 | -1.79648300 |
| H | -2.27340500 | 4.22298800 | -2.74072700 |
| C | -2.88930300 | 4.12298700 | -0.66431200 |
| C | -2.75252000 | 3.40979900 | 0.53441800 |
| H | -3.31018200 | 3.74459300 | 1.40330800 |
| C | -1.92109800 | 2.29886700 | 0.59699300 |
| H | -1.83357300 | 1.75813400 | 1.53064500 |
| C | -3.90503300 | 5.95307100 | -1.81407300 |
| H | -4.59992900 | 6.75636800 | -1.56339100 |
| H | -4.33692000 | 5.34114400 | -2.61673600 |
| H | -2.96200100 | 6.39011100 | -2.16791200 |
| C | -2.28151400 | -1.02236400 | 0.02177600 |
| C | -2.85235400 | -0.92334800 | 1.30040900 |
| H | -2.23377600 | -0.63189700 | 2.14126200 |
| C | -4.19234600 | -1.21935300 | 1.51897200 |
| H | -4.62839700 | -1.14913700 | 2.51022200 |
| C | -5.00839900 | -1.62670800 | 0.45535800 |
| C | -4.45924200 | -1.73845000 | -0.82710900 |
| H | -5.06186600 | -2.05680000 | -1.66945800 |
| C | -3.11085100 | -1.43950400 | -1.02789600 |

A82

| | | | |
|---|---|---|---|
| H | -2.69438000 | -1.53646900 | -2.02612600 |
| C | -7.17463400 | -2.32716000 | -0.26576000 |
| H | -8.14878500 | -2.48634800 | 0.19968500 |
| H | -6.83159600 | -3.26864500 | -0.71422600 |
| H | -7.27264900 | -1.57078600 | -1.05550100 |
| C | 1.89634200 | 1.15586300 | 1.99355200 |
| C | 3.45785700 | 2.71332200 | 2.56990200 |
| H | 4.40018400 | 3.23424200 | 2.51043100 |
| C | 2.38019000 | 2.91434600 | 3.36352300 |
| H | 2.19473900 | 3.64365900 | 4.13602600 |
| C | 4.11322200 | 1.10985200 | 0.78196700 |
| H | 4.63920700 | 1.94093900 | 0.30796200 |
| H | 3.58972600 | 0.54619900 | 0.01551200 |
| H | 4.83213700 | 0.45817300 | 1.28889900 |
| C | 0.14906800 | 1.85724600 | 3.67340900 |
| H | -0.33352300 | 2.83768000 | 3.70059600 |
| H | 0.27808100 | 1.48604500 | 4.69450400 |
| H | -0.47326500 | 1.16209200 | 3.11762700 |
| H | 2.50798300 | -1.19506100 | 1.35476800 |
| H | 2.82746500 | -2.34786300 | -1.01379100 |
| O | 3.24613100 | -2.74226400 | -0.13959200 |
| H | 2.70623400 | -1.85392800 | 0.70561000 |
| C | 4.67517900 | -2.63870400 | -0.20461200 |
| H | 5.03089700 | -2.38952700 | 0.80301500 |
| H | 4.95399600 | -1.81560400 | -0.87533200 |
| C | 5.28238300 | -3.95223000 | -0.67581100 |
| H | 6.37580300 | -3.88375400 | -0.69301900 |
| H | 4.93775600 | -4.19885500 | -1.68448000 |
| H | 4.99438200 | -4.76775500 | -0.00654500 |

**TS21**

| | | | |
|---|---|---|---|
| Ru | 0.55214900 | -1.21529800 | 0.93599000 |

| | | | |
|---|---|---|---|
| N | 3.58339300 | -1.42042300 | 1.43950900 |
| N | 2.78340800 | 0.09644300 | 2.74157400 |
| O | -0.85374500 | -1.30219000 | 3.62805700 |
| O | 0.90417000 | -2.65492400 | -2.06546900 |
| O | 0.39823300 | 6.18781900 | -0.24776900 |
| O | -6.07550400 | 2.20493100 | 0.82012000 |
| C | -0.30380800 | -1.26676300 | 2.59950100 |
| C | 0.41519100 | -1.62077300 | -1.48102800 |
| C | 1.10677700 | -0.37813500 | -1.19378700 |
| C | 0.18378800 | 0.51655600 | -0.49725500 |
| C | -1.05785700 | -0.20863600 | -0.30030300 |
| C | -0.90240900 | -1.54124500 | -0.81827300 |
| C | 2.46217000 | -0.04956400 | -1.69198200 |
| C | 2.95031000 | -0.65681300 | -2.86599200 |
| H | 2.33202200 | -1.38714100 | -3.37305400 |
| C | 4.21938800 | -0.34846800 | -3.35756400 |
| H | 4.57049400 | -0.83167600 | -4.26558700 |
| C | 5.03353700 | 0.57162000 | -2.69590500 |
| H | 6.02095900 | 0.81052100 | -3.08128200 |
| C | 4.56281200 | 1.18251700 | -1.53078500 |
| H | 5.18390400 | 1.90153500 | -1.00294300 |
| C | 3.29714500 | 0.87624900 | -1.03543200 |
| H | 2.94876000 | 1.35876000 | -0.12955500 |
| C | -1.96063900 | -2.57030700 | -0.94514100 |
| C | -2.06874300 | -3.32310900 | -2.13110300 |
| H | -1.34865700 | -3.16012700 | -2.92491800 |
| C | -3.07335400 | -4.28064800 | -2.28123300 |
| H | -3.13529400 | -4.84928100 | -3.20520900 |
| C | -3.99433300 | -4.50646200 | -1.25730500 |
| H | -4.77531500 | -5.25222300 | -1.37549500 |
| C | -3.89733800 | -3.76787900 | -0.07513100 |
| H | -4.60356200 | -3.93729700 | 0.73302800 |
| C | -2.89091900 | -2.81673400 | 0.08206900 |
| H | -2.81778300 | -2.26045300 | 1.01001000 |

| | | | |
|---|---|---|---|
| C | 0.28706300 | 1.99565200 | -0.41667000 |
| C | 0.69998400 | 2.73130900 | -1.53722500 |
| H | 0.98586400 | 2.20615700 | -2.44229300 |
| C | 0.75379000 | 4.12680200 | -1.52652200 |
| H | 1.08203900 | 4.64846500 | -2.41786700 |
| C | 0.38018700 | 4.82753300 | -0.37479600 |
| C | -0.05134900 | 4.11278400 | 0.75143300 |
| H | -0.34953300 | 4.66743900 | 1.63538000 |
| C | -0.09588100 | 2.72492800 | 0.72450500 |
| H | -0.44496000 | 2.19119400 | 1.60079500 |
| C | 0.81533900 | 6.95737200 | -1.36313800 |
| H | 0.75338600 | 8.00116500 | -1.05072800 |
| H | 0.16147600 | 6.80212000 | -2.23124600 |
| H | 1.84977600 | 6.72841900 | -1.65125400 |
| C | -2.36964700 | 0.41431600 | 0.03956600 |
| C | -2.80312500 | 0.72042600 | 1.33945700 |
| H | -2.17405800 | 0.47761200 | 2.18764100 |
| C | -4.03884400 | 1.31442200 | 1.56695300 |
| H | -4.37320900 | 1.54441800 | 2.57339000 |
| C | -4.88418100 | 1.62334000 | 0.49298500 |
| C | -4.47393200 | 1.32348700 | -0.81102300 |
| H | -5.10541000 | 1.54599200 | -1.66294700 |
| C | -3.23074100 | 0.72477900 | -1.02142000 |
| H | -2.92497900 | 0.49324000 | -2.03758400 |
| C | -6.97146200 | 2.53173000 | -0.22932000 |
| H | -7.84588800 | 2.97734700 | 0.24779500 |
| H | -7.28230100 | 1.64074400 | -0.79033000 |
| H | -6.53293000 | 3.25751800 | -0.92658900 |
| C | 2.41078000 | -0.80482600 | 1.78350500 |
| C | 4.65000700 | -0.91361900 | 2.16421200 |
| H | 5.65833000 | -1.26970500 | 2.02738900 |
| C | 4.14847500 | 0.04113700 | 2.98392100 |
| H | 4.63226500 | 0.68369900 | 3.70189000 |
| C | 3.73215300 | -2.50984100 | 0.47502200 |

| H | 4.76486300 | -2.51563800 | 0.12191800 |
|---|---|---|---|
| H | 3.07130800 | -2.35835100 | -0.37608200 |
| H | 3.50106900 | -3.46992400 | 0.94458900 |
| C | 1.88883400 | 1.02820000 | 3.42126600 |
| H | 2.48472900 | 1.64397600 | 4.09721200 |
| H | 1.13683900 | 0.48950200 | 3.99892700 |
| H | 1.39396500 | 1.67097100 | 2.69326200 |
| H | 1.07599000 | -2.83705100 | 1.29246400 |
| H | 0.75853500 | -3.78372200 | -1.16405800 |
| O | 0.67097100 | -4.40304500 | -0.31627100 |
| H | 0.83120500 | -3.42169700 | 0.59351700 |
| H | -0.27407500 | -4.61430300 | -0.26705100 |

**TS22**

| Ru | 0.55214900 | -1.21529800 | 0.93599000 |
|---|---|---|---|
| N | 3.58339300 | -1.42042300 | 1.43950900 |
| N | 2.78340800 | 0.09644300 | 2.74157400 |
| O | -0.85374500 | -1.30219000 | 3.62805700 |
| O | 0.90417000 | -2.65492400 | -2.06546900 |
| O | 0.39823300 | 6.18781900 | -0.24776900 |
| O | -6.07550400 | 2.20493100 | 0.82012000 |
| C | -0.30380800 | -1.26676300 | 2.59950100 |
| C | 0.41519100 | -1.62077300 | -1.48102800 |
| C | 1.10677700 | -0.37813500 | -1.19378700 |
| C | 0.18378800 | 0.51655600 | -0.49725500 |
| C | -1.05785700 | -0.20863600 | -0.30030300 |
| C | -0.90240900 | -1.54124500 | -0.81827300 |
| C | 2.46217000 | -0.04956400 | -1.69198200 |
| C | 2.95031000 | -0.65681300 | -2.86599200 |
| H | 2.33202200 | -1.38714100 | -3.37305100 |
| C | 4.21938800 | -0.34846800 | -3.35756400 |
| H | 4.57049400 | -0.83167600 | -4.26558700 |

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|---|---|---|---|
| C | 5.03353700 | 0.57162000 | -2.69590500 |
| H | 6.02095900 | 0.81052100 | -3.08128200 |
| C | 4.56281200 | 1.18251700 | -1.53078500 |
| H | 5.18390400 | 1.90153500 | -1.00294300 |
| C | 3.29714500 | 0.87624900 | -1.03543200 |
| H | 2.94876000 | 1.35876000 | -0.12955500 |
| C | -1.96063900 | -2.57030700 | -0.94514100 |
| C | -2.06874300 | -3.32310900 | -2.13110300 |
| H | -1.34865700 | -3.16012700 | -2.92491800 |
| C | -3.07335400 | -4.28064800 | -2.28123300 |
| H | -3.13529400 | -4.84928100 | -3.20520900 |
| C | -3.99433300 | -4.50646200 | -1.25730500 |
| H | -4.77531500 | -5.25222300 | -1.37549500 |
| C | -3.89733800 | -3.76787900 | -0.07513100 |
| H | -4.60356200 | -3.93729700 | 0.73302800 |
| C | -2.89091900 | -2.81673400 | 0.08206900 |
| H | -2.81778300 | -2.26045300 | 1.01001000 |
| C | 0.28706300 | 1.99565200 | -0.41667000 |
| C | 0.69998400 | 2.73130900 | -1.53722500 |
| H | 0.98586400 | 2.20615700 | -2.44229300 |
| C | 0.75379000 | 4.12680200 | -1.52652200 |
| H | 1.08203900 | 4.64846500 | -2.41786700 |
| C | 0.38018700 | 4.82753300 | -0.37479600 |
| C | -0.05134900 | 4.11278400 | 0.75143300 |
| H | -0.34953300 | 4.66743900 | 1.63538000 |
| C | -0.09588100 | 2.72492800 | 0.72450500 |
| H | -0.44496000 | 2.19119400 | 1.60079500 |
| C | 0.81533900 | 6.95737200 | -1.36313800 |
| H | 0.75338600 | 8.00116500 | -1.05072800 |
| H | 0.16147600 | 6.80212000 | -2.23124600 |
| H | 1.84977600 | 6.72841900 | -1.65125400 |
| C | -2.36964700 | 0.41431600 | 0.03956600 |
| C | -2.80312500 | 0.72042600 | 1.33945700 |
| H | -2.17405800 | 0.47761200 | 2.18764100 |

| C | -4.03884400 | 1.31442200 | 1.56695300 |
|---|---|---|---|
| H | -4.37320900 | 1.54441800 | 2.57339000 |
| C | -4.88418100 | 1.62334000 | 0.49298500 |
| C | -4.47393200 | 1.32348700 | -0.81102300 |
| H | -5.10541000 | 1.54599200 | -1.66294700 |
| C | -3.23074100 | 0.72477900 | -1.02142000 |
| H | -2.92497900 | 0.49324000 | -2.03758400 |
| C | -6.97146200 | 2.53173000 | -0.22932000 |
| H | -7.84588800 | 2.97734700 | 0.24779500 |
| H | -7.28230100 | 1.64074400 | -0.79033000 |
| H | -6.53293000 | 3.25751800 | -0.92658900 |
| C | 2.41078000 | -0.80482600 | 1.78350500 |
| C | 4.65000700 | -0.91361900 | 2.16421200 |
| H | 5.65833000 | -1.26970500 | 2.02738900 |
| C | 4.14847500 | 0.04113700 | 2.98392100 |
| H | 4.63226500 | 0.68369900 | 3.70189000 |
| C | 3.73215300 | -2.50984100 | 0.47502200 |
| H | 4.76486300 | -2.51563800 | 0.12191800 |
| H | 3.07130800 | -2.35835100 | -0.37608200 |
| H | 3.50106900 | -3.46992400 | 0.94458900 |
| C | 1.88883400 | 1.02820000 | 3.42126600 |
| H | 2.48472900 | 1.64397600 | 4.09721200 |
| H | 1.13683900 | 0.48950200 | 3.99892700 |
| H | 1.39396500 | 1.67097100 | 2.69326200 |
| H | 1.07599000 | -2.83705100 | 1.29246400 |
| H | 0.75853500 | -3.78372200 | -1.16405800 |
| O | 0.67097100 | -4.40304500 | -0.31627100 |
| H | 0.83120500 | -3.42169700 | 0.59351700 |
| H | -0.27407500 | -4.61430300 | -0.26705100 |

**TS23E**

| Ru | -0.86231100 | -0.13739200 | 0.65244200 |
|---|---|---|---|

| N | -2.08287600 | -2.90919500 | 1.33425700 |
|---|---|---|---|
| N | -0.76733500 | -2.29897500 | 2.92530100 |
| O | -0.81667400 | 1.63552900 | 3.09867400 |
| O | -1.98280600 | -0.33753900 | -2.44039700 |
| O | 6.24559500 | -2.65669600 | 0.51690300 |
| O | 4.59330800 | 4.94141400 | 0.81020700 |
| C | -0.85898200 | 0.91854500 | 2.17584200 |
| C | -0.86686200 | -0.11527100 | -1.72534900 |
| C | 0.03672200 | -1.14309100 | -1.31374800 |
| C | 1.11018600 | -0.49807400 | -0.57272600 |
| C | 0.81513700 | 0.91791700 | -0.51748100 |
| C | -0.42390100 | 1.16361500 | -1.21392800 |
| C | -0.04831100 | -2.57118900 | -1.69778000 |
| C | -0.61163400 | -2.94513700 | -2.93147900 |
| H | -0.99697000 | -2.18109500 | -3.59581500 |
| C | -0.69654000 | -4.28822500 | -3.30060900 |
| H | -1.14038700 | -4.55138200 | -4.25662700 |
| C | -0.21525200 | -5.28677100 | -2.45286500 |
| H | -0.28153200 | -6.33177800 | -2.74222200 |
| C | 0.35701700 | -4.92807300 | -1.22908000 |
| H | 0.73964100 | -5.69462600 | -0.56060600 |
| C | 0.43968800 | -3.58829700 | -0.85581600 |
| H | 0.87974600 | -3.32301100 | 0.09861500 |
| C | -1.03490800 | 2.47290300 | -1.53802300 |
| C | -1.58407200 | 2.69550000 | -2.81394000 |
| H | -1.57581500 | 1.89584500 | -3.54665200 |
| C | -2.14375200 | 3.93027500 | -3.14546100 |
| H | -2.56758300 | 4.07623100 | -4.13492000 |
| C | -2.15853300 | 4.96972400 | -2.21540500 |
| H | -2.59527400 | 5.93014100 | -2.47363600 |
| C | -1.61073200 | 4.76317400 | -0.94654700 |
| H | -1.61981400 | 5.56365600 | -0.21205000 |
| C | -1.05998900 | 3.52912600 | -0.60898400 |
| H | -0.65094600 | 3.37575100 | 0.38347200 |

| C | 2.43580900 | -1.09391300 | -0.27474700 |
| C | 3.14214100 | -1.76056900 | -1.28666900 |
| H | 2.69342600 | -1.86340200 | -2.26947500 |
| C | 4.41227800 | -2.29756300 | -1.06909400 |
| H | 4.91799400 | -2.80380800 | -1.88280900 |
| C | 5.01307800 | -2.16991600 | 0.18831900 |
| C | 4.32723600 | -1.49968300 | 1.21122900 |
| H | 4.80614900 | -1.40401700 | 2.18039100 |
| C | 3.06319000 | -0.97464600 | 0.97815800 |
| H | 2.54966500 | -0.45592500 | 1.77928400 |
| C | 6.98622800 | -3.33539400 | -0.48437200 |
| H | 7.92562200 | -3.63301000 | -0.01568900 |
| H | 7.20183200 | -2.68403500 | -1.34124500 |
| H | 6.46147700 | -4.23152300 | -0.84051900 |
| C | 1.78590400 | 1.98118800 | -0.13359400 |
| C | 2.13485700 | 2.29865000 | 1.18913700 |
| H | 1.65368500 | 1.78069700 | 2.01029000 |
| C | 3.06982500 | 3.28682900 | 1.47116400 |
| H | 3.33219900 | 3.53522600 | 2.49436900 |
| C | 3.68999200 | 3.99169000 | 0.43044600 |
| C | 3.35425900 | 3.69436900 | -0.89545000 |
| H | 3.81244100 | 4.22387800 | -1.72226100 |
| C | 2.41094300 | 2.70055400 | -1.16092400 |
| H | 2.15541400 | 2.48192200 | -2.19359000 |
| C | 5.24219300 | 5.69284400 | -0.20293500 |
| H | 5.90833300 | 6.38498900 | 0.31458600 |
| H | 4.52523000 | 6.26536100 | -0.80555000 |
| H | 5.83536300 | 5.05104100 | -0.86723900 |
| C | -1.26309600 | -1.87926900 | 1.71717400 |
| C | -2.09311500 | -3.92829700 | 2.27395400 |
| H | -2.67451400 | -4.82650000 | 2.13963600 |
| C | -1.26880300 | -3.54383100 | 3.27647700 |
| H | -0.99347200 | -4.03675000 | 4.19516000 |
| C | -2.85235400 | -2.99952300 | 0.09651200 |

| | | | |
|---|---|---|---|
| H | -2.53715200 | -3.87828800 | -0.47014100 |
| H | -2.67608900 | -2.11420200 | -0.50740100 |
| H | -3.91825200 | -3.07453800 | 0.32832600 |
| C | 0.16940300 | -1.56203200 | 3.76595500 |
| H | 0.63075000 | -2.26156300 | 4.46567400 |
| H | -0.33745900 | -0.77330000 | 4.32608600 |
| H | 0.94192100 | -1.11617800 | 3.14181600 |
| H | -2.61211400 | 0.09085700 | 0.55234100 |
| H | -2.76829800 | 0.14246000 | -2.04961900 |
| C | -3.97185900 | 0.41214500 | 0.35835000 |
| C | -4.30429000 | 0.61034400 | -1.00229800 |
| C | -4.10065000 | 1.57805700 | 1.34613900 |
| H | -4.99815500 | 2.14595300 | 1.06903500 |
| H | -3.25665200 | 2.26620800 | 1.22942200 |
| H | -4.34307300 | -0.53370500 | 0.76448700 |
| H | -4.24320100 | 1.60887900 | -1.43349100 |
| C | -5.01153500 | -0.39138700 | -1.76425400 |
| H | -5.14035900 | -1.36383900 | -1.22436400 |
| O | -5.47076700 | -0.25322900 | -2.89520700 |
| C | -4.23314000 | 1.12639300 | 2.80575900 |
| H | -3.39387200 | 0.47119900 | 3.06627800 |
| H | -5.14215300 | 0.51687200 | 2.90425200 |
| C | -4.29155700 | 2.29842900 | 3.78990400 |
| H | -4.42921900 | 1.94830300 | 4.81831700 |
| H | -5.12260600 | 2.97350600 | 3.55490300 |
| H | -3.36531000 | 2.88140600 | 3.75759600 |

**TS23Z**

| | | | |
|---|---|---|---|
| Ru | -0.82883400 | 0.10270200 | 0.63341200 |
| N | -2.73094400 | -2.32637600 | 0.96071300 |
| N | -1.34268900 | -2.27987000 | 2.60619600 |
| O | -0.47905500 | 1.51388500 | 3.28678400 |

A91

| | | | |
|---|---|---|---|
| O | -1.87797500 | 0.41421700 | -2.46935200 |
| O | 5.51240100 | -3.93862700 | 0.44701400 |
| O | 5.62585700 | 3.78832500 | 1.26847000 |
| C | -0.63301400 | 0.94391900 | 2.27817200 |
| C | -0.76005000 | 0.31831000 | -1.72978900 |
| C | -0.12218800 | -0.91689200 | -1.39941900 |
| C | 1.04275300 | -0.59743100 | -0.58847700 |
| C | 1.07564900 | 0.84175700 | -0.41822700 |
| C | -0.04976900 | 1.41758200 | -1.10776700 |
| C | -0.51844600 | -2.25096800 | -1.90723400 |
| C | -1.09574200 | -2.38121200 | -3.18348900 |
| H | -1.26393300 | -1.49642400 | -3.78564500 |
| C | -1.47108300 | -3.63264800 | -3.67383100 |
| H | -1.91922900 | -3.70641800 | -4.66070400 |
| C | -1.27314300 | -4.78130200 | -2.90634100 |
| H | -1.56603200 | -5.75474100 | -3.28944800 |
| C | -0.69080500 | -4.66695500 | -1.64089600 |
| H | -0.52772700 | -5.55323000 | -1.03370600 |
| C | -0.31756200 | -3.41857800 | -1.14742700 |
| H | 0.12752700 | -3.34199200 | -0.16203600 |
| C | -0.32794400 | 2.85380500 | -1.33489900 |
| C | -0.72953500 | 3.29530100 | -2.60880300 |
| H | -0.85910900 | 2.57317200 | -3.40782700 |
| C | -0.97080200 | 4.64791100 | -2.85217100 |
| H | -1.28619000 | 4.96527800 | -3.84197800 |
| C | -0.80889100 | 5.58659600 | -1.83276100 |
| H | -0.99874000 | 6.63913000 | -2.02225700 |
| C | -0.40615300 | 5.16095300 | -0.56437100 |
| H | -0.28129500 | 5.88222600 | 0.23841100 |
| C | -0.17292900 | 3.81016900 | -0.31556400 |
| H | 0.12517500 | 3.48812800 | 0.67618900 |
| C | 2.18644000 | -1.49996300 | -0.31158500 |
| C | 2.74262600 | -2.26540300 | -1.34685300 |
| H | 2.30631100 | -2.21608200 | -2.33917400 |

A92

| | | | |
|---|---|---|---|
| C | 3.84876200 | -3.09209000 | -1.14068200 |
| H | 4.24212300 | -3.66454600 | -1.97239000 |
| C | 4.43422800 | -3.16415000 | 0.12821800 |
| C | 3.90020400 | -2.39814000 | 1.17440600 |
| H | 4.36737500 | -2.45838700 | 2.15211000 |
| C | 2.79769900 | -1.58403500 | 0.95285800 |
| H | 2.40250700 | -0.99340000 | 1.77142000 |
| C | 6.09759000 | -4.72608200 | -0.57729600 |
| H | 6.93120300 | -5.25511500 | -0.11264800 |
| H | 6.47804500 | -4.10551100 | -1.39895600 |
| H | 5.38713800 | -5.45833400 | -0.98266500 |
| C | 2.25210500 | 1.62153000 | 0.06176400 |
| C | 2.58471000 | 1.81248100 | 1.41257700 |
| H | 1.94495500 | 1.40553000 | 2.18669300 |
| C | 3.71113000 | 2.53712300 | 1.78220400 |
| H | 3.96230200 | 2.68892600 | 2.82689800 |
| C | 4.54561400 | 3.09565500 | 0.80438700 |
| C | 4.23076000 | 2.92068500 | -0.54812400 |
| H | 4.85293300 | 3.34318500 | -1.32807400 |
| C | 3.09418300 | 2.19193500 | -0.90195800 |
| H | 2.85769400 | 2.06681800 | -1.95462000 |
| C | 6.49753300 | 4.38450800 | 0.32138600 |
| H | 7.27739600 | 4.88182800 | 0.90026900 |
| H | 5.97775100 | 5.12816200 | -0.29647700 |
| H | 6.95871700 | 3.63444700 | -0.33419700 |
| C | -1.68926300 | -1.59539300 | 1.46973800 |
| C | -3.01567100 | -3.42620500 | 1.75484000 |
| H | -3.79940100 | -4.12444600 | 1.50781200 |
| C | -2.14569500 | -3.39574900 | 2.79180600 |
| H | -2.02527500 | -4.05753100 | 3.63457800 |
| C | -3.45324400 | -2.06734600 | -0.28231200 |
| H | -3.25964500 | -2.86854700 | -0.99853400 |
| H | -3.11703700 | -1.12732300 | -0.71099700 |
| H | -4.52535100 | -2.00974700 | -0.07774400 |

| C | -0.26153000 | -1.92206400 | 3.51864200 |
| H | -0.06250700 | -2.77644800 | 4.16819000 |
| H | -0.53124800 | -1.06008100 | 4.13170100 |
| H | 0.63589800 | -1.68921200 | 2.94694300 |
| H | -2.47837700 | 0.78803100 | 0.54348000 |
| H | -2.55430000 | 1.01718500 | -2.03930700 |
| C | -3.53167600 | 1.64672900 | 0.39435300 |
| C | -3.88223600 | 1.84160100 | -0.97569700 |
| C | -4.54840000 | 1.06265300 | 1.38538900 |
| H | -5.45640200 | 1.67466200 | 1.29760000 |
| H | -4.84359300 | 0.05049300 | 1.08998000 |
| H | -3.00195200 | 2.50342500 | 0.81486700 |
| H | -3.45107300 | 2.69545700 | -1.49694600 |
| C | -4.95198500 | 1.16704500 | -1.66332100 |
| H | -5.44682100 | 0.34651800 | -1.09081900 |
| O | -5.34237200 | 1.42687400 | -2.80271300 |
| C | -4.10141000 | 1.05598000 | 2.85104300 |
| H | -3.77439100 | 2.06494300 | 3.13504100 |
| H | -3.22833100 | 0.40646500 | 2.96749400 |
| C | -5.21253800 | 0.59275800 | 3.79956200 |
| H | -4.87502000 | 0.60003200 | 4.84111300 |
| H | -5.53759200 | -0.42736500 | 3.56284800 |
| H | -6.09287100 | 1.24201600 | 3.73107900 |

