Reaction Prediction using Density Functional Theory Calculations: A Study into the Synthesis of Safranal *via* Diels-Alder Reactions

Gabriele Wagner[a,b], Nadia Vahdati[b], Ashley Howkins[b], and Louisa Cubitt[b]

[a] Institute of Inorganic Chemistry, University of Ulm, Albert-Einstein-Allee 11, 89081 Ulm, Germany
[b] Chemical Sciences, FHMS, University of Surrey, Guildford, Surrey, GU2 7XH, UK

Reprint requests to Dr. Gabriele Wagner. Fax: +49 (0) 73150 22733.
E-mail: gabriele.wagner@uni-ulm.de

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Two pathways for the synthesis of safranal (2,6,6-trimethyl-cyclohexa-1,3-diene-1-carbaldehyde) *via* a Diels-Alder reaction are proposed and analyzed for their feasibility by Density Functional Theory (DFT) calculations on a B3LYP/6-31G* level of theory. Pathway **A** involving the reaction of 3-methyl-2-butenal with 4-methoxypenta-1,3-diene is predicted to produce the desired regioisomers, although with low stereoselectivity. Due to the high activation barrier (23 kcal mol^{-1}), the reaction will require harsher conditions than the related known reaction of *Z*-2-butenal and 1-methoxy-1,3-butadiene with a calculated ΔE^{a} of 17 kcal mol^{-1}. Replacement of the methoxy group at the diene by OAc, $OSiMe_3$ or pyrrolidinyl does not enhance the reactivity any further. Preliminary experiments confirm these results, although the reaction conditions need to be improved for the reaction to be of synthetic use.

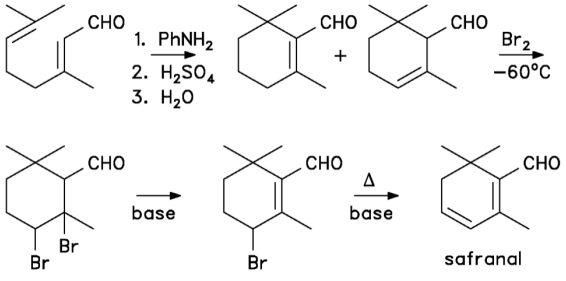
In the reaction of methoxyethene with 3-formyl-2,4-dimethylpenta-1,3-diene (pathway **B**), the homo- and hetero-Diels-Alder pathways were compared. The desired homo-Diels-Alder reaction is predicted to give the correct regioisomer in an exothermic reaction. However, the activation barrier is high (30 kcal mol^{-1}) and the reaction unlikely to proceed. The hetero-Diels-Alder reaction requires less activation energy (23 kcal mol^{-1}) and is expected to dominate, although the thermodynamic driving force is low. The preferred regioisomeric product is the 2-methoxy-3,4-dihydropyran, in agreement with related reactions studied experimentally.

Key words: Cycloaddition, Diels-Alder Reaction, hetero-Diels-Alder Reaction, DFT Calculations, Safranal

Introduction

Modern quantum-chemical methods have significantly improved their accuracy in recent years, and computational facilities allow for efficient calculation of the physical properties of molecules and mechanistic details of chemical reactions. With increasing reliability, quantum chemistry can not only be used to validate and explain experimental results but also to predict the potential outcome of new reactions for which no experimental results exist. This is particularly promising if the prediction is based on a comparison of calculated data for a known and an unknown reaction, as long as the two are chemically sufficiently similar.

Safranal, the main flavor component of saffron, is used in food, tobacco and perfumes, and also serves as a useful starting material for the synthesis of organic and pharmacologically relevant compounds such as retinals [1], coumarins [2], terpenoids [3], or taxoids [4]. Its synthesis was first accomplished by Kuhn and Wendt [5], and since then a number of synthetic processes have been developed. Most of them are lengthy or involve toxic reagents such as Hg salts or

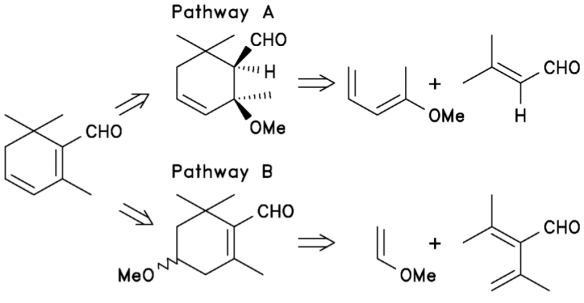


Scheme 1. Synthesis of safranal, according to Könst [7] and Cainelli [8].

organoselenium compounds [6]. The best strategy uses the cyclization of citral followed by bromination/dehydrobromination steps (Scheme 1) [7, 8], although the overall yield is quite low.

In the framework of our project on cycloadditions with poorly reactive functional groups [9, 10] we considered that the synthesis of safranal could be made more efficient and economical by using Diels-Alder reactions as a key step, as shown in Scheme 2.

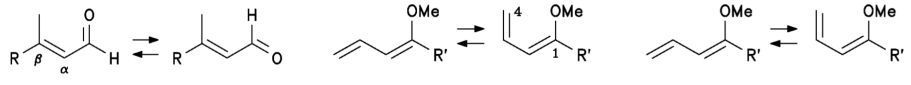
Pathway **A** suggests a Diels-Alder reaction between 3-methyl-2-butenal and 4-methoxypenta-1,3-diene, to provide a suitable precursor from which safranal could be formed by elimination of MeOH. The choice of the reagents has obvious advantages: (a) 3-methyl-2-butenal is commercially available. (b) The synthesis of 4-methoxypenta-1,3-diene is possible in no more than two steps, starting from commercially available materials following published methods [11]. (c) Similar Diels-Alder reactions of electron-rich dienes with electron-deficient dienophiles, *e. g.* of 1-methoxybutadiene with acrolein or (*Z*)-2-butenal, are described in the literature [12 – 14], and also for the subsequent elimination of methanol there is precedence [12].



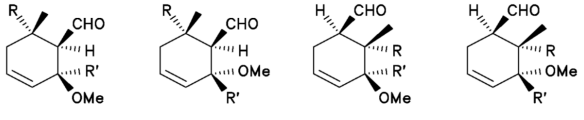
Scheme 2. Proposed retrosynthetic Diels-Alder approaches to safranal.

However, there are issues that are likely to complicate the reaction: (a) the 1,3-diene can undergo double bond shift by [1,5]-sigmatropic H-migration [15], leading to side products in the Diels-Alder reaction. (b) The diene can exist as two stereoisomers, with the methoxy group in *Z* or *E* position. Moreover, the double bond system can adopt a *s-cis* or a *s-trans* conformation, and only the former is suitable for a Diels-Alder reaction. (c) The Diels-Alder reaction may be disfavored by the electronic and steric effects of the methyl substituents, leading to high activation barriers which require harsh reaction conditions. (d) Four different products can be formed, *i. e.* two pairs of stereoisomers differing in their regiochemistry, as shown in Scheme 3. Compound **11a** and **11b** are suited as precursors for safranal, and the elimination of methanol leads to the same product. The Diels-Alder reaction thus needs to be highly regioselective to be of practical use, while the stereoselectivity is less relevant.

Alternatively, the reaction of 2,4-dimethylpenta-1,3-diene-3-carbaldehyde with methoxyethene (pathway **B** in Scheme 2) is proposed, for which there are no stereochemical issues and where the control of the regiochemistry is sufficient. Additionally, a double bond shift of the diene does not change its identity. On the other hand, the synthesis of the diene is less straightforward and may require unjustifiable efforts, and the inverse electron demand of the starting materials is less favorable for a Diels-Alder reaction. Also, the terminal C=C bond of the diene is conjugated with the carbonyl group. Hence, a hetero-Diels-Alder reaction across the C=C–C=O moiety of the molecule can occur as a potential side reaction. Precedence for an involvement of α,β-unsaturated aldehydes in such kind of reactions exists in the literature [16].



R = H	**1c**	**1t**	R' = H	**3Zt**	**3Zc**	**3Et**	**3Ec**
R = Me	**2c**	**2t**	R' = Me	**4Zt**	**4Zc**	**4Et**	**4Ec**



A-1: R = H; R' = H	**5a**	**5b**	**6a**	**6b**
A-2: R = H; R' = Me	**7a**	**7b**	**8a**	**8b**
A-3: R = Me; R' = H	**9a**	**9b**	**10a**	**10b**
A-4: R = Me; R' = Me	**11a**	**11b**	**12a**	**12b**

Scheme 3. Reactants and products of the Diels-Alder reaction proposed as pathway **A**.

Considering the factors mentioned above, we decided to use DFT calculations to predict the reactivity and assess the suitability of the two proposed reactions for the synthesis of safranal. The results of this work are expected to provide guidance for the choice of the synthetic strategy and promising reaction conditions.

Results and Discussion

For an assessment of the Diels-Alder reaction proposed in pathway **A** the reactions shown in Scheme 3 have been calculated. The experimental conditions for reaction **A-1** are known [12] and can be used to assess the quality of the computational results for this type of reactions. Our target reaction **A-4** differs from **A-1** in the presence of two more methyl groups, one attached to the diene and the other to the dienophile. These were introduced stepwise in **A-2** and **A-3** to study their effect on the reactivity, selectivity and reaction mechanism separately.

Analysis of the reactants

The unsaturated aldehydes **1** and **2** can exist as two conformers with different relative orientation of the C=O and the C=C bond. The energy of the *s-cis* and *s-trans* forms of (*Z*)-2-butenal differs by 0.6 kcal mol^{-1}, the *s-cis* form being more stable. For 3-methyl-2-butenal, these forms are energetically equivalent. Interconversion between the two forms is easily possible as the activation barrier for the rotation around the C–C bond is low (6.8 kcal mol^{-1} for **1**, and 8.0 kcal mol^{-1} for **2**). The dienes **3** and **4** can form *Z*- and *E*-stereoisomers, each of which can adopt a *s-cis* or *s-trans* conformation (Scheme 3). The *s-cis* forms relevant for the Diels-Alder reaction are slightly higher in energy than the *s-trans* ones (2.7 kcal mol^{-1} for **3Z**, 3.6 kcal mol^{-1} for **3E**, 3.0 kcal mol^{-1} for **4Z**, and 3.3 kcal mol^{-1} for **4E**). However, the low rotational barriers (*s-trans* → *s-cis*: 4.3 to 7.6 kcal mol^{-1}) suggest equilibrium between the two forms, so that a continuous provision of the *s-cis* conformer for the Diels-Alder reaction is ensured.

The global electrophilicity index [17] ω of the reactants and $\Delta\omega$ of the reaction can be used as a measure for the reactivity, *e. g.* in Diels-Alder reactions and other cycloadditions [18]. For reaction **A-1**, known to proceed at 150 °C within 3 h, the value for $\Delta\omega$ is comparatively small and justifies the rather harsh experimental reaction conditions (Table 1). In **A-2** $\Delta\omega$ is larger, suggesting a higher reactivity due to the additional methyl group that activates the diene by making it more nucleophilic. For **A-3**, in contrast, a lower reactivity is expected because the dienophile is less electrophilic. In the target reaction **A-4**, the two effects cancel each other, and the reactivity should be very similar to **A-1**. However, one should be aware that ω is based on the HOMO/LUMO energies of the reactants, thus reflecting their individual electronic properties but not the steric factors or secondary electronic interactions that come into play when the two reagents approach each other. Therefore, a DFT study was undertaken to assess the reaction paths in more detail.

Table 1. Global electrophilicity index ω of the starting materials and $\Delta\omega$ of the reactions.

Reaction		$\Delta\omega$ (eV)	Reaction		$\Delta\omega$ (eV)
A1	**1c+3Ec**	1.73 – 0.83 = 0.90	**A3**	**2c+3Ec**	1.64 – 0.83 = 0.81
	1c+3Zc	1.73 – 0.77 = 0.96		**2c+3Zc**	1.64 – 0.77 = 0.87
A2	**1c+4Ec**	1.73 – 0.73 = 1.00	**A4**	**2c+4Ec**	1.64 – 0.73 = 0.91
	1c+4Zc	1.73 – 0.68 = 1.05		**2c+4Zc**	1.64 – 0.68 = 0.96

*Reaction of (Z)-2-butenal with 1-methoxybuta-1,3-diene (reaction **A-1**)*

This reaction was reported to proceed at 150 °C within 3 h to provide 70 % of the regioisomers with the aldehyde and methoxy groups in vicinal positions on the ring. The stereoselectivity is low, and a 70 : 30 *cis* : *trans* mixture is obtained [12]. Four products can be formed from the reaction of **1** with **3Zc** or **3Ec**, *via* eight different pathways. Products **5a** and **5b** bear the aldehyde and the methoxy group in 1,2-position of the six-membered ring. In **5a**, these substituents are *cis* to each other whereas **5b** is in the *trans* configuration. Products **6a** and **6b** are the corresponding *cis/trans* regioisomers with the functional groups in 1,3-position. The relative energies of all products are similar (−25.1 to −28.2 kcal mol^{-1}, Table 2), suggesting poor regio- and stereoselectivity under thermodynamic control of the reaction.