**TS24E**

| Ru | -0.88677900 | -0.03753600 | 0.61896200 |
| N | -2.54671100 | -2.65220300 | 0.81565900 |
| N | -1.22435500 | -2.51458700 | 2.50985100 |
| O | -0.71523300 | 1.32616300 | 3.31260000 |
| O | -1.90867700 | 0.31276000 | -2.48779800 |
| O | 5.77973600 | -3.54102100 | 0.36305500 |
| O | 5.22505400 | 4.12689900 | 1.55712900 |

| C | -0.79733800 | 0.77059700 | 2.28751800 |
|---|---|---|---|
| C | -0.79440300 | 0.27948300 | -1.73003600 |
| C | -0.06122000 | -0.91197700 | -1.44066900 |
| C | 1.06294800 | -0.53241100 | -0.59743300 |
| C | 0.97465100 | 0.89370400 | -0.36906400 |
| C | -0.18398300 | 1.40526200 | -1.05713700 |
| C | -0.32889000 | -2.25029900 | -2.01568300 |
| C | -0.87419400 | -2.37202000 | -3.30686900 |
| H | -1.11257600 | -1.47821000 | -3.87092900 |
| C | -1.12693500 | -3.62763500 | -3.86088100 |
| H | -1.55162800 | -3.69511700 | -4.85861600 |
| C | -0.83520600 | -4.78883500 | -3.14368400 |
| H | -1.03190200 | -5.76561400 | -3.57656200 |
| C | -0.28238300 | -4.68206900 | -1.86434800 |
| H | -0.04619100 | -5.57770400 | -1.29616400 |
| C | -0.03163600 | -3.42975600 | -1.30735600 |
| H | 0.39166100 | -3.35972200 | -0.31195500 |
| C | -0.55931000 | 2.82469800 | -1.24565000 |
| C | -0.92937700 | 3.28368800 | -2.52191800 |
| H | -0.97605800 | 2.58355900 | -3.34911900 |
| C | -1.25584000 | 4.62379700 | -2.73156300 |
| H | -1.55508400 | 4.95236400 | -3.72224000 |
| C | -1.21040300 | 5.53194200 | -1.67397100 |
| H | -1.46875200 | 6.57438400 | -1.83633900 |
| C | -0.83990000 | 5.08874600 | -0.40115600 |
| H | -0.80704200 | 5.78661200 | 0.43089600 |
| C | -0.52211700 | 3.74945500 | -0.18695600 |
| H | -0.24941300 | 3.41079300 | 0.80668800 |
| C | 2.27354000 | -1.35039300 | -0.34080600 |
| C | 2.91825700 | -1.99877300 | -1.40433600 |
| H | 2.50262300 | -1.92350100 | -2.40399000 |
| C | 4.08660200 | -2.74004400 | -1.21739800 |
| H | 4.54771500 | -3.22295100 | -2.07085300 |
| C | 4.64596500 | -2.84242100 | 0.06116200 |

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|---|---|---|---|
| C | 4.02260700 | -2.19333300 | 1.13640500 |
| H | 4.46971700 | -2.27610900 | 2.12182300 |
| C | 2.85900500 | -1.46364900 | 0.93317800 |
| H | 2.39402500 | -0.96283500 | 1.77459100 |
| C | 6.45650200 | -4.20651700 | -0.69072800 |
| H | 7.32228100 | -4.69044400 | -0.23577200 |
| H | 6.80023000 | -3.50331700 | -1.46039800 |
| H | 5.82356100 | -4.96975900 | -1.16210300 |
| C | 2.07074300 | 1.74676400 | 0.17125300 |
| C | 2.38040000 | 1.87286300 | 1.53506300 |
| H | 1.77779500 | 1.35575000 | 2.27243900 |
| C | 3.43347700 | 2.67076800 | 1.96485300 |
| H | 3.66622000 | 2.77208100 | 3.01989000 |
| C | 4.21504000 | 3.37121000 | 1.03594600 |
| C | 3.92152500 | 3.26318500 | -0.32829800 |
| H | 4.50364300 | 3.79543800 | -1.07111900 |
| C | 2.85862400 | 2.45900600 | -0.74258300 |
| H | 2.63714100 | 2.38739900 | -1.80341000 |
| C | 6.03860200 | 4.86748000 | 0.66188000 |
| H | 6.76712900 | 5.39356100 | 1.28089700 |
| H | 5.45249400 | 5.60096300 | 0.09314400 |
| H | 6.56965000 | 4.21218300 | -0.04077200 |
| C | -1.59917200 | -1.83549900 | 1.37845600 |
| C | -2.74678200 | -3.79602600 | 1.57322800 |
| H | -3.44753900 | -4.56195800 | 1.28147900 |
| C | -1.91896400 | -3.70830200 | 2.64070200 |
| H | -1.76120000 | -4.37785800 | 3.47109700 |
| C | -3.25324500 | -2.43379100 | -0.44392000 |
| H | -2.96040300 | -3.19416400 | -1.17071400 |
| H | -2.99923700 | -1.45417800 | -0.83962000 |
| H | -4.33158600 | -2.48845600 | -0.27175900 |
| C | -0.22084200 | -2.07489400 | 3.47342100 |
| H | 0.06531600 | -2.93057800 | 4.08786700 |
| H | -0.61064000 | -1.28390800 | 4.11729700 |

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| H | 0.65495000 | -1.70469000 | 2.94264200 |
| H | -2.56491600 | 0.47242800 | 0.54863900 |
| H | -2.62806000 | 0.84543600 | -2.05036600 |
| C | -3.80358800 | 1.18254300 | 0.40778900 |
| C | -4.20581900 | 1.28411300 | -0.94176200 |
| H | -4.80205200 | 0.49109000 | -1.39240600 |
| C | -4.68059200 | 0.39552200 | 1.38407400 |
| H | -4.83140600 | -0.62490900 | 1.01322800 |
| H | -5.67024800 | 0.87262500 | 1.34183000 |
| C | -4.14278600 | 2.53504600 | -1.66430100 |
| H | -3.62586300 | 3.35566700 | -1.11622500 |
| H | -3.42250500 | 2.11689600 | 0.82779500 |
| O | -4.62061700 | 2.73808300 | -2.77977600 |
| C | -4.22202700 | 0.36270900 | 2.84481200 |
| H | -4.04476800 | 1.38914500 | 3.19171000 |
| H | -3.26243900 | -0.15633600 | 2.91957900 |
| C | -5.24471900 | -0.31777500 | 3.76155200 |
| H | -4.90369800 | -0.32420900 | 4.80195000 |
| H | -5.41566600 | -1.35861900 | 3.46180000 |
| H | -6.21253600 | 0.19587500 | 3.73287300 |

**TS24Z**

| Ru | -0.67126400 | -0.46448300 | 0.72596800 |
| N | -1.04436800 | -3.49427100 | 1.32759200 |
| N | 0.13160500 | -2.59771400 | 2.89202900 |
| O | -1.10524000 | 1.10997400 | 3.27908400 |
| O | -1.83346500 | -0.87639900 | -2.30764400 |
| O | 6.81770400 | -0.81865400 | 0.35204100 |
| O | 3.10655200 | 5.94777400 | 0.94564800 |
| C | -0.94727400 | 0.47787700 | 2.31017100 |
| C | -0.79825400 | -0.37411500 | -1.64340100 |
| C | 0.37753300 | -1.11493100 | -1.28324900 |

| C | 1.24643400 | -0.21608500 | -0.54294000 |
|---|---|---|---|
| C | 0.56487600 | 1.06332800 | -0.43316100 |
| C | -0.71098000 | 0.96739800 | -1.08679600 |
| C | 0.68680900 | -2.49542400 | -1.72384600 |
| C | 0.21018000 | -2.96816700 | -2.96036300 |
| H | -0.39889100 | -2.31990600 | -3.57866600 |
| C | 0.49584400 | -4.26544300 | -3.38782200 |
| H | 0.11329900 | -4.60783400 | -4.34530100 |
| C | 1.26747100 | -5.11754700 | -2.59655300 |
| H | 1.48958200 | -6.12688800 | -2.93133900 |
| C | 1.75570200 | -4.65699700 | -1.37055700 |
| H | 2.36168000 | -5.30774300 | -0.74589500 |
| C | 1.46957700 | -3.36327800 | -0.93930400 |
| H | 1.85038300 | -3.02005900 | 0.01578600 |
| C | -1.67355400 | 2.06131500 | -1.34911400 |
| C | -2.29733400 | 2.15671500 | -2.60585900 |
| H | -2.10149400 | 1.40155200 | -3.35858800 |
| C | -3.17881500 | 3.20104100 | -2.88694400 |
| H | -3.65803800 | 3.24728500 | -3.86030600 |
| C | -3.45077600 | 4.17193200 | -1.92310800 |
| H | -4.13998300 | 4.98256100 | -2.14162600 |
| C | -2.83720400 | 4.08806300 | -0.67033600 |
| H | -3.04668100 | 4.83446900 | 0.09082000 |
| C | -1.96161900 | 3.04303600 | -0.38380200 |
| H | -1.50197600 | 2.97976300 | 0.59624300 |
| C | 2.69620800 | -0.41217500 | -0.29727100 |
| C | 3.52805900 | -0.84521800 | -1.33997800 |
| H | 3.09456700 | -1.06929900 | -2.30918900 |
| C | 4.90562200 | -0.99520700 | -1.16994500 |
| H | 5.50697900 | -1.33237900 | -2.00587600 |
| C | 5.48737300 | -0.70443700 | 0.06914400 |
| C | 4.67393800 | -0.26053800 | 1.12170700 |
| H | 5.13867800 | -0.03238200 | 2.07548300 |
| C | 3.30561200 | -0.11835200 | 0.93571300 |

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|---|---|---|---|
| H | 2.69339100 | 0.23476400 | 1.75732700 |
| C | 7.68757000 | -1.25331900 | -0.68078600 |
| H | 8.68802500 | -1.27062000 | -0.24558000 |
| H | 7.67843000 | -0.56460900 | -1.53546600 |
| H | 7.42961900 | -2.26107900 | -1.03154500 |
| C | 1.21383000 | 2.34417000 | -0.03393800 |
| C | 1.45527800 | 2.73482000 | 1.29298100 |
| H | 1.12866400 | 2.09957000 | 2.10794100 |
| C | 2.08543600 | 3.93762400 | 1.58692800 |
| H | 2.26414800 | 4.24107200 | 2.61331100 |
| C | 2.49736700 | 4.79136000 | 0.55436900 |
| C | 2.26330100 | 4.42290800 | -0.77551200 |
| H | 2.56508400 | 5.06271700 | -1.59614800 |
| C | 1.62662200 | 3.21232600 | -1.05319500 |
| H | 1.44539000 | 2.93995800 | -2.08881900 |
| C | 3.53044100 | 6.85571600 | -0.05862900 |
| H | 3.97950800 | 7.69947900 | 0.46766000 |
| H | 2.68720800 | 7.21505200 | -0.66251500 |
| H | 4.27971400 | 6.40544100 | -0.72261400 |
| C | -0.51856800 | -2.29193500 | 1.72461100 |
| C | -0.73029500 | -4.50632400 | 2.22142700 |
| H | -1.05102600 | -5.52475100 | 2.07057100 |
| C | 0.00728700 | -3.94265800 | 3.20675600 |
| H | 0.45314700 | -4.37056300 | 4.09042100 |
| C | -1.81722200 | -3.75710300 | 0.11585000 |
| H | -1.32954000 | -4.54457500 | -0.46271700 |
| H | -1.86445300 | -2.85959800 | -0.49335600 |
| H | -2.83128800 | -4.06920500 | 0.38089400 |
| C | 0.87092300 | -1.65759300 | 3.72769600 |
| H | 1.53477300 | -2.22509400 | 4.38265500 |
| H | 0.19416000 | -1.05359600 | 4.33577600 |
| H | 1.46574200 | -1.00162700 | 3.09465900 |
| H | -2.48945600 | -0.74907700 | 0.63542500 |
| H | -2.74693900 | -0.80842500 | -1.78969000 |

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|---|---|---|---|
| C | -3.72698400 | -0.90592200 | 0.52678700 |
| C | -4.13437100 | -1.06947800 | -0.86062900 |
| H | -4.24447500 | -2.08787400 | -1.23435000 |
| C | -4.29154900 | 0.24652100 | 1.36852500 |
| H | -3.74097500 | 0.28632300 | 2.31571300 |
| H | -4.10865400 | 1.20532500 | 0.87151000 |
| C | -4.86826600 | -0.08412300 | -1.62372200 |
| H | -4.88313900 | 0.94270700 | -1.19705800 |
| H | -3.79671800 | -1.84622200 | 1.08381500 |
| O | -5.43527200 | -0.30508800 | -2.69445100 |
| C | -5.79073400 | 0.09102200 | 1.67207700 |
| H | -5.96157400 | -0.88166200 | 2.15401300 |
| H | -6.35851900 | 0.06961200 | 0.73539500 |
| C | -6.32309500 | 1.20988400 | 2.57354100 |
| H | -7.38954600 | 1.07778000 | 2.78416700 |
| H | -6.19669700 | 2.19069700 | 2.10134800 |
| H | -5.79379700 | 1.23509900 | 3.53321600 |

**TS25E**

| | | | |
|---|---|---|---|
| Ru | 0.68100500 | 0.02259600 | -0.49011600 |
| N | 2.40301400 | -2.54460900 | -0.78565300 |
| N | 1.06888600 | -2.37344600 | -2.46770000 |
| O | 0.82021100 | 1.48915500 | -3.13678400 |
| O | 1.45166300 | 0.14337100 | 2.71517400 |
| O | -6.05026100 | -3.28983200 | -1.01548600 |
| O | -5.26842300 | 4.37943800 | -1.56951000 |
| C | 0.76613900 | 0.90537000 | -2.12606700 |
| C | 0.42756100 | 0.17414700 | 1.88133300 |
| C | -0.30013700 | -0.97513100 | 1.42408200 |
| C | -1.34259900 | -0.51146700 | 0.51937100 |
| C | -1.21401400 | 0.93060000 | 0.40971500 |
| C | -0.10682900 | 1.36120400 | 1.22067900 |

| C | -0.07599800 | -2.36169000 | 1.89562700 |
|---|---|---|---|
| C | 0.38225900 | -2.59836700 | 3.20509600 |
| H | 0.59308000 | -1.75512700 | 3.85124300 |
| C | 0.59000100 | -3.89920600 | 3.66564900 |
| H | 0.94660800 | -4.05530600 | 4.68017800 |
| C | 0.34228500 | -4.99304700 | 2.83494500 |
| H | 0.50472800 | -6.00500600 | 3.19542600 |
| C | -0.11879400 | -4.77236100 | 1.53439900 |
| H | -0.31710400 | -5.61391300 | 0.87604300 |
| C | -0.32559600 | -3.47474900 | 1.07069700 |
| H | -0.67872300 | -3.31759900 | 0.05800900 |
| C | 0.29991000 | 2.75212100 | 1.52207700 |
| C | 0.69587200 | 3.09979000 | 2.82684100 |
| H | 0.73636700 | 2.33154000 | 3.59033900 |
| C | 1.04667700 | 4.41281200 | 3.14021400 |
| H | 1.35009600 | 4.65697500 | 4.15455800 |
| C | 1.01002600 | 5.40707500 | 2.16192900 |
| H | 1.28485100 | 6.42902000 | 2.40745200 |
| C | 0.62452500 | 5.07426500 | 0.86131500 |
| H | 0.59898300 | 5.83676900 | 0.08770600 |
| C | 0.27837100 | 3.76255300 | 0.54292200 |
| H | -0.00794700 | 3.51509900 | -0.47315400 |
| C | -2.54881900 | -1.27174700 | 0.11079100 |
| C | -3.25050900 | -2.03614200 | 1.05459900 |
| H | -2.88045700 | -2.09515800 | 2.07277100 |
| C | -4.41928400 | -2.72541900 | 0.72490300 |
| H | -4.92449300 | -3.30318600 | 1.48991400 |
| C | -4.92197300 | -2.65552500 | -0.57890300 |
| C | -4.24325600 | -1.88628200 | -1.53476500 |
| H | -4.64739700 | -1.83366000 | -2.54061300 |
| C | -3.08057800 | -1.20995200 | -1.19077000 |
| H | -2.57540700 | -0.61191700 | -1.94051700 |
| C | -6.77922400 | -4.07316000 | -0.08513800 |
| H | -7.62918500 | -4.48176500 | -0.63421300 |

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|---|---|---|---|
| H | -7.14930800 | -3.46851400 | 0.75310300 |
| H | -6.17538100 | -4.89993300 | 0.31139800 |
| C | -2.25848700 | 1.83949500 | -0.14436900 |
| C | -2.40566600 | 2.14817000 | -1.50635500 |
| H | -1.71179300 | 1.73365800 | -2.22857700 |
| C | -3.41461800 | 2.99484700 | -1.94935500 |
| H | -3.52228200 | 3.23642800 | -3.00180300 |
| C | -4.31389100 | 3.56185200 | -1.03614300 |
| C | -4.18357200 | 3.27045500 | 0.32646900 |
| H | -4.86021700 | 3.69570500 | 1.05813400 |
| C | -3.16318600 | 2.41932300 | 0.75441400 |
| H | -3.06909000 | 2.20386500 | 1.81480100 |
| C | -6.19751100 | 4.98816700 | -0.68784100 |
| H | -6.85700600 | 5.59165400 | -1.31367300 |
| H | -5.69836400 | 5.63900400 | 0.04181300 |
| H | -6.79593800 | 4.24151600 | -0.14966300 |
| C | 1.43550100 | -1.73293600 | -1.31271200 |
| C | 2.62157700 | -3.65478100 | -1.58555800 |
| H | 3.34224400 | -4.41375700 | -1.32637800 |
| C | 1.78690600 | -3.54641600 | -2.64626800 |
| H | 1.64231300 | -4.18532400 | -3.50275900 |
| C | 3.09942300 | -2.36783300 | 0.48859200 |
| H | 2.66862200 | -3.03008900 | 1.24299400 |
| H | 3.02187400 | -1.33938900 | 0.83113700 |
| H | 4.15520900 | -2.60948800 | 0.34601300 |
| C | 0.05687600 | -1.91143600 | -3.41146700 |
| H | -0.18842800 | -2.73566400 | -4.08401200 |
| H | 0.42216900 | -1.06592200 | -3.99777000 |
| H | -0.83897300 | -1.61263300 | -2.86907800 |
| C | 4.40497000 | 1.04561100 | -0.60404100 |
| C | 3.32881900 | 1.23471400 | 0.41020500 |
| H | 2.32887100 | 0.46360000 | -0.26117100 |
| H | 2.77679800 | 2.18106600 | 0.29370800 |
| O | 3.50288400 | 0.77849000 | 1.60548200 |

| H | 2.36895000 | 0.54879100 | 2.28080300 |
|---|---|---|---|
| C | 5.58404200 | 0.47961300 | -0.31799900 |
| C | 6.72479000 | 0.31931700 | -1.28075300 |
| H | 6.42368100 | 0.65691400 | -2.28077100 |
| H | 6.97340500 | -0.74948200 | -1.37437800 |
| H | 5.74102000 | 0.13416100 | 0.70361600 |
| H | 4.19069900 | 1.42948100 | -1.60093300 |
| C | 7.99541000 | 1.07308700 | -0.84014500 |
| H | 8.27594900 | 0.74581700 | 0.16962000 |
| H | 7.76378900 | 2.14234300 | -0.76021300 |
| C | 9.17355700 | 0.86445300 | -1.79616900 |
| H | 10.06039300 | 1.41218000 | -1.46124900 |
| H | 8.93076700 | 1.21152300 | -2.80705900 |
| H | 9.44420300 | -0.19545600 | -1.86750100 |

**TS25Z**

| Ru | -0.60536500 | 0.06981800 | 0.74904000 |
|---|---|---|---|
| N | -2.39875900 | -2.41636900 | 1.24295500 |
| N | -0.82250100 | -2.36242800 | 2.70943700 |
| O | -0.27775300 | 1.46167800 | 3.41963600 |
| O | -1.83172700 | 0.34411300 | -2.29916100 |
| O | 5.92377400 | -3.61536400 | 0.18318200 |
| O | 5.67753000 | 4.06579700 | 1.04655300 |
| C | -0.40339700 | 0.90651900 | 2.39935200 |
| C | -0.69544400 | 0.29021400 | -1.62785000 |
| C | 0.02243500 | -0.91219000 | -1.31349800 |
| C | 1.21213300 | -0.53631900 | -0.56262300 |
| C | 1.18538600 | 0.90630700 | -0.39788200 |
| C | -0.00207600 | 1.42323500 | -1.02316400 |
| C | -0.35232600 | -2.26802300 | -1.77891200 |
| C | -1.01390100 | -2.43628300 | -3.00956100 |
| H | -1.26634800 | -1.56241500 | -3.59742800 |

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|---|---|---|---|
| C | -1.36732300 | -3.70774100 | -3.46337300 |
| H | -1.87983600 | -3.81074000 | -4.41600200 |
| C | -1.06642900 | -4.83986800 | -2.70468000 |
| H | -1.34254800 | -5.82885400 | -3.05971400 |
| C | -0.40420700 | -4.68748500 | -1.48357800 |
| H | -0.16232900 | -5.55952700 | -0.88191800 |
| C | -0.05142100 | -3.41931000 | -1.02668000 |
| H | 0.45673800 | -3.31512000 | -0.07487600 |
| C | -0.36803200 | 2.84332500 | -1.22391800 |
| C | -0.92050300 | 3.25832800 | -2.44963900 |
| H | -1.10887800 | 2.52178200 | -3.22224500 |
| C | -1.23733500 | 4.59823700 | -2.67218800 |
| H | -1.66391900 | 4.89496000 | -3.62641500 |
| C | -1.01014800 | 5.55253400 | -1.67986100 |
| H | -1.25876200 | 6.59555300 | -1.85440000 |
| C | -0.46762700 | 5.15291400 | -0.45637700 |
| H | -0.29294900 | 5.88415000 | 0.32801500 |
| C | -0.15472500 | 3.81432000 | -0.22820600 |
| H | 0.25440900 | 3.51459500 | 0.73015300 |
| C | 2.41878300 | -1.37405300 | -0.35744100 |
| C | 2.92386100 | -2.14880300 | -1.41201800 |
| H | 2.40210500 | -2.15784800 | -2.36317900 |
| C | 4.08604000 | -2.91114800 | -1.27769900 |
| H | 4.43512800 | -3.49380500 | -2.12205500 |
| C | 4.78252400 | -2.90692400 | -0.06429700 |
| C | 4.30243400 | -2.12860400 | 0.99866900 |
| H | 4.85597000 | -2.12724800 | 1.93216700 |
| C | 3.14356600 | -1.37890700 | 0.84902500 |
| H | 2.79442700 | -0.77505800 | 1.67870900 |
| C | 6.45638200 | -4.41184900 | -0.86213500 |
| H | 7.35329300 | -4.88282700 | -0.45645200 |
| H | 6.73165400 | -3.80551500 | -1.73492200 |
| H | 5.75143900 | -5.19190000 | -1.17830500 |
| C | 2.35064200 | 1.73882100 | 0.01830900 |

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|---|---|---|---|
| C | 2.70709500 | 2.00167900 | 1.35085600 |
| H | 2.09905600 | 1.60720700 | 2.15677200 |
| C | 3.81708000 | 2.77801500 | 1.66109400 |
| H | 4.08678000 | 2.98450200 | 2.69173300 |
| C | 4.61017900 | 3.31819900 | 0.63963200 |
| C | 4.27110700 | 3.07185600 | -0.69565500 |
| H | 4.86137300 | 3.47833100 | -1.50829100 |
| C | 3.15169100 | 2.29127200 | -0.98948200 |
| H | 2.89583900 | 2.11048700 | -2.02946700 |
| C | 6.50751800 | 4.64489500 | 0.05303800 |
| H | 7.28387200 | 5.19255400 | 0.58980100 |
| H | 5.95024300 | 5.34284900 | -0.58525600 |
| H | 6.97793400 | 3.88058500 | -0.57922300 |
| C | -1.32128900 | -1.67046600 | 1.63664700 |
| C | -2.55654400 | -3.53705100 | 2.04254000 |
| H | -3.34841700 | -4.25019700 | 1.87836600 |
| C | -1.56880500 | -3.50235800 | 2.96808400 |
| H | -1.33314200 | -4.17314100 | 3.77876600 |
| C | -3.26998600 | -2.16478100 | 0.09546800 |
| H | -3.15015500 | -1.14583400 | -0.26206800 |
| H | -4.30859100 | -2.30578800 | 0.40401300 |
| H | -3.02782000 | -2.85854800 | -0.71293500 |
| C | 0.34257300 | -1.98066800 | 3.50026700 |
| H | 0.63458900 | -2.83328900 | 4.11634500 |
| H | 0.11749500 | -1.13059400 | 4.14730900 |
| H | 1.16563500 | -1.71973500 | 2.83649200 |
| C | -4.18509200 | 1.27693400 | 1.48004900 |
| C | -3.29210900 | 1.43201000 | 0.29507300 |
| H | -2.24978300 | 0.59663700 | 0.77350300 |
| H | -2.68217500 | 2.34878000 | 0.35582000 |
| O | -3.66112900 | 1.03959600 | -0.88103300 |
| H | -2.64966800 | 0.78129500 | -1.72232400 |
| C | -5.45559600 | 0.84281300 | 1.51883300 |
| C | -6.33092800 | 0.37075700 | 0.39117300 |

| H | -6.56734800 | -0.69419700 | 0.55136200 |
|---|---|---|---|
| H | -5.79073500 | 0.44104800 | -0.55441000 |
| H | -5.94160100 | 0.86360300 | 2.49696700 |
| H | -3.72261400 | 1.60959300 | 2.40861000 |
| C | -7.65862200 | 1.14930300 | 0.31882600 |
| H | -7.43910600 | 2.21009000 | 0.14464500 |
| H | -8.16859000 | 1.09807400 | 1.29096000 |
| C | -8.59096600 | 0.62788100 | -0.77876900 |
| H | -9.52369900 | 1.20036500 | -0.81632800 |
| H | -8.85220300 | -0.42362100 | -0.61073900 |
| H | -8.11703800 | 0.69657800 | -1.76417400 |

**TS26E**

| Ru | 0.72199800 | -0.61432700 | -0.33792000 |
|---|---|---|---|
| N | 0.78156200 | -3.67741000 | -0.91403800 |
| N | 0.03095100 | -2.62577800 | -2.63688100 |
| O | 1.83776000 | 0.82783000 | -2.74893500 |
| O | 1.05305500 | -1.16680900 | 2.91372200 |
| O | -6.65851000 | 0.16413000 | -1.63830400 |
| O | -1.99139300 | 6.29472500 | -1.15430200 |
| C | 1.40815700 | 0.24645900 | -1.82967100 |
| C | 0.30406200 | -0.53541900 | 2.00968200 |
| C | -0.85651100 | -1.08950100 | 1.37998100 |
| C | -1.39881000 | -0.07465700 | 0.48828200 |
| C | -0.53296800 | 1.08397300 | 0.57004400 |
| C | 0.53956200 | 0.80174900 | 1.48942000 |
| C | -1.44262100 | -2.41610700 | 1.68457200 |
| C | -1.32687600 | -2.96331600 | 2.97572200 |
| H | -0.78351200 | -2.41552300 | 3.73563600 |
| C | -1.88078100 | -4.20818100 | 3.27688500 |
| H | -1.77507100 | -4.61024400 | 4.28079600 |
| C | -2.56600100 | -4.93348600 | 2.30110800 |

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|---|---|---|---|
| H | -2.99665400 | -5.90248700 | 2.53764300 |
| C | -2.69457900 | -4.39830900 | 1.01648900 |
| H | -3.22694700 | -4.95029500 | 0.24652500 |
| C | -2.14100500 | -3.15638500 | 0.71197400 |
| H | -2.24298600 | -2.75605600 | -0.29019700 |
| C | 1.55143900 | 1.75306700 | 2.00264500 |
| C | 1.91348200 | 1.72771100 | 3.36203500 |
| H | 1.47605000 | 0.97968300 | 4.01296700 |
| C | 2.83469300 | 2.64248200 | 3.87250700 |
| H | 3.10047700 | 2.60158100 | 4.92527600 |
| C | 3.41146700 | 3.60356900 | 3.04165800 |
| H | 4.12949200 | 4.31456800 | 3.44047500 |
| C | 3.06220000 | 3.63804900 | 1.68950700 |
| H | 3.50967700 | 4.37556700 | 1.02901000 |
| C | 2.14742400 | 2.72194100 | 1.17446500 |
| H | 1.89726900 | 2.74942000 | 0.11991700 |
| C | -2.76969300 | -0.05221400 | -0.07901900 |
| C | -3.86674300 | -0.39220200 | 0.72620500 |
| H | -3.69759600 | -0.70659100 | 1.75077900 |
| C | -5.17813600 | -0.33661600 | 0.24990400 |
| H | -5.99168000 | -0.61036800 | 0.91133200 |
| C | -5.42205800 | 0.07574800 | -1.06463900 |
| C | -4.34073300 | 0.43328100 | -1.88240100 |
| H | -4.54340000 | 0.75938400 | -2.89748700 |
| C | -3.04285800 | 0.36882400 | -1.39347900 |
| H | -2.22124900 | 0.66040100 | -2.03742100 |
| C | -7.78717300 | -0.17592600 | -0.85015700 |
| H | -8.65800900 | -0.03557600 | -1.49265000 |
| H | -7.87975200 | 0.47513400 | 0.02888800 |
| H | -7.75015200 | -1.22136600 | -0.51684900 |
| C | -0.89115500 | 2.44779100 | 0.08399400 |
| C | -0.72287100 | 2.89448300 | -1.23662100 |
| H | -0.27727200 | 2.23691900 | -1.97381300 |
| C | -1.09733800 | 4.17733500 | -1.61769900 |

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|---|---|---|---|
| H | -0.96031400 | 4.52180200 | -2.63757700 |
| C | -1.65681200 | 5.05822200 | -0.68223600 |
| C | -1.83086400 | 4.63489600 | 0.64033900 |
| H | -2.25698100 | 5.29286400 | 1.38834400 |
| C | -1.44732300 | 3.34362600 | 1.00648700 |
| H | -1.58300800 | 3.02788600 | 2.03679600 |
| C | -2.55145500 | 7.22931400 | -0.24648300 |
| H | -2.73747400 | 8.13659400 | -0.82355600 |
| H | -1.86149600 | 7.46038700 | 0.57550900 |
| H | -3.49963000 | 6.86926100 | 0.17368000 |
| C | 0.51001000 | -2.41395300 | -1.36864300 |
| C | 0.47799700 | -4.63540500 | -1.86846100 |
| H | 0.61749300 | -5.68879900 | -1.68522800 |
| C | 0.00996900 | -3.97564600 | -2.95342900 |
| H | -0.33105700 | -4.33691100 | -3.91044600 |
| C | 1.26850000 | -4.06143200 | 0.41090200 |
| H | 0.48723100 | -4.60909200 | 0.94278800 |
| H | 1.54856900 | -3.18686900 | 0.99060900 |
| H | 2.14992500 | -4.69847600 | 0.29672000 |
| C | -0.41759300 | -1.59500700 | -3.56676000 |
| H | -1.00166600 | -2.07395000 | -4.35499500 |
| H | 0.42872600 | -1.07057200 | -4.01454900 |
| H | -1.04709800 | -0.87924600 | -3.04087600 |
| C | 3.51601600 | -1.55198700 | 0.75913100 |
| H | 2.31199400 | -1.12369300 | 0.00163700 |
| O | 3.18285800 | -1.92118100 | 1.93066500 |
| H | 2.01674800 | -1.36199200 | 2.57601100 |
| H | 3.70593700 | -2.34393000 | 0.00918200 |
| C | 4.42893500 | -0.32725600 | 0.58773800 |
| H | 3.95500600 | 0.53685100 | 1.06374600 |
| C | 4.83038700 | -0.03574400 | -0.82936000 |
| C | 6.01219600 | -0.36415000 | -1.36198200 |
| H | 6.75854700 | -0.85243200 | -0.73010500 |
| H | 4.09442800 | 0.46179400 | -1.45799200 |

A108

| H | 5.31850100 | -0.57102800 | 1.18540300 |
|---|---|---|---|
| C | 6.43355900 | -0.08816300 | -2.78002400 |
| H | 5.59638100 | 0.35621400 | -3.33147900 |
| H | 6.66849200 | -1.03854100 | -3.28162200 |
| C | 7.66416000 | 0.83085400 | -2.86914900 |
| H | 7.96703000 | 0.98639600 | -3.91007200 |
| H | 8.51844800 | 0.40130900 | -2.33369800 |
| H | 7.45333500 | 1.80928100 | -2.42572000 |

**TS26Z**

| Ru | 0.83736400 | -0.27288000 | -0.41033200 |
|---|---|---|---|
| N | 1.85990600 | -3.18765600 | -0.82377900 |
| N | 0.74286900 | -2.55504000 | -2.55282500 |
| O | 1.31713400 | 1.28225700 | -2.95776500 |
| O | 1.47236500 | -0.46125000 | 2.83691900 |
| O | -6.45379400 | -1.98561600 | -1.26219400 |
| O | -3.99278800 | 5.33092500 | -1.41977800 |
| C | 1.14297500 | 0.65677600 | -1.98564900 |
| C | 0.51986400 | -0.16600600 | 1.95060600 |
| C | -0.42752800 | -1.10389800 | 1.42893700 |
| C | -1.30707200 | -0.38105800 | 0.52177500 |
| C | -0.85798300 | 0.99557500 | 0.48549700 |
| C | 0.28824600 | 1.13609900 | 1.34717100 |
| C | -0.54150400 | -2.52280200 | 1.84063500 |
| C | -0.19940600 | -2.91258500 | 3.14862700 |
| H | 0.17158000 | -2.16845500 | 3.84251800 |
| C | -0.30996300 | -4.24463100 | 3.54947800 |
| H | -0.03662500 | -4.52076600 | 4.56422400 |
| C | -0.76803600 | -5.21673900 | 2.65898100 |
| H | -0.85358100 | -6.25326200 | 2.97310800 |
| C | -1.11847600 | -4.84175100 | 1.35904200 |
| H | -1.47878200 | -5.58695000 | 0.65490700 |

| | | | |
|---|---|---|---|
| C | -1.00731000 | -3.51286900 | 0.95508200 |
| H | -1.27680800 | -3.23613100 | -0.05767900 |
| C | 0.96213900 | 2.39405500 | 1.74179600 |
| C | 1.37808200 | 2.58072600 | 3.07292200 |
| H | 1.23665400 | 1.77997700 | 3.78945800 |
| C | 1.97888200 | 3.77466600 | 3.47245700 |
| H | 2.29396800 | 3.89422500 | 4.50544700 |
| C | 2.17444400 | 4.80895600 | 2.55668900 |
| H | 2.64332900 | 5.73774400 | 2.86913700 |
| C | 1.76765900 | 4.63579300 | 1.23151900 |
| H | 1.92080300 | 5.42955600 | 0.50562000 |
| C | 1.17321400 | 3.44229500 | 0.82702400 |
| H | 0.87624600 | 3.31557900 | -0.20795900 |
| C | -2.63613800 | -0.83779700 | 0.04550400 |
| C | -3.52932300 | -1.44563600 | 0.94013200 |
| H | -3.22305800 | -1.61088700 | 1.96784400 |
| C | -4.80888300 | -1.84543900 | 0.54954100 |
| H | -5.46137600 | -2.31170600 | 1.27833100 |
| C | -5.23016500 | -1.63343500 | -0.76769900 |
| C | -4.35795100 | -1.01543200 | -1.67490900 |
| H | -4.69910900 | -0.84938500 | -2.69170000 |
| C | -3.08765400 | -0.62757900 | -1.27036700 |
| H | -2.43240300 | -0.14156400 | -1.98386700 |
| C | -7.37757200 | -2.60457000 | -0.38234000 |
| H | -8.27504200 | -2.79694700 | -0.97259500 |
| H | -7.63497500 | -1.95128000 | 0.46154400 |
| H | -6.99241800 | -3.55571300 | 0.00804600 |
| C | -1.65736300 | 2.13569600 | -0.04879000 |
| C | -1.70715000 | 2.51072900 | -1.40113000 |
| H | -1.11113500 | 1.97408500 | -2.12993000 |
| C | -2.49148400 | 3.57627800 | -1.82606500 |
| H | -2.52294200 | 3.86774800 | -2.87088200 |
| C | -3.25643300 | 4.30347600 | -0.90405600 |
| C | -3.21944100 | 3.94893600 | 0.44933000 |

| H | -3.79613000 | 4.49328000 | 1.18766200 |
|---|---|---|---|
| C | -2.42452300 | 2.87718500 | 0.85923900 |
| H | -2.40025500 | 2.61428400 | 1.91277200 |
| C | -4.77650700 | 6.10674700 | -0.52811600 |
| H | -5.27174600 | 6.86216100 | -1.14038100 |
| H | -4.15669000 | 6.60571900 | 0.22817000 |
| H | -5.53729900 | 5.49852500 | -0.02167600 |
| C | 1.17708100 | -2.11258000 | -1.32873800 |
| C | 1.84459000 | -4.25707800 | -1.70533900 |
| H | 2.32348900 | -5.19512500 | -1.47423000 |
| C | 1.14654800 | -3.85943100 | -2.79443300 |
| H | 0.90338500 | -4.37696800 | -3.70861700 |
| C | 2.49805900 | -3.30069200 | 0.48766700 |
| H | 1.95334400 | -4.02375100 | 1.09894000 |
| H | 2.51154300 | -2.34160900 | 0.99702700 |
| H | 3.52994000 | -3.63730600 | 0.35448100 |
| C | -0.04640100 | -1.78804600 | -3.51035900 |
| H | -0.48761200 | -2.48295600 | -4.22753200 |
| H | 0.57314100 | -1.06477000 | -4.04427700 |
| H | -0.84243000 | -1.26183400 | -2.98647700 |
| C | 3.83254200 | -0.18100400 | 0.54811300 |
| H | 2.51668100 | -0.21914500 | -0.14970900 |
| O | 3.69363300 | -0.54642000 | 1.75758000 |
| H | 2.42807700 | -0.35282900 | 2.45142700 |
| H | 4.22720200 | -0.92469500 | -0.17115300 |
| C | 4.28635200 | 1.25598100 | 0.24068700 |
| H | 3.58748400 | 1.95531700 | 0.70785100 |
| C | 4.46596000 | 1.55906900 | -1.22113300 |
| C | 5.58307300 | 1.39156400 | -1.94265900 |
| H | 5.53817900 | 1.64777800 | -3.00266200 |
| H | 3.58798500 | 1.93594400 | -1.73890500 |
| H | 5.23485700 | 1.35487300 | 0.78450900 |
| C | 6.92220300 | 0.88308500 | -1.47748100 |
| H | 6.91968000 | 0.70334000 | -0.39754500 |

| | | | |
|---|---|---|---|
| H | 7.68024900 | 1.65875900 | -1.66034300 |
| C | 7.35187300 | -0.40105300 | -2.20899200 |
| H | 8.34971500 | -0.72165700 | -1.89139400 |
| H | 7.37872300 | -0.24788100 | -3.29369300 |
| H | 6.65123900 | -1.21833700 | -2.00826100 |

**20E**

| | | | |
|---|---|---|---|
| C | -2.62539100 | 0.33491600 | -0.19367000 |
| H | -2.57441700 | 0.49299300 | -1.28288900 |
| C | -1.24347000 | 0.33403400 | 0.38579100 |
| H | -1.18611700 | 0.13083800 | 1.45516600 |
| C | -0.13078600 | 0.57520200 | -0.31043100 |
| H | -0.21430900 | 0.75949800 | -1.38375800 |
| C | 1.26174300 | 0.60541900 | 0.25459200 |
| H | 1.22493400 | 0.44657100 | 1.33976600 |
| H | 1.69690800 | 1.60494700 | 0.10169600 |
| C | 2.19644300 | -0.43578300 | -0.38961300 |
| H | 2.21033600 | -0.28365700 | -1.47716900 |
| H | 1.77844900 | -1.43687500 | -0.22755200 |
| C | 3.62568500 | -0.37241700 | 0.15584800 |
| H | 4.26703100 | -1.12252600 | -0.31786800 |
| H | 3.64602300 | -0.55291200 | 1.23658000 |
| H | 4.07566800 | 0.61096600 | -0.02261600 |
| O | -3.25521700 | -0.90572200 | 0.12977400 |
| H | -4.18895600 | -0.82962700 | -0.10515900 |
| H | -3.19916400 | 1.17734300 | 0.23050300 |

**20Z**

| | | | |
|---|---|---|---|
| C | -2.11136100 | -0.36010100 | 0.47045900 |
| H | -2.62263500 | -0.11375100 | 1.41785900 |

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|---|---|---|---|
| C | -1.41626600 | 0.86588400 | -0.04432100 |
| H | -2.09566200 | 1.60278900 | -0.47003600 |
| C | -0.10757400 | 1.13844200 | -0.01331400 |
| H | 0.21015900 | 2.09930200 | -0.42076000 |
| C | 1.01313400 | 0.28294400 | 0.51322000 |
| H | 0.64013600 | -0.68767600 | 0.85931900 |
| H | 1.45175000 | 0.77092900 | 1.39733900 |
| C | 2.12919500 | 0.06276600 | -0.52490800 |
| H | 2.49029900 | 1.03839600 | -0.87675100 |
| H | 1.70500100 | -0.43918900 | -1.40324300 |
| C | 3.30359300 | -0.75176100 | 0.02404000 |
| H | 4.08089400 | -0.89167200 | -0.73396600 |
| H | 2.97851400 | -1.74534900 | 0.35305100 |
| H | 3.76404200 | -0.25379000 | 0.88508000 |
| O | -3.06001400 | -0.77095100 | -0.51518000 |
| H | -3.59302300 | -1.47856300 | -0.13084400 |
| H | -1.39368500 | -1.16285700 | 0.69333100 |

**21**

| | | | |
|---|---|---|---|
| C | 2.72947300 | 0.19212800 | 0.28144400 |
| C | 1.42799700 | -0.56736100 | 0.17169200 |
| H | 1.49500700 | -1.24860300 | -0.68216100 |
| C | 0.21413400 | 0.37329200 | 0.05562000 |
| H | 0.22706300 | 1.08939800 | 0.88908700 |
| C | -1.12454900 | -0.37464800 | 0.04875200 |
| H | -1.21291300 | -0.96746000 | 0.97034200 |
| H | -1.13229500 | -1.09743100 | -0.77888100 |
| C | -2.33886000 | 0.55354000 | -0.07692100 |
| H | -2.24770700 | 1.14488800 | -0.99791900 |
| H | -2.32866200 | 1.27653700 | 0.74997200 |
| C | -3.67307300 | -0.19842400 | -0.08224000 |
| H | -4.51913100 | 0.49007000 | -0.17343600 |

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|---|---|---|---|
| H | -3.80911800 | -0.77164800 | 0.84179800 |
| H | -3.72706800 | -0.90404600 | -0.91889800 |
| O | 3.68148400 | 0.04881000 | -0.45334700 |
| H | 2.76320900 | 0.93303700 | 1.11538500 |
| H | 0.30602100 | 0.96884600 | -0.86200700 |
| H | 1.32299600 | -1.17523300 | 1.08340600 |

**TS27**

| | | | |
|---|---|---|---|
| Ru | 0.71832800 | 0.19926300 | -0.39933900 |
| N | 2.77924200 | -2.11920400 | -0.47511800 |
| N | 1.58414100 | -2.16134000 | -2.26692800 |
| O | 0.75074600 | 1.59144600 | -3.08767200 |
| O | 1.30499300 | 0.47070800 | 2.83076300 |
| O | -5.40753600 | -4.08996600 | -1.20419700 |
| O | -5.76096400 | 3.58375500 | -1.87217000 |
| C | 0.73860000 | 1.03270500 | -2.06164800 |
| C | 0.32139800 | 0.34155600 | 1.94767100 |
| C | -0.21192500 | -0.90713900 | 1.48991200 |
| C | -1.25970900 | -0.61662000 | 0.52069500 |
| C | -1.34339900 | 0.82502900 | 0.39121700 |
| C | -0.35691300 | 1.42715600 | 1.24846600 |
| C | 0.17001800 | -2.23869400 | 2.01425900 |
| C | 0.57047000 | -2.38043700 | 3.35594700 |
| H | 0.62415200 | -1.50165700 | 3.98692400 |
| C | 0.92055300 | -3.62997300 | 3.86909000 |
| H | 1.22886400 | -3.71314000 | 4.90771500 |
| C | 0.87587800 | -4.76586000 | 3.05916300 |
| H | 1.14928900 | -5.73779700 | 3.46033200 |
| C | 0.47398400 | -4.63995600 | 1.72674800 |
| H | 0.43343400 | -5.51560000 | 1.08449200 |
| C | 0.12465500 | -3.39354400 | 1.21082900 |
| H | -0.18027500 | -3.30880600 | 0.17407700 |

A114

| C | -0.19156200 | 2.86638900 | 1.55046900 |
|---|---|---|---|
| C | 0.09346000 | 3.27887400 | 2.86529900 |
| H | 0.22912300 | 2.53039800 | 3.63745100 |
| C | 0.21454000 | 4.63272900 | 3.17817100 |
| H | 0.43558400 | 4.92692400 | 4.20049100 |
| C | 0.05390100 | 5.60398000 | 2.18932700 |
| H | 0.14960000 | 6.65794900 | 2.43458800 |
| C | -0.22300900 | 5.20790500 | 0.87875400 |
| H | -0.34259900 | 5.95310800 | 0.09717100 |
| C | -0.33956700 | 3.85624600 | 0.56097700 |
| H | -0.54272400 | 3.56131600 | -0.46240900 |
| C | -2.31558600 | -1.55455000 | 0.06558800 |
| C | -2.96771600 | -2.38130600 | 0.99205100 |
| H | -2.66613200 | -2.35426400 | 2.03397800 |
| C | -4.00072000 | -3.24201700 | 0.61505600 |
| H | -4.47229200 | -3.86201900 | 1.36839500 |
| C | -4.41405400 | -3.28658200 | -0.72083500 |
| C | -3.78440600 | -2.45870000 | -1.66105300 |
| H | -4.11920200 | -2.49695200 | -2.69269900 |
| C | -2.75618000 | -1.61174700 | -1.26956900 |
| H | -2.28784000 | -0.97191300 | -2.00881100 |
| C | -6.08412900 | -4.93891000 | -0.29202700 |
| H | -6.82724100 | -5.48186100 | -0.87842500 |
| H | -6.59394400 | -4.36654400 | 0.49390200 |
| H | -5.40043300 | -5.65813900 | 0.17777900 |
| C | -2.48134700 | 1.55735000 | -0.23523100 |
| C | -2.60736500 | 1.80507200 | -1.61178000 |
| H | -1.82641400 | 1.47988900 | -2.28936100 |
| C | -3.70753100 | 2.48081300 | -2.12556700 |
| H | -3.79933500 | 2.67606500 | -3.18907400 |
| C | -4.72303700 | 2.93145400 | -1.27127000 |
| C | -4.61629300 | 2.69835700 | 0.10456100 |
| H | -5.38233300 | 3.03726000 | 0.79184000 |
| C | -3.50340700 | 2.01955000 | 0.60404700 |

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|---|---|---|---|
| H | -3.42942300 | 1.84821900 | 1.67402300 |
| C | -6.81181300 | 4.06871200 | -1.05259500 |
| H | -7.52263400 | 4.55002600 | -1.72628100 |
| H | -6.45100700 | 4.80574600 | -0.32338500 |
| H | -7.31786900 | 3.25483100 | -0.51712600 |
| C | 1.76518500 | -1.45115500 | -1.10831500 |
| C | 3.20476700 | -3.21070800 | -1.21559600 |
| H | 3.99049200 | -3.86400700 | -0.87152000 |
| C | 2.45793200 | -3.23574800 | -2.34459500 |
| H | 2.46973400 | -3.90808900 | -3.18750300 |
| C | 3.33768500 | -1.82320100 | 0.84472400 |
| H | 2.93745500 | -2.52065700 | 1.58306700 |
| H | 3.09812400 | -0.80571400 | 1.14250400 |
| H | 4.42443200 | -1.92301700 | 0.79437600 |
| C | 0.60449200 | -1.86228100 | -3.30606600 |
| H | 0.52829200 | -2.72851800 | -3.96602600 |
| H | 0.90364500 | -0.99049000 | -3.89106700 |
| H | -0.36616800 | -1.67326800 | -2.84977000 |
| C | 4.15813800 | 2.11012800 | -0.40262400 |
| C | 3.01936300 | 1.89649500 | 0.59248500 |
| H | 4.67239100 | 3.01929300 | -0.05298400 |
| H | 2.26304600 | 0.90755600 | -0.13845500 |
| H | 2.25261600 | 2.68354900 | 0.52341300 |
| O | 3.29061100 | 1.42343500 | 1.75682300 |
| H | 2.14887200 | 0.99817500 | 2.43558100 |
| C | 5.16800000 | 0.96725100 | -0.50928500 |
| H | 5.49308900 | 0.69244200 | 0.50094100 |
| C | 6.38567200 | 1.31725500 | -1.37354200 |
| H | 6.89251700 | 2.19647200 | -0.95044500 |
| H | 6.05053500 | 1.61562400 | -2.37757300 |
| H | 4.66562700 | 0.08689500 | -0.93146100 |
| H | 3.72953600 | 2.35127400 | -1.38278600 |
| C | 7.39343100 | 0.16756500 | -1.50013700 |
| H | 6.88762300 | -0.70998100 | -1.92662100 |

| H | 7.72641200 | -0.13193900 | -0.49690300 |
|---|---|---|---|
| C | 8.61210700 | 0.52091900 | -2.35868500 |
| H | 9.31101900 | -0.31918200 | -2.43025800 |
| H | 9.15871600 | 1.37273400 | -1.93811100 |
| H | 8.31338700 | 0.79283100 | -3.37765600 |

**TS28**

| Ru | 0.48328100 | -0.85191900 | -0.42500800 |
|---|---|---|---|
| N | -0.31129100 | -3.77473100 | -1.17171800 |
| N | -0.76501800 | -2.45321400 | -2.81039300 |
| O | 1.91271700 | 0.38149500 | -2.78633500 |
| O | 0.73814200 | -1.63621800 | 2.78577700 |
| O | -6.47011900 | 1.90694900 | -1.38247800 |
| O | -0.34711100 | 6.55514000 | -0.85229900 |
| C | 1.35620600 | -0.11778200 | -1.88757400 |
| C | 0.15962200 | -0.78741900 | 1.93920000 |
| C | -1.12135800 | -0.98549000 | 1.32867600 |
| C | -1.39954300 | 0.18030400 | 0.50269200 |
| C | -0.25804000 | 1.06613800 | 0.60131200 |
| C | 0.72595300 | 0.46639800 | 1.46625900 |
| C | -2.03047700 | -2.12424500 | 1.59812800 |
| C | -2.02578300 | -2.75570400 | 2.85563900 |
| H | -1.33206700 | -2.41656300 | 3.61489500 |
| C | -2.88313900 | -3.82389100 | 3.12228100 |
| H | -2.85790700 | -4.29661500 | 4.10033200 |
| C | -3.76736500 | -4.28395900 | 2.14539300 |
| H | -4.43413100 | -5.11568900 | 2.35523000 |
| C | -3.78774300 | -3.66079500 | 0.89459700 |
| H | -4.47214400 | -4.00607100 | 0.12428700 |
| C | -2.93150100 | -2.59526400 | 0.62437800 |
| H | -2.95389700 | -2.12480800 | -0.35187700 |
| C | 1.96670000 | 1.09266900 | 1.97716200 |