The transition states for the eight different reaction pathways were located. As shown in Table 2, the activation energies are lower for the transition states involving the *Ec*-methoxybutadiene **3Ec**, which is expected to react faster than **3Zc**. This is in contrast to the electrophilicity considerations discussed above (Table 1), which predict **3Zc** as more reactive. The reason for this discrepancy might be the dipolar interaction between the reagents in the transition state, which is not accounted for in ω, but leads to a destabilization of transition states involving **3Zc** where the elec-

	Reaction	TS	Prod.	Reaction	TS	Prod.
A-1	**1c + 3Ec → [TS-5aE] → 5a**	+17.7	−27.5	**1c + 3Ec → [TS-6aE] → 6a**	+21.8	−25.8
	1c + 3Zc → [TS-5aZ] → 5a	+22.5	−26.8	**1c + 3Zc → [TS-6aZ] → 6a**	+29.6	−25.1
	1c + 3Ec → [TS-5bE] → 5b	+15.9	−27.6	**1c + 3Ec → [TS-6bE] → 6b**	+24.3	−28.2
	1c + 3Zc → [TS-5bZ] → 5b	+22.9	−26.9	**1c + 3Zc → [TS-6bZ] → 6b**	+27.2	−27.5
A-2	**1c + 4Ec → [TS-7aE] → 7a**	+21.1	−26.1	**1c + 4Ec → [TS-8aE] → 8a**	+26.0	−25.8
	1c + 4Zc → [TS-7aZ] → 7a	+18.6	−25.4	**1c + 4Zc → [TS-8aZ] → 8a**	+27.8	−25.1
	1c + 4Ec → [TS-7bE] → 7b	+17.0	−26.1	**1c + 4Ec → [TS-8bE] → 8b**	+29.6	−27.0
	1c + 4Zc → [TS-7bZ] → 7b	+19.9	−25.4	**1c + 4Zc → [TS-8bZ] → 8b**	+25.1	−26.3
A-3	**2c + 3Ec → [TS-9aE] → 9a**	+22.5	−20.2	**2c + 3Ec → [TS-10aE] → 10a**	+27.6	−20.8
	2c + 3Zc → [TS-9aZ] → 9a	+27.4	−19.5	**2c + 3Zc → [TS-10aZ] → 10a**	+34.0	−20.1
	2c + 3Ec → [TS-9bE] → 9b	+20.0	−20.2	**2c + 3Ec → [TS-10bE] → 10b**	+28.4	−20.4
	2c + 3Zc → [TS-9bZ] → 9b	+28.2	−19.5	**2c + 3Zc → [TS-10bZ] → 10b**	+33.3	−19.7
A-4	**2c + 4Ec → [TS-11aE] → 11a**	+26.1	−16.0	**2c + 4Ec → [TS-12aE] → 12a**	+33.2	−17.6
	2c + 4Zc → [TS-11aZ] → 11a	+23.5	−15.3	**2c + 4Zc → [TS-12aZ] → 12a**	+32.7	−16.9
	2c + 4Ec → [TS-11bE] → 11b	+21.7	−17.7	**2c + 4Ec → [TS-12bE] → 12b**	+34.3	−18.8
	2c + 4Zc → [TS-11bZ] → 11b	+24.8	−17.0	**2c + 4Zc → [TS-12bZ] → 12b**	+32.3	−18.2

Table 2. Relative energies (kcal mol^{-1}) of transition states and products of reactions **A-1** to **A-4**.

Reaction	TS	C1–Cα	C4–Cβ	$\lvert\Delta\rvert$	TS	C4–Cα	C1–Cβ	$\lvert\Delta\rvert$
A-1	**TS-5aE**	2.811	2.000	0.811	**TS-6aE**	2.320	2.160	0.160
	TS-5aZ	2.993	2.000	0.993	**TS-6aZ**	2.444	2.109	0.335
	TS-5bE	2.993	1.894	1.099	**TS-6bE**	2.270	2.200	0.07
	TS-5bZ	2.774	1.938	0.836	**TS-6bZ**	2.513	2.064	0.449
A-2	**TS-7aE**	2.961	1.954	1.007	**TS-8aE**	2.319	2.182	0.137
	TS-7aZ	3.132	1.883	1.249	**TS-8aZ**	2.221	2.277	0.056
	TS-7bE	3.157	1.963	1.194	**TS-8bE**	2.316	2.198	0.118
	TS-7bZ	2.941	1.896	1.045	**TS-8bZ**	2.350	2.142	0.208
A-3	**TS-9aE**	2.771	1.996	0.775	**TS-10aE**	2.209	2.258	0.049
	TS-9aZ	3.033	1.880	1.153	**TS-10aZ**	2.409	2.130	0.279
	TS-9bE	2.911	1.995	0.916	**TS-10bE**	2.192	2.272	0.080
	TS-9bZ	2.728	1.947	0.781	**TS-10bZ**	2.439	2.122	0.317
A-4	**TS-11aE**	2.944	1.949	0.995	**TS-12aE**	2.229	2.294	0.065
	TS-11aZ	3.178	1.868	1.310	**TS-12aZ**	2.132	2.380	0.248
	TS-11bE	3.202	1.939	1.263	**TS-12bE**	2.212	2.296	0.084
	TS-11bZ	2.943	1.881	1.062	**TS-12bZ**	2.162	2.353	0.191

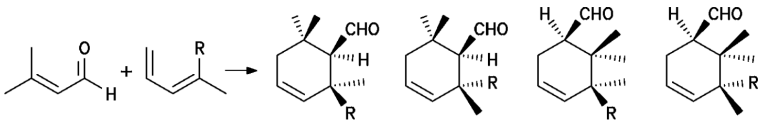
Table 3. Relevant bond lengths of the transition states **TS-5**–**TS-12** and asynchronicity parameter $\lvert\Delta\rvert = \lvert(\text{C–C}\alpha) - (\text{C–C}\beta)\rvert$ (Å). (For atom numbering used see Scheme 3).

tronegative oxygen-containing moieties of diene and dienophile come fairly close to each other. The reaction with **3Ec** and **3Zc** is regioselective in favor of the formation of the 1,2-disubstituted products **5a** and **5b** since the activation energies leading to **5a/5b** are 4–6 kcal mol^{-1} lower than for the formation of **6a/6b**. However, the stereoselectivity is low. This agrees well with the experimental observations [12].

A mechanistic difference in the formation of **5** and **6** is noticeable from the newly formed bonds in the transition state and the asynchronicity parameter $\lvert\Delta\rvert = \lvert(\text{C–C}\alpha) - (\text{C–C}\beta)\rvert$ where Cα and Cβ refer to the Cα and Cβ carbons of the unsaturated aldehyde, and C to the C1 or C4 atom of the diene moiety that is about to form a bond with Cα and Cβ (see Table 3). These two bonds are almost equally advanced in the transition states leading to **6**, so these reactions are concerted and nearly synchronous. The transition states leading to **5**, however, are much less symmetric. The overall reaction, although still concerted, resembles a Michael addition of the terminal C4 of the diene to the β-carbon atom of the unsaturated aldehyde, followed by ring closure between the α-carbon atom of the aldehyde with the methoxy-substituted C1 of the diene. Analogous results have been obtained before for the reaction of butadiene with acrolein or methyl acrylate [19].

*Reaction of (Z)-2-butenal with 4-methoxypenta-1,3-diene (reaction **A-2**)*

The influence of an additional methyl group at the diene was studied by comparing **A-2** with **A-1**. Both reactions are equally exothermic, and no regio- or stereoselectivity is expected under thermodynamic control. The activation barriers resemble those in **A-1** ($\sim$ 1 kcal mol^{-1} higher), but now the **Zc**- and **Ec**-forms of the diene are similar in reactivity. Kinetic control clearly favours the 1,2-disubstituted products **7**, and the reaction is less synchronous. Overall, the introduction of an additional methyl at the diene manifests itself in some change of the reaction mechanism but there



11a **11b** **12a** **12b**

Scheme 4. Reactants and products of the Diels-Alder reaction **A-4** (R = -OMe), **A-4ac** (R = -OCOMe), **A-4si** (R = -$OSiMe_3$) and **A-4N** (R = -$N(CH_2)_4$).

is little effect on the energy profile of the reaction. 4-Methoxypenta-1,3-diene is expected to be equally reactive as 1-methoxybuta-1,3-diene, whereas the electrophilicities would have predicted a higher reactivity of the former. The electronic activation of the methyl group appears to be compensated by its desactivating steric effects.

*Reaction of 3-methyl-2-butenal with 1-methoxybuta-1,3-diene (reaction **A-3**)*

In reaction **A-3**, the methyl group was placed onto the dienophile. Compared to **A-1** and **A-2**, the relative product energies are now by 6 – 7 kcal mol^{-1} higher, making the reaction less exothermic. Again, there is no thermodynamic control of the regio- and stereochemistry, because the product energies are all similar. The activation barriers of **A-3** are approximately 5 kcal mol^{-1} higher than for the reactions **A-1** and **A-2**, suggesting a lower reactivity. The kinetic regioselectivity remains in favor of the 1,2-disubstituted product **9**, again with poor stereoselectivity. Overall, if an additional methyl group is attached to the dienophile both steric and electronic factors work together to desactivate the substrate. However, the reaction mechanism remains unaffected, and the degree of asynchronicity is similar as in **A-1**.

*Reaction of 3-methyl-2-butenal with 4-methoxypenta-1,3-diene (reaction **A-4**) and other 2-substituted penta-1,3-dienes (**A-4ac**, **A-4si** and **A-4N**, Scheme 4)*

The reactions of 3-methyl-2-butenal and 4-methoxypenta-1,3-diene (**A-4**) and other 4-substituted penta-1,3-dienes with an acetoxy (**A-4ac**), trimethylsilyloxy (**A-4si**) or pyrrolidinyl moiety (**A-4N**) were calculated. Relative energies of **A-4** are given in Table 2, relevant bond lengths of the transition states in Table 3, and transition state structures in Fig. 1.

A-4 shows a combination of the trends observed for **A-2** and **A-3**. The thermodynamic driving force is about 10 kcal mol^{-1} lower and the activation barriers are about 3 – 7 kcal mol^{-1} higher than in **A-1**, but similar to **A-3**. The methyl group attached to the

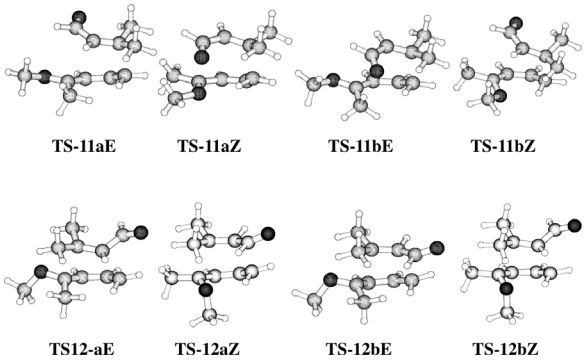


Fig. 1. Transition states of reactions **A-4**.

dienophile thus dominates the energy profile of the reaction. Also here, the agreement between the DFT activation barriers to the transition states and the electrophilicity of the starting materials is moderate. Under thermodynamic control no regio- or stereoselectivity is expected, but kinetic conditions clearly favor the desired product **11**, although with poor stereoselectivity. Mechanistically, the reaction resembles **A-2** more closely, and the formation of **11** is even more asynchronous and comes very close to a two-step reaction. Formation of **12**, however, remains a concerted synchronous process. This is clearly seen in the IRC of the reactions **2c + 4Ec** → [**TS-12aE**] → **12a** and **2c + 4Ec** → [**TS-11bE**] → **11b** shown in Fig. 2.

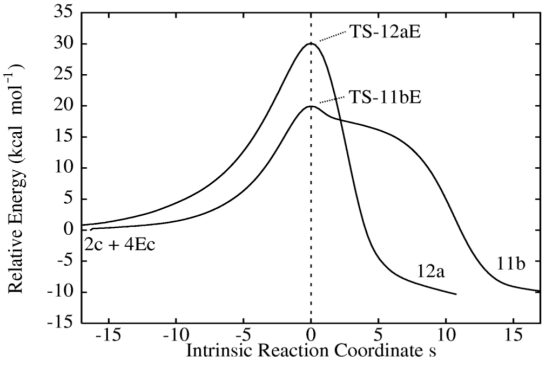


Fig. 2. Energy profile of the synchronous and asynchronous reactions **2c + 4Ec** → [**TS-12aE**] → **12a** and **2c + 4Ec** → [**TS-11bE**] → **11b**. Energy values are not ZPE-corrected.

Reaction **A-4** appears promising for the synthesis of safranal since the correct precursor product is predicted to be formed. Elimination of methanol to produce the target molecule safranal should pose no serious problem and may occur during the cycloaddition already [12]. Harsher reaction conditions (*i. e.* T > 150 °C applied for **A-1**) will be required to pass an activation barrier that is 6 – 7 kcal mol^{-1} higher than for the model reaction **A-1**. Since DFT methods tend to slightly underestimate the activation barriers, the calculated E^a of 21.7 kcal mol^{-1} for **A-4** is comparable to experimental values of feasible reactions: *e. g.* the reaction of butadiene with ethylene (E^a_{expt} = 27.5 kcal mol^{-1}) can be achieved at 165 °C, 900 atm, 17 h [20a, b], and the reaction of anthracene with methyl crotonate (E^a_{expt} = 25 kcal mol^{-1}) occurs at 200 °C [20c].

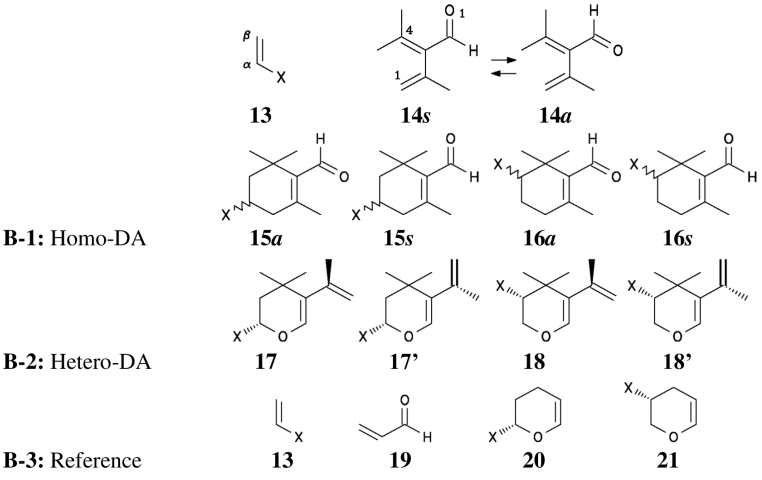
Diels-Alder reactions like the ones discussed in this section are known to proceed faster with electron-rich dienes. Thus, replacement of the methoxy by a more donating group should enhance the reactivity. The ω values for a series of 1-substituted 1,3-butadienes decrease in the order OAc > OMe > $OSiMe_3$ > NMe_2 (1.10 > 0.77 > 0.73 > 0.54) [21]. A similar decrease of ω and an increase of the reactivity is expected for the 4-substituted 1,3-pentadienes. Indeed, 1-acetoxypenta-1,3-diene is less reactive than 1-methoxypenta-1,3-diene (see Tables S3, S4 of the Supplementary Information; see the note at the end of the paper for availability), and the activation barriers for the formation of **11** from reaction **A-4ac** are 5 kcal mol^{-1} higher than those from reaction **A-4**. But reactions **A-4ac** leading to **11** tend to be less synchronous, where one might have expected the opposite trend.