A117

| | | | |
|---|---|---|---|
| C | 2.36112500 | 0.88644300 | 3.31197600 |
| H | 1.77011100 | 0.23386900 | 3.94379800 |
| C | 3.50640500 | 1.49923000 | 3.82119100 |
| H | 3.79167200 | 1.32220800 | 4.85460100 |
| C | 4.28055200 | 2.33359000 | 3.01448900 |
| H | 5.17218900 | 2.80970800 | 3.41251800 |
| C | 3.90086100 | 2.54584400 | 1.68675900 |
| H | 4.49657300 | 3.18923300 | 1.04504000 |
| C | 2.76166600 | 1.92999000 | 1.17230000 |
| H | 2.48817600 | 2.09169300 | 0.13583900 |
| C | -2.73179500 | 0.59206600 | -0.00518300 |
| C | -3.85258200 | 0.52002100 | 0.83524700 |
| H | -3.73986700 | 0.12526700 | 1.83959300 |
| C | -5.11617100 | 0.94447000 | 0.41973500 |
| H | -5.95088800 | 0.86729900 | 1.10643700 |
| C | -5.28423800 | 1.46621300 | -0.86756500 |
| C | -4.17453900 | 1.55931200 | -1.71936300 |
| H | -4.31605800 | 1.97320100 | -2.71258300 |
| C | -2.92585500 | 1.12941000 | -1.29069900 |
| H | -2.07834600 | 1.22058800 | -1.95993300 |
| C | -7.62169500 | 1.84482300 | -0.55740100 |
| H | -8.44384000 | 2.24151200 | -1.15537200 |
| H | -7.50677100 | 2.45628900 | 0.34707400 |
| H | -7.85552500 | 0.81335900 | -0.26278200 |
| C | -0.25878100 | 2.49849000 | 0.18612300 |
| C | -0.02948300 | 2.94921800 | -1.12389300 |
| H | 0.19768100 | 2.23394000 | -1.90573200 |
| C | -0.06497800 | 4.30241400 | -1.43810700 |
| H | 0.11905200 | 4.64824400 | -2.45009400 |
| C | -0.33433500 | 5.25258800 | -0.44374300 |
| C | -0.56300300 | 4.82578200 | 0.86938100 |
| H | -0.77035500 | 5.53527500 | 1.66161200 |
| C | -0.52144200 | 3.46282600 | 1.16792500 |
| H | -0.69592700 | 3.14393400 | 2.19138600 |

A118

| | | | |
|---|---|---|---|
| C | -0.60412400 | 7.55853600 | 0.11644400 |
| H | -0.56512300 | 8.50992300 | -0.41657500 |
| H | 0.15349200 | 7.55944000 | 0.91087900 |
| H | -1.59691500 | 7.44046400 | 0.56990200 |
| C | -0.22951600 | -2.45947800 | -1.54664600 |
| C | -0.88083200 | -4.55143700 | -2.16840100 |
| H | -1.03620400 | -5.61163200 | -2.04780400 |
| C | -1.16246400 | -3.72299800 | -3.20075800 |
| H | -1.60263500 | -3.91678800 | -4.16586500 |
| C | 0.07292100 | -4.36096800 | 0.11254900 |
| H | -0.82068400 | -4.69354600 | 0.64539600 |
| H | 0.60781100 | -3.64105000 | 0.72542300 |
| H | 0.73003300 | -5.21599500 | -0.06922600 |
| C | -0.91312900 | -1.28681700 | -3.67359300 |
| H | -1.64661800 | -1.52150900 | -4.44747700 |
| H | 0.03512400 | -1.02010300 | -4.14495800 |
| H | -1.27086300 | -0.44371500 | -3.08580500 |
| C | 2.93443600 | -2.56927800 | 0.53757000 |
| H | 1.88201500 | -1.79455000 | -0.16219200 |
| O | 2.50796300 | -2.92897900 | 1.68571600 |
| H | 1.59191200 | -2.09694600 | 2.39155900 |
| H | 2.90402100 | -3.33283700 | -0.26470700 |
| C | 4.12408800 | -1.61788600 | 0.43854600 |
| H | 3.87115600 | -0.66286700 | 0.90861000 |
| C | 4.67246000 | -1.41505600 | -0.97554900 |
| H | 4.90763300 | -2.39355700 | -1.41969600 |
| C | 5.92755300 | -0.53272800 | -1.00675100 |
| H | 6.70766000 | -0.98238500 | -0.37533500 |
| H | 5.69385200 | 0.44020800 | -0.55221900 |
| H | 3.90330900 | -0.96446600 | -1.61196400 |
| H | 4.89781100 | -2.07560400 | 1.07283200 |
| C | 6.48298300 | -0.31290300 | -2.41941600 |
| H | 5.70240800 | 0.13820200 | -3.04674100 |
| H | 6.71231100 | -1.28683200 | -2.87374000 |

A119

| C | 7.73499500 | 0.56973600 | -2.44638700 |
| H | 8.10699500 | 0.70856100 | -3.46705100 |
| H | 8.54497500 | 0.12767800 | -1.85456000 |
| H | 7.52812900 | 1.56252400 | -2.03041800 |

**TS29E**

| Ru | -0.85493100 | -0.02476700 | 0.70826500 |
| N | -2.02343400 | -2.72707700 | 1.72765300 |
| N | -0.67643500 | -1.92065200 | 3.19913400 |
| O | -0.87843200 | 1.98080700 | 2.96550000 |
| O | -2.05265500 | -0.17993900 | -2.37092500 |
| O | 6.06631400 | -3.03920400 | 0.41695000 |
| O | 4.94046600 | 4.62926300 | 0.69552800 |
| C | -0.89222400 | 1.17713900 | 2.11482400 |
| C | -0.91585300 | -0.05808900 | -1.69796400 |
| C | -0.08167900 | -1.14251500 | -1.24681100 |
| C | 1.05389700 | -0.55643400 | -0.55840200 |
| C | 0.85960000 | 0.87566400 | -0.52649000 |
| C | -0.37262900 | 1.19281100 | -1.20782700 |
| C | -0.25600700 | -2.56851000 | -1.60428800 |
| C | -0.85906300 | -2.93152400 | -2.82292700 |
| H | -1.19637600 | -2.15477400 | -3.49881600 |
| C | -1.02694100 | -4.27290100 | -3.16935200 |
| H | -1.49944000 | -4.52511600 | -4.11470100 |
| C | -0.58635000 | -5.28445100 | -2.31500500 |
| H | -0.71521900 | -6.32831300 | -2.58678200 |
| C | 0.02984800 | -4.93894200 | -1.10881900 |
| H | 0.38586000 | -5.71546700 | -0.43690100 |
| C | 0.19184500 | -3.60034200 | -0.75717000 |
| H | 0.66439000 | -3.34616300 | 0.18475100 |
| C | -0.89262300 | 2.53788500 | -1.54797000 |
| C | -1.46083700 | 2.77267300 | -2.81357200 |

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|---|---|---|---|
| H | -1.54440700 | 1.95306500 | -3.51795800 |
| C | -1.92681300 | 4.04001100 | -3.16445600 |
| H | -2.36379600 | 4.19530500 | -4.14714900 |
| C | -1.83078100 | 5.10218700 | -2.26475100 |
| H | -2.19391100 | 6.08865600 | -2.53899200 |
| C | -1.26697500 | 4.88323900 | -1.00564000 |
| H | -1.19009500 | 5.69971400 | -0.29287200 |
| C | -0.80712300 | 3.61695200 | -0.64918600 |
| H | -0.38408500 | 3.45909600 | 0.33640100 |
| C | 2.34639600 | -1.23494200 | -0.28707300 |
| C | 2.98671500 | -1.94142400 | -1.31562700 |
| H | 2.51000600 | -2.01243900 | -2.28811500 |
| C | 4.22492200 | -2.55843700 | -1.12772400 |
| H | 4.67964100 | -3.09288200 | -1.95347200 |
| C | 4.85946100 | -2.47392200 | 0.11656100 |
| C | 4.23950800 | -1.76644500 | 1.15592500 |
| H | 4.74416700 | -1.70580800 | 2.11485700 |
| C | 3.00634300 | -1.16144400 | 0.95188300 |
| H | 2.54215500 | -0.61777900 | 1.76599600 |
| C | 6.73939400 | -3.75958000 | -0.60212000 |
| H | 7.66811800 | -4.11873500 | -0.15560700 |
| H | 6.97731800 | -3.12018400 | -1.46221600 |
| H | 6.15070800 | -4.61892600 | -0.94912500 |
| C | 1.91245600 | 1.87040900 | -0.17709200 |
| C | 2.28802300 | 2.19133700 | 1.13734500 |
| H | 1.76717300 | 1.72912100 | 1.96815000 |
| C | 3.29656100 | 3.11119000 | 1.39631400 |
| H | 3.57991600 | 3.36296600 | 2.41315000 |
| C | 3.96559500 | 3.74222700 | 0.33873100 |
| C | 3.60430700 | 3.44129500 | -0.97951200 |
| H | 4.09914700 | 3.91563700 | -1.81865400 |
| C | 2.58719000 | 2.51626300 | -1.22123400 |
| H | 2.31226700 | 2.29412600 | -2.24817700 |
| C | 5.64045400 | 5.30549700 | -0.33580700 |

A121

| | | | |
|---|---|---|---|
| H | 6.35910500 | 5.95716200 | 0.16389600 |
| H | 4.96690400 | 5.91661600 | -0.95063300 |
| H | 6.18103100 | 4.60562800 | -0.98637000 |
| C | -1.20886000 | -1.64771100 | 1.96278700 |
| C | -1.99547900 | -3.62960800 | 2.78015700 |
| H | -2.56607100 | -4.54461500 | 2.76732200 |
| C | -1.15105300 | -3.12107100 | 3.70735300 |
| H | -0.84275100 | -3.50113500 | 4.66829100 |
| C | -2.84812200 | -2.95130000 | 0.54616900 |
| H | -2.58916700 | -3.90838600 | 0.08862300 |
| H | -2.66196200 | -2.15833200 | -0.17191400 |
| H | -3.90580400 | -2.95165600 | 0.82567400 |
| C | 0.25337400 | -1.07357900 | 3.93568800 |
| H | 0.82924500 | -1.69892600 | 4.62120600 |
| H | -0.27688300 | -0.30532800 | 4.50407600 |
| H | 0.92793200 | -0.58879900 | 3.23316900 |
| H | -2.57718100 | 0.15572500 | 0.58831000 |
| H | -2.93957600 | 0.17356000 | -1.79007000 |
| C | -4.00230500 | 0.46353500 | 0.26410800 |
| C | -4.25640700 | 0.41712600 | -1.12460100 |
| C | -4.13529400 | 1.77285700 | 1.04286100 |
| H | -5.01392100 | 2.30544300 | 0.65422900 |
| H | -3.27587100 | 2.42178800 | 0.84232500 |
| H | -4.33236700 | -0.41378400 | 0.82645300 |
| H | -4.40262600 | 1.38016700 | -1.62003700 |
| C | -5.04326200 | -0.73979600 | -1.72296000 |
| H | -4.93556500 | -1.62447200 | -1.07066300 |
| C | -4.31117400 | 1.56557900 | 2.55263000 |
| H | -3.48762000 | 0.95314100 | 2.93644100 |
| H | -5.23163000 | 0.99028700 | 2.72512800 |
| C | -4.37463000 | 2.88212600 | 3.33223400 |
| H | -4.54333700 | 2.70482600 | 4.39958800 |
| H | -5.18776900 | 3.52138700 | 2.96884300 |
| H | -3.43776600 | 3.43963600 | 3.23151600 |

| O | -4.72034000 | -1.04884300 | -3.07129900 |
| H | -3.76156200 | -1.17486600 | -3.11426900 |
| H | -6.11553300 | -0.49921100 | -1.73921500 |

**TS29Z**

| Ru | -0.80429200 | 0.17895000 | 0.67857700 |
| N | -2.60901300 | -2.27957000 | 1.28679500 |
| N | -1.20509600 | -1.99973200 | 2.89445200 |
| O | -0.52364100 | 1.85840200 | 3.17565500 |
| O | -1.89321200 | 0.52319700 | -2.41456100 |
| O | 5.38858800 | -4.12933000 | 0.30052300 |
| O | 5.79180200 | 3.55645600 | 1.22429000 |
| C | -0.64839200 | 1.18610900 | 2.22645900 |
| C | -0.77388000 | 0.35531700 | -1.71985200 |
| C | -0.19085800 | -0.90740500 | -1.35068900 |
| C | 1.00931900 | -0.62477800 | -0.58352700 |
| C | 1.10522700 | 0.81014900 | -0.42902500 |
| C | -0.00726700 | 1.42520900 | -1.10911200 |
| C | -0.63712300 | -2.23367300 | -1.83341800 |
| C | -1.27175500 | -2.36162000 | -3.08295600 |
| H | -1.43697000 | -1.47652900 | -3.68543600 |
| C | -1.69698300 | -3.60676700 | -3.54768800 |
| H | -2.18745800 | -3.67688800 | -4.51477500 |
| C | -1.49047500 | -4.75582900 | -2.78289100 |
| H | -1.82006600 | -5.72495500 | -3.14669400 |
| C | -0.84856600 | -4.64601900 | -1.54602600 |
| H | -0.67524600 | -5.53238600 | -0.94151700 |
| C | -0.42831400 | -3.40296800 | -1.07692200 |
| H | 0.05964800 | -3.33140100 | -0.11165900 |
| C | -0.22819100 | 2.87120100 | -1.34433900 |
| C | -0.65235500 | 3.31846700 | -2.60909200 |
| H | -0.84802600 | 2.59237200 | -3.39011800 |

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|---|---|---|---|
| C | -0.83600800 | 4.67812700 | -2.86239700 |
| H | -1.16709800 | 4.99886300 | -3.84636000 |
| C | -0.59413300 | 5.62111700 | -1.86263900 |
| H | -0.73757700 | 6.67963400 | -2.06042600 |
| C | -0.17023000 | 5.19039100 | -0.60319100 |
| H | 0.01709600 | 5.91339000 | 0.18594900 |
| C | 0.00668100 | 3.83250800 | -0.34483700 |
| H | 0.32200100 | 3.51051300 | 0.64133300 |
| C | 2.12942200 | -1.56827600 | -0.34115600 |
| C | 2.65077500 | -2.31716700 | -1.40626200 |
| H | 2.20345300 | -2.22352300 | -2.39066800 |
| C | 3.73351700 | -3.18286700 | -1.23998900 |
| H | 4.10001500 | -3.74036900 | -2.09389800 |
| C | 4.32990500 | -3.31281400 | 0.01909200 |
| C | 3.82970200 | -2.56639800 | 1.09517500 |
| H | 4.30427800 | -2.67330400 | 2.06536300 |
| C | 2.74960800 | -1.71301700 | 0.91240500 |
| H | 2.37818600 | -1.14091700 | 1.75451900 |
| C | 5.93789400 | -4.89950300 | -0.75555900 |
| H | 6.76066500 | -5.46817700 | -0.31900400 |
| H | 6.32743900 | -4.26422200 | -1.56172700 |
| H | 5.20139200 | -5.59682900 | -1.17603400 |
| C | 2.31924400 | 1.53997800 | 0.03405000 |
| C | 2.68079800 | 1.69309500 | 1.38227200 |
| H | 2.03415800 | 1.29565900 | 2.15628000 |
| C | 3.83937700 | 2.36769500 | 1.74702200 |
| H | 4.11289900 | 2.49091000 | 2.78993400 |
| C | 4.67812000 | 2.91304500 | 0.76552600 |
| C | 4.33494500 | 2.77632600 | -0.58438400 |
| H | 4.95998700 | 3.19053300 | -1.36655800 |
| C | 3.16606900 | 2.09726000 | -0.93277600 |
| H | 2.90756000 | 2.00139000 | -1.98330900 |
| C | 6.66862400 | 4.13760200 | 0.27337800 |
| H | 7.47635200 | 4.59497900 | 0.84716300 |

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|---|---|---|---|
| H | 6.16678800 | 4.91145400 | -0.32201200 |
| H | 7.09060400 | 3.38377700 | -0.40409900 |
| C | -1.58911200 | -1.45578300 | 1.69355000 |
| C | -2.84262500 | -3.29442800 | 2.20251800 |
| H | -3.59949700 | -4.04635500 | 2.04536400 |
| C | -1.96304500 | -3.11640700 | 3.21571800 |
| H | -1.80576200 | -3.67708000 | 4.12335300 |
| C | -3.37670000 | -2.16820000 | 0.05131600 |
| H | -3.21358200 | -3.05001800 | -0.57152000 |
| H | -3.04851200 | -1.28678900 | -0.49290900 |
| H | -4.44078200 | -2.07821800 | 0.28727900 |
| C | -0.14933100 | -1.49038600 | 3.76131100 |
| H | 0.20307500 | -2.30481700 | 4.39761300 |
| H | -0.51196900 | -0.67192100 | 4.38792200 |
| H | 0.67283000 | -1.12754800 | 3.14764800 |
| H | -2.43122900 | 0.79444900 | 0.54979000 |
| H | -2.66726400 | 1.06782600 | -1.82986500 |
| C | -3.57396200 | 1.67726100 | 0.24025100 |
| C | -3.85355200 | 1.69920000 | -1.14897500 |
| C | -4.58526700 | 1.13581400 | 1.24954100 |
| H | -5.50521300 | 1.72449000 | 1.10761400 |
| H | -4.86147000 | 0.10388600 | 1.00675800 |
| H | -3.04600800 | 2.56061600 | 0.59986800 |
| H | -3.60992400 | 2.63117300 | -1.66369100 |
| C | -4.99531000 | 0.92366300 | -1.77456400 |
| H | -5.14482900 | -0.03237100 | -1.24539000 |
| C | -4.16942100 | 1.22758200 | 2.72092400 |
| H | -3.86848900 | 2.25864500 | 2.94804800 |
| H | -3.28417300 | 0.60678100 | 2.88868500 |
| C | -5.28851100 | 0.79847500 | 3.67577300 |
| H | -4.97107000 | 0.87689800 | 4.72066600 |
| H | -5.58702800 | -0.24148300 | 3.49720100 |
| H | -6.18157800 | 1.42214500 | 3.55285000 |
| O | -4.82670900 | 0.71032100 | -3.17239200 |

| H | -3.95731000 | 0.30412500 | -3.29641500 |
| H | -5.94445200 | 1.47280200 | -1.68540900 |

**TS30E**

| Ru | -0.87929500 | -0.01541900 | 0.68443700 |
| N | -2.44068600 | -2.68549600 | 1.04190800 |
| N | -1.03877900 | -2.43715700 | 2.65673500 |
| O | -0.84533600 | 1.42609300 | 3.34074400 |
| O | -1.96599600 | 0.48321500 | -2.38324600 |
| O | 5.71508800 | -3.63754500 | 0.17675300 |
| O | 5.38121200 | 3.93696100 | 1.55153400 |
| C | -0.86556100 | 0.84568700 | 2.32433000 |
| C | -0.84115600 | 0.36504600 | -1.67973300 |
| C | -0.14409100 | -0.86662700 | -1.41227800 |
| C | 1.02294700 | -0.53964200 | -0.61127400 |
| C | 0.98405100 | 0.87818700 | -0.33595300 |
| C | -0.17497200 | 1.44346000 | -0.97720200 |
| C | -0.47696700 | -2.18503300 | -1.99987800 |
| C | -1.11348600 | -2.26751200 | -3.25249300 |
| H | -1.37460000 | -1.35486200 | -3.77403000 |
| C | -1.42970600 | -3.50455200 | -3.81551700 |
| H | -1.92417000 | -3.53967700 | -4.78249400 |
| C | -1.11219000 | -4.68883900 | -3.14859900 |
| H | -1.35737000 | -5.65106100 | -3.58943000 |
| C | -0.47053500 | -4.62235900 | -1.90855600 |
| H | -0.21339400 | -5.53538200 | -1.37809100 |
| C | -0.15818900 | -3.38839400 | -1.34142100 |
| H | 0.33133900 | -3.35200700 | -0.37517900 |
| C | -0.48410500 | 2.88330300 | -1.13586900 |
| C | -0.69113900 | 3.40564100 | -2.42457300 |
| H | -0.63842500 | 2.74062600 | -3.28081900 |
| C | -0.95761000 | 4.76170400 | -2.61371000 |

A126

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|---|---|---|---|
| H | -1.12416400 | 5.14106700 | -3.61779600 |
| C | -1.01070700 | 5.62585900 | -1.51911100 |
| H | -1.21930200 | 6.68185700 | -1.66512500 |
| C | -0.79647100 | 5.12168500 | -0.23418700 |
| H | -0.83691400 | 5.78512200 | 0.62530100 |
| C | -0.54120400 | 3.76433100 | -0.04314100 |
| H | -0.39467000 | 3.37710200 | 0.95928800 |
| C | 2.22300900 | -1.38660200 | -0.40285300 |
| C | 2.79168500 | -2.08437800 | -1.47821500 |
| H | 2.32196600 | -2.03205700 | -2.45490100 |
| C | 3.95209300 | -2.84767000 | -1.33199200 |
| H | 4.35216000 | -3.36999300 | -2.19307800 |
| C | 4.58180300 | -2.92055900 | -0.08487700 |
| C | 4.03849200 | -2.21723800 | 0.99982200 |
| H | 4.54201700 | -2.27429500 | 1.95956900 |
| C | 2.88211900 | -1.46653400 | 0.83792100 |
| H | 2.48381400 | -0.91778800 | 1.68391400 |
| C | 6.31061300 | -4.35864100 | -0.88880300 |
| H | 7.18890500 | -4.85067200 | -0.46756900 |
| H | 6.62667500 | -3.69353000 | -1.70306700 |
| H | 5.63124000 | -5.11985400 | -1.29443700 |
| C | 2.12672100 | 1.67903800 | 0.19141600 |
| C | 2.32735200 | 1.97364300 | 1.54928200 |
| H | 1.61579400 | 1.61741600 | 2.28515900 |
| C | 3.41745000 | 2.72582100 | 1.97064200 |
| H | 3.56821500 | 2.95587100 | 3.02043700 |
| C | 4.34567400 | 3.20903600 | 1.03874200 |
| C | 4.16364800 | 2.92917400 | -0.32039400 |
| H | 4.86234000 | 3.29023200 | -1.06573700 |
| C | 3.06273300 | 2.17282600 | -0.72628800 |
| H | 2.93112900 | 1.96302900 | -1.78392600 |
| C | 6.34415200 | 4.45776800 | 0.65041300 |
| H | 7.06781000 | 4.99978100 | 1.26149600 |
| H | 5.89207900 | 5.15038100 | -0.07147500 |

A127

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|---|---|---|---|
| H | 6.86196400 | 3.65940600 | 0.10282000 |
| C | -1.49696600 | -1.81300400 | 1.52336800 |
| C | -2.55577500 | -3.80812900 | 1.84760800 |
| H | -3.23936300 | -4.61041100 | 1.61969100 |
| C | -1.67783000 | -3.65036800 | 2.86582700 |
| H | -1.44992900 | -4.28333100 | 3.70860500 |
| C | -3.23256600 | -2.52926500 | -0.17412900 |
| H | -2.96238400 | -3.30017700 | -0.89847600 |
| H | -3.03374900 | -1.55246500 | -0.60645900 |
| H | -4.29526500 | -2.61201300 | 0.06981900 |
| C | -0.01533000 | -1.91828100 | 3.55713300 |
| H | 0.38514400 | -2.74847700 | 4.14237700 |
| H | -0.42829600 | -1.16550400 | 4.23249400 |
| H | 0.78462600 | -1.46957800 | 2.97123100 |
| H | -2.54525200 | 0.41729800 | 0.58900400 |
| H | -2.85712900 | 0.70647700 | -1.75676700 |
| C | -3.83925500 | 1.16364700 | 0.30697600 |
| C | -4.12411600 | 1.18520300 | -1.07359200 |
| H | -4.83725900 | 0.43889900 | -1.43511400 |
| C | -4.76412000 | 0.43163900 | 1.27279300 |
| H | -4.98450800 | -0.57233500 | 0.89122900 |
| H | -5.72105600 | 0.97488800 | 1.22464200 |
| C | -4.16413900 | 2.51168500 | -1.82562800 |
| H | -3.44142700 | 3.20832900 | -1.37342400 |
| H | -3.43245000 | 2.09286100 | 0.71186500 |
| C | -4.32587000 | 0.36018800 | 2.73850600 |
| H | -4.06488500 | 1.36756300 | 3.08793700 |
| H | -3.41327800 | -0.23673300 | 2.82046300 |
| C | -5.41199300 | -0.23019200 | 3.64444100 |
| H | -5.08062600 | -0.27119700 | 4.68711300 |
| H | -5.67341900 | -1.25058300 | 3.33945400 |
| H | -6.33035300 | 0.36748200 | 3.61158800 |
| O | -3.96845900 | 2.39080000 | -3.22695200 |
| H | -3.09289000 | 1.99678900 | -3.35086200 |