In the cycloaddition of 3-methyl-2-butenal with 1-trimethylsiloxypenta-1,3-diene (**A-4si**) the $OSiMe_3$-substituted diene is expected to be more reactive than the methoxy derivative, according to its position on the ω scale and other theoretical calculations on similar systems [22]. Although the reactions leading to **11** are less synchronous than in reaction **A-4**, the activation barriers are in fact higher. The bulkiness of the Me_3SiO moiety, not included in ω, certainly plays a role. Additionally, the *s-trans* form of the Me_3SiO-substituted diene is significantly more populated (ΔE(*s-trans*/*s-cis*) = 3.3 and 5.2 kcal mol^{-1} for the *Z* and *E* isomer, respectively). The low availability of the *s-cis* form further disfavors the Diels-Alder reaction.

1-(1-methylbuta-1,3-dienyl)-pyrrolidine, the diene component in reaction **A-4N**, ought to be most reactive according to its position on the ω scale. This is confirmed insofar as the trend towards a very polar mechanism for the reactions leading to **11** is concerned. The activation barriers, however, suggest a similar reactivity of the enamide and the methoxy-substituted diene. Moreover, the reaction products of **A-4N** are less stable and the reaction has very little thermodynamic motivation to occur. Overall, the methoxy-substituted diene in **A-4** appears to be the most promising reagent, offering the best balance between steric and electronic factors.

*Reaction of 2,4-dimethylpenta-1,3-diene-3-carbaldehyde with methoxyethene (**B-1**, **B-2**)*

In search of a Diels-Alder reaction with a more favorable energy profile pathway **B** was calculated (Scheme 5). From the global electrophilicity indices of the starting materials $\Delta\omega$ (1.53 – 0.43 = 1.10) is



Scheme 5. Reactants and products of the homo-Diels-Alder reaction proposed as pathway **B-1**, and the competing hetero-Diels-Alder reaction **B-2**, together with the reference hetero-Diels-Alder reaction **B-3** (X = OMe).

	Reaction	TS	Prod.	Reaction	TS	Prod.
B-1	**13 + 14a → [TS-15a1] → 15a**	+31.0	−30.6	**13 + 14a → [TS-16a1] → 16a**	+36.2	−25.4
	13 + 14a → [TS-15a2] → 15a	+31.2	−30.6	**13 + 14a → [TS-16a2] → 16a**	+33.8	−25.4
B-2	**13 + 14s → [TS-17s1] → 177**	+24.1	−18.5	**13 + 14s → [TS-18s1] → 188**	+38.9	−10.4
	13 + 14s → [TS-17s2] → 177	+22.7	−18.5	**13 + 14s → [TS-18s2] → 188**	+35.0	−10.4
B-3	**13 + 19 → [TS-20-1] → 200**	+15.4	−27.1	**13 + 19 → [TS-21-1] → 211**	+29.3	−19.2
	13 + 19 → [TS-20-2] → 200	+15.3	−27.1	**13 + 19 → [TS-21-2] → 211**	+30.0	−19.2

Table 4. Relative energies (kcal mol^{-1}) of selected transition states and products of reactions **B-1** (homo-Diels-Alder), **B-2** (hetero-Diels-Alder) and **B-3** (reference reaction).

Reaction	TS	C1–Cα	C4–Cβ	$\lvert\Delta\rvert$	TS	C4–Cα	C1–Cβ	$\lvert\Delta\rvert$
B-1	**TS-15a1**	2.551	2.087	0.464	**TS-16a1**	2.293	2.242	0.051
	TS-15a2	2.583	2.056	0.527	**TS-16a2**	2.676	2.003	0.673
Reaction	TS	O1–Cα	C4–Cβ	$\lvert\Delta\rvert$	TS	C4–Cα	O1–Cβ	$\lvert\Delta\rvert$
B-2	**TS-17s1**	2.371	2.035	0.336	**TS-18s1**	2.156	2.018	0.138
	TS-17s2	2.392	2.009	0.383	**TS-18s2**	2.097	2.086	0.011
B-3	**TS-20-1**	2.553	1.946	0.607	**TS-21-1**	2.018	2.169	0.151
	TS-20-2	2.478	1.989	0.489	**TS-21-2**	2.026	2.139	0.113

Table 5. Relevant bond lengths of selected transition states **TS15** – **TS21** and asynchronicity parameters $\lvert\Delta\rvert = \lvert$(C–C$\alpha$) − (C–C$\beta\rvert$ (Å). (For atom numbering used see Scheme 5).

slightly higher than for reactions **A1** and **A4**, suggesting that the reaction should be feasible. To gain a more detailed insight, a DFT study was undertaken of the products and transition states, whose relative energies are given in Table 4, the relevant transition state bond lengths in Table 5. Dienophile **13** has been subject to DFT calculations before, and the conformer with the methoxy group *syn* to the alkene is 2.3 kcal mol^{-1} more stable than the *anti* form [23]. However, all previously calculated cycloaddition transition states derived from the *anti* form are lower in energy than the *syn* ones [23]. Based on these results, we used the *anti* form only. The diene **14** was geometry-optimized starting from the *s-cis* or *s-trans* conformation. Both converged to the same structure in which the two C=C bonds adopt a dihedral angle of 70.8° relative to each other. The conformers **14s** and **14a** with the aldehyde *syn* or *anti* to the conjugated C=C bond are energetically equivalent (ΔE = 0.02 kcal mol^{-1}). The non-planarity of the diene might reduce the reactivity in the Diels-Alder reaction. However, even the classical 1,3-butadiene is not planar, its energy minimum being a *gauche* conformation with a dihedral angle of 37.9° between its terminal ends [24].

Combination of the reactants can produce two regioisomeric homo-Diels-Alder products **15** and **16**, each with the aldehyde in *syn/anti* conformation as indicated by the descriptors *s* and *a*. The desired products **15*s/a*** are more stable than **16*s/a***, whereas the energy difference between the conformers ($\sim$ 1 kcal mol^{-1}) is negligible. Thermodynamic control is expected to lead to **15** with a ΔE of −30 to −31 kcal mol^{-1}, which is much larger than the one predicted for reaction **A-4** described above. The transition state structures for relevant relative orientations of the reactants are shown in Fig. 3. Those producing **15** are by 3 – 5 kcal mol^{-1} lower in energy than those leading to **16**, so that **15** is also the preferred kinetic product. However, the ΔE^{a} in a range of 31 kcal mol^{-1} are much higher than those for reaction **A-4** (22 – 26 kcal mol^{-1}), indicating the need for extreme reaction conditions, or that the reaction may not occur at all.

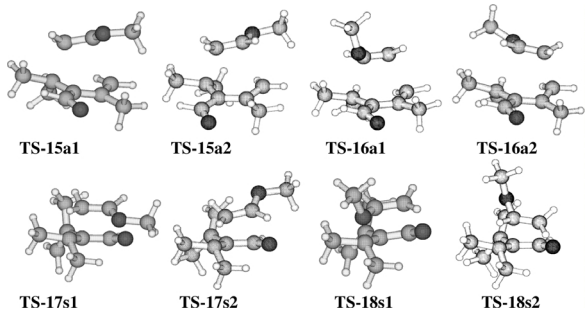


Fig. 3. Selected transition states of the homo-Diels-Alder reactions **B-1** and **B-2**.

The carbonyl group in the dienes **14s** and **14a** is coplanar with the conjugated C=C bond, suggesting that **14s**, where these groups are in a *cisoid* arrangement, might undergo hetero-Diels-Alder reaction with the dienophile, as in the reaction of acrolein with methoxyethene [16] or related substrates [25]. This would lead to products **17** and **18**, which are less stable than the homo-Diels-Alder adducts **15** and **16**, *i. e.* thermodynamic control favors the homo-Diels-Alder pathway. Kinetic control, however, leads to the hetero Diels-Alder adduct **17**, because the transition state leading to it is much lower in energy than for the homo-Diels-Alder ones.

The hetero-Diels-Alder reaction of acrolein with ethene has been studied before, using DFT meth-

ods [26], and identified as a concerted reaction with reverse electron demand, on the basis of FMO considerations and the fact that the C–C bond forms at an earlier stage than the C–O bond. The product is -23.4 kcal mol^{-1} lower in energy than the starting materials, and the calculated ΔE^a of 24.0 kcal mol^{-1}[26] translates into experimental reaction conditions of 1 atm/230 °C or 14 kbar/80 °C [27]. Compared to this, acrolein **19** reacts with the electron-rich methoxyethene **13** (reference reaction **B-3**) with a higher thermodynamic driving force (ΔE = -27.1 kcal mol^{-1}) and a lower activation barrier (ΔE^a = 15.3 kcal mol^{-1}), in agreement with the milder experimental reaction conditions (135 °C, 12 h, 81 %) described in the literature [16a]. The energy profile of our target hetero-Diels-Alder reaction (**13** + **14** → **17**), with a calculated ΔE^a = 22.7 to 24.1 kcal mol^{-1} and ΔE = -18.5 to -19.3 kcal mol^{-1}, is still in a range where the reaction should be feasible, although diene **14**, due to the combination of electron-donating and steric effects of the Me and -CMe=CH_2 groups, is less reactive than acrolein.

Experimental verification of the computational results

Encouraged by the computational results obtained for reaction path **A**, some preliminary experiments were undertaken, in which a mixture of equimolar amounts of 3-methyl-2-butenal and 4-methoxypenta-1,3-diene was heated in a sealed tube in a microwave reactor, in the presence of 2 mol-% of hydroquinone as a stabilizer to prevent radical polymerization. The reaction time and temperature were varied from 5 to 45 min and 130 to 210 °C. The crude reaction mixtures were analyzed by NMR spectroscopy and LCMS, and the signals were assigned by comparison with a reference sample of safranal synthesized by the Könst/Cainelli method [7, 8]. Safranal was only detected when the reaction temperature was above 180 °C, and when the heating and cooling occurred rapidly to prevent thermal decomposition of the product. But even at the best reaction conditions (200 °C for 30 min) the sample was heavily contaminated with polymeric material, and also some starting 3-methyl-2-butenal was still present, suggesting that it is mainly the diene which undergoes unwanted side reactions. The estimated yield of safranal in the crude mixture was in a range of 10 – 15 %. After purification by steam distillation and extraction with diethyl ether, 5 % of product was isolated. This shows that the prediction from our calculations is correct, but the experimental reaction conditions need to be thoroughly optimized for the reaction to be of synthetic use. One way forward could involve Lewis acid catalysis, which has been well established for other Diels-Alder reactions [28].

Conclusion

In summary, the DFT analysis of two new retrosynthetic routes to safranal can aid synthetic chemists with the prediction of new reactions together with plausible reaction conditions, and also help to identify potential side reactions that could compete with the desired target reaction. The latter part, however, still relies strongly on user-based chemical knowledge or intuition. Thus, pathway **B** could be ruled out because an obvious side reaction with a more favorable energy profile was identified. Pathway **A** is potentially feasible although harsh reaction conditions will be required under which other side reactions might occur. In the present case, the strong asynchronicity of the cycloaddition suggests the transient existence of reactive species which might induce a polymerization of the reactants. This side reaction has not been addressed in the calculations, but seems to play a significant role in the experiment, as well as the thermal decomposition of the product. For a further optimization of the reaction conditions, a combined DFT and experimental study of the Lewis acid-catalyzed Diels-Alder reaction of pathway **A** is currently in progress in our group.

Experimental Section

Computational methods

Calculations were carried out with GAUSSIAN 03 [29] (pathway **A**) and the PC GAMESS version [30] of the GAMESS(US) [31] quantum chemistry package (pathway **B**). Results were visualized with MOLDEN [32] and MOLEKEL [33]. Molecular geometries were fully optimized using the B3LYP hybrid functional [34], based on the VWN3 formula in GAUSSIAN and the VWN1 formula in GAMESS [35]. The standard 6-31G* basis set [36] was used for all atoms. The relative energies were zero-point energy corrected and are given relative to the most stable conformations of the reactants. Harmonic vibrational frequencies were computed for all stationary points in order to characterize them as local minima (no imaginary frequency) or transition states (one imaginary frequency along the reaction coordinate). Intrinsic reaction pathways were traced from the transition states, forward to product, and in the opposite direction towards the reactants, along the imaginary vibrational mode using the algorithm developed by González and Schlegel [37]. All transition states correctly connected

the starting materials with the products. The global electrophilicity index ω, introduced by Parr *et al.* [17], was calculated from the one-electron energies of the frontier molecular orbitals HOMO and LUMO, εH and εL, obtained from the Kohn-Sham scheme [38], according to the following equation: $\omega = (\mu^2/2\eta)$, where the chemical hardness is $\eta \approx (\varepsilon L - \varepsilon H)$ and the electronic chemical potential $\mu \approx (\varepsilon H + \varepsilon L)/2$.

Synthesis of safranal

A mixture of 3-methyl-2-butenal (0.84 g, 0.01 mol), 4-methoxypenta-1,3-diene (0.98 g, 0.01 mol) and hydroquinone (11 mg, 2 mol-%) was heated in a microwave reactor to 200 °C for 30 min. The product was steam-distilled from the brown oily crude product and extracted from the aqueous phase with diethyl ether. Yield: 90 mg (5 %). – LCMS (ESI): m/z = 151 $[M+H]^+$. – ^{1}H NMR ($CDCl_3$), δ (ppm) = 1.15 (s, 6H, gem. CH_3), 2.08 (m, 2H, CH_2), 2.16 (s, 3H, CH_3), 5.89 (dt, ^3J = 9.6 and 4.5 Hz, 1H, =CH), 6.12 (dt, ^3J = 9.5, ^4J = 2.1 Hz, 1H, =CH), 10.10 (s, 1H, CHO). Analytical data agree with the literature [7, 8].

Supplementary information

Tables S3 (Relative energies (kcal mol^{-1}) of transition states and products of reactions **A-4ac**, **A-4si** and **A-4N**) and S4 (relevant bond lengths of the transition states **TS11**–**TS12** and asynchronicity parameter $|\Delta| = |(C\text{–}C\alpha) - (C\text{–}C\beta)|$ (Å)), tables of absolute energies (a. u.), zero point energies (a. u.), Cartesian coordinates and imaginary vibrational frequencies of all compounds are given as Supplementary Information available online (http://www.znaturforsch.com/ab/v66b/c66b.htm).

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Supplementary Material

Reaction Prediction using Density Functional Theory Calculations: A Study into the Synthesis of Safranal via Diels-Alder Reaction.

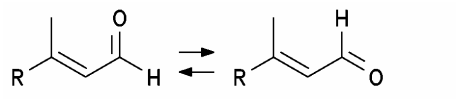
Gabriele Wagner,[a,b*] Nadia Vahdati,[b] Ashley Howkins,[b] Louisa Cubitt[b]

[a]: Institute of Inorganic Chemistry, University of Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany.

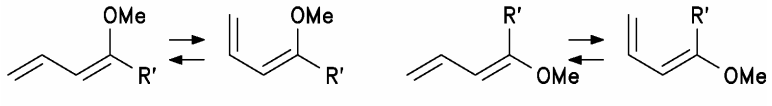
[b]: Chemical Sciences, FHMS, University of Surrey, Guildford, Surrey, GU2 7XH, United Kingdom.

Content:

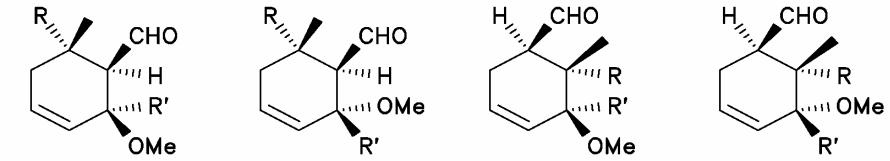
Reactants and products for all reactions, and compound numbering



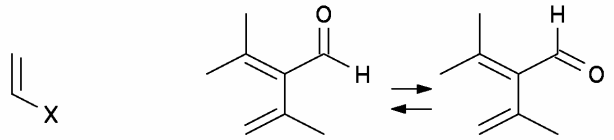
R = H **1c** **1t**
R = Me **2c** **2t**



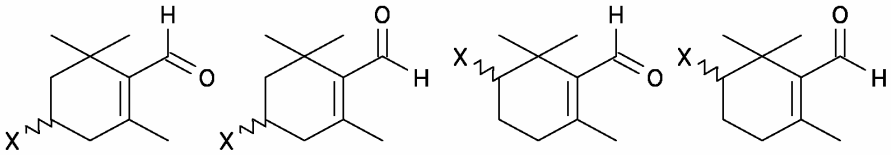
R' = H **3Zt** **3Zc** **3Et** **3Ec**
R' = Me **4Zt** **4Zc** **4Et** **4Ec**



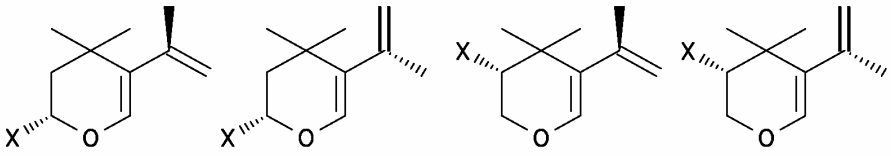
A-1: R = H; R' = H **5a** **5b** **6a** **6b**
A-2: R = H; R' = Me **7a** **7b** **8a** **8b**
A-3: R = Me; R' = H **9a** **9b** **10a** **10b**
A-4: R = Me; R' = Me **11a** **11b** **12a** **12b**



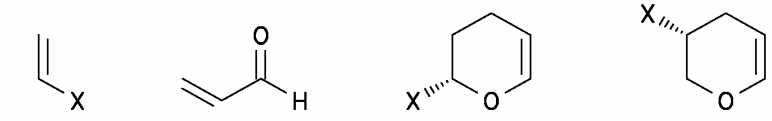
13 **14s** **14a**



B-1: Homo-DA **15** **15'** **16** **16'**



B-2: Hetero-DA **17** **17'** **18** **18'**



1 - **B-3:** Reference **13** **19** **20** **21**

Table S3. Relative energies (kcal/mol) of transition states and products of reactions **A-4ac**, **A-4si** and **A-4N**.

Reaction		TS	Prod.	Reaction	TS	Prod.
A-4ac	**2c+4Ec(ac)→[TS-11aE(ac)]→11a(ac)**	+30.3	-17.3	**2c+4Ec(ac)→[TS-12aE(ac)]→12a(ac)**	+40.9	-18.3
	2c+4Zc(ac)→[TS-11aZ(ac)]→11a(ac)	+28.0	-16.7	**2c+4Zc(ac)→[TS-12aZ(ac)]→12a(ac)**	+35.0	-17.7
	2c+4Ec(ac)→[TS-11bE(ac)]→11b(ac)	+29.8	-18.6	**2c+4Ec(ac)→[TS-12bE(ac)]→12b(ac)**	+41.8	-19.1
	2c+4Zc(ac)→[TS-11bZ(ac)]→11b(ac)	+30.1	-17.9	**2c+4Zc(ac)→[TS-12bZ(ac)]→12b(ac)**	+34.5	-18.4
A-4si	**2c+4Ec(si)→[TS-11aE(si)]→11a(si)**	+28.5	-14.6	**2c+4Ec(si)→[TS-12aE(si)]→12a(si)**	+34.5	-15.3
	2c+4Zc(si)→[TS-11aZ(si)]→11a(si)	+24.8	-12.6	**2c+4Zc(si)→[TS-12aZ(si)]→12a(si)**	+36.2	-13.3
	2c+4Ec(si)→[TS-11bE(si)]→11b(si)	+24.4	-14.3	**2c+4Ec(si)→[TS-12bE(si)]→12b(si)**	+35.8	-16.3
	2c+4Zc(si)→[TS-11bZ(si)]→11b(si)	+29.2	-12.3	**2c+4Zc(si)→[TS-12bZ(si)]→12b(si)**	+35.9	-14.3
A-4N	**2c+4Ec(N)→[TS-11aE(N)]→11a(N)**	+21.6	-1.7	**2c+4Ec(N)→[TS-12aE(N)]→12a(N)**	+38.1	-3.2
	2c+4Zc(N)→[TS-11aZ(N)]→11a(N)	+20.7	-3.9	**2c+4Zc(N)→[TS-12aZ(N)]→12a(N)**	+39.1	-5.3
	2c+4Ec(N)→[TS-11bE(N)]→11b(N)	+18.8	-6.6	**2c+4Ec(N)→[TS-12bE(N)]→12b(N)**	+37.4	-4.4
	2c+4Zc(N)→[TS-11bZ(N)]→11b(N)	+26.5	-8.7	**2c+4Zc(N)→[TS-12bZ(N)]→12b(N)**	+38.6	-6.6

Table S4. Relevant bond lengths of the transition states TS11 - TS12 and asynchronicity parameter $|\Delta| = |(C–C\alpha) – (C–C\beta)|$ (Å)

Reaction	TS	C1–Cα	C4–Cβ	|Δ|	TS	C4–Cα	C1–Cβ	|Δ|
A-4ac	**TS-11aE(ac)**	2.781	1.940	0.841	**TS-12aE(ac)**	2.206	2.310	0.104
	TS-11aZ(ac)	3.152	1.867	1.285	**TS-12aZ(ac)**	2.168	2.359	0.145
	TS-11bE(ac)	2.999	1.879	1.120	**TS-12bE(ac)**	2.191	2.313	0.122
	TS-11bZ(ac)	2.781	1.910	0.871	**TS-12bZ(ac)**	2.191	2.338	0.147
A-4si	**TS-11aE(si)**	2.986	1.915	1.071	**TS-12aE(si)**	2.189	2.329	0.140
	TS-11aZ(si)	3.199	1.881	1.318	**TS-12aZ(si)**	2.084	2.409	0.325
	TS-11bE(si)	3.380	1.643	1.737	**TS-12bE(si)**	2.153	2.344	0.191
	TS-11bZ(si)	2.899	1.869	1.030	**TS-12bZ(si)**	2.111	2.382	0.271
A-4N	**TS-11aE(N)**	3.234	2.014	1.220	**TS-12aE(N)**	1.920	2.674	0.754
	TS-11aZ(N)	3.317	2.012	1.305	**TS-12aZ(N)**	1.876	2.773	0.897
	TS-11bE(N)	3.360	1.989	1.371	**TS-12bE(N)**	1.840	2.903	1.063
	TS-11bZ(N)	3.181	1.928	1.253	**TS-12bZ(N)**	1.902	2.644	0.742

Table of absolute energies and zero point energies, compounds pathway A

Compound	Absolute Energy (a.u.)	Zero point energy (a.u.)	Compound	Absolute Energy (a.u.)	Zero point energy (a.u.)
1c	-231.2286246	0.089932	**TS-10aE**	-541.019206	0.239878
1t	-231.2276468	0.089868	**TS-10aZ**	-541.009893	0.239706
2c	-270.5508252	0.118417	**10a**	-541.100944	0.244566
2t	-270.5507398	0.118333	**TS-10bE**	-541.017756	0.239812
3Zt	-270.5148972	0.118687	**TS-10bZ**	-541.011142	0.239786
3Zc	-270.5108622	0.118922	**10b**	-541.100411	0.244712
3Et	-270.5150644	0.118494	**TS-11aE**	-580.334647	0.267984
3Ec	-270.5089884	0.118164	**TS-11aZ**	-580.340361	0.268498
4Zt	-309.8282648	0.146607	**11a**	-580.406920	0.273099
4Zc	-309.8237586	0.146799	**TS-11bE**	-580.342462	0.268739
4Et	-309.8275949	0.146517	**TS-11bZ**	-580.338126	0.268364
4Ec	-309.8229047	0.147034	**11b**	-580.409270	0.272845
4Zt(ac)	-423.1918037	0.156337	**TS-12aE**	-580.323274	0.267892
4Zc(ac)	-423.1860207	0.156457	**TS-12aZ**	-580.324912	0.267646
4Et(ac)	-423.1901786	0.156240	**12a**	-580.409135	0.272832
4Ec(ac)	-423.1848570	0.156325	**TS-12bE**	-580.321560	0.267981
4Zt(si)	-679.2480058	0.220803	**TS-12bZ**	-580.325597	0.267672
4Zc(si)	-679.2428658	0.220902	**12b**	-580.410885	0.272576
4Et(si)	-679.2477441	0.220644	**TS-11aE(ac)**	-693.690012	0.277406
4Ec(si)	-679.2397467	0.220955	**TS-11aZ(ac)**	-693.694999	0.277367
4Zt(N)	-406.6999331	0.225148	**11a(ac)**	-693.771137	0.282606
4Zc(N)	-406.6952555	0.225101	**TS-11bE(ac)**	-693.690767	0.277367
4Et(N)	-406.7047785	0.224928	**TS-11bZ(ac)**	-693.691434	0.277450
4Ec(N)	-406.6986143	0.225040	**11b(ac)**	-693.773148	0.282609
TS-5aE	-501.713207	0.211832	**TS-12aE(ac)**	-693.673127	0.277319

TS-5aZ	-501.707243	0.212413	**TS-12aZ(ac)**	-693.683082	0.276848
5a	-501.790056	0.21668	**12a(ac)**	-693.772479	0.282331
TS-5bE	-501.716378	0.212265	**TS-12bE(ac)**	-693.671637	0.277361
TS-5bZ	-501.706339	0.212254	**TS-12bZ(ac)**	-693.683979	0.277014
5b	-501.790447	0.216868	**12b(ac)**	-693.773898	0.282564
TS-6aE	-501.706543	0.211734	**TS-11aE(si)**	-949.747676	0.341903
TS-6aZ	-501.695269	0.211740	**TS-11aZ(si)**	-949.757108	0.342274
6a	-501.787516	0.216809	**11a(si)**	-949.821390	0.346867
TS-6bE	-501.702467	0.211609	**TS-11bE(si)**	-949.755927	0.343666
TS-6bZ	-501.698967	0.211724	**TS-11bZ(si)**	-949.749578	0.341694
6b	-501.791196	0.216812	**11b(si)**	-949.820555	0.346591
TS-7aE	-541.021270	0.240401	**TS-12aE(si)**	-949.738035	0.341839
TS-7aZ	-541.026453	0.240495	**TS-12aZ(si)**	-949.738036	0.341359
7a	-541.100774	0.24458	**12a(si)**	-949.822182	0.346639
TS-7bE	-541.028116	0.240660	**TS-12bE(si)**	-949.736091	0.341860
TS-7bZ	-541.024781	0.240380	**TS-12bZ(si)**	-949.738718	0.341534
7b	-541.100972	0.244765	**12b(si)**	-949.823578	0.346477
TS-8aE	-541.013105	0.240045	**TS-11aE(N)**	-677.217957	0.346466
TS-8aZ	-541.011061	0.239717	**TS-11aZ(N)**	-677.216132	0.346622
8a	-541.100331	0.244702	**11a(N)**	-677.2595502	0.350831
TS-8bE	-541.007356	0.239982	**TS-11bE(N)**	-677.222806	0.346842
TS-8bZ	-541.015467	0.239801	**TS-11bZ(N)**	-677.206457	0.346080
8b	-541.102531	0.244917	**11b(N)**	-677.266945	0.350522
TS-9aE	-541.027104	0.239786	**TS-12aE(N)**	-677.191288	0.346068
TS-9aZ	-541.021046	0.240288	**TS-12aZ(N)**	-677.185969	0.345644
9a	-541.100134	0.24468	**12a(N)**	-677.261621	0.350591
TS-9bE	-541.031558	0.240211	**TS-12bE(N)**	-677.191754	0.345376
TS-9bZ	-541.019654	0.240172	**TS-12bZ(N)**	-677.186649	0.345664
9b	-541.100193	0.244737	**12b(N)**	-677.263844	0.350781