A128

| | | | |
|---|---|---|---|
| H | -5.15849700 | 2.96781500 | -1.71735000 |

**TS30Z**

| | | | |
|---|---|---|---|
| Ru | -0.70041700 | -0.41974900 | 0.77822900 |
| N | -1.07953400 | -3.43100000 | 1.48972000 |
| N | 0.12650300 | -2.47022800 | 2.99146900 |
| O | -1.23986400 | 1.14815100 | 3.30524100 |
| O | -1.93708100 | -0.72449800 | -2.25647700 |
| O | 6.78493700 | -1.11361400 | 0.23496400 |
| O | 3.40987500 | 5.78639600 | 0.97781500 |
| C | -1.03110100 | 0.52522500 | 2.33599800 |
| C | -0.85425300 | -0.30279800 | -1.61048900 |
| C | 0.28732600 | -1.11282400 | -1.26716300 |
| C | 1.22934400 | -0.26045600 | -0.56453500 |
| C | 0.61719700 | 1.04115500 | -0.41431800 |
| C | -0.67985500 | 1.01925800 | -1.04032500 |
| C | 0.50669600 | -2.51045500 | -1.70763400 |
| C | -0.04797000 | -2.97247000 | -2.91584700 |
| H | -0.65145300 | -2.29912600 | -3.51212600 |
| C | 0.15174000 | -4.28691400 | -3.33970300 |
| H | -0.29029400 | -4.61867500 | -4.27528400 |
| C | 0.91509300 | -5.16989800 | -2.57455500 |
| H | 1.07153400 | -6.19223900 | -2.90724400 |
| C | 1.48042700 | -4.72194800 | -1.37723700 |
| H | 2.08087900 | -5.39606900 | -0.77210500 |
| C | 1.27830900 | -3.41145600 | -0.94877600 |
| H | 1.71640100 | -3.07982900 | -0.01447800 |
| C | -1.56527000 | 2.17806800 | -1.29762100 |
| C | -2.06383400 | 2.39489600 | -2.59452900 |
| H | -1.80481100 | 1.69833200 | -3.38508000 |
| C | -2.87797900 | 3.49239300 | -2.87545600 |
| H | -3.25711600 | 3.63468400 | -3.88346900 |

A129

| C | -3.20202300 | 4.40313600 | -1.86885900 |
| H | -3.83613000 | 5.25778000 | -2.08675900 |
| C | -2.70580100 | 4.20485800 | -0.57828800 |
| H | -2.95211100 | 4.90619000 | 0.21417800 |
| C | -1.90109000 | 3.10241900 | -0.29366600 |
| H | -1.53649600 | 2.94682100 | 0.71558200 |
| C | 2.67238800 | -0.52664100 | -0.34739200 |
| C | 3.45812800 | -1.04827700 | -1.38525800 |
| H | 2.99241800 | -1.29241300 | -2.33437100 |
| C | 4.83018600 | -1.26233900 | -1.23645900 |
| H | 5.39415700 | -1.66864000 | -2.06784400 |
| C | 5.45448500 | -0.94391500 | -0.02568400 |
| C | 4.68952800 | -0.40748700 | 1.02006300 |
| H | 5.18756400 | -0.15661700 | 1.95115700 |
| C | 3.32601000 | -0.20491300 | 0.85661100 |
| H | 2.75254900 | 0.22274200 | 1.67124200 |
| C | 7.60519800 | -1.64256100 | -0.79334900 |
| H | 8.61395500 | -1.69278000 | -0.38004900 |
| H | 7.61170500 | -0.99634700 | -1.68085500 |
| H | 7.28672300 | -2.65072300 | -1.08949400 |
| C | 1.34040500 | 2.28418600 | -0.01810900 |
| C | 1.43654400 | 2.75636300 | 1.30065800 |
| H | 0.95266400 | 2.20858700 | 2.10127900 |
| C | 2.13044900 | 3.92256700 | 1.60052800 |
| H | 2.19964800 | 4.28805000 | 2.62001300 |
| C | 2.75328200 | 4.65627900 | 0.58192000 |
| C | 2.66780000 | 4.20521300 | -0.74016900 |
| H | 3.13639000 | 4.75126800 | -1.55030600 |
| C | 1.96601000 | 3.03208500 | -1.02365800 |
| H | 1.90517400 | 2.69243800 | -2.05362900 |
| C | 4.05058800 | 6.57080000 | -0.01456000 |
| H | 4.50262900 | 7.41328800 | 0.51150000 |
| H | 3.33578000 | 6.95099200 | -0.75598200 |
| H | 4.83678700 | 6.00679400 | -0.53333800 |

| | | | |
|---|---|---|---|
| C | -0.54774700 | -2.21059100 | 1.82455300 |
| C | -0.74520600 | -4.40577100 | 2.41778200 |
| H | -1.06499300 | -5.43044700 | 2.31442000 |
| C | 0.01006700 | -3.80105900 | 3.36427400 |
| H | 0.47416400 | -4.19181200 | 4.25578300 |
| C | -1.87778900 | -3.74100000 | 0.30809400 |
| H | -1.39712600 | -4.53969100 | -0.26097000 |
| H | -1.94700600 | -2.85894500 | -0.32080600 |
| H | -2.88167200 | -4.05669400 | 0.60799500 |
| C | 0.88331400 | -1.49694700 | 3.77115000 |
| H | 1.59071400 | -2.03517800 | 4.40532300 |
| H | 0.22281700 | -0.89255700 | 4.39691200 |
| H | 1.42974900 | -0.84238600 | 3.09459700 |
| H | -2.39868600 | -0.71330000 | 0.70349700 |
| H | -2.82674900 | -0.87895400 | -1.59184700 |
| C | -3.83548000 | -0.87167600 | 0.48865700 |
| C | -4.13857400 | -1.02127000 | -0.88859900 |
| H | -4.32777500 | -2.04182200 | -1.23033000 |
| C | -4.32184900 | 0.31467100 | 1.31216200 |
| H | -3.75701400 | 0.35964800 | 2.24910700 |
| H | -4.11859300 | 1.25346100 | 0.78604700 |
| C | -4.85990700 | 0.03484500 | -1.71467900 |
| H | -4.56361200 | 1.04369800 | -1.39317800 |
| H | -3.83455600 | -1.80183500 | 1.05908000 |
| C | -5.82418600 | 0.21741800 | 1.64136900 |
| H | -6.02154200 | -0.73650500 | 2.14917800 |
| H | -6.40983400 | 0.19686600 | 0.71510500 |
| C | -6.30108700 | 1.37559500 | 2.52446600 |
| H | -7.36781200 | 1.28686200 | 2.75553700 |
| H | -6.14644900 | 2.34006800 | 2.02794200 |
| H | -5.75410800 | 1.40177400 | 3.47373800 |
| O | -4.66267600 | -0.13479200 | -3.11350700 |
| H | -3.71042600 | -0.05948800 | -3.27040300 |
| H | -5.94706400 | -0.03945100 | -1.57216600 |

**22**

| | | | |
|---|---|---|---|
| C | -1.18136800 | 0.39944000 | -0.15934400 |
| C | 0.19904900 | -0.08942100 | 0.29360300 |
| H | -1.19054100 | 0.49698900 | -1.25447500 |
| H | -1.36076400 | 1.41057700 | 0.23478400 |
| C | 1.34245500 | 0.83587600 | -0.13877700 |
| H | 0.38737700 | -1.09268000 | -0.10555400 |
| H | 0.20911400 | -0.18686600 | 1.38917500 |
| C | 2.72172700 | 0.33722700 | 0.27481700 |
| H | 1.19752100 | 1.83781900 | 0.28756100 |
| H | 1.33279200 | 0.95364400 | -1.23015100 |
| O | 2.96771300 | -0.90091200 | -0.38707800 |
| H | 2.75798000 | 0.21428200 | 1.37030400 |
| H | 3.48268800 | 1.08695800 | 0.00431900 |
| H | 3.81431800 | -1.24408400 | -0.07574400 |
| C | -2.32903200 | -0.52101900 | 0.27374100 |
| H | -2.32159800 | -0.61736800 | 1.36809500 |
| H | -2.14885600 | -1.53063400 | -0.11950200 |
| C | -3.70541200 | -0.03133800 | -0.18602800 |
| H | -4.50185200 | -0.70886300 | 0.13882000 |
| H | -3.75572000 | 0.04071700 | -1.27849100 |
| H | -3.92867800 | 0.96221400 | 0.21941200 |

**23**

| | | | |
|---|---|---|---|
| Ru | -1.93805000 | 0.02286000 | -1.29340200 |
| O | -2.64262300 | 2.07655400 | -3.46276200 |
| O | -2.39368500 | -2.31584500 | -3.21935700 |
| O | -0.24906400 | 0.35628800 | 1.69828900 |
| O | -7.83675500 | -4.17971800 | 0.10875400 |
| O | -8.36255800 | 3.52461000 | -0.41709800 |
| C | -2.34845700 | 1.29463000 | -2.66610200 |

| | | | |
|---|---|---|---|
| C | -2.16763300 | -1.43277500 | -2.50923400 |
| C | -1.36780300 | 0.20715900 | 1.12902000 |
| C | -2.03504600 | -1.04429000 | 0.74568000 |
| C | -3.35712400 | -0.70403600 | 0.24911100 |
| C | -3.45987800 | 0.74147300 | 0.17897800 |
| C | -2.20559300 | 1.30732800 | 0.62494600 |
| C | -1.62166600 | -2.39360500 | 1.19719500 |
| C | -1.05064100 | -2.54915200 | 2.47289200 |
| H | -0.85666200 | -1.66910300 | 3.07571100 |
| C | -0.74080400 | -3.81639900 | 2.96815900 |
| H | -0.29704500 | -3.91130800 | 3.95509000 |
| C | -0.99925500 | -4.95340700 | 2.20229700 |
| H | -0.76040500 | -5.94027300 | 2.58875700 |
| C | -1.56298900 | -4.81134500 | 0.93234200 |
| H | -1.76043100 | -5.68742200 | 0.32152200 |
| C | -1.86693900 | -3.54680200 | 0.43369900 |
| H | -2.29602900 | -3.45472700 | -0.55737000 |
| C | -1.93171900 | 2.74255900 | 0.87318800 |
| C | -1.31699100 | 3.13622600 | 2.07564700 |
| H | -0.99732700 | 2.37766600 | 2.77974700 |
| C | -1.11422000 | 4.48572000 | 2.36511900 |
| H | -0.63897600 | 4.76551900 | 3.30137100 |
| C | -1.51794900 | 5.46951600 | 1.46244700 |
| H | -1.35754500 | 6.52012400 | 1.68766900 |
| C | -2.12488100 | 5.09129700 | 0.26308200 |
| H | -2.43709600 | 5.84634200 | -0.45280700 |
| C | -2.32851100 | 3.74467600 | -0.02857900 |
| H | -2.79832500 | 3.46918700 | -0.96585300 |
| C | -4.51274700 | -1.63848400 | 0.17630000 |
| C | -4.94856700 | -2.24303200 | 1.36300000 |
| H | -4.41352500 | -2.04963900 | 2.28760500 |
| C | -6.05383200 | -3.09420600 | 1.38929400 |
| H | -6.35582200 | -3.53950200 | 2.32965200 |
| C | -6.74889700 | -3.36242500 | 0.20415400 |

| C  | -6.32172600 | -2.77096800 | -0.99285700 |
|----|-------------|-------------|-------------|
| H  | -6.86460800 | -2.99481900 | -1.90520100 |
| C  | -5.22216600 | -1.92280400 | -1.00168000 |
| H  | -4.89998100 | -1.48648400 | -1.94009300 |
| C  | -8.30590600 | -4.81323800 | 1.28825800 |
| H  | -9.16718500 | -5.41154100 | 0.98699300 |
| H  | -8.62188200 | -4.08176000 | 2.04327900 |
| H  | -7.54429400 | -5.47201300 | 1.72510400 |
| C  | -4.72631300 | 1.49436600 | -0.01603400 |
| C  | -5.48770200 | 1.45419100 | -1.19588100 |
| H  | -5.12451100 | 0.89191500 | -2.04839300 |
| C  | -6.69051800 | 2.13947500 | -1.29928300 |
| H  | -7.27399200 | 2.11389300 | -2.21366300 |
| C  | -7.17328400 | 2.88815500 | -0.21635800 |
| C  | -6.42863100 | 2.94292700 | 0.96762700 |
| H  | -6.77218300 | 3.51628500 | 1.82025100 |
| C  | -5.21878300 | 2.25311600 | 1.05422400 |
| H  | -4.64725600 | 2.30993800 | 1.97526800 |
| C  | -8.89245100 | 4.30722200 | 0.64108900 |
| H  | -9.83130700 | 4.72058700 | 0.26938100 |
| H  | -8.21886500 | 5.12997000 | 0.91340800 |
| H  | -9.09430900 | 3.69986900 | 1.53287500 |
| Ru | 1.93807800 | 0.02263400 | 1.29330500 |
| O  | 2.64306400 | 2.07588300 | 3.46291500 |
| O  | 2.39366600 | -2.31541700 | 3.22014300 |
| O  | 0.24915600 | 0.35564100 | -1.69865100 |
| O  | 7.83759200 | -4.17876000 | -0.10888700 |
| O  | 8.36206600 | 3.52532600 | 0.41676100 |
| C  | 2.34868300 | 1.29420400 | 2.66609500 |
| C  | 2.16763000 | -1.43275100 | 2.50952600 |
| C  | 1.36782400 | 0.20676900 | -1.12910600 |
| C  | 2.03530100 | -1.04451100 | -0.74586800 |
| C  | 3.35727800 | -0.70395400 | -0.24916200 |
| C  | 3.45968000 | 0.74162200 | -0.17904600 |

| C | 2.20526200 | 1.30712300 | -0.62490900 |
|---|---|---|---|
| C | 1.62214300 | -2.39392500 | -1.19729400 |
| C | 1.05002700 | -2.54957400 | -2.47247800 |
| H | 0.85512500 | -1.66958500 | -3.07507300 |
| C | 0.74014000 | -3.81690700 | -2.96751900 |
| H | 0.29547500 | -3.91190400 | -3.95403400 |
| C | 0.99970100 | -4.95388400 | -2.20199600 |
| H | 0.76083900 | -5.94080000 | -2.58832200 |
| C | 1.56460500 | -4.81171800 | -0.93256700 |
| H | 1.76298800 | -5.68776900 | -0.32201400 |
| C | 1.86855000 | -3.54710100 | -0.43411700 |
| H | 2.29856200 | -3.45494200 | 0.55654300 |
| C | 1.93101300 | 2.74231200 | -0.87298500 |
| C | 1.31627400 | 3.13600400 | -2.07542400 |
| H | 0.99686500 | 2.37746100 | -2.77965800 |
| C | 1.11318500 | 4.48549700 | -2.36470300 |
| H | 0.63794400 | 4.76530700 | -3.30095400 |
| C | 1.51658200 | 5.46925600 | -1.46185000 |
| H | 1.35593100 | 6.51985800 | -1.68691800 |
| C | 2.12352800 | 5.09100400 | -0.26249300 |
| H | 2.43549700 | 5.84601700 | 0.45353600 |
| C | 2.32748600 | 3.74439500 | 0.02896900 |
| H | 2.79728300 | 3.46887500 | 0.96624500 |
| C | 4.51316400 | -1.63809500 | -0.17642800 |
| C | 4.94956600 | -2.24192100 | -1.36326700 |
| H | 4.41484200 | -2.04814300 | -2.28797900 |
| C | 6.05499800 | -3.09288300 | -1.38955900 |
| H | 6.35744400 | -3.53765000 | -2.33002200 |
| C | 6.74963200 | -3.36160400 | -0.20428500 |
| C | 6.32186900 | -2.77087800 | 0.99287800 |
| H | 6.86443400 | -2.99511800 | 1.90531500 |
| C | 5.22214500 | -1.92292900 | 1.00170200 |
| H | 4.89947800 | -1.48713400 | 1.94019100 |
| C | 8.30752500 | -4.81131700 | -1.28859700 |

| | | | |
|---|---|---|---|
| H | 9.16891500 | -5.40946300 | -0.98733800 |
| H | 8.62352800 | -4.07921600 | -2.04300000 |
| H | 7.54637600 | -5.47012300 | -1.72620600 |
| C | 4.72602600 | 1.49469300 | 0.01587800 |
| C | 5.48775800 | 1.45410600 | 1.19547600 |
| H | 5.12493100 | 0.89138300 | 2.04784300 |
| C | 6.69052000 | 2.13951900 | 1.29883700 |
| H | 7.27425000 | 2.11359000 | 2.21304300 |
| C | 7.17283700 | 2.88875500 | 0.21611800 |
| C | 6.42780100 | 2.94396600 | -0.96762200 |
| H | 6.77102800 | 3.51778200 | -1.82006900 |
| C | 5.21803500 | 2.25403000 | -1.05418400 |
| H | 4.64620000 | 2.31119400 | -1.97501500 |
| C | 8.89153700 | 4.30845000 | -0.64125600 |
| H | 9.83048400 | 4.72172400 | -0.26967700 |
| H | 8.21779600 | 5.13126800 | -0.91298200 |
| H | 9.09314300 | 3.70151000 | -1.53337900 |

**24**

| | | | |
|---|---|---|---|
| Ru | -0.00014600 | -1.52627600 | 1.34733000 |
| O | -2.23979200 | -1.16777900 | 3.41137600 |
| O | 2.23861500 | -1.16792900 | 3.41246400 |
| O | -0.00029700 | -3.38756200 | -1.42700300 |
| O | 3.83970700 | 4.61187100 | 0.02382100 |
| O | -3.83842900 | 4.61283100 | 0.02338600 |
| C | -1.38228300 | -1.35229000 | 2.65971400 |
| C | 1.38152400 | -1.35236600 | 2.66031300 |
| C | -0.00023500 | -2.22425400 | -1.02288000 |
| C | 1.19521600 | -1.41386600 | -0.62276200 |
| C | 0.73673500 | -0.11899400 | -0.24248700 |
| C | -0.73668400 | -0.11885500 | -0.24234200 |
| C | -1.19546400 | -1.41369800 | -0.62256300 |

| | | | |
|---|---|---|---|
| C | 2.59195300 | -1.85954700 | -0.82575500 |
| C | 2.89093200 | -2.80883500 | -1.82139800 |
| H | 2.08616800 | -3.23262900 | -2.40800300 |
| C | 4.20566500 | -3.21986100 | -2.04015600 |
| H | 4.41230400 | -3.95368000 | -2.81417000 |
| C | 5.24796200 | -2.69984600 | -1.27288500 |
| H | 6.27037900 | -3.02504000 | -1.44307000 |
| C | 4.96392800 | -1.76150200 | -0.27755800 |
| H | 5.76429700 | -1.35401200 | 0.33352400 |
| C | 3.65381000 | -1.34626900 | -0.05598700 |
| H | 3.45307000 | -0.62216600 | 0.72498300 |
| C | -2.59233500 | -1.85907100 | -0.82551500 |
| C | -2.89154000 | -2.80844800 | -1.82101200 |
| H | -2.08687500 | -3.23253600 | -2.40753400 |
| C | -4.20637100 | -3.21918300 | -2.03972900 |
| H | -4.41317600 | -3.95307300 | -2.81363200 |
| C | -5.24855700 | -2.69879200 | -1.27256200 |
| H | -6.27105100 | -3.02376000 | -1.44271400 |
| C | -4.96430300 | -1.76035900 | -0.27738600 |
| H | -5.76457700 | -1.35256900 | 0.33361900 |
| C | -3.65408500 | -1.34540700 | -0.05586200 |
| H | -3.45321400 | -0.62121300 | 0.72498600 |
| C | 1.56542100 | 1.10930700 | -0.14341300 |
| C | 2.23969500 | 1.55082000 | -1.28927900 |
| H | 2.16804400 | 0.97386100 | -2.20639700 |
| C | 3.00530500 | 2.71723000 | -1.28193900 |
| H | 3.50827400 | 3.02573700 | -2.19048700 |
| C | 3.11677500 | 3.46428000 | -0.10281900 |
| C | 2.45582400 | 3.02818300 | 1.05521300 |
| H | 2.56138300 | 3.61221600 | 1.96339000 |
| C | 1.68977000 | 1.87091100 | 1.03032900 |
| H | 1.19870400 | 1.53718100 | 1.93758200 |
| C | 4.53995300 | 5.09608100 | -1.11219000 |
| H | 5.04315000 | 6.00846500 | -0.78898600 |

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|---|---|---|---|
| H | 3.85679300 | 5.33400400 | -1.93756600 |
| H | 5.28957600 | 4.37537500 | -1.46302300 |
| C | -1.56510800 | 1.10962700 | -0.14343100 |
| C | -1.68901000 | 1.87156000 | 1.03014400 |
| H | -1.19784800 | 1.53791700 | 1.93737800 |
| C | -2.45476300 | 3.02903500 | 1.05490000 |
| H | -2.55998500 | 3.61332600 | 1.96295000 |
| C | -3.11583600 | 3.46501100 | -0.10310800 |
| C | -3.00480900 | 2.71763000 | -1.28206400 |
| H | -3.50789200 | 3.02603200 | -2.19058300 |
| C | -2.23950500 | 1.55101800 | -1.28927200 |
| H | -2.16820200 | 0.97380300 | -2.20625400 |
| C | -4.53878900 | 5.09693300 | -1.11260200 |
| H | -5.04166300 | 6.00954200 | -0.78953300 |
| H | -5.28868600 | 4.37634000 | -1.46308100 |
| H | -3.85574300 | 5.33444800 | -1.93819000 |

**25**

| | | | |
|---|---|---|---|
| Ru | -1.06741300 | 0.57459500 | 1.05264700 |
| O | 0.08303300 | 2.60229800 | 3.03381200 |
| O | -1.56684900 | -1.53141900 | 3.21062700 |
| O | -2.31369400 | 1.22299400 | -2.11948300 |
| O | 2.75145500 | -5.71823100 | 0.44672700 |
| O | 6.27940400 | 1.23165000 | 0.50490000 |
| C | -0.39345900 | 1.83630000 | 2.31048400 |
| C | -1.40404600 | -0.70791000 | 2.41301800 |
| C | -1.34091300 | 0.75411000 | -1.46075800 |
| C | -1.25215100 | -0.61796700 | -0.91163300 |
| C | 0.06819400 | -0.78333300 | -0.33503900 |
| C | 0.71243900 | 0.51084300 | -0.31930300 |
| C | -0.19334100 | 1.48544700 | -0.91861000 |
| C | -2.26133000 | -1.67029100 | -1.18015200 |

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|---|---|---|---|
| C | -3.03772700 | -1.63000700 | -2.35899400 |
| H | -2.86485800 | -0.83458200 | -3.07439500 |
| C | -4.00769400 | -2.60503100 | -2.61578200 |
| H | -4.58405700 | -2.55355000 | -3.53589700 |
| C | -4.21993500 | -3.64710300 | -1.71409300 |
| H | -4.97054000 | -4.40575700 | -1.91575300 |
| C | -3.44940000 | -3.70700500 | -0.54854700 |
| H | -3.60016500 | -4.51425600 | 0.16267300 |
| C | -2.49058500 | -2.73324300 | -0.28236800 |
| H | -1.91313600 | -2.79328900 | 0.63267800 |
| C | 0.10310600 | 2.90878400 | -1.20636900 |
| C | -0.44724300 | 3.53237900 | -2.34256800 |
| H | -1.10993900 | 2.96570700 | -2.98395100 |
| C | -0.15962200 | 4.86563400 | -2.63659600 |
| H | -0.59715500 | 5.32205300 | -3.52068400 |
| C | 0.68070400 | 5.61020000 | -1.80897900 |
| H | 0.90098000 | 6.64902000 | -2.03855400 |
| C | 1.23242100 | 5.00477400 | -0.67769700 |
| H | 1.88519300 | 5.57078100 | -0.01876900 |
| C | 0.94831200 | 3.67415300 | -0.38012500 |
| H | 1.38474200 | 3.22820900 | 0.50565100 |
| C | 0.74440600 | -2.08524600 | -0.09732600 |
| C | 0.84767900 | -2.98866700 | -1.16379000 |
| H | 0.40606400 | -2.73356800 | -2.12236700 |
| C | 1.50975500 | -4.21020500 | -1.03038600 |
| H | 1.56754400 | -4.87668100 | -1.88268900 |
| C | 2.08592800 | -4.55355800 | 0.19805800 |
| C | 1.98691100 | -3.66368900 | 1.27731000 |
| H | 2.43070100 | -3.94744400 | 2.22589200 |
| C | 1.32731900 | -2.45132200 | 1.12797900 |
| H | 1.24857600 | -1.78311600 | 1.97756200 |
| C | 2.87829700 | -6.65728500 | -0.60873000 |
| H | 3.43585500 | -7.50015600 | -0.19732800 |
| H | 3.43261000 | -6.23945700 | -1.45913400 |

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|---|---|---|---|
| H | 1.89911900 | -7.00934300 | -0.95859100 |
| C | 2.16577000 | 0.72008900 | -0.07561500 |
| C | 2.76550800 | 0.64150400 | 1.19183800 |
| H | 2.14595900 | 0.45943700 | 2.06337900 |
| C | 4.13419700 | 0.81513100 | 1.35355000 |
| H | 4.59535300 | 0.75971600 | 2.33420200 |
| C | 4.94920300 | 1.07513000 | 0.24307700 |
| C | 4.37070700 | 1.16315500 | -1.02871600 |
| H | 4.97323400 | 1.36875400 | -1.90543200 |
| C | 2.99369900 | 0.98841500 | -1.17352300 |
| H | 2.55490900 | 1.06665500 | -2.16381700 |
| C | 7.14838700 | 1.51033000 | -0.58085400 |
| H | 8.14797000 | 1.59890000 | -0.15230800 |
| H | 6.88544500 | 2.45213700 | -1.07974600 |
| H | 7.14489200 | 0.70033400 | -1.32184100 |
| O | -3.09822000 | 1.30890600 | 1.08192300 |
| C | -3.63711200 | 1.82763600 | 2.26525100 |
| H | -3.60197500 | 1.08783700 | 3.08631300 |
| H | -3.06414700 | 2.70456900 | 2.61555500 |
| C | -5.09243200 | 2.25143600 | 2.05364900 |
| H | -5.52338100 | 2.67073400 | 2.97013000 |
| H | -5.70926700 | 1.39042400 | 1.76201300 |
| H | -5.16013000 | 3.01623400 | 1.26994200 |
| Na | -4.00463400 | 0.83512700 | -0.79319900 |

**TS31**

| | | | |
|---|---|---|---|
| Ru | -1.02391300 | 0.73439300 | 1.14685200 |
| O | 0.14178900 | 2.66323500 | 3.21477200 |
| O | -1.84932200 | -1.31696100 | 3.26048300 |
| O | -2.39552300 | 1.74341700 | -1.67834600 |
| O | 2.03241100 | -5.89317300 | 0.46382800 |
| O | 6.32880000 | 0.87088400 | 0.38866500 |