Table of absolute energies and zero point energies, compounds pathway B

Compound	Absolute Energy (a.u.)	Zero point energy (a.u.)	Compound	Absolute Energy (a.u.)	Zero point energy (a.u.)
13	-193.110422	0.084694	**TS-17s2**	-580.337861	0.268011
14a	-387.260055	0.179699	**17**	-580.408939	0.273394
14s	-387.259337	0.179049	**TS-17s3**	-580.337250	0.267851
19	-191.909327	0.061729	**TS-17s4**	-580.335496	0.267732
TS-15a1	-580.325018	0.268407	**17‘**	-580.410496	0.273639
TS-15a2	-580.324693	0.268385	**TS-18s1**	-580.311540	0.267455
15	-580.427936	0.273183	**TS-18s2**	-580.317381	0.267079
TS-15s1	-580.325292	0.268487	**18**	-580.395725	0.273163
TS-15s2	-580.325573	0.268417	**TS-18s3**	-580.314451	0.267455
15‘	-580.430057	0.273390	**TS-18s4**	-580.316541	0.267258
TS-16a1	-580.316341	0.267976	**18‘**	-580.397244	0.273139
TS-16a2	-580.319865	0.267700	**TS-20-1**	-384.999373	0.150524
16	-580.420255	0.273714	**TS-20-2**	-384.999172	0.150215
TS-16s1	-580.315637	0.267799	**20**	-385.072567	0.155993
TS-16s2	-580.320550	0.267704	**TS-21-1**	-384.976096	0.149534
16‘	-580.421645	0.273788	**TS-21-2**	-384.9751557	0.149687
TS-17s1	-580.334948	0.267362	**21**	-385.059712	0.155721

Cartesian coordinates and imaginary frequencies of compounds pathway A

Compound 1c: (No imaginary frequency)

C	1.187070	0.468218	0.000000
C	1.403477	-1.017426	0.000000
C	0.000000	1.107625	0.000000
C	-1.309870	0.438032	0.000000
O	-1.486280	-0.770482	0.000000
H	-2.182970	1.127524	0.000000
H	-0.022288	2.195929	0.000000
H	2.469463	-1.261142	0.000000
H	0.930027	-1.483820	0.871267
H	0.930027	-1.483820	-0.871267
H	2.081915	1.090488	0.000000

Compound 1t: (No imaginary frequency)

C	1.288038	0.403920	0.000000
C	1.812834	-1.012482	0.000000
C	0.000000	0.793109	0.000000
C	-1.147481	-0.124983	0.000000
O	-2.308193	0.246952	0.000000
H	-0.905400	-1.209556	0.000000
H	-0.255769	1.850406	0.000000
H	2.905931	-1.020117	0.000000
H	1.478708	-1.571392	0.882043
H	1.478708	-1.571392	-0.882043
H	2.043025	1.189057	0.000000

Compound 2c: (No imaginary frequency)

C	-0.633704	1.460152	-0.000035
C	-0.793372	-0.035643	-0.000020
C	-2.215474	-0.532824	-0.000043
C	0.234205	-0.916323	0.000153
C	1.676823	-0.621761	-0.000229
O	2.215678	0.474402	0.000038
H	2.308094	-1.538601	0.000072
H	0.001296	-1.980576	0.000423
H	-1.138122	1.888968	-0.877127
H	-1.133512	1.888153	0.880151
H	0.412576	1.759640	-0.002385
H	-2.755628	-0.153745	0.878208
H	-2.754693	-0.155823	-0.879774
H	-2.276303	-1.624833	0.001175

Compound 2t: (No imaginary frequency)

C	-0.869867	-0.050655	-0.000087
C	-1.244148	1.410126	-0.000148
C	0.392956	-0.530627	-0.000067
C	1.629938	0.257186	0.000350
C	2.741037	-0.247158	-0.000225
O	-2.043786	-0.995394	0.000080
H	1.524161	1.362137	0.001326

H	0.556632	-1.606810	-0.000391
H	-1.859643	1.640456	-0.880034
H	-1.862230	1.640064	0.878009
H	-0.389420	2.087773	0.001202
H	-2.677540	-0.825441	0.881282
H	-2.680957	-0.822070	-0.877947
H	-1.729859	-2.042661	-0.002418

Compound 3Zt: (No imaginary frequency)

C	-2.944010	-0.327981	0.000309
C	-1.602746	-0.384647	0.000030
C	-0.731017	0.776652	0.000051
C	0.613648	0.733191	-0.000353
O	1.308903	-0.436586	-0.001243
C	2.723741	-0.308448	0.000834
H	3.127809	-1.322542	-0.001179
H	3.078664	0.222785	-0.892721
H	3.076447	0.218364	0.897870
H	-1.189473	1.762570	0.000369
H	-1.109949	-1.355058	-0.000213
H	-3.551984	-1.227629	0.000317
H	-3.476886	0.620718	0.000537
H	1.216456	1.640872	-0.000258

Compound 3Zc: (No imaginary frequency)

H	-2.923491	0.613043	0.001348
C	-1.933499	0.156354	0.000386
C	-0.834907	1.117264	-0.000090
C	0.490297	0.881545	-0.000280
O	1.028862	-0.366199	-0.000240
C	2.449896	-0.419096	0.000339
H	2.721801	-1.476147	-0.000198
H	2.866694	0.061761	-0.894619
H	2.865926	0.060657	0.896246
H	-1.110763	2.168568	-0.000246
H	1.208490	1.701472	-0.000534
C	-1.865693	-1.185926	-0.000215
H	-2.774042	-1.782104	0.000290
H	-0.922075	-1.718509	-0.001209

Compound 3Et: (No imaginary frequency)

C	-3.146500	-0.097990	0.000478
C	-1.906741	0.417229	-0.000105
C	-0.680809	-0.357898	-0.000068
C	0.537387	0.209974	-0.000683
O	1.677824	-0.528025	-0.000876
C	2.888552	0.216296	0.000887
H	3.700800	-0.512959	-0.000473
H	2.970814	0.849247	-0.893135
H	2.970497	0.845580	0.897517
H	-0.750976	-1.443934	0.000507
H	-1.789930	1.502326	-0.000690
H	-4.026797	0.537175	0.000381

H	-3.317958	-1.171994	0.001018
H	0.669631	1.293090	-0.001167

Compound 3Ec: (No imaginary frequency)

C	-2.690458	0.497056	0.000241
O	-1.658541	-0.480482	-0.000495
C	-0.389845	0.007075	0.000214
C	0.676638	-0.809770	-0.000182
C	2.079277	-0.394191	0.000397
C	2.589530	0.847909	-0.000313
H	2.786001	-1.223782	0.001505
H	-3.635122	-0.049856	-0.000264
H	-2.641060	1.130727	0.896058
H	-2.640945	1.132184	-0.894537
H	0.478020	-1.879126	-0.000868
H	-0.302642	1.093672	0.001172
H	3.662912	1.009582	0.000408
H	1.970305	1.741979	-0.001663

Compound 4Zt: (No imaginary frequency)

C	-3.194691	-0.242230	0.000095
C	-1.866356	-0.444747	0.000008
C	-0.873413	0.611883	0.000050
C	0.466147	0.431884	-0.000120
O	0.934861	-0.857917	-0.000476
C	2.323486	-1.135900	0.000292
H	2.402142	-2.225344	0.000215
H	2.826852	-0.747303	-0.894798
H	2.825851	-0.747477	0.896016
H	-1.232012	1.639204	0.000220
H	-1.485312	-1.463801	-0.000094
H	-3.897000	-1.070353	0.000074
H	-3.621232	0.758919	0.000184
C	1.426617	1.603700	-0.000005
H	2.475476	1.303981	-0.000229
H	1.267674	2.234168	-0.882113
H	1.267938	2.233798	0.882415

Compound 4Zc: (No imaginary frequency)

C	1.828378	-1.459259	0.000116
O	0.558526	-0.828628	-0.000043
C	0.439273	0.534970	-0.000031
C	-0.803505	1.068660	0.000019
C	-2.098849	0.400385	0.000137
C	-2.385901	-0.913919	-0.000136
H	-2.942301	1.092120	0.000493
H	1.621040	-2.531535	0.000176
H	2.413777	-1.213779	-0.895350
H	2.413641	-1.213651	0.895633
H	-0.835991	2.155861	0.000011
C	1.673911	1.415875	-0.000079
H	-3.420624	-1.246014	0.000015
H	-1.618966	-1.678015	-0.000513

H	2.607963	0.852306	-0.000243
H	1.686604	2.065815	-0.882280
H	1.686808	2.065647	0.882245

Compound 4Et: (No imaginary frequency)

C	-3.272387	-0.349116	0.000127
C	-2.052496	0.216226	0.000070
C	-0.802613	-0.515651	-0.000048
C	0.428675	0.042134	-0.000132
O	1.482206	-0.839465	-0.000409
C	2.822919	-0.383854	0.000350
H	3.436173	-1.287740	0.000351
H	3.065622	0.204486	-0.894675
H	3.064813	0.203942	0.895942
H	-0.853383	-1.602506	-0.000104
H	-1.992361	1.304435	0.000120
H	-4.177548	0.250255	0.000222
H	-3.400472	-1.429244	0.000084
C	0.676783	1.535068	-0.000097
H	1.736847	1.791126	0.000095
H	0.228854	2.006049	-0.882374
H	0.228519	2.006063	0.881998

Compound 4Ec: (No imaginary frequency)

C	-2.786542	0.048663	0.000024
O	-1.593370	-0.714580	-0.000184
C	-0.360326	-0.108933	-0.000004
C	0.695236	-0.957164	-0.000003
C	2.120233	-0.663005	0.000157
C	2.798731	0.501925	-0.000188
H	2.732033	-1.565878	0.000625
H	-3.597907	-0.682479	-0.000175
H	-2.880234	0.677401	0.895416
H	-2.880231	0.677891	-0.895024
H	0.433758	-2.012719	-0.000061
C	-0.248108	1.392066	0.000154
H	3.884836	0.493033	0.000047
H	2.334868	1.480552	-0.000762
H	-1.213805	1.899108	0.000750
H	0.309626	1.734057	0.880607
H	0.308674	1.734362	-0.880789

Compound 4Zt(ac): (No imaginary frequency)

C	3.434251	-1.035129	0.222448
C	2.141356	-0.768869	-0.016787
C	1.576540	0.570317	-0.014501
C	0.290134	0.883838	-0.238714
C	-0.290293	2.263213	-0.260463
O	-0.592498	-0.151009	-0.597018
C	-1.675011	-0.415043	0.198233
C	-2.515421	-1.505602	-0.421196
O	-1.903940	0.150898	1.239420
H	2.255977	1.396654	0.182951

H	1.456893	-1.586655	-0.230456
H	3.817871	-2.050749	0.211329
H	4.150370	-0.245423	0.439159
H	-0.769786	2.462890	-1.227737
H	-1.050318	2.379086	0.518765
H	0.493475	3.008935	-0.102244
H	-3.353719	-1.733952	0.237519
H	-2.887508	-1.182360	-1.399139
H	-1.911094	-2.403879	-0.583490

Compound 4Zc(ac): (No imaginary frequency)

C	1.512812	-0.311051	0.189447
O	0.384125	-0.095353	-0.557493
C	-0.470826	0.965302	-0.220935
C	0.114422	2.334484	-0.387227
C	-1.740412	0.697688	0.126231
C	-2.415896	-0.588122	0.307460
C	-2.020393	-1.813588	-0.071599
H	-3.380147	-0.505012	0.808892
C	2.297643	-1.466321	-0.383270
O	1.810510	0.332805	1.165449
H	-2.354592	1.574270	0.319301
H	-2.645201	-2.678457	0.132634
H	-1.091812	-1.990033	-0.601222
H	0.516533	2.459352	-1.401170
H	-0.648519	3.099739	-0.221759
H	0.935056	2.496056	0.318792
H	3.232487	-1.575961	0.167182
H	1.713470	-2.389394	-0.301293
H	2.501555	-1.300529	-1.445650

Compound 4Et(ac): (No imaginary frequency)

C	-3.770806	-0.849668	0.260662
O	-2.740989	-0.007998	0.083790
C	-1.373434	-0.444604	-0.144173
C	-0.303804	0.346988	-0.325830
C	-0.232326	1.841267	-0.366083
O	0.907560	-0.307247	-0.625408
C	1.961009	-0.189475	0.238729
C	3.162716	-0.919826	-0.311036
O	1.915533	0.411526	1.285004
H	-1.201360	-1.518834	-0.173302
H	-2.931085	1.063097	0.115156
H	-4.779662	-0.486833	0.430951
H	-3.635935	-1.928800	0.242756
H	0.400710	2.215645	0.444670
H	0.208879	2.170230	-1.315563
H	-1.221670	2.293568	-0.273664
H	3.986174	-0.848198	0.400055
H	2.915023	-1.970409	-0.493578
H	3.459981	-0.483803	-1.270604

Compound 4Ec(ac): (No imaginary frequency)

C	1.933892	0.064036	-0.248918
O	0.952324	-0.560970	0.467455
C	-0.368897	-0.077105	0.379323
C	-0.574921	1.315426	0.887426
O	-1.286286	-0.970332	-0.023914
C	-2.734056	-0.780396	-0.133790
C	-3.387201	0.331413	-0.502138
H	-3.324762	-1.672166	0.080651
C	3.270221	-0.578188	0.037298
O	1.740081	0.989613	-1.000109
H	-0.913388	-1.965675	-0.259323
H	-4.472469	0.353333	-0.544363
H	-2.870480	1.238792	-0.800036
H	0.067081	1.488052	1.759329
H	-0.308820	2.060320	0.130508
H	-1.617758	1.464101	1.179144
H	4.041223	-0.091083	-0.560307
H	3.510495	-0.487194	1.101812
H	3.233135	-1.646760	-0.197910

Compound 4Zt(si): (No imaginary frequency)

C	4.102289	-1.041889	0.048982
C	2.805889	-0.729773	-0.110147
C	2.263153	0.611702	-0.002469
C	0.961741	0.939116	-0.150465
C	0.445556	2.347200	-0.051028
O	0.046670	-0.026688	-0.469626
Si	-1.539157	-0.337295	0.023273
C	-1.864803	-2.080889	-0.597163
C	-1.663160	-0.252981	1.903801
C	-2.748480	0.867913	-0.781773
H	2.959827	1.420075	0.206767
H	2.092315	-1.518493	-0.339665
H	4.457672	-2.063842	-0.043585
H	4.850255	-0.284727	0.275669
H	-0.049052	2.646247	-0.984290
H	-0.294800	2.451882	0.753903
H	1.260152	3.048257	0.148633
H	-3.781975	0.579988	-0.550134
H	-2.609876	1.898860	-0.438149
H	-2.641660	0.861356	-1.872907
H	-2.664078	-0.554678	2.237269
H	-0.938050	-0.926139	2.375431
H	-1.479515	0.756018	2.290916
H	-2.887787	-2.400313	-0.363440
H	-1.735901	-2.141399	-1.683819
H	-1.175796	-2.799856	-0.139841

Compound 4Zc(si): (No imaginary frequency)

Si	1.389644	-0.281615	0.036807
O	-0.207169	0.016973	-0.436362
C	-1.095107	1.012597	-0.146840

C	-0.551630	2.415608	-0.159558
C	-2.395890	0.731714	0.084528
C	-3.066770	-0.564322	0.125238
C	-2.596164	-1.778696	-0.208416
H	-4.099550	-0.508679	0.471951
C	1.687942	-2.062303	-0.484060
C	2.591753	0.858809	-0.867834
C	1.554808	-0.086963	1.905541
H	-3.030408	1.593063	0.276871
H	-3.232864	-2.655014	-0.120696
H	-1.592252	-1.929845	-0.584963
H	-0.090233	2.644521	-1.128937
H	-1.343801	3.145373	0.026197
H	0.222878	2.556940	0.606659
H	2.563258	-0.367253	2.234970
H	1.375713	0.942300	2.237455
H	0.840720	-0.733230	2.428644
H	3.626910	0.565092	-0.651073
H	2.452319	0.795184	-1.953457
H	2.480592	1.909084	-0.576962
H	2.714834	-2.372672	-0.255291
H	1.007097	-2.746623	0.034247
H	1.533464	-2.190084	-1.561610

Compound 4Et(si): (No imaginary frequency)

C	-3.788919	-1.427570	-0.000149
C	-3.104351	-0.271633	-0.000073
C	-1.655589	-0.175902	0.000319
C	-0.923783	0.961974	0.000266
C	-1.457191	2.366080	0.000018
O	0.441400	0.978078	0.000565
Si	1.627472	-0.232778	0.000016
C	3.235505	0.739990	-0.001984
C	1.496424	-1.285047	1.559477
C	1.493844	-1.286604	-1.558182
H	-1.126517	-1.126661	0.000624
H	-3.670591	0.658116	-0.000334
H	-4.874282	-1.445735	-0.000461
H	-3.284871	-2.391748	0.000097
H	-1.087426	2.904539	0.881244
H	-1.087256	2.904336	-0.881251
H	-2.547287	2.405072	-0.000072
H	4.103598	0.069464	0.000993
H	3.309640	1.379373	-0.888896
H	3.308076	1.385173	0.880849
H	2.310459	-2.020139	1.594104
H	1.575902	-0.661097	2.457377
H	0.550823	-1.833729	1.621089
H	2.311740	-2.017225	-1.596529
H	0.551029	-1.840547	-1.614988
H	1.565508	-0.662647	-2.456742

Compound 4Ec(si): (No imaginary frequency)

Si	-1.771377	-0.058621	-0.008237
O	-0.192086	-0.524363	-0.374882
C	1.060983	-0.057810	-0.080372
C	1.187086	1.416687	0.180022
C	2.064916	-0.960416	-0.054038
C	3.492133	-0.730655	0.163824
C	4.246584	0.304011	-0.240466
H	3.997739	-1.538276	0.697171
C	-2.811367	-1.471913	-0.681205
C	-2.000547	0.102188	1.858386
C	-2.230645	1.552405	-0.878313
H	1.763616	-1.998665	-0.183421
H	5.304906	0.351244	0.000495
H	3.850363	1.117205	-0.841700
H	0.417285	1.753278	0.885222
H	2.165454	1.656031	0.600566
H	1.057591	1.998977	-0.741914
H	-3.300625	1.760421	-0.749580
H	-1.679411	2.415909	-0.490563
H	-2.035614	1.486771	-1.955196
H	-3.055307	0.286297	2.099312
H	-1.699304	-0.818708	2.371091
H	-1.418854	0.926299	2.286933
H	-3.881165	-1.289269	-0.522024
H	-2.650183	-1.600719	-1.757517
H	-2.555390	-2.418179	-0.191528

Compound 4Zt(N): (No imaginary frequency)

C	-0.292949	2.456493	0.205035
C	-0.540381	0.969768	0.049537
C	-1.832606	0.521699	0.068566
C	-2.395328	-0.790417	-0.185165
C	-3.709916	-1.074414	-0.114029
N	0.603290	0.200744	-0.082572
C	1.940661	0.775025	-0.284269
C	2.859780	-0.450334	-0.386684
H	-1.728594	-1.593817	-0.484949
H	-2.575158	1.288698	0.278045
H	-4.090526	-2.066113	-0.338583
H	-4.443459	-0.321366	0.166727
H	0.339990	2.677680	1.074336
H	0.210474	2.879704	-0.673497
H	-1.238868	2.986979	0.329129
H	3.882529	-0.227870	-0.067746
C	2.152155	-1.486508	0.497527
H	2.900524	-0.805522	-1.423474
C	0.671999	-1.238301	0.180536
H	1.982217	1.395067	-1.188199
H	2.238887	1.411450	0.563003
H	2.458739	-2.516473	0.290911
H	2.350409	-1.280159	1.556363

H	0.366153	-1.828502	-0.697316
H	0.003156	-1.503027	1.006924

Compound 4Zc(N): (No imaginary frequency)

C	0.521529	2.517788	-0.068371
C	0.736704	1.018533	-0.090405
C	1.994414	0.530875	-0.310188
C	2.547818	-0.805743	-0.133996
C	2.198345	-1.746783	0.763689
N	-0.401853	0.246312	0.065481
C	-1.677759	0.790655	0.547617
C	-2.632977	-0.408332	0.483431
H	3.408595	-1.024147	-0.770209
H	2.724156	1.275406	-0.623614
H	2.727787	-2.693845	0.818245
H	1.412731	-1.583495	1.495705
H	-0.199616	2.844468	-0.829224
H	0.137029	2.855199	0.902729
H	1.466024	3.037514	-0.243005
H	-3.678027	-0.100900	0.379179
C	-2.100409	-1.199088	-0.720085
H	-2.547132	-1.008009	1.397660
C	-0.579097	-1.062532	-0.569350
H	-1.581853	1.194646	1.563108
H	-2.042269	1.605669	-0.096920
H	-2.427605	-2.243443	-0.731223
H	-2.434699	-0.731412	-1.654651
H	-0.163889	-1.876350	0.043049
H	-0.039666	-1.087725	-1.523242

Compound 4Et(N): (No imaginary frequency)

C	-0.772198	2.034373	0.095387
C	-0.577379	0.537765	0.029190
C	-1.612793	-0.354084	-0.024234
C	-3.027428	-0.050161	-0.011546
C	-4.012751	-0.965252	-0.081832
N	0.740015	0.120188	0.014321
C	1.906443	1.004393	0.031335
C	3.064875	0.074651	-0.353469
H	-3.323478	0.995825	0.058182
H	-1.375518	-1.412422	-0.093900
H	-5.058977	-0.675991	-0.068214
H	-3.801248	-2.029956	-0.156406
H	-0.415575	2.525101	-0.819392
H	-1.821989	2.296849	0.220025
H	-0.217530	2.471272	0.934470
H	4.029796	0.433534	0.017648
C	2.640092	-1.271968	0.251266
H	3.130466	-0.004504	-1.445256
C	1.118375	-1.291263	0.038458
H	1.794188	1.834866	-0.673707
H	2.074062	1.442036	1.030132

H	3.137139	-2.130282	-0.210523
H	2.869250	-1.291404	1.323587
H	0.843475	-1.784795	-0.907524
H	0.592424	-1.822174	0.843291

Compound 4Ec(N): (No imaginary frequency)

C	-1.126849	1.683281	-0.003029
C	-0.652625	0.254718	-0.114927
C	-1.504605	-0.803224	-0.280262
C	-2.961075	-0.813341	-0.257584
C	-3.827594	-0.037374	0.421318
N	0.716410	0.070534	-0.064217
C	1.716133	1.142605	-0.071165
C	3.055481	0.398140	-0.200716
H	-3.398801	-1.607131	-0.867794
H	-1.059605	-1.770667	-0.498422
H	-4.899376	-0.178151	0.312612
H	-3.512004	0.732243	1.119294
H	-0.526337	2.352470	-0.628284
H	-2.166720	1.763382	-0.320575
H	-1.056881	2.057232	1.027383
H	3.880217	0.943975	0.267494
C	2.773182	-0.962834	0.452126
H	3.303748	0.261416	-1.260106
C	1.327813	-1.252503	0.028564
H	1.565874	1.839232	-0.904735
H	1.676989	1.732997	0.857920
H	3.469179	-1.746085	0.136842
H	2.832659	-0.879542	1.544004
H	1.291004	-1.782270	-0.938209
H	0.786017	-1.869644	0.756148

TS-5aE: (one imaginary frequency, -422.27 cm^{-1})

H	4.306361	0.694547	-0.204120
C	3.360756	0.388910	-0.653773
H	2.859705	1.262080	-1.089208
O	2.575810	-0.166662	0.398144
C	1.418836	-0.746032	0.032835
H	1.278861	-0.912266	-1.030090
C	0.588383	-1.277559	0.992305
C	-0.676367	-1.810430	0.701708
C	-1.262381	-1.787267	-0.570938
H	3.552987	-0.354388	-1.438231
C	-1.780537	0.109297	-0.937026
H	-2.129981	-0.157296	-1.936568
C	-0.621528	0.918641	-0.949789
C	-0.197055	1.808308	0.106429
O	-0.718721	1.957926	1.211186
C	-2.915643	0.366891	0.041041
H	-0.046652	0.976903	-1.873122
H	0.698372	2.420152	-0.162895
H	-0.619417	-1.891820	-1.441329

H	-2.218643	-2.291783	-0.691060
H	-1.299257	-2.083651	1.550290
H	0.897225	-1.168144	2.028284
H	-2.552562	0.433628	1.065586
H	-3.387779	1.329180	-0.194116
H	-3.682708	-0.411808	-0.034804

TS-5aZ: (one imaginary frequency, -396.65 cm^{-1})

H	-3.572703	-0.727373	-0.191568
C	-2.650910	-0.994783	-0.722106
H	-2.196443	-1.895818	-0.310175
O	-1.710084	0.093664	-0.659902
C	-1.633327	0.772229	0.482075
H	-2.368909	0.502951	1.241684
C	-0.866793	1.916003	0.646262
C	0.255643	2.278430	-0.102257
C	0.973891	1.362613	-0.904280
H	-2.866290	-1.138780	-1.781720
C	1.887215	0.163046	0.242167
C	2.596833	-0.727224	-0.779681
C	1.008996	-0.439205	1.194706
C	0.226751	-1.616237	0.997811
O	0.069485	-2.247724	-0.060443
H	2.573981	0.872651	0.707777
H	0.917935	0.025846	2.173232
H	-0.307314	-1.958068	1.915976
H	0.402006	0.617351	-1.447307
H	1.797204	1.779260	-1.482730
H	0.734664	3.221261	0.157315
H	-1.131864	2.518081	1.512917
H	3.119118	-0.132431	-1.536815
H	3.344501	-1.340240	-0.261663
H	1.889104	-1.401440	-1.262328

Compound 5a: (No imaginary frequency)

C	-0.627177	1.745355	0.292300
C	-1.102635	0.486456	-0.390797
C	0.001161	-0.599686	-0.305305
C	1.308981	-0.014027	-0.887202
C	1.796865	1.153063	-0.004334
C	0.667146	2.036404	0.461786
O	-2.333858	0.100426	0.217655
C	-3.132934	-0.757758	-0.574308
C	0.113517	-1.117458	1.124717
O	1.147486	-1.432070	1.678233
C	2.403551	-1.057920	-1.140147
H	1.032372	0.415913	-1.862274
H	-0.310238	-1.466955	-0.910921
H	-0.856534	-1.213786	1.652996
H	2.529845	1.753044	-0.562479
H	2.335073	0.760377	0.869934
H	0.941269	2.961145	0.967946