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|---|---|---|---|
| C | -0.30448300 | 1.92066100 | 2.44915200 |
| C | -1.53798700 | -0.52687800 | 2.47663000 |
| C | -1.40628700 | 1.05033100 | -1.17959300 |
| C | -1.41047000 | -0.36487400 | -0.83947200 |
| C | -0.07065800 | -0.70041400 | -0.38728300 |
| C | 0.72093200 | 0.50637500 | -0.36390400 |
| C | -0.12624200 | 1.60788900 | -0.79557100 |
| C | -2.52684500 | -1.29197600 | -1.15127000 |
| C | -3.25446500 | -1.11783100 | -2.34137400 |
| H | -3.01516600 | -0.28579000 | -2.99378500 |
| C | -4.28826400 | -1.99177400 | -2.67872400 |
| H | -4.83979300 | -1.83627500 | -3.60163800 |
| C | -4.61516000 | -3.05527900 | -1.83758900 |
| H | -5.42282900 | -3.73295900 | -2.09917400 |
| C | -3.89986000 | -3.23769800 | -0.65154000 |
| H | -4.14915800 | -4.05812300 | 0.01549900 |
| C | -2.86824400 | -2.36579900 | -0.31106200 |
| H | -2.32666600 | -2.51654500 | 0.61606300 |
| C | 0.28822700 | 2.99543800 | -1.12238400 |
| C | 1.45023500 | 3.23131200 | -1.87507200 |
| H | 2.06767200 | 2.39496100 | -2.18439400 |
| C | 1.81692300 | 4.52895100 | -2.23239300 |
| H | 2.72133500 | 4.68941500 | -2.81242900 |
| C | 1.02677800 | 5.61380900 | -1.85132600 |
| H | 1.31385400 | 6.62422500 | -2.12803800 |
| C | -0.13787700 | 5.39051100 | -1.11391500 |
| H | -0.76338100 | 6.22720600 | -0.81590600 |
| C | -0.50378300 | 4.09468100 | -0.75526700 |
| H | -1.41122800 | 3.92688500 | -0.18604200 |
| C | 0.44635000 | -2.07202100 | -0.14948600 |
| C | 0.27469400 | -3.05774500 | -1.12987300 |
| H | -0.27003500 | -2.82055500 | -2.03799000 |
| C | 0.78982900 | -4.34621900 | -0.96976900 |
| H | 0.63365900 | -5.07874700 | -1.75256700 |

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|---|---|---|---|
| C | 1.49204300 | -4.67076200 | 0.19626800 |
| C | 1.67305900 | -3.69318400 | 1.18771100 |
| H | 2.21567500 | -3.96215900 | 2.08794400 |
| C | 1.16002400 | -2.41681500 | 1.01326900 |
| H | 1.30616800 | -1.67134500 | 1.78809100 |
| C | 1.86201900 | -6.92787700 | -0.49251700 |
| H | 2.35680300 | -7.80686600 | -0.07677200 |
| H | 2.32781700 | -6.67277300 | -1.45317400 |
| H | 0.80118100 | -7.15516000 | -0.65819500 |
| C | 2.18689900 | 0.57142000 | -0.13650400 |
| C | 2.77665300 | 1.51720600 | 0.72359200 |
| H | 2.14840900 | 2.20022800 | 1.28367000 |
| C | 4.15256200 | 1.59039500 | 0.87776300 |
| H | 4.60369200 | 2.31448500 | 1.54806800 |
| C | 4.99289300 | 0.71977800 | 0.16606000 |
| C | 4.42887400 | -0.22134800 | -0.70195500 |
| H | 5.05005200 | -0.90454600 | -1.26867600 |
| C | 3.04089400 | -0.28609000 | -0.84352000 |
| H | 2.61988700 | -1.02006100 | -1.52236400 |
| C | 7.22630200 | 0.01042700 | -0.29562900 |
| H | 8.22691000 | 0.29775700 | 0.03070300 |
| H | 7.15345100 | 0.13191000 | -1.38408600 |
| H | 7.05161900 | -1.04256900 | -0.04012200 |
| H | -3.33594100 | 1.70045800 | -1.04647000 |
| H | -4.82447900 | 0.61954600 | 2.20773500 |
| O | -4.24119500 | 1.64023200 | -0.15508100 |
| H | -2.54011000 | 1.45388900 | 1.33882500 |
| C | -3.84716400 | 2.08908300 | 0.97468300 |
| C | -4.62536200 | 1.69313300 | 2.21050900 |
| H | -4.09810000 | 1.97423200 | 3.12531500 |
| H | -5.58853800 | 2.21848100 | 2.18530900 |
| H | -3.39452200 | 3.09555600 | 1.00669600 |

**26**

| Ru | -0.16196700 | -1.46650100 | 1.41402700 |
|----|-------------|-------------|------------|
| O | -2.31787500 | -1.03762600 | 3.51936200 |
| O | -0.33622000 | -3.39461000 | -1.34691400 |
| O | 4.33976600 | 4.21464000 | 0.21584700 |
| O | -3.79801400 | 4.82435900 | -0.00142600 |
| C | -1.48407600 | -1.19001300 | 2.73124600 |
| C | -0.23098600 | -2.13758100 | -0.86894100 |
| C | 1.01012200 | -1.48010100 | -0.61610900 |
| C | 0.67885200 | -0.08420300 | -0.29567700 |
| C | -0.74257100 | 0.05535000 | -0.28982100 |
| C | -1.32211500 | -1.25809600 | -0.56999600 |
| C | 2.35360800 | -2.04791700 | -0.89475000 |
| C | 2.55385600 | -2.83746200 | -2.03997500 |
| H | 1.71616200 | -3.05052600 | -2.69452500 |
| C | 3.81366100 | -3.35861600 | -2.33676400 |
| H | 3.94385100 | -3.97037600 | -3.22513400 |
| C | 4.89913800 | -3.09669700 | -1.50082800 |
| H | 5.87924000 | -3.50483800 | -1.73059200 |
| C | 4.71343400 | -2.30968700 | -0.36196000 |
| H | 5.54878100 | -2.10338000 | 0.30109500 |
| C | 3.45559800 | -1.79155800 | -0.06146600 |
| H | 3.32519900 | -1.18993600 | 0.83090200 |
| C | -2.72716300 | -1.60523500 | -0.89980100 |
| C | -3.43759500 | -0.86672400 | -1.86228800 |
| H | -2.97422200 | 0.00500600 | -2.31239900 |
| C | -4.72595000 | -1.24314900 | -2.23750500 |
| H | -5.26174700 | -0.65565000 | -2.97758800 |
| C | -5.32525700 | -2.37242800 | -1.67372500 |
| H | -6.32855900 | -2.66372600 | -1.97035100 |
| C | -4.63010900 | -3.11812800 | -0.72177200 |
| H | -5.09126700 | -3.99009200 | -0.26699900 |
| C | -3.34450800 | -2.73474600 | -0.33229500 |

A143

| | | | |
|---|---|---|---|
| H | -2.82487000 | -3.28686000 | 0.44683300 |
| C | 1.66348300 | 1.01791300 | -0.15087100 |
| C | 2.60768200 | 1.25046500 | -1.15934200 |
| H | 2.63633300 | 0.59760300 | -2.02595500 |
| C | 3.51998700 | 2.30580600 | -1.08035000 |
| H | 4.23505400 | 2.44771300 | -1.88190100 |
| C | 3.49820200 | 3.15730500 | 0.02956700 |
| C | 2.55790500 | 2.93851000 | 1.04868000 |
| H | 2.55856100 | 3.60349000 | 1.90607900 |
| C | 1.65910000 | 1.88621500 | 0.95676500 |
| H | 0.94163300 | 1.72279200 | 1.75455800 |
| C | 5.32716600 | 4.46873400 | -0.77053800 |
| H | 5.88667500 | 5.33763800 | -0.42061500 |
| H | 4.87750000 | 4.69873600 | -1.74528800 |
| H | 6.01346600 | 3.61982500 | -0.88507800 |
| C | -1.51333400 | 1.31907800 | -0.18576300 |
| C | -2.66888700 | 1.43240000 | 0.61126300 |
| H | -2.98861300 | 0.59201800 | 1.21726900 |
| C | -3.40478000 | 2.60713500 | 0.65113800 |
| H | -4.28866700 | 2.69384600 | 1.27441500 |
| C | -3.01075400 | 3.71638800 | -0.11305300 |
| C | -1.87128800 | 3.62348700 | -0.91920700 |
| H | -1.54339300 | 4.46003900 | -1.52471600 |
| C | -1.14064900 | 2.43341800 | -0.95005300 |
| H | -0.26251300 | 2.37631100 | -1.58420500 |
| C | -3.43513300 | 5.98264600 | -0.73595500 |
| H | -4.18242300 | 6.73983100 | -0.49374300 |
| H | -3.44782200 | 5.79743700 | -1.81793600 |
| H | -2.44197400 | 6.35043000 | -0.44770600 |
| C | 1.21702600 | -1.44807000 | 2.70924300 |
| H | -0.30290400 | -3.01193000 | 1.80380300 |
| H | -1.27704000 | -3.63190400 | -1.37456100 |
| O | 2.07460700 | -1.44977100 | 3.48470000 |

**TS32**

| | | | |
|---|---|---|---|
| Ru | 0.03707600 | -1.56156200 | 1.33203900 |
| O | -2.09677800 | -1.03654600 | 3.48321400 |
| O | 0.06669100 | -3.48461400 | -1.00317900 |
| O | 3.77064700 | 4.72945500 | 0.07985400 |
| O | -3.94799100 | 4.58870200 | 0.03212600 |
| C | -1.27412900 | -1.24160400 | 2.70212000 |
| C | 0.04783800 | -2.18919400 | -0.87510700 |
| C | 1.21141500 | -1.34813000 | -0.62533400 |
| C | 0.71982100 | -0.03777500 | -0.20417900 |
| C | -0.72980200 | -0.06270000 | -0.22793900 |
| C | -1.16131400 | -1.39719900 | -0.58383600 |
| C | 2.60859300 | -1.75461500 | -0.89853600 |
| C | 2.86028300 | -2.75279600 | -1.85746500 |
| H | 2.02475400 | -3.24399500 | -2.34152300 |
| C | 4.16616200 | -3.13362600 | -2.16159300 |
| H | 4.33679700 | -3.90793500 | -2.90429700 |
| C | 5.24725800 | -2.53175100 | -1.51617900 |
| H | 6.26405900 | -2.83288200 | -1.75167600 |
| C | 5.00945300 | -1.54419900 | -0.55821500 |
| H | 5.84093900 | -1.07295200 | -0.04178100 |
| C | 3.70609600 | -1.15849400 | -0.25174800 |
| H | 3.54316300 | -0.39378900 | 0.49848700 |
| C | -2.54142200 | -1.87975800 | -0.82362600 |
| C | -2.77578200 | -2.83382000 | -1.82948600 |
| H | -1.93623400 | -3.23914900 | -2.38153300 |
| C | -4.06909300 | -3.28289600 | -2.09547500 |
| H | -4.22762100 | -4.02209700 | -2.87563100 |
| C | -5.15160500 | -2.79392900 | -1.36366800 |
| H | -6.15761400 | -3.14846500 | -1.56918000 |
| C | -4.92961200 | -1.85144600 | -0.35680400 |
| H | -5.76237000 | -1.47002200 | 0.22724700 |
| C | -3.63977700 | -1.39942800 | -0.08838400 |

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|---|---|---|---|
| H | -3.48428300 | -0.67337400 | 0.70172000 |
| C | 1.53229200 | 1.20326200 | -0.10564800 |
| C | 2.06241300 | 1.74828600 | -1.28206000 |
| H | 1.88987700 | 1.24518600 | -2.22896800 |
| C | 2.81215900 | 2.92522400 | -1.26857900 |
| H | 3.20292200 | 3.31420500 | -2.20112300 |
| C | 3.05116000 | 3.58026600 | -0.05422300 |
| C | 2.53431400 | 3.04137600 | 1.13311200 |
| H | 2.73646600 | 3.55512500 | 2.06706900 |
| C | 1.78634800 | 1.87179100 | 1.10295100 |
| H | 1.40567400 | 1.45679900 | 2.03062100 |
| C | 4.32701800 | 5.31600500 | -1.08704800 |
| H | 4.85332900 | 6.21097100 | -0.75215900 |
| H | 3.54903900 | 5.60298200 | -1.80604300 |
| H | 5.03933200 | 4.64139700 | -1.57899400 |
| C | -1.59526600 | 1.13720300 | -0.12628500 |
| C | -1.64053400 | 1.96738200 | 1.00676800 |
| H | -1.06076100 | 1.70611500 | 1.88485300 |
| C | -2.43335300 | 3.10599300 | 1.02934800 |
| H | -2.47659500 | 3.74246800 | 1.90684300 |
| C | -3.20499300 | 3.45364100 | -0.08978100 |
| C | -3.17379300 | 2.63817800 | -1.22753300 |
| H | -3.76123900 | 2.87822300 | -2.10552300 |
| C | -2.37781800 | 1.49222400 | -1.23331200 |
| H | -2.36704600 | 0.86421300 | -2.11871300 |
| C | -4.76053500 | 4.98326100 | -1.06315500 |
| H | -5.26175500 | 5.90046200 | -0.75073300 |
| H | -5.51499200 | 4.22283400 | -1.30179000 |
| H | -4.16061800 | 5.18736900 | -1.95924100 |
| C | 1.50687500 | -1.51040000 | 2.57144600 |
| H | -0.15635100 | -3.41303400 | 1.33044300 |
| H | -0.09767500 | -3.56753600 | 0.37433900 |
| O | 2.42286400 | -1.47154400 | 3.26976900 |

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**TS33**

| | | | |
|---|---|---|---|
| Ru | 0.01358600 | -1.35739400 | 1.33867100 |
| O | -2.27315400 | -1.19293800 | 3.38093800 |
| O | 0.04570100 | -3.24812400 | -1.46311400 |
| O | 3.63630100 | 4.88878100 | 0.18591600 |
| O | -4.34697200 | 4.44695000 | 0.01033800 |
| C | -1.40007100 | -1.24690800 | 2.62845800 |
| C | 0.00911900 | -2.06002700 | -1.02457100 |
| C | 1.15981500 | -1.21899500 | -0.63358700 |
| C | 0.64932400 | 0.09501900 | -0.28435000 |
| C | -0.79686500 | 0.03387700 | -0.27708600 |
| C | -1.19278100 | -1.32206700 | -0.62025200 |
| C | 2.57237400 | -1.60258700 | -0.88762500 |
| C | 2.88593500 | -2.39283600 | -2.01069600 |
| H | 2.08588600 | -2.72872700 | -2.65993100 |
| C | 4.20592900 | -2.76021900 | -2.27986400 |
| H | 4.42208200 | -3.37129000 | -3.15178200 |
| C | 5.24044500 | -2.34710600 | -1.44005000 |
| H | 6.26637400 | -2.63580900 | -1.64952200 |
| C | 4.94325200 | -1.56186400 | -0.32311900 |
| H | 5.73802700 | -1.23602300 | 0.34193500 |
| C | 3.62690600 | -1.19616100 | -0.04841200 |
| H | 3.41502800 | -0.59043900 | 0.82527900 |
| C | -2.55680600 | -1.82546300 | -0.91704100 |
| C | -3.44086800 | -1.08594200 | -1.71950700 |
| H | -3.14015300 | -0.11339800 | -2.09401000 |
| C | -4.70026800 | -1.59072200 | -2.04444900 |
| H | -5.37059900 | -1.00085300 | -2.66338900 |
| C | -5.09574300 | -2.84636600 | -1.58233200 |
| H | -6.07733200 | -3.23790100 | -1.83390600 |
| C | -4.21882700 | -3.59764500 | -0.79678200 |
| H | -4.51409700 | -4.57891400 | -0.43612300 |
| C | -2.96172300 | -3.09337200 | -0.46934000 |

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|---|---|---|---|
| H | -2.28232400 | -3.68101000 | 0.13857700 |
| C | 1.45959700 | 1.33202500 | -0.14159900 |
| C | 2.36907200 | 1.68196400 | -1.14801900 |
| H | 2.50003600 | 1.02639700 | -2.00294100 |
| C | 3.11485500 | 2.86143400 | -1.08295500 |
| H | 3.80726200 | 3.09368600 | -1.88321000 |
| C | 2.95989600 | 3.71843100 | 0.01220000 |
| C | 2.05152600 | 3.38174500 | 1.02860100 |
| H | 1.94619400 | 4.05447600 | 1.87329100 |
| C | 1.31446400 | 2.21009200 | 0.94845900 |
| H | 0.61690500 | 1.96261700 | 1.74172400 |
| C | 4.58302300 | 5.27150400 | -0.79978900 |
| H | 5.00516500 | 6.21852000 | -0.46041700 |
| H | 4.11103900 | 5.41792600 | -1.77991400 |
| H | 5.38775500 | 4.53156800 | -0.89682900 |
| C | -1.70114000 | 1.20805800 | -0.16488500 |
| C | -2.84201300 | 1.21262300 | 0.65958400 |
| H | -3.06208300 | 0.35272200 | 1.28067100 |
| C | -3.69814700 | 2.30242200 | 0.69785500 |
| H | -4.57164400 | 2.30604600 | 1.34132000 |
| C | -3.44804300 | 3.42915900 | -0.10118000 |
| C | -2.32804000 | 3.44035400 | -0.93930800 |
| H | -2.11025000 | 4.29150400 | -1.57324700 |
| C | -1.47122300 | 2.33762200 | -0.96217800 |
| H | -0.60903000 | 2.36255900 | -1.61979400 |
| C | -4.14043900 | 5.61531200 | -0.76849000 |
| H | -4.96110500 | 6.29056700 | -0.52196900 |
| H | -4.16537200 | 5.39512500 | -1.84350700 |
| H | -3.18713700 | 6.10122000 | -0.52415600 |
| C | 1.32969300 | -0.87657700 | 2.64382200 |
| H | 0.12863200 | -3.03513500 | 1.81638300 |
| H | 0.81341100 | -4.09199600 | -0.47470100 |
| O | 1.23723300 | -4.43150400 | 0.40164100 |
| H | 0.64525400 | -3.53945800 | 1.20523400 |

| O | 2.13924300 | -0.55431900 | 3.40188700 |
| H | 2.16413000 | -4.15010200 | 0.35350800 |

**TS34**

| Ru | -0.87775100 | -0.80397800 | 1.25584500 |
| O | -2.09349200 | 1.17684900 | 3.25810100 |
| O | -2.15509900 | -1.84914200 | -1.75574300 |
| O | 6.40668900 | -0.02410300 | 0.27517000 |
| O | 1.60387500 | 6.07007300 | 0.18843500 |
| C | -1.63885200 | 0.41000100 | 2.52373500 |
| C | -1.27010800 | -1.14911600 | -1.19235000 |
| C | 0.04452900 | -1.61582900 | -0.70171400 |
| C | 0.77887000 | -0.45555700 | -0.24052600 |
| C | -0.11643100 | 0.68315900 | -0.23831500 |
| C | -1.41212900 | 0.24298500 | -0.72766700 |
| C | 0.59011300 | -2.97209200 | -0.95511600 |
| C | 0.15678500 | -3.70699100 | -2.07384000 |
| H | -0.60417300 | -3.28650700 | -2.71910700 |
| C | 0.68035500 | -4.97256900 | -2.34088900 |
| H | 0.32912100 | -5.52177300 | -3.21021700 |
| C | 1.64315600 | -5.53293100 | -1.50182000 |
| H | 2.04617000 | -6.52010300 | -1.70978300 |
| C | 2.07946400 | -4.81433700 | -0.38609600 |
| H | 2.82400500 | -5.23993300 | 0.28087300 |
| C | 1.55975500 | -3.55100000 | -0.11574800 |
| H | 1.90773900 | -3.01141400 | 0.75768200 |
| C | -2.57287500 | 1.10970700 | -1.04846600 |
| C | -3.34714200 | 0.85173400 | -2.19570100 |
| H | -3.10444800 | -0.00401000 | -2.81341400 |
| C | -4.42549300 | 1.67289400 | -2.52862000 |
| H | -5.00680300 | 1.45379900 | -3.42025900 |
| C | -4.75683600 | 2.76678400 | -1.72903300 |

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|---|---|---|---|
| H | -5.59813700 | 3.40311800 | -1.98864300 |
| C | -3.99591100 | 3.03432700 | -0.58838400 |
| H | -4.24211900 | 3.88135600 | 0.04585400 |
| C | -2.91861200 | 2.21756500 | -0.25228400 |
| H | -2.34196900 | 2.44253700 | 0.63747300 |
| C | 2.25214700 | -0.37218400 | -0.06949200 |
| C | 3.06850700 | -0.70350200 | -1.15927600 |
| H | 2.61246600 | -1.05221900 | -2.08061900 |
| C | 4.45832100 | -0.59853300 | -1.09188200 |
| H | 5.05114400 | -0.86384400 | -1.95899200 |
| C | 5.06252100 | -0.15915400 | 0.09199300 |
| C | 4.25977400 | 0.16943600 | 1.19409900 |
| H | 4.74296400 | 0.49927800 | 2.10780000 |
| C | 2.87817300 | 0.06511800 | 1.10995800 |
| H | 2.27496400 | 0.30989300 | 1.97671900 |
| C | 7.26878800 | -0.35707300 | -0.80168600 |
| H | 8.28331800 | -0.18162900 | -0.44069000 |
| H | 7.08415500 | 0.27577800 | -1.67931900 |
| H | 7.16625100 | -1.41061500 | -1.09187400 |
| C | 0.31517400 | 2.09974400 | -0.09541100 |
| C | 0.69648600 | 2.68454900 | 1.12319300 |
| H | 0.64487800 | 2.09978800 | 2.03521900 |
| C | 1.11977700 | 4.00574400 | 1.18611600 |
| H | 1.40861200 | 4.45842500 | 2.12890000 |
| C | 1.17590100 | 4.78613000 | 0.02256500 |
| C | 0.79549100 | 4.22336400 | -1.20161800 |
| H | 0.82292000 | 4.80205800 | -2.11711600 |
| C | 0.36888200 | 2.89544300 | -1.24731500 |
| H | 0.07034000 | 2.47211400 | -2.20175900 |
| C | 1.67410800 | 6.90820200 | -0.95442100 |
| H | 2.03479300 | 7.87420500 | -0.59787500 |
| H | 0.68947400 | 7.04084900 | -1.42101300 |
| H | 2.37495300 | 6.51563400 | -1.70242400 |
| C | 0.18524400 | -1.66881300 | 2.59661100 |

| H | -2.10623900 | -1.99501300 | 1.67096200 |
|---|---|---|---|
| H | -3.21493800 | -2.38989200 | -0.69927500 |
| O | -3.71962600 | -2.57825100 | 0.15306400 |
| H | -2.72123700 | -2.16039600 | 1.01136500 |
| C | -4.84795600 | -1.67999100 | 0.23532700 |
| H | -5.31825200 | -1.63729100 | -0.75271500 |
| H | -4.49777700 | -0.66931600 | 0.47896400 |
| C | -5.81285200 | -2.19798000 | 1.28612000 |
| H | -6.68218800 | -1.53643300 | 1.35618900 |
| H | -5.33499300 | -2.23737100 | 2.27007800 |
| H | -6.15869700 | -3.20388300 | 1.03202100 |
| O | 0.85790200 | -2.18887200 | 3.37666500 |

**TS35E**

| Ru | -1.09335300 | -0.27564700 | 0.83801200 |
|---|---|---|---|
| O | -1.39718700 | 1.90418800 | 2.95976800 |
| O | -1.09062100 | -2.53014100 | 2.90334700 |
| O | -2.30764400 | -0.68874700 | -2.24617300 |
| O | 5.72926000 | -3.08490400 | 1.04721600 |
| O | 4.25345300 | 4.75403800 | 0.83092400 |
| C | -1.28508900 | 1.06684400 | 2.16892500 |
| C | -1.08937900 | -1.66256800 | 2.13863200 |
| C | -1.24216100 | -0.43530900 | -1.55960400 |
| C | -0.32191800 | -1.42162600 | -1.01788200 |
| C | 0.79455700 | -0.70660200 | -0.42085900 |
| C | 0.51134000 | 0.70860300 | -0.49400800 |
| C | -0.78253100 | 0.88612200 | -1.12534700 |
| C | -0.41095700 | -2.86647000 | -1.34388700 |
| C | 0.69003900 | -3.54808500 | -1.88829500 |
| H | 1.62691100 | -3.02259200 | -2.03689300 |
| C | 0.59086600 | -4.89292600 | -2.24553800 |
| H | 1.45594600 | -5.40151900 | -2.66193900 |

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|---|---|---|---|
| C | -0.61121900 | -5.57991500 | -2.07401200 |
| H | -0.68748600 | -6.62773300 | -2.35052100 |
| C | -1.71700000 | -4.90808800 | -1.54867300 |
| H | -2.66041600 | -5.43062000 | -1.41742100 |
| C | -1.62009300 | -3.56512500 | -1.18873200 |
| H | -2.48779800 | -3.05092700 | -0.79003200 |
| C | -1.45214200 | 2.15766600 | -1.49470200 |
| C | -2.11496900 | 2.26415100 | -2.73148500 |
| H | -2.15043400 | 1.40291200 | -3.38752100 |
| C | -2.73762500 | 3.45582700 | -3.10635000 |
| H | -3.24349700 | 3.51393900 | -4.06617500 |
| C | -2.71281000 | 4.56424500 | -2.25998800 |
| H | -3.19922000 | 5.49028300 | -2.55325900 |
| C | -2.06028500 | 4.47049300 | -1.02793800 |
| H | -2.03753400 | 5.32383700 | -0.35582000 |
| C | -1.43958400 | 3.28251000 | -0.64862400 |
| H | -0.94336800 | 3.22501400 | 0.31364500 |
| C | 2.09135000 | -1.30009400 | -0.00500400 |
| C | 3.28380000 | -0.83789100 | -0.57821900 |
| H | 3.25254900 | -0.02124200 | -1.29175500 |
| C | 4.52043600 | -1.40364200 | -0.25894200 |
| H | 5.41641100 | -1.01357900 | -0.72686000 |
| C | 4.58239600 | -2.45968700 | 0.65637100 |
| C | 3.39726100 | -2.93828000 | 1.23658200 |
| H | 3.46051500 | -3.75697300 | 1.94577000 |
| C | 2.17658800 | -2.36912600 | 0.90683000 |
| H | 1.27456000 | -2.75518300 | 1.36742000 |
| C | 6.95879900 | -2.63682400 | 0.49902600 |
| H | 7.73356000 | -3.26233100 | 0.94501400 |
| H | 7.15482800 | -1.58617800 | 0.74903600 |
| H | 6.98349500 | -2.75568900 | -0.59194900 |
| C | 1.46254800 | 1.79087900 | -0.13478700 |
| C | 2.08875400 | 1.85876100 | 1.12352600 |
| H | 1.84159800 | 1.12147800 | 1.88029200 |