H	-1.408491	2.418764	0.637106
H	2.724197	-1.524771	-0.206255
H	2.045393	-1.846220	-1.814022
H	3.275709	-0.590198	-1.613202
H	-4.076456	-0.892026	-0.039184
H	-3.340730	-0.315863	-1.561504
H	-2.673803	-1.746201	-0.726450
H	-1.297477	0.693356	-1.459054

TS-5bE: (one imaginary frequency, -413.86 cm^{-1})

C	0.819576	-0.669961	1.046320
C	1.923471	0.117997	0.649115
C	1.322773	1.456915	-0.731289
C	0.346255	2.276115	-0.157816
C	-0.965484	1.871531	0.144359
C	-1.471007	0.635877	-0.187707
H	-0.978191	-0.045665	-0.873536
O	-2.708781	0.301951	0.205866
C	-3.167250	-0.999177	-0.170294
H	-4.237161	-1.019162	0.041147
H	-2.994465	-1.184612	-1.236458
H	-2.656003	-1.768562	0.418994
H	-1.604196	2.526679	0.732014
H	0.656410	3.246099	0.227342
H	2.269168	1.926443	-0.987350
H	2.254722	0.821951	1.412597
C	3.081144	-0.501094	-0.127517
H	3.766089	0.260559	-0.513254
H	3.654371	-1.146110	0.550859
H	2.717075	-1.117145	-0.950043
H	1.026175	0.673559	-1.424915
H	0.326579	-0.442779	1.987903
C	0.318595	-1.808981	0.329856
O	0.577947	-2.123904	-0.839408
H	-0.402345	-2.430964	0.912869

TS-5bZ: (one imaginary frequency, -438.27 cm^{-1})

C	3.093997	0.505158	-0.866256
O	2.210167	-0.371746	-0.174013
C	1.510776	0.172996	0.843329
C	0.566128	-0.524626	1.574476
C	-0.229822	-1.568714	1.097286
C	-0.315930	-1.891645	-0.272513
H	1.918561	1.105606	1.235163
C	-1.241913	-0.406411	-1.104239
C	-2.683794	-0.545506	-0.629172
H	-1.093419	-0.813993	-2.107106
C	-0.538315	0.815804	-0.911729
C	-0.875213	1.852796	0.031002
O	-1.749800	1.818877	0.899612
H	3.706862	-0.121949	-1.515316
H	3.739629	1.046558	-0.162722

H	2.530893	1.225619	-1.471523
H	0.258500	1.057853	-1.612120
H	-0.252116	2.773187	-0.083080
H	0.594319	-1.844951	-0.857594
H	-0.962890	-2.724527	-0.542940
H	-0.994502	-1.950105	1.770250
H	0.317898	-0.086801	2.537202
H	-2.784282	-0.278984	0.422081
H	-3.324504	0.140292	-1.197129
H	-3.053375	-1.563960	-0.793061

Compound 5b: (No imaginary frequency)

C	0.415883	2.115807	0.143837
C	-0.746912	1.648305	0.608802
C	-1.166857	0.205397	0.491470
C	0.041683	-0.706393	0.142475
C	0.866650	-0.090731	-1.005339
C	1.435180	1.274329	-0.577355
H	-1.597527	-0.121213	1.454499
C	0.807700	-1.027591	1.413770
O	2.001338	-0.911210	1.589213
C	1.944463	-1.028775	-1.561182
H	0.136445	0.101289	-1.803543
H	-0.373991	-1.675800	-0.181338
H	0.162444	-1.416158	2.238061
H	1.790180	1.817014	-1.464848
H	2.316365	1.134360	0.063655
H	0.656955	3.169025	0.284712
H	-1.460274	2.316277	1.086627
H	2.702546	-1.255044	-0.806753
H	1.505499	-1.975117	-1.901480
H	2.444471	-0.569792	-2.422622
O	-2.193064	0.130870	-0.502436
C	-3.065927	-0.972421	-0.361356
H	-3.812845	-0.887169	-1.154816
H	-2.550206	-1.939481	-0.471416
H	-3.577440	-0.963025	0.614317

TS-6aE: (one imaginary frequency, -501.52 cm^{-1})

C	1.191077	1.703330	-0.570191
C	0.444601	1.948361	0.573649
C	-0.833323	1.418758	0.763012
C	-1.405767	0.524704	-0.147977
C	0.035615	-1.083535	-0.103618
C	1.246436	-0.614241	-0.650672
C	2.528759	-0.585125	0.065407
O	3.619828	-0.597811	-0.483794
H	2.458812	-0.558817	1.173801
C	-0.095988	-1.565550	1.325844
H	-1.151698	-1.646992	1.603495
H	0.388322	-0.890291	2.036673
H	0.360621	-2.557276	1.447324

H	-0.594655	-1.624296	-0.808785
O	-2.614277	-0.023780	0.193855
H	-1.240630	0.641714	-1.216902
H	-1.322894	1.517934	1.728690
H	0.930099	2.421909	1.424877
H	0.705096	1.564401	-1.529413
H	2.226835	2.022260	-0.632820
H	1.364107	-0.652230	-1.732219
C	-3.356982	-0.587948	-0.878140
H	-4.270949	-0.995958	-0.442448
H	-3.620717	0.174858	-1.623272
H	-2.803320	-1.397010	-1.373365

TS-6aZ: (one imaginary frequency, -517.18 cm^{-1})

C	-0.331127	1.879761	0.468550
C	0.573692	2.122593	-0.547704
C	1.448275	1.141413	-1.032978
C	1.462142	-0.179075	-0.564688
O	1.333070	-0.470506	0.790838
C	2.587845	-0.525502	1.462313
H	2.100923	-0.895245	-1.091035
C	-1.429173	-0.020273	-0.606720
C	-0.442720	-0.882985	-1.132835
C	-0.290507	-2.323987	-0.665744
H	-0.270177	-0.760500	-2.200421
C	-2.212178	-0.306503	0.596544
O	-3.261919	0.252866	0.882034
H	-0.123060	1.151732	1.237078
H	-1.139720	2.577778	0.666118
H	0.456969	3.026195	-1.144227
H	1.916268	1.309882	-2.001448
H	2.374078	-0.794333	2.499511
H	3.100958	0.444622	1.429625
H	3.242845	-1.289878	1.018435
H	-0.183195	-2.400171	0.417774
H	0.590667	-2.789003	-1.120313
H	-1.164652	-2.913912	-0.968509
H	-1.875035	0.724203	-1.257862
H	-1.793570	-1.082901	1.271860

Compound 6a: (No imaginary frequency)

C	-0.153111	2.156586	0.096879
C	-1.225702	1.389646	-0.115808
C	-1.141702	-0.096891	-0.392964
C	0.178604	-0.697859	0.130067
C	1.342582	0.179304	-0.423625
C	1.259438	1.631047	0.085653
O	-2.223528	-0.807137	0.208703
C	0.188389	-0.849727	1.659344
C	2.680535	-0.463199	-0.102784
H	1.257783	0.171234	-1.518057
H	0.283687	-1.696372	-0.311657

H	0.104165	0.115504	2.169027
H	1.893380	2.278004	-0.537064
H	1.680889	1.704793	1.101059
H	-0.278878	3.219032	0.301790
H	-2.221059	1.829011	-0.092713
H	3.163261	-0.125211	0.843701
H	-1.183937	-0.264736	-1.484700
O	3.209378	-1.306510	-0.793139
H	-0.657842	-1.465012	1.973414
H	1.108153	-1.338686	2.000150
C	-3.423978	-0.777273	-0.535596
H	-4.148205	-1.390690	0.006987
H	-3.834287	0.238886	-0.638428
H	-3.284232	-1.196397	-1.545033

TS-6bE: (one imaginary frequency, -517.26 cm^{-1})

C	-1.159072	1.622662	0.696289
C	-0.200298	2.257999	-0.080170
C	1.037203	1.673282	-0.363565
C	1.373249	0.394202	0.080864
C	-0.229394	-0.868901	-0.741938
C	-1.475323	-0.226839	-0.581008
H	-1.847062	0.381014	-1.399600
H	0.221101	-0.766967	-1.725654
C	0.138574	-2.163066	-0.041943
O	2.528986	-0.180234	-0.393171
H	1.062745	0.045601	1.065306
H	1.683191	2.117162	-1.117658
H	-0.490648	3.138855	-0.649594
H	-0.866289	0.971259	1.513778
H	-2.157540	2.039682	0.788403
C	-2.543035	-0.733401	0.293323
C	3.450942	-0.591193	0.610916
H	4.257281	-1.120014	0.098143
H	3.864636	0.274036	1.146225
H	2.979319	-1.268010	1.337172
O	-3.724407	-0.452677	0.168887
H	-2.216822	-1.408293	1.115233
H	1.209672	-2.356421	-0.150866
H	-0.101264	-2.159308	1.026870
H	-0.392027	-3.013768	-0.490095

TS-6bZ: (one imaginary frequency, -486.88 cm^{-1})

C	-0.232319	-1.743209	0.610618
C	0.272090	-0.979717	1.642576
C	1.112870	0.126763	1.443579
C	1.445879	0.634044	0.179539
C	-0.383580	1.243260	-0.557174
C	-1.148736	0.096606	-0.835660
C	-2.438702	-0.226499	-0.224421
O	-3.249966	-1.006035	-0.705886
H	-2.672735	0.310154	0.720333

C	-0.858293	2.314486	0.407639
H	-0.070757	3.053047	0.591903
H	-1.156757	1.896148	1.373207
H	-1.724221	2.849581	-0.002386
H	0.165345	1.621507	-1.418692
H	2.002050	1.577158	0.155775
O	1.762026	-0.196986	-0.894965
C	3.137080	-0.569236	-0.909897
H	3.788713	0.315563	-0.965666
H	3.283567	-1.178745	-1.804771
H	3.404629	-1.150743	-0.017918
H	1.266571	0.802470	2.282542
H	-0.137488	-1.119833	2.641910
H	0.282193	-1.821382	-0.334507
H	-1.028649	-2.458507	0.793581
H	-0.936668	-0.451239	-1.749303

Compound 6b: (No imaginary frequency)

C	-0.142164	2.276889	-0.195449
C	-1.248767	1.631657	0.184881
C	-1.312565	0.137929	0.399262
C	0.089138	-0.494963	0.542911
C	0.979739	0.062759	-0.582556
C	1.170057	1.588962	-0.468356
H	-1.888645	-0.064853	1.318339
C	0.661071	-0.280036	1.953571
C	2.302497	-0.651921	-0.746488
H	0.441048	-0.113924	-1.529922
H	-0.004829	-1.575795	0.386305
H	0.745552	0.782872	2.205646
H	1.610397	1.983778	-1.394394
H	1.890218	1.834095	0.328026
H	-0.164929	3.358695	-0.321115
H	-2.177162	2.179616	0.331678
H	3.006009	-0.159818	-1.459526
O	-2.034665	-0.404816	-0.716427
C	-2.690416	-1.628790	-0.444459
H	-3.213349	-1.917174	-1.360327
H	-1.991298	-2.433652	-0.172208
H	-3.427118	-1.520928	0.367596
O	2.618082	-1.685824	-0.197081
H	0.006922	-0.742095	2.702510
H	1.648308	-0.740617	2.045550

TS-7aE: (one imaginary frequency, -426.61 cm^{-1})

H	-3.929146	1.385982	-0.497347
C	-3.261520	0.818535	0.152428
H	-2.731442	1.506409	0.822213
O	-2.345013	0.170224	-0.725267
C	-1.379510	-0.645779	-0.231025
C	-1.668062	-1.328503	1.077422
C	-0.431274	-1.000432	-1.182844

C	0.809936	-1.623556	-1.013260
C	1.508802	-1.810604	0.194869
H	-3.851036	0.107024	0.740800
C	2.038136	-0.032051	0.807135
H	2.503638	-0.453604	1.701374
C	0.878933	0.733600	1.096402
C	0.382272	1.849082	0.333715
O	0.800799	2.276772	-0.743828
C	3.057020	0.454322	-0.211369
H	0.379970	0.556364	2.047971
H	-0.469638	2.375118	0.834184
H	0.971497	-2.079651	1.096680
H	2.464556	-2.327747	0.119336
H	1.388502	-1.739015	-1.927743
H	-0.648306	-0.611599	-2.175390
H	2.583291	0.706572	-1.159189
H	3.535001	1.369972	0.157971
H	3.839874	-0.295727	-0.371739
H	-0.902961	-2.060819	1.321819
H	-1.766302	-0.635256	1.917083
H	-2.622198	-1.867668	0.983894

TS-7aZ: (one imaginary frequency, -374.67 cm^{-1})

H	-1.520023	-1.750237	-2.140124
C	-2.024218	-1.318780	-1.276820
H	-3.062898	-1.077225	-1.530219
O	-1.294154	-0.120762	-0.975791
C	-1.576340	0.607972	0.108303
C	-2.734591	0.209818	0.981291
C	-0.909202	1.815971	0.307467
C	0.284862	2.237295	-0.282900
C	1.217252	1.380016	-0.911796
H	-1.972596	-2.034724	-0.456758
C	2.092516	0.359028	0.406064
C	3.016357	-0.496338	-0.464370
C	1.179582	-0.301317	1.286682
C	0.521483	-1.537968	1.041378
O	0.527602	-2.206350	-0.008597
H	2.638543	1.160741	0.908038
H	0.927883	0.188207	2.224920
H	-0.084210	-1.902989	1.906513
H	0.822452	0.552502	-1.491067
H	2.059156	1.877346	-1.392261
H	0.620819	3.238247	-0.014218
H	-1.357047	2.464549	1.056506
H	3.556156	0.110112	-1.199895
H	3.759926	-0.985166	0.176934
H	2.447995	-1.275478	-0.973293
H	-2.837939	0.909862	1.812281
H	-3.677465	0.200357	0.418579