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|---|---|---|---|
| C | 3.00959200 | 2.85439000 | 1.41367200 |
| H | 3.48663600 | 2.91181300 | 2.38650700 |
| C | 3.33949400 | 3.81755900 | 0.44706900 |
| C | 2.73119200 | 3.76503000 | -0.81199300 |
| H | 2.96500600 | 4.49395700 | -1.57870900 |
| C | 1.80249500 | 2.75892600 | -1.08863200 |
| H | 1.33660600 | 2.73051600 | -2.06853300 |
| C | 4.61288100 | 5.76309600 | -0.09959300 |
| H | 5.33857200 | 6.39868400 | 0.41012300 |
| H | 3.74671600 | 6.36920800 | -0.39471300 |
| H | 5.07557400 | 5.33846500 | -0.99994100 |
| H | -3.36968700 | -0.88020700 | -1.59906300 |
| O | -4.21873300 | -1.09498100 | -0.86847800 |
| H | -2.76443900 | -0.41086200 | 0.81237000 |
| C | -4.21195100 | -0.27130600 | 0.12047000 |
| C | -5.01698400 | -0.59570400 | 1.30024200 |
| H | -5.25449700 | -1.64797800 | 1.43962500 |
| H | -4.03209600 | 0.79146600 | -0.08387700 |
| C | -5.47830900 | 0.34808500 | 2.13574800 |
| H | -5.21105000 | 1.38828000 | 1.94308300 |
| C | -6.34473500 | 0.09453100 | 3.32848400 |
| H | -5.85470700 | 0.45000900 | 4.24380400 |
| H | -6.57075200 | -0.96826300 | 3.44881700 |
| H | -7.29107200 | 0.64415400 | 3.24921700 |

**TS35Z**

| | | | |
|---|---|---|---|
| Ru | -0.99334900 | -0.52429700 | 0.93043700 |
| O | -1.56832500 | 1.61138800 | 3.03988100 |
| O | -0.48662700 | -2.69888200 | 3.01884800 |
| O | -2.21387900 | -1.28751300 | -2.09572200 |
| O | 6.25971300 | -1.87368100 | 0.90637700 |
| O | 3.18298500 | 5.49581900 | 0.54191900 |

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|---|---|---|---|
| C | -1.35491500 | 0.79015600 | 2.25207900 |
| C | -0.67920700 | -1.86019100 | 2.24637000 |
| C | -1.20179900 | -0.79930100 | -1.45928500 |
| C | -0.07933800 | -1.55521200 | -0.93073800 |
| C | 0.88940300 | -0.60631700 | -0.40395400 |
| C | 0.31817400 | 0.71766400 | -0.50197000 |
| C | -1.00899700 | 0.60329300 | -1.07529100 |
| C | 0.11823000 | -2.99860400 | -1.21214400 |
| C | 1.30951200 | -3.45884400 | -1.79695300 |
| H | 2.10894300 | -2.75754100 | -2.00955200 |
| C | 1.47436800 | -4.80768800 | -2.11241000 |
| H | 2.40530800 | -5.14279400 | -2.56126900 |
| C | 0.45025300 | -5.72028100 | -1.85777000 |
| H | 0.57982500 | -6.77093100 | -2.10175500 |
| C | -0.74437200 | -5.27143500 | -1.29071100 |
| H | -1.55124800 | -5.97173600 | -1.09377200 |
| C | -0.91057900 | -3.92479500 | -0.97230600 |
| H | -1.84498100 | -3.58521100 | -0.53865200 |
| C | -1.94812600 | 1.69385700 | -1.43551100 |
| C | -2.67416700 | 1.62182000 | -2.63902300 |
| H | -2.55279000 | 0.75511200 | -3.27731700 |
| C | -3.55562800 | 2.64161400 | -3.00253200 |
| H | -4.10487600 | 2.56337400 | -3.93672600 |
| C | -3.73234600 | 3.75230600 | -2.17774600 |
| H | -4.41963200 | 4.54404600 | -2.46213800 |
| C | -3.01983500 | 3.83458700 | -0.97826300 |
| H | -3.15050400 | 4.69162300 | -0.32334600 |
| C | -2.14079100 | 2.81834800 | -0.61020800 |
| H | -1.60020800 | 2.89526900 | 0.32649300 |
| C | 2.29567500 | -0.90821200 | -0.03281500 |
| C | 3.34524700 | -0.23123500 | -0.66858400 |
| H | 3.11998800 | 0.53719000 | -1.40058700 |
| C | 4.68292100 | -0.52061500 | -0.38869700 |
| H | 5.46140500 | 0.02890900 | -0.90432200 |

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|---|---|---|---|
| C | 4.99497600 | -1.51041100 | 0.54924900 |
| C | 3.95620700 | -2.20239600 | 1.19142300 |
| H | 4.21300400 | -2.96676100 | 1.91738700 |
| C | 2.63314500 | -1.90636300 | 0.90078600 |
| H | 1.84750700 | -2.45287900 | 1.40974000 |
| C | 7.34946000 | -1.19994800 | 0.29687500 |
| H | 8.25233700 | -1.63732500 | 0.72576400 |
| H | 7.33216000 | -0.12383500 | 0.51250300 |
| H | 7.35975400 | -1.34679900 | -0.79092300 |
| C | 1.03726100 | 1.98502600 | -0.21547600 |
| C | 1.69155500 | 2.22280200 | 1.00754500 |
| H | 1.63962700 | 1.47517100 | 1.79215200 |
| C | 2.39453900 | 3.39765900 | 1.22845300 |
| H | 2.89218100 | 3.58473800 | 2.17429900 |
| C | 2.47035800 | 4.37706900 | 0.22549700 |
| C | 1.83058400 | 4.15804900 | -0.99952300 |
| H | 1.87115500 | 4.89462500 | -1.79303800 |
| C | 1.12287400 | 2.97157600 | -1.20637700 |
| H | 0.63013800 | 2.81477500 | -2.16068100 |
| C | 3.27974100 | 6.52746800 | -0.42739700 |
| H | 3.87747200 | 7.31679600 | 0.03094900 |
| H | 2.29299500 | 6.92915300 | -0.69141500 |
| H | 3.78055300 | 6.18046800 | -1.34051300 |
| H | -3.20715000 | -1.67239300 | -1.39834800 |
| O | -3.97097200 | -1.99224100 | -0.62877900 |
| H | -2.61070700 | -0.95677600 | 0.98455300 |
| C | -4.08514900 | -1.09329400 | 0.28629300 |
| C | -4.82710600 | -1.44438300 | 1.49695300 |
| H | -4.95726800 | -2.51235200 | 1.65077900 |
| H | -4.04302900 | -0.04434600 | -0.02030500 |
| C | -5.36842100 | -0.56522200 | 2.36019800 |
| H | -5.93460900 | -0.97945000 | 3.19355200 |
| C | -5.28102500 | 0.93029800 | 2.32934400 |
| H | -6.28478000 | 1.37157300 | 2.36095500 |

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| H | -4.76161300 | 1.32313700 | 1.45352200 |
|---|---|---|---|
| H | -4.75285100 | 1.29205400 | 3.22028500 |

**TS36E**

| Ru | 0.91979300 | -0.35728600 | 1.19265500 |
|---|---|---|---|
| O | 0.36304300 | -2.60813100 | 3.18650500 |
| O | 2.62764000 | -0.82447800 | -1.59070000 |
| O | -4.05889600 | 4.97143000 | 0.45434300 |
| O | -5.97460000 | -2.82185700 | 0.15513300 |
| C | 0.59257600 | -1.74536600 | 2.45206600 |
| C | 1.44438100 | -0.48977200 | -1.11063200 |
| C | 0.99112800 | 0.84855600 | -0.77764200 |
| C | -0.39443500 | 0.73205200 | -0.37155600 |
| C | -0.76049300 | -0.66868000 | -0.38039400 |
| C | 0.40451600 | -1.43491000 | -0.78264500 |
| C | 1.78094200 | 2.08220800 | -1.01915600 |
| C | 2.59546900 | 2.16946400 | -2.16206600 |
| H | 2.65803200 | 1.32647300 | -2.84028700 |
| C | 3.33957000 | 3.32177500 | -2.41939100 |
| H | 3.97097800 | 3.36265700 | -3.30179200 |
| C | 3.28103300 | 4.40767200 | -1.54639300 |
| H | 3.86481600 | 5.30174800 | -1.74493600 |
| C | 2.47272200 | 4.33350300 | -0.40887900 |
| H | 2.42417900 | 5.17051400 | 0.28177600 |
| C | 1.73224200 | 3.18350800 | -0.14598500 |
| H | 1.11637200 | 3.13695200 | 0.74515900 |
| C | 0.47350100 | -2.87935200 | -1.11936100 |
| C | -0.50592000 | -3.46128600 | -1.94015500 |
| H | -1.33628400 | -2.85946300 | -2.29365100 |
| C | -0.41912400 | -4.80394200 | -2.30778500 |
| H | -1.18776500 | -5.23669900 | -2.94167200 |
| C | 0.64953200 | -5.58611000 | -1.86825600 |

A156

| | | | |
|---|---|---|---|
| H | 0.71560000 | -6.63196700 | -2.15379100 |
| C | 1.63508400 | -5.01472200 | -1.06095000 |
| H | 2.47323400 | -5.61380700 | -0.71687900 |
| C | 1.54816700 | -3.67378300 | -0.69117500 |
| H | 2.31713000 | -3.23447200 | -0.06473400 |
| C | -1.32777700 | 1.86285600 | -0.14128500 |
| C | -1.44153600 | 2.87630800 | -1.10165400 |
| H | -0.81874700 | 2.84531600 | -1.98991400 |
| C | -2.34256400 | 3.93205000 | -0.94662300 |
| H | -2.39916300 | 4.69542200 | -1.71324500 |
| C | -3.15163600 | 3.98955700 | 0.19399800 |
| C | -3.04916800 | 2.98017500 | 1.16502200 |
| H | -3.68009300 | 3.04217900 | 2.04548000 |
| C | -2.15413600 | 1.93501900 | 0.99561200 |
| H | -2.08459700 | 1.16232600 | 1.75424300 |
| C | -4.19200300 | 6.03140400 | -0.48088500 |
| H | -4.95346700 | 6.69803400 | -0.07368000 |
| H | -4.51992700 | 5.66634700 | -1.46263200 |
| H | -3.25251000 | 6.58587000 | -0.59979100 |
| C | -2.13455800 | -1.20163400 | -0.21031400 |
| C | -2.41562300 | -2.30855600 | 0.61336800 |
| H | -1.61901900 | -2.76870800 | 1.18654300 |
| C | -3.69958100 | -2.82098900 | 0.71525200 |
| H | -3.91572000 | -3.66808900 | 1.35770100 |
| C | -4.75226800 | -2.24632500 | -0.01490000 |
| C | -4.49310900 | -1.15189500 | -0.84751800 |
| H | -5.28277200 | -0.68908500 | -1.42710500 |
| C | -3.19586200 | -0.64284700 | -0.93585300 |
| H | -3.01166000 | 0.20455400 | -1.58756000 |
| C | -7.08006500 | -2.27700400 | -0.54966000 |
| H | -7.94442500 | -2.87853900 | -0.26492000 |
| H | -6.93839400 | -2.34075000 | -1.63612600 |
| H | -7.26060700 | -1.23076800 | -0.27189300 |
| C | 0.95168300 | 0.95956200 | 2.56809800 |

| H | 2.69267500 | -0.56944600 | 1.36582600 |
|---|---|---|---|
| H | 3.43274600 | -0.66910600 | -0.92171600 |
| C | 3.98028300 | -0.56771400 | 1.46898200 |
| C | 4.61863900 | -0.71783300 | 0.19286500 |
| C | 4.18846200 | -1.66250100 | 2.51228000 |
| H | 3.97491200 | -2.65179500 | 2.09646500 |
| H | 3.54947400 | -1.51193100 | 3.38715100 |
| H | 5.23358600 | -1.65805000 | 2.84035800 |
| H | 4.08875400 | 0.43744600 | 1.88607700 |
| H | 4.93236600 | -1.71370700 | -0.12178000 |
| C | 5.33301500 | 0.39804000 | -0.41319400 |
| H | 5.09791900 | 1.39100300 | 0.03904000 |
| O | 6.12372600 | 0.31084500 | -1.34346800 |
| O | 0.94070800 | 1.78334000 | 3.37894500 |

**TS36Z**

| Ru | 0.97567500 | -0.13969300 | 1.23491900 |
|---|---|---|---|
| O | 0.43799100 | -2.25982700 | 3.37208300 |
| O | 2.69815000 | -0.34797600 | -1.58805800 |
| O | -4.73205500 | 4.46707900 | 0.18706800 |
| O | -5.64090700 | -3.31655100 | 0.24551900 |
| C | 0.66272100 | -1.44874600 | 2.57953700 |
| C | 1.48175600 | -0.21297600 | -1.09555500 |
| C | 0.86011500 | 1.04993200 | -0.75721400 |
| C | -0.48330600 | 0.74945500 | -0.30297600 |
| C | -0.65045200 | -0.68767300 | -0.29270800 |
| C | 0.58679400 | -1.29555500 | -0.73738000 |
| C | 1.43648400 | 2.38747000 | -1.04057800 |
| C | 2.26730700 | 2.57198000 | -2.16001600 |
| H | 2.50877400 | 1.72636800 | -2.79227400 |
| C | 2.79547600 | 3.82927000 | -2.45416000 |
| H | 3.43845300 | 3.94753000 | -3.32157900 |

A158

| | | | |
|---|---|---|---|
| C | 2.50407800 | 4.92557100 | -1.64254400 |
| H | 2.91889700 | 5.90295100 | -1.87160700 |
| C | 1.67745900 | 4.75499000 | -0.52952200 |
| H | 1.44553300 | 5.59936500 | 0.11325000 |
| C | 1.14929300 | 3.50117400 | -0.23119300 |
| H | 0.51247800 | 3.38566700 | 0.63837600 |
| C | 0.84618800 | -2.73327900 | -0.99715800 |
| C | 1.60340100 | -3.11683800 | -2.11851800 |
| H | 2.01865100 | -2.35601200 | -2.76855500 |
| C | 1.83600100 | -4.46498400 | -2.39241800 |
| H | 2.42667100 | -4.73826700 | -3.26205000 |
| C | 1.31729600 | -5.45479100 | -1.55774100 |
| H | 1.50233100 | -6.50369400 | -1.77060500 |
| C | 0.56148600 | -5.08569000 | -0.44232700 |
| H | 0.15544900 | -5.84646400 | 0.21815100 |
| C | 0.32835500 | -3.74104700 | -0.16413600 |
| H | -0.25594600 | -3.47111300 | 0.70821600 |
| C | -1.58235700 | 1.73767600 | -0.15190100 |
| C | -2.00529600 | 2.45025800 | -1.28141300 |
| H | -1.50711200 | 2.28778400 | -2.23255800 |
| C | -3.05427400 | 3.36838200 | -1.21667300 |
| H | -3.35094200 | 3.89705100 | -2.11453400 |
| C | -3.70212500 | 3.59393900 | 0.00393400 |
| C | -3.28462400 | 2.89418900 | 1.14565800 |
| H | -3.78983300 | 3.08778800 | 2.08608800 |
| C | -2.24186400 | 1.98130400 | 1.06442600 |
| H | -1.91879900 | 1.46063800 | 1.95949300 |
| C | -5.19022700 | 5.21224300 | -0.93085700 |
| H | -6.00370900 | 5.83862200 | -0.56199000 |
| H | -5.57102200 | 4.55763000 | -1.72526600 |
| H | -4.39954000 | 5.85280600 | -1.34199400 |
| C | -1.94501800 | -1.39650000 | -0.12564700 |
| C | -2.66614200 | -1.41820100 | 1.08001900 |
| H | -2.25168000 | -0.93644500 | 1.95876800 |

A159

| | | | |
|---|---|---|---|
| C | -3.89078100 | -2.06519200 | 1.17239600 |
| H | -4.44479700 | -2.08827600 | 2.10493800 |
| C | -4.43538600 | -2.71166800 | 0.05291000 |
| C | -3.73012200 | -2.70437900 | -1.15662600 |
| H | -4.12268800 | -3.19835000 | -2.03726300 |
| C | -2.49812300 | -2.05345600 | -1.23258100 |
| H | -1.95856500 | -2.05859300 | -2.17488200 |
| C | -6.23731100 | -3.99406600 | -0.85008600 |
| H | -7.17998000 | -4.39731700 | -0.47738700 |
| H | -5.60786500 | -4.81925700 | -1.20699900 |
| H | -6.44195900 | -3.31172800 | -1.68501000 |
| C | 1.06027600 | 1.25334700 | 2.52799900 |
| H | 2.73961100 | -0.43324700 | 1.39252300 |
| H | 3.44305100 | -0.63027800 | -0.88569900 |
| C | 4.00047100 | -0.70641100 | 1.49492800 |
| C | 4.58403700 | -0.97813200 | 0.20702400 |
| C | 4.49798300 | 0.46104300 | 2.34664900 |
| H | 5.54757300 | 0.30161000 | 2.61642300 |
| H | 3.91490600 | 0.53751100 | 3.26821300 |
| H | 4.42554300 | 1.41708300 | 1.82363800 |
| H | 3.86334300 | -1.61327900 | 2.08751200 |
| H | 4.62473900 | -2.01923600 | -0.11437800 |
| C | 5.54459000 | -0.10436800 | -0.45343100 |
| H | 5.59289600 | 0.93855800 | -0.07134400 |
| O | 6.26031600 | -0.44956000 | -1.38657600 |
| O | 1.07286300 | 2.12426500 | 3.28787000 |

**TS37E**

| | | | |
|---|---|---|---|
| Ru | 0.96927600 | -0.25066500 | 1.17655800 |
| O | 0.38142700 | -2.37488500 | 3.28620200 |
| O | 2.57949800 | -0.50928800 | -1.72291200 |
| O | -4.39948900 | 4.80820300 | 0.45107900 |

A160

| | | | |
|---|---|---|---|
| O | -5.90223500 | -2.89748100 | 0.30533300 |
| C | 0.62320600 | -1.56259200 | 2.49729600 |
| C | 1.39695800 | -0.29039500 | -1.18518600 |
| C | 0.87677600 | 1.00058000 | -0.78657400 |
| C | -0.47266800 | 0.78687800 | -0.29891900 |
| C | -0.74604200 | -0.62890900 | -0.32801800 |
| C | 0.43398300 | -1.31221800 | -0.81868000 |
| C | 1.52991600 | 2.30370200 | -1.06232500 |
| C | 2.30522000 | 2.46662900 | -2.22459600 |
| H | 2.44623500 | 1.62410900 | -2.89106200 |
| C | 2.90068100 | 3.69386600 | -2.51827300 |
| H | 3.49474700 | 3.79669000 | -3.42226200 |
| C | 2.73346000 | 4.78297400 | -1.66256700 |
| H | 3.19847400 | 5.73759100 | -1.89178400 |
| C | 1.96337300 | 4.63417200 | -0.50676800 |
| H | 1.82703600 | 5.47280100 | 0.17011000 |
| C | 1.36836500 | 3.40998500 | -0.20963700 |
| H | 0.77679100 | 3.31062300 | 0.69323100 |
| C | 0.57359300 | -2.75736200 | -1.12410500 |
| C | 1.24304100 | -3.16578200 | -2.29152500 |
| H | 1.68149300 | -2.41807500 | -2.94155200 |
| C | 1.35890100 | -4.51915300 | -2.61027900 |
| H | 1.88154500 | -4.81154100 | -3.51685200 |
| C | 0.80836200 | -5.49138000 | -1.77498100 |
| H | 0.90112200 | -6.54478600 | -2.02346100 |
| C | 0.13948900 | -5.09799600 | -0.61343700 |
| H | -0.29039100 | -5.84445100 | 0.04845200 |
| C | 0.02344800 | -3.74775100 | -0.29096300 |
| H | -0.49407300 | -3.45917600 | 0.61690900 |
| C | -1.48851700 | 1.85118000 | -0.08376300 |
| C | -1.93601000 | 2.59032900 | -1.18605700 |
| H | -1.51884600 | 2.38803700 | -2.16819100 |
| C | -2.90710400 | 3.58465900 | -1.05627900 |
| H | -3.22571200 | 4.13171200 | -1.93552600 |

A161

| | | | |
|---|---|---|---|
| C | -3.45048000 | 3.86019100 | 0.20410100 |
| C | -3.00793700 | 3.13420600 | 1.31929100 |
| H | -3.43202700 | 3.36601700 | 2.29074400 |
| C | -2.04258300 | 2.14676900 | 1.17301200 |
| H | -1.69680200 | 1.60417400 | 2.04667800 |
| C | -4.87925200 | 5.57870400 | -0.63927700 |
| H | -5.61839900 | 6.26420500 | -0.22188500 |
| H | -5.36012500 | 4.94983600 | -1.39968100 |
| H | -4.07544000 | 6.15882000 | -1.11075900 |
| C | -2.08429900 | -1.24580700 | -0.14007200 |
| C | -2.78052700 | -1.22022000 | 1.08036000 |
| H | -2.31348800 | -0.77213700 | 1.95054900 |
| C | -4.04688700 | -1.77698400 | 1.19707700 |
| H | -4.58174100 | -1.76297100 | 2.14099500 |
| C | -4.65942100 | -2.37929600 | 0.08842900 |
| C | -3.98103500 | -2.41870800 | -1.13540200 |
| H | -4.42641000 | -2.88027000 | -2.00857200 |
| C | -2.70729500 | -1.85686000 | -1.23598900 |
| H | -2.18954500 | -1.89664200 | -2.18961000 |
| C | -6.56594900 | -3.52765000 | -0.77869200 |
| H | -7.52736400 | -3.86509100 | -0.38846300 |
| H | -6.00349400 | -4.39398900 | -1.15016800 |
| H | -6.73874000 | -2.83053900 | -1.60883100 |
| C | 1.27283400 | 1.07286900 | 2.49928800 |
| H | 2.63358000 | -0.65072100 | 1.26391700 |
| H | 3.38921400 | -0.69030800 | -0.98579500 |
| C | 4.06486100 | -0.95930500 | 1.23587600 |
| C | 4.56552600 | -0.84544500 | -0.07585000 |
| C | 4.03989600 | -2.30849600 | 1.92635200 |
| H | 3.67315900 | -3.09009100 | 1.25466800 |
| H | 3.41583100 | -2.30241900 | 2.82305800 |
| H | 5.06307200 | -2.57122800 | 2.22109300 |
| H | 4.26858500 | -0.11312100 | 1.89298700 |
| H | 4.87875700 | -1.77459100 | -0.55685400 |

A162

| | | | |
|---|---|---|---|
| C | 5.31009000 | 0.40319300 | -0.47520000 |
| H | 4.71184600 | 1.28800400 | -0.20488800 |
| O | 1.44853300 | 1.90336400 | 3.28627500 |
| O | 6.57540900 | 0.42277100 | 0.19718300 |
| H | 7.03549300 | 1.22980700 | -0.07026700 |
| H | 5.44649100 | 0.42607600 | -1.56678200 |

**TS37Z**

| | | | |
|---|---|---|---|
| Ru | 0.87908600 | -0.37482700 | 1.17969700 |
| O | 0.34585500 | -2.53388800 | 3.27113900 |
| O | 2.51406100 | -0.91755500 | -1.65340800 |
| O | -3.98558900 | 5.07104200 | 0.41620800 |
| O | -6.09137100 | -2.70727000 | 0.33153400 |
| C | 0.55368300 | -1.70235200 | 2.49279500 |
| C | 1.35168300 | -0.56322700 | -1.14694600 |
| C | 0.93552300 | 0.78873500 | -0.82194200 |
| C | -0.44772800 | 0.71721600 | -0.39132500 |
| C | -0.84722600 | -0.66896800 | -0.36832400 |
| C | 0.29184000 | -1.47240900 | -0.76893200 |
| C | 1.73721500 | 2.00349100 | -1.11382800 |
| C | 2.49857900 | 2.06377300 | -2.29483600 |
| H | 2.51124100 | 1.20955600 | -2.96180900 |
| C | 3.24369700 | 3.20239200 | -2.60574200 |
| H | 3.82413500 | 3.22709400 | -3.52393900 |
| C | 3.24184300 | 4.30302400 | -1.74829600 |
| H | 3.82269700 | 5.18837900 | -1.99077300 |
| C | 2.48810900 | 4.25545900 | -0.57307700 |
| H | 2.48112700 | 5.10364000 | 0.10562700 |
| C | 1.74531400 | 3.11923600 | -0.25833600 |
| H | 1.17035900 | 3.09499800 | 0.66048100 |
| C | 0.31071100 | -2.92384200 | -1.08086900 |
| C | -0.67009600 | -3.47632400 | -1.92055200 |

A163

| | | | |
|---|---|---|---|
| H | -1.46536600 | -2.84417200 | -2.30150400 |
| C | -0.63106100 | -4.82602400 | -2.26963100 |
| H | -1.40104100 | -5.23465400 | -2.91793800 |
| C | 0.39153000 | -5.64702300 | -1.79213700 |
| H | 0.42028500 | -6.69863700 | -2.06267900 |
| C | 1.37676100 | -5.10727500 | -0.96328300 |
| H | 2.17682000 | -5.73753600 | -0.58535900 |
| C | 1.33629600 | -3.75869000 | -0.61182900 |
| H | 2.09887900 | -3.34681400 | 0.04081300 |
| C | -1.34793200 | 1.87742800 | -0.16992700 |
| C | -1.47114900 | 2.86324700 | -1.15726200 |
| H | -0.88003900 | 2.78862200 | -2.06454200 |
| C | -2.34075100 | 3.94618800 | -1.00614100 |
| H | -2.40486700 | 4.68685700 | -1.79428200 |
| C | -3.10954400 | 4.05854800 | 0.15753900 |
| C | -2.99758800 | 3.07819700 | 1.15626500 |
| H | -3.59655700 | 3.18299800 | 2.05489300 |
| C | -2.13222800 | 2.00716800 | 0.99128100 |
| H | -2.05188400 | 1.25809000 | 1.77230500 |
| C | -4.12591600 | 6.10136600 | -0.54912100 |
| H | -4.85823300 | 6.79947900 | -0.14078400 |
| H | -4.49438900 | 5.71223700 | -1.50717900 |
| H | -3.17885100 | 6.62973000 | -0.71825400 |
| C | -2.22829400 | -1.17079500 | -0.15758800 |
| C | -2.51175800 | -2.25438900 | 0.69551200 |
| H | -1.71028900 | -2.71606400 | 1.26101300 |
| C | -3.80273000 | -2.73994900 | 0.83738000 |
| H | -4.01975100 | -3.56941100 | 1.50227600 |
| C | -4.86092300 | -2.15920400 | 0.12096700 |
| C | -4.60065500 | -1.08704500 | -0.73917500 |
| H | -5.39494600 | -0.61959400 | -1.30879600 |
| C | -3.29555200 | -0.60675300 | -0.86953100 |
| H | -3.11009400 | 0.22350500 | -1.54271200 |
| C | -7.20103400 | -2.15167100 | -0.35627900 |

A164

| | | | |
|---|---|---|---|
| H | -8.07147000 | -2.72832800 | -0.03973400 |
| H | -7.08805700 | -2.23813300 | -1.44474400 |
| H | -7.35255800 | -1.09646700 | -0.09489700 |
| C | 1.05703500 | 0.96297500 | 2.51121400 |
| H | 2.55787500 | -0.70329000 | 1.32083400 |
| H | 3.31424500 | -1.06442100 | -0.89265200 |
| C | 3.99094500 | -0.97767700 | 1.34060100 |
| C | 4.46710200 | -1.23193700 | 0.03373500 |
| C | 4.44075100 | 0.23821100 | 2.13108100 |
| H | 5.51304900 | 0.14501400 | 2.33166300 |
| H | 3.89920100 | 0.31895500 | 3.07639200 |
| H | 4.29104200 | 1.16527600 | 1.57193100 |
| H | 3.82473900 | -1.86610200 | 1.94997100 |
| H | 4.61738700 | -2.28324400 | -0.21751700 |
| C | 5.39047500 | -0.26695800 | -0.66926500 |
| H | 4.97511700 | 0.75115600 | -0.63381000 |
| O | 1.14025800 | 1.80171100 | 3.30486200 |
| O | 6.67989600 | -0.31320500 | -0.04200200 |
| H | 7.24671500 | 0.32762100 | -0.49197300 |
| H | 5.46723100 | -0.54548100 | -1.73080600 |

**TS38**

| | | | |
|---|---|---|---|
| Ru | 1.14726200 | 0.06619700 | 0.77272600 |
| O | 1.05069900 | -2.10567200 | 2.92248700 |
| O | 1.47963800 | 2.32538500 | 2.80779100 |
| O | 2.36009200 | 0.21582700 | -2.32099800 |
| O | -5.14484200 | 3.92457300 | 1.03816100 |
| O | -4.91327900 | -4.06224800 | 0.99062700 |
| C | 1.10634500 | -1.27366800 | 2.12167000 |
| C | 1.35196800 | 1.45783300 | 2.05478000 |
| C | 1.26665300 | 0.15599800 | -1.60904800 |
| C | 0.52493200 | 1.28743600 | -1.09444300 |

| | | | |
|---|---|---|---|
| C | -0.67704000 | 0.76887300 | -0.45690000 |
| C | -0.62515700 | -0.67391500 | -0.50796300 |
| C | 0.61001100 | -1.06605300 | -1.16191400 |
| C | 0.82949400 | 2.69396600 | -1.45793700 |
| C | -0.16753100 | 3.51832400 | -2.00564300 |
| H | -1.17480500 | 3.13543700 | -2.12702900 |
| C | 0.12513200 | 4.82338600 | -2.40134400 |
| H | -0.66120200 | 5.44499000 | -2.82037000 |
| C | 1.41933000 | 5.32635600 | -2.26452600 |
| H | 1.64652500 | 6.34349200 | -2.57106300 |
| C | 2.42120600 | 4.51013300 | -1.73576600 |
| H | 3.43434700 | 4.88825300 | -1.63225900 |
| C | 2.13234200 | 3.20579600 | -1.33736100 |
| H | 2.92304500 | 2.57873100 | -0.93915000 |
| C | 1.05250300 | -2.43257800 | -1.53641300 |
| C | 1.61092600 | -2.65773700 | -2.80743600 |
| H | 1.74104800 | -1.82247400 | -3.48496000 |
| C | 2.01432300 | -3.93731900 | -3.19142500 |
| H | 2.44498500 | -4.08753100 | -4.17747200 |
| C | 1.86861400 | -5.01597400 | -2.31911400 |
| H | 2.18555100 | -6.01083500 | -2.61887900 |
| C | 1.31657500 | -4.80450000 | -1.05325600 |
| H | 1.20295100 | -5.63435800 | -0.36141900 |
| C | 0.91445100 | -3.52832900 | -0.66544600 |
| H | 0.49369400 | -3.38023900 | 0.32275800 |
| C | -1.85463500 | 1.56892600 | -0.03224600 |
| C | -3.11773400 | 1.28315700 | -0.56826400 |
| H | -3.23081700 | 0.45325900 | -1.25776800 |
| C | -4.24346000 | 2.04271700 | -0.24180900 |
| H | -5.20001800 | 1.78487400 | -0.68033300 |
| C | -4.11900800 | 3.11910600 | 0.64316900 |
| C | -2.86012200 | 3.42294300 | 1.18482300 |
| H | -2.77836400 | 4.26036800 | 1.86977800 |
| C | -1.75077900 | 2.66248200 | 0.84787700 |

| | | | |
|---|---|---|---|
| H | -0.78909400 | 2.91785200 | 1.27733500 |
| C | -6.44272300 | 3.65911000 | 0.52915900 |
| H | -7.09952900 | 4.40865800 | 0.97307000 |
| H | -6.79235000 | 2.65848100 | 0.81398500 |
| H | -6.47611700 | 3.75268600 | -0.56397100 |
| C | -1.72378500 | -1.58751600 | -0.10398000 |
| C | -2.32869000 | -1.52497000 | 1.16510300 |
| H | -1.95895000 | -0.81374300 | 1.89636900 |
| C | -3.38435600 | -2.36000300 | 1.49831000 |
| H | -3.84527300 | -2.31809500 | 2.47963500 |
| C | -3.87578100 | -3.28713300 | 0.56547000 |
| C | -3.29154000 | -3.36125200 | -0.70388600 |
| H | -3.64869700 | -4.06590100 | -1.44528800 |
| C | -2.22582700 | -2.51694500 | -1.02407900 |
| H | -1.78074300 | -2.58658300 | -2.01142900 |
| C | -5.43837000 | -5.03222100 | 0.09754400 |
| H | -6.24112100 | -5.53605000 | 0.63794100 |
| H | -4.67879000 | -5.77001100 | -0.19095900 |
| H | -5.84951600 | -4.56863100 | -0.80851100 |
| H | 3.32337100 | 0.34609900 | -1.72945400 |
| H | 4.86255400 | 1.26078600 | 1.54094100 |
| O | 4.28401600 | 0.53650800 | -0.92780200 |
| H | 2.83590100 | -0.03680500 | 0.73452200 |
| C | 4.21036700 | -0.19668900 | 0.11607900 |
| C | 5.04443500 | 0.20321300 | 1.32080100 |
| H | 6.08754000 | 0.13933400 | 0.97386800 |
| H | 4.06112600 | -1.28123400 | -0.02111100 |
| C | 4.86670000 | -0.67097100 | 2.56434400 |
| H | 5.00502400 | -1.72555900 | 2.29057200 |
| H | 3.83831300 | -0.58050300 | 2.93126600 |
| C | 5.84374000 | -0.30253400 | 3.68587900 |
| H | 5.69387600 | -0.93792500 | 4.56420600 |
| H | 5.70991000 | 0.73827800 | 4.00122200 |
| H | 6.88444300 | -0.41944000 | 3.36301900 |

A167

**Dimethyl N-Heterocyclic carbene**

| | | | |
|---|---|---|---|
| N | -1.06248100 | 0.11892400 | -0.00000900 |
| N | 1.06249500 | 0.11892600 | 0.00006600 |
| C | 0.00001500 | 0.98774900 | 0.00002900 |
| C | -0.67832100 | -1.21869400 | -0.00003700 |
| H | -1.38167100 | -2.03788400 | -0.00013200 |
| C | 0.67821900 | -1.21866800 | 0.00001700 |
| H | 1.38153200 | -2.03787200 | 0.00021600 |
| C | -2.44146400 | 0.57458900 | -0.00000900 |
| H | -2.97284800 | 0.22228000 | 0.89068200 |
| H | -2.97339200 | 0.22077300 | -0.88976400 |
| H | -2.42242700 | 1.66398400 | -0.00087300 |
| C | 2.44151400 | 0.57452400 | -0.00005300 |
| H | 2.97294100 | 0.22185200 | -0.89057200 |
| H | 2.97342400 | 0.22100600 | 0.88985600 |
| H | 2.42257200 | 1.66391000 | 0.00050400 |

**27**

| | | | |
|---|---|---|---|
| Ru | -0.21442400 | -0.15450800 | 1.69665900 |
| N | 6.38861100 | -1.23539900 | -0.62879000 |
| N | 7.37903800 | 0.63694500 | -0.33520400 |
| O | -1.36781200 | -2.25752200 | 3.62137000 |
| O | -0.83440300 | 2.17211400 | 3.60498800 |
| O | 2.23605800 | -0.52567500 | -0.46636400 |
| O | -5.18331700 | 4.60411600 | -0.35753900 |
| O | -6.22838300 | -3.45554800 | -0.87975900 |
| C | -0.91055000 | -1.45901900 | 2.93008000 |
| C | -0.57056300 | 1.28201200 | 2.92138400 |
| C | 0.99581900 | -0.35895700 | -0.38333600 |
| C | 0.31021600 | 0.94092700 | -0.23947500 |
| C | -1.10182100 | 0.70190300 | -0.18466100 |

| | | | |
|---|---|---|---|
| C | -1.31358300 | -0.76200500 | -0.20487600 |
| C | -0.02847400 | -1.40305100 | -0.20935300 |
| C | 1.05797100 | 2.21079800 | -0.43843200 |
| C | 1.77710900 | 2.37428400 | -1.64259400 |
| H | 1.71422200 | 1.60367100 | -2.40693300 |
| C | 2.54216400 | 3.52180700 | -1.87588600 |
| H | 3.07210800 | 3.63353200 | -2.81779700 |
| C | 2.59779800 | 4.53355700 | -0.91183900 |
| H | 3.18291500 | 5.42988600 | -1.09298500 |
| C | 1.87866700 | 4.39008700 | 0.27676900 |
| H | 1.90598100 | 5.17484500 | 1.02662400 |
| C | 1.12130500 | 3.24013800 | 0.51394600 |
| H | 0.57559200 | 3.14430600 | 1.44502400 |
| C | 0.28520000 | -2.84246500 | -0.38668900 |
| C | -0.29361400 | -3.57397300 | -1.43633100 |
| H | -1.00993200 | -3.09373500 | -2.09517500 |
| C | 0.04317700 | -4.91221600 | -1.63701800 |
| H | -0.41573700 | -5.46484300 | -2.45133500 |
| C | 0.96422300 | -5.53973400 | -0.79605000 |
| H | 1.22004200 | -6.58371700 | -0.94987500 |
| C | 1.55312400 | -4.81866200 | 0.24458100 |
| H | 2.26740400 | -5.30069700 | 0.90570700 |
| C | 1.21997200 | -3.47910900 | 0.44438100 |
| H | 1.67965600 | -2.92195200 | 1.25528700 |
| C | -2.15722600 | 1.73524700 | -0.23076600 |
| C | -2.06282100 | 2.79968200 | -1.13928600 |
| H | -1.21236900 | 2.86393500 | -1.80959500 |
| C | -3.05472200 | 3.77696300 | -1.22356400 |
| H | -2.95066000 | 4.57671300 | -1.94653600 |
| C | -4.16736300 | 3.71135300 | -0.37350500 |
| C | -4.27219300 | 2.65150700 | 0.54682200 |
| H | -5.13629000 | 2.61994600 | 1.20169800 |
| C | -3.28995000 | 1.67954900 | 0.60902200 |
| H | -3.38484500 | 0.87129300 | 1.32584400 |

| | | | |
|---|---|---|---|
| C | -5.14087100 | 5.71110900 | -1.25343000 |
| H | -6.04595600 | 6.28633600 | -1.05846200 |
| H | -5.13934100 | 5.37995700 | -2.29880300 |
| H | -4.26293200 | 6.34138900 | -1.06833600 |
| C | -2.62016000 | -1.42818900 | -0.34997100 |
| C | -2.93425300 | -2.61582800 | 0.34612200 |
| H | -2.22554000 | -3.03297400 | 1.05149200 |
| C | -4.14347500 | -3.25827700 | 0.15517800 |
| H | -4.39282300 | -4.16051000 | 0.70303100 |
| C | -5.08136000 | -2.75077600 | -0.76420000 |
| C | -4.77885400 | -1.58589000 | -1.48325900 |
| H | -5.47496400 | -1.17903400 | -2.20632600 |
| C | -3.56537100 | -0.93603700 | -1.26597700 |
| H | -3.34839300 | -0.03945100 | -1.83529800 |
| C | -7.22965500 | -2.99918200 | -1.78584100 |
| H | -8.05101500 | -3.71091100 | -1.70362300 |
| H | -6.85943100 | -2.98909000 | -2.81778700 |
| H | -7.58655800 | -1.99864900 | -1.51484600 |
| C | 6.13329800 | 0.09498500 | -0.46148600 |
| C | 7.74834000 | -1.51048800 | -0.60950900 |
| H | 8.14442600 | -2.50724700 | -0.72690900 |
| C | 8.37745400 | -0.32296800 | -0.42216900 |
| H | 9.42678600 | -0.08492600 | -0.34213200 |
| C | 5.36950000 | -2.26403500 | -0.82824100 |
| H | 5.44274700 | -2.68198500 | -1.83644900 |
| H | 4.37750500 | -1.83267200 | -0.69325100 |
| H | 5.50539900 | -3.06857200 | -0.10071000 |
| C | 7.64798700 | 2.05394200 | -0.12548800 |
| H | 8.25781000 | 2.45367900 | -0.94052300 |
| H | 8.17161100 | 2.20971100 | 0.82187900 |
| H | 6.69877500 | 2.58913900 | -0.09739700 |
| Na | 3.86355700 | 0.96603100 | -0.45112700 |

A170

**TS39**

| | | | |
|---|---|---|---|
| Ru | -0.16051100 | -0.49705600 | 1.31541100 |
| N | 6.92604500 | -0.99765100 | -0.35543700 |
| N | 6.96641600 | 1.13904400 | -0.35730400 |
| O | -1.75809900 | -2.08447000 | 3.38850600 |
| O | 0.85188800 | 1.50687100 | 3.39164800 |
| O | 1.65166600 | -1.08080600 | -1.35699200 |
| O | -4.13576300 | 5.65798500 | 0.21629000 |
| O | -7.32603500 | -1.60949700 | -0.10503000 |
| C | -1.14393100 | -1.48067000 | 2.62397600 |
| C | 0.45863500 | 0.73852500 | 2.62608500 |
| C | 0.45054900 | -0.62919300 | -0.94457400 |
| C | 0.18852400 | 0.73919600 | -0.62107400 |
| C | -1.21973800 | 0.82458300 | -0.24482700 |
| C | -1.79041400 | -0.49865700 | -0.35527100 |
| C | -0.73382200 | -1.42709500 | -0.72191200 |
| C | 1.13567700 | 1.85894800 | -0.84923200 |
| C | 1.95669800 | 1.85023900 | -1.99577800 |
| H | 1.88131500 | 1.03063800 | -2.70320800 |
| C | 2.83635700 | 2.90573300 | -2.25458800 |
| H | 3.44605000 | 2.88595600 | -3.15329500 |
| C | 2.90502200 | 3.99318000 | -1.38112200 |
| H | 3.57525900 | 4.82155100 | -1.58979400 |
| C | 2.08703500 | 4.01796000 | -0.24810700 |
| H | 2.12378800 | 4.86392200 | 0.43146000 |
| C | 1.21381400 | 2.96416800 | 0.01733500 |
| H | 0.58141200 | 3.00537800 | 0.89591500 |
| C | -0.83657800 | -2.87482700 | -1.03690000 |
| C | -0.27237900 | -3.36230500 | -2.22890200 |
| H | 0.23816000 | -2.67991900 | -2.90035700 |
| C | -0.37022500 | -4.71431600 | -2.56082200 |
| H | 0.06949200 | -5.07203400 | -3.48699200 |
| C | -1.03357100 | -5.60005400 | -1.71142300 |

A171

| | | | |
|---|---|---|---|
| H | -1.10885900 | -6.65191500 | -1.96961500 |
| C | -1.60215600 | -5.12541600 | -0.52654700 |
| H | -2.12164900 | -5.80704600 | 0.14016900 |
| C | -1.50456200 | -3.77681400 | -0.19098900 |
| H | -1.95177700 | -3.42009900 | 0.73039500 |
| C | -1.98538100 | 2.09293800 | -0.10548200 |
| C | -2.41650400 | 2.74686400 | -1.26698600 |
| H | -2.19079900 | 2.31808300 | -2.23937800 |
| C | -3.13869300 | 3.93932700 | -1.20821200 |
| H | -3.45735600 | 4.41148200 | -2.12952200 |
| C | -3.44347500 | 4.50575300 | 0.03702300 |
| C | -3.01501700 | 3.86232800 | 1.20942400 |
| H | -3.25892000 | 4.31257100 | 2.16579500 |
| C | -2.29898800 | 2.67591600 | 1.13424300 |
| H | -1.97795700 | 2.18972000 | 2.05061400 |
| C | -4.61491100 | 6.35256400 | -0.92998100 |
| H | -5.13979700 | 7.22920700 | -0.54976100 |
| H | -5.31219500 | 5.73616200 | -1.51020400 |
| H | -3.79059500 | 6.67658000 | -1.57710600 |
| C | -3.22974300 | -0.82565000 | -0.26396200 |
| C | -4.04755000 | -0.36479000 | 0.78575000 |
| H | -3.61277200 | 0.21107100 | 1.59475100 |
| C | -5.40354500 | -0.64561300 | 0.81146100 |
| H | -6.03322400 | -0.30092600 | 1.62465700 |
| C | -5.99425400 | -1.39142600 | -0.22356100 |
| C | -5.19737900 | -1.85156900 | -1.28042900 |
| H | -5.62463900 | -2.42379900 | -2.09475500 |
| C | -3.83150600 | -1.57076900 | -1.28851300 |
| H | -3.23066700 | -1.93158500 | -2.11678400 |
| C | -7.98854800 | -2.36458000 | -1.11395300 |
| H | -9.03460700 | -2.41363900 | -0.81092700 |
| H | -7.58330900 | -3.38121500 | -1.18472900 |
| H | -7.91731700 | -1.87522000 | -2.09285400 |
| C | 6.09754300 | 0.08730800 | -0.38162600 |

| | | | |
|---|---|---|---|
| C | 8.26420600 | -0.63268300 | -0.32002200 |
| H | 9.06671600 | -1.35364800 | -0.30181900 |
| C | 8.29011100 | 0.72384700 | -0.31746200 |
| H | 9.11900500 | 1.41385800 | -0.28702300 |
| C | 6.47466300 | -2.38520500 | -0.41176900 |
| H | 6.62366800 | -2.80126600 | -1.41285200 |
| H | 5.41598700 | -2.43034500 | -0.15429500 |
| H | 7.03705800 | -2.98549300 | 0.30772100 |
| C | 6.56736700 | 2.54096500 | -0.32605800 |
| H | 7.11790600 | 3.10470000 | -1.08384100 |
| H | 6.76594000 | 2.97863000 | 0.65692700 |
| H | 5.50101900 | 2.61080600 | -0.54039100 |
| Na | 3.65575800 | -0.08185800 | -0.44116000 |
| H | 2.02362900 | -1.80990700 | -0.73721400 |
| H | 1.17042800 | -1.46269300 | 1.68840600 |
| C | 2.29814100 | -2.46878200 | 1.50178300 |
| C | 2.97113000 | -2.26057700 | 2.83995000 |
| H | 3.73562200 | -3.04048500 | 2.95113800 |
| H | 2.26296900 | -2.35598800 | 3.66582400 |
| H | 3.46743300 | -1.28831500 | 2.89066200 |
| H | 1.58577200 | -3.30576600 | 1.45776500 |
| O | 2.92186000 | -2.17057700 | 0.42516500 |

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| | | | |
|---|---|---|---|
| Ru | 0.31200200 | -0.60000600 | 1.09273100 |
| N | 6.71954600 | -0.08582600 | -0.32098800 |
| N | 6.07791600 | -1.16899900 | 1.40643000 |
| O | -0.54235400 | -2.63443100 | 3.20783100 |
| O | 1.19619700 | 1.40941300 | 3.20866600 |
| O | 1.67159700 | -1.28894900 | -1.82232400 |
| O | -3.47655900 | 5.74652600 | 0.55237100 |
| O | -7.03481200 | -1.49852500 | 0.74149600 |

| | | | |
|---|---|---|---|
| C | -0.22216300 | -1.85639000 | 2.42124900 |
| C | 0.85430800 | 0.63753800 | 2.42149900 |
| C | 0.54263100 | -0.77110700 | -1.23850100 |
| C | 0.42290500 | 0.60850100 | -0.87467100 |
| C | -0.92937100 | 0.76746700 | -0.32627900 |
| C | -1.56575700 | -0.51601200 | -0.31760600 |
| C | -0.62188600 | -1.49745600 | -0.85937500 |
| C | 1.39499400 | 1.67716500 | -1.22859300 |
| C | 2.07622700 | 1.63060100 | -2.46191900 |
| H | 1.87611200 | 0.82133100 | -3.15608100 |
| C | 2.98924100 | 2.62985700 | -2.81222600 |
| H | 3.49136700 | 2.58153900 | -3.77407200 |
| C | 3.23174600 | 3.69666400 | -1.94575400 |
| H | 3.93338200 | 4.47764800 | -2.22194400 |
| C | 2.55425300 | 3.75963500 | -0.72437400 |
| H | 2.72904600 | 4.58958300 | -0.04668000 |
| C | 1.64894500 | 2.76212600 | -0.36654800 |
| H | 1.12693300 | 2.82778900 | 0.58117200 |
| C | -0.85633100 | -2.91906100 | -1.21746400 |
| C | -0.55886200 | -3.34888200 | -2.52535900 |
| H | -0.21471700 | -2.63108100 | -3.26659900 |
| C | -0.75526200 | -4.67975300 | -2.90286900 |
| H | -0.52305700 | -4.99078300 | -3.91689100 |
| C | -1.26469500 | -5.59698900 | -1.98519300 |
| H | -1.42041100 | -6.63117800 | -2.27593700 |
| C | -1.58301900 | -5.17594500 | -0.69056400 |
| H | -1.98735900 | -5.88349100 | 0.02677700 |
| C | -1.37901800 | -3.85252100 | -0.30764800 |
| H | -1.62510700 | -3.54092800 | 0.70091200 |
| C | -1.57974300 | 2.07902600 | -0.07296100 |
| C | -1.85970700 | 2.90887500 | -1.16736400 |
| H | -1.58691900 | 2.58657900 | -2.16833500 |
| C | -2.49402700 | 4.14100900 | -1.00758300 |
| H | -2.69834400 | 4.74914500 | -1.88033700 |

| | | | |
|---|---|---|---|
| C | -2.85987300 | 4.57130000 | 0.27522500 |
| C | -2.57762900 | 3.75406700 | 1.38197400 |
| H | -2.86058800 | 4.10394700 | 2.36901300 |
| C | -1.94961300 | 2.52962400 | 1.20625800 |
| H | -1.73264400 | 1.91693300 | 2.07499100 |
| C | -3.80489100 | 6.61699300 | -0.52478400 |
| H | -4.29366000 | 7.48013600 | -0.07241900 |
| H | -4.49452400 | 6.13893400 | -1.23095900 |
| H | -2.90738300 | 6.94906300 | -1.06099300 |
| C | -2.98988900 | -0.79902000 | -0.02162100 |
| C | -3.58183700 | -0.52580000 | 1.22476600 |
| H | -2.97442000 | -0.13170200 | 2.03219900 |
| C | -4.92811100 | -0.77006600 | 1.44747800 |
| H | -5.38461500 | -0.56614800 | 2.41015400 |
| C | -5.73237900 | -1.29703200 | 0.42314300 |
| C | -5.15915700 | -1.57990500 | -0.82389700 |
| H | -5.75335300 | -1.98744100 | -1.63263600 |
| C | -3.80212500 | -1.33301300 | -1.03175100 |
| H | -3.37467900 | -1.55357000 | -2.00523400 |
| C | -7.90552600 | -2.03344600 | -0.24903700 |
| H | -8.88548400 | -2.10657700 | 0.22311800 |
| H | -7.58302000 | -3.03132600 | -0.57056200 |
| H | -7.97280900 | -1.37391000 | -1.12281700 |
| C | 5.58967700 | -0.51417500 | 0.31328200 |
| C | 7.87216300 | -0.46397300 | 0.35291700 |
| H | 8.86235200 | -0.21609700 | 0.00332100 |
| C | 7.46464900 | -1.15021200 | 1.45008100 |
| H | 8.03098500 | -1.61255900 | 2.24359000 |
| C | 6.73436800 | 0.65766000 | -1.57531000 |
| H | 7.37381000 | 1.53915800 | -1.48199600 |
| H | 5.72017000 | 0.98485100 | -1.80581000 |
| H | 7.10565300 | 0.03259100 | -2.39292200 |
| C | 5.25626200 | -1.80744400 | 2.42957700 |
| H | 5.42852900 | -1.34108900 | 3.40347000 |

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| H  | 5.49107500 | -2.87325600 | 2.49664200  |
|----|------------|-------------|-------------|
| H  | 4.20502300 | -1.69234500 | 2.16447500  |
| Na | 3.24804100 | -0.21842500 | -0.30175300 |
| H  | 1.55019200 | -2.24953400 | -1.91729000 |
| H  | 1.76816900 | -1.29121200 | 1.27820100  |

**H$_2$**

| H | 0.00000000 | 0.00000000 | 0.37145000  |
|---|------------|------------|-------------|
| H | 0.00000000 | 0.00000000 | -0.37145000 |