H	-2.594544	-0.793375	1.397380

Compound 7a: (No imaginary frequency)

C	0.491756	1.437361	-0.957173
C	1.003128	0.470872	0.090089
C	-0.142921	-0.526122	0.482565
C	-1.453314	0.236963	0.795145
C	-1.931699	1.052412	-0.422625
C	-0.799008	1.700445	-1.172717
C	1.531424	1.251622	1.309356
O	2.083385	-0.220954	-0.573591
C	2.943089	-1.022773	0.217053
C	-0.284773	-1.604037	-0.588132
O	-1.266271	-1.793197	-1.275159
C	-2.560159	-0.667870	1.353988
H	-1.201137	0.956685	1.585445
H	0.176225	-1.063225	1.390845
H	0.598610	-2.264825	-0.698891
H	-2.642666	1.821510	-0.087229
H	-2.487981	0.403069	-1.110764
H	-1.069371	2.412592	-1.951506
H	1.269784	1.926650	-1.539270
H	-2.879238	-1.408636	0.616310
H	-2.222056	-1.198294	2.253076
H	-3.435260	-0.069180	1.634338
H	0.754942	1.897485	1.726006
H	1.881278	0.585050	2.105741
H	2.366524	1.889717	0.999844
H	3.596923	-1.545204	-0.486670
H	3.567853	-0.427581	0.896420
H	2.403519	-1.775845	0.811010

TS-7bE: (one imaginary frequency, -409.85 cm^{-1})

C	1.200379	0.075873	1.498557
C	1.459079	0.667640	0.150005
O	2.553198	0.283124	-0.541271
C	3.285347	-0.880154	-0.149650
C	0.802522	1.763627	-0.405531
C	-0.476171	2.240889	-0.101523
C	-1.495853	1.537570	0.568788
C	-2.167059	0.113918	-0.604628
C	-3.169897	-0.553610	0.330442
C	-1.098817	-0.643500	-1.155024
C	-0.476123	-1.789893	-0.585859
O	-0.624025	-2.247881	0.565108
H	3.960805	-1.087987	-0.980856
H	3.875955	-0.697915	0.755359
H	2.619311	-1.733969	0.008181
H	0.650943	0.788599	2.115925
H	2.147043	-0.142848	2.003077
H	0.617314	-0.859618	1.450012
H	1.333381	2.235487	-1.230397

H	-0.777162	3.137534	-0.642023
H	-2.408464	2.096438	0.769787
H	-2.645871	0.765572	-1.336871
H	-3.804207	0.180008	0.839726
H	-3.826051	-1.206388	-0.259273
H	-2.658535	-1.174947	1.066491
H	-1.240379	0.850684	1.367318
H	-0.702480	-0.333012	-2.119118
H	0.244575	-2.293756	-1.271498

TS-7bZ: (one imaginary frequency, -395.03 cm^{-1})

C	2.699589	-0.661603	-1.343010
O	1.870332	-0.936139	-0.216876
C	1.484842	0.077044	0.597065
C	0.501978	-0.160567	1.550036
C	-0.505197	-1.127598	1.502570
C	-0.838356	-1.869493	0.346379
C	2.343664	1.310617	0.658420
C	-1.674671	-0.661518	-0.851996
C	-3.043884	-0.381762	-0.237663
H	-1.733115	-1.399369	-1.656943
C	-0.820032	0.429451	-1.195664
C	-0.856430	1.745027	-0.623994
O	-1.568498	2.144589	0.304530
H	2.863052	-1.625145	-1.828290
H	3.665959	-0.239370	-1.047768
H	2.197642	0.018248	-2.041770
H	-0.112044	0.284777	-2.009937
H	-0.148634	2.459761	-1.112255
H	-0.020568	-2.201959	-0.281248
H	-1.616087	-2.622494	0.467826
H	-1.222126	-1.109575	2.320728
H	0.442536	0.579087	2.342835
H	-2.961699	0.268196	0.632365
H	-3.672093	0.138497	-0.971113
H	-3.550280	-1.314258	0.036959
H	1.917599	2.026126	1.363615
H	3.364546	1.063564	0.984259
H	2.421618	1.808717	-0.313356

Compound 7b: (No imaginary frequency)

C	1.657682	0.189021	1.364362
C	0.598134	-0.666940	2.001341
C	-0.604825	-0.891733	1.467880
C	-1.064533	-0.331821	0.137145
C	0.178545	0.140505	-0.702479
C	1.113974	1.000909	0.174935
O	-1.861124	0.822421	0.487307
C	-2.678616	1.397731	-0.515709
C	0.851601	-1.019479	-1.415382
O	1.971151	-1.437616	-1.206342
C	2.232149	1.683795	-0.622396

C	-1.922253	-1.384773	-0.586010
H	0.465986	1.783039	0.590178
H	-0.221615	0.762418	-1.519718
H	0.232866	-1.489214	-2.212878
H	2.069504	0.876561	2.117258
H	2.492649	-0.445698	1.040548
H	0.843982	-1.124998	2.959007
H	-1.337155	-1.497223	1.999291
H	2.917553	0.952373	-1.060532
H	1.821545	2.298186	-1.433719
H	2.815981	2.346013	0.028159
H	-3.095592	2.308216	-0.076873
H	-2.116003	1.678098	-1.419403
H	-3.508683	0.742194	-0.812951
H	-2.198158	-1.079903	-1.601214
H	-1.392266	-2.339926	-0.652317
H	-2.841958	-1.551855	-0.014673

TS-8aE: (one imaginary frequency, -506.70 cm^{-1})

C	1.466286	1.718100	-0.018481
C	0.580101	1.733366	1.054298
C	-0.706571	1.201147	1.063039
C	-1.340330	0.500219	0.012194
C	0.169928	-1.055720	-0.230516
C	1.383952	-0.500548	-0.687544
C	2.683597	-0.677130	-0.025730
O	3.759549	-0.597400	-0.599639
H	2.641768	-0.909786	1.059513
C	0.068768	-1.798259	1.084550
H	-0.977977	-1.931428	1.372410
H	0.571523	-1.263209	1.895254
H	0.528965	-2.792954	1.009183
H	-0.458475	-1.460636	-1.022770
O	-2.464043	-0.168002	0.478099
C	-1.446592	1.025663	-1.405447
H	-1.190929	1.086239	2.030429
H	0.989272	1.994557	2.029344
H	1.150899	1.847342	-1.042874
H	2.505928	1.983322	0.152269
H	1.478814	-0.299554	-1.753094
C	-3.287811	-0.883463	-0.431043
H	-4.062704	-1.350552	0.180322
H	-3.766075	-0.226269	-1.167025
H	-2.732643	-1.669313	-0.959448
H	-1.547263	0.230827	-2.150834
H	-2.334206	1.668329	-1.476360
H	-0.588909	1.636058	-1.675922

TS-8aZ: (one imaginary frequency, -532.02 cm^{-1})

C	0.786980	-1.723421	0.142425
C	-0.170200	-1.948821	-0.844927
C	-1.206938	-1.053955	-1.102999

C	-1.462810	0.110108	-0.360989
O	-1.313950	0.112583	1.030382
C	-2.162250	-0.807573	1.720369
C	-2.512397	1.088071	-0.837205
C	1.565516	0.216021	-0.610160
C	0.525329	1.170988	-0.688762
C	0.389529	2.290521	0.324405
H	0.218163	1.433176	-1.698027
C	2.612067	0.264822	0.426081
O	3.722365	-0.224972	0.299911
H	0.516345	-1.242933	1.072383
H	1.681160	-2.339734	0.174008
H	0.043104	-2.696834	-1.606707
H	-1.710515	-1.131088	-2.065207
H	-2.001201	-0.626709	2.785971
H	-1.909325	-1.846900	1.480689
H	-3.219814	-0.631347	1.483105
H	-3.504062	0.812985	-0.450694
H	-2.305011	2.100999	-0.482267
H	-2.570042	1.106192	-1.929820
H	0.314086	1.914860	1.347735
H	-0.501179	2.894197	0.131607
H	1.250877	2.969993	0.270420
H	1.908390	-0.239000	-1.534391
H	2.332746	0.780688	1.369434

Compound 8a: (No imaginary frequency)

C	-1.397310	1.652199	-0.319809
C	0.019413	2.157327	-0.398692
C	1.090921	1.406893	-0.125757
C	1.043119	-0.055059	0.290273
C	-0.347098	-0.669907	-0.054059
C	-1.454409	0.298203	0.415540
O	1.987860	-0.818634	-0.489685
C	3.368269	-0.633571	-0.247447
C	-0.486213	-1.022161	-1.545928
C	-2.850368	-0.292879	0.388600
O	-3.119615	-1.467482	0.265359
H	-1.296215	0.524919	1.484048
H	-0.452308	-1.600598	0.516142
H	-0.319362	-0.151899	-2.189730
H	-2.033176	2.387515	0.193012
H	-1.811573	1.561004	-1.335580
H	0.154419	3.192794	-0.709421
H	2.079603	1.856000	-0.199094
H	-3.664473	0.457611	0.530727
C	1.358456	-0.206648	1.791773
H	0.248979	-1.778718	-1.823626
H	-1.484529	-1.421897	-1.744140
H	3.887040	-1.220376	-1.010729
H	3.687460	0.414127	-0.346313
H	3.678317	-0.999397	0.741377

H	1.469755	-1.267538	2.044088
H	2.281233	0.314584	2.067449
H	0.560195	0.214422	2.409443

TS-8bE: (one imaginary frequency, -517.09 cm^{-1})

C	-1.276287	1.819830	0.397960
C	-0.176113	2.230965	-0.341634
C	1.000153	1.493502	-0.473822
C	1.256905	0.229998	0.092815
C	-0.396362	-0.888908	-0.827306
C	-1.627761	-0.210290	-0.658629
H	-2.008290	0.375789	-1.488466
H	0.065235	-0.749043	-1.801385
C	-0.124906	-2.269417	-0.257510
H	0.945161	-2.490373	-0.292383
H	-0.472331	-2.396755	0.771374
H	-0.637556	-3.024873	-0.867956
O	2.325900	-0.445238	-0.504261
C	1.048418	-0.120829	1.556963
H	1.671357	1.771065	-1.284959
H	-0.324421	3.038474	-1.057247
H	-1.172448	1.295182	1.336205
H	-2.233926	2.316341	0.269098
C	-2.673097	-0.636222	0.278184
C	3.603091	-0.252087	0.096375
H	4.319061	-0.797189	-0.523108
H	3.875294	0.812818	0.113632
H	3.645684	-0.646658	1.120047
H	1.411546	-1.133236	1.751390
H	1.599069	0.570705	2.207090
H	0.001391	-0.086173	1.857555
O	-3.844441	-0.297007	0.204190
H	-2.340745	-1.297372	1.109308

TS-8bZ: (one imaginary frequency, -513.35 cm^{-1})

C	-0.676912	-1.702543	0.607890
C	-0.010965	-1.026203	1.619236
C	0.987714	-0.078425	1.376482
C	1.401289	0.334929	0.096357
C	-0.452531	1.127516	-0.626473
C	-1.369454	0.067787	-0.773424
C	-2.683829	0.017196	-0.122354
O	-3.629856	-0.636859	-0.535539
H	-2.789341	0.635662	0.795116
C	-0.745928	2.317527	0.266371
H	0.110686	2.996251	0.314707
H	-0.992936	2.013415	1.288401
H	-1.596882	2.895307	-0.117775
H	0.102752	1.356796	-1.533819
C	2.396687	1.467937	-0.044651
H	2.320431	2.180777	0.781262
H	2.246634	2.004959	-0.987015

H	3.424004	1.080142	-0.056425
O	1.510427	-0.591228	-0.953805
C	2.498259	-1.602000	-0.748857
H	3.496207	-1.169335	-0.597424
H	2.508602	-2.203581	-1.661044
H	2.250932	-2.238952	0.108880
H	1.283570	0.561707	2.205064
H	-0.416816	-1.071985	2.628645
H	-0.184865	-1.944978	-0.320907
H	-1.572824	-2.273366	0.834198
H	-1.300694	-0.540453	-1.670567

Compound 8b: (No imaginary frequency)

C	1.380039	1.567430	-0.584309
C	0.040872	2.253163	-0.514220
C	-1.095138	1.625492	-0.199297
C	-1.187621	0.150915	0.153377
C	0.212576	-0.408148	0.540571
C	1.209033	0.035980	-0.548268
O	-1.629439	-0.470301	-1.083230
C	-2.124739	-1.796615	-1.016244
C	0.666313	-0.015930	1.957811
C	2.541403	-0.676412	-0.507208
O	2.799312	-1.655426	0.160808
C	-2.235610	-0.036487	1.261887
H	0.765854	-0.247910	-1.517602
H	0.161103	-1.502814	0.511029
H	0.653199	1.069131	2.109771
H	1.902960	1.868051	-1.502914
H	2.018608	1.911526	0.244310
H	0.021048	3.318588	-0.740649
H	-2.036132	2.173181	-0.200110
H	3.314499	-0.243251	-1.185930
H	-2.282948	-2.110236	-2.051946
H	-1.418075	-2.496154	-0.546851
H	-3.083655	-1.861433	-0.483687
H	0.018278	-0.464202	2.717243
H	1.680539	-0.381064	2.141531
H	-2.275746	-1.069395	1.623689
H	-2.015331	0.609216	2.116456
H	-3.225954	0.236240	0.880437

TS-9aE: (one imaginary frequency, -425.10 cm^{-1})

C	1.106465	-1.708506	-0.202392
C	0.304617	-1.504019	-1.337415
C	-1.001598	-1.003989	-1.282812
C	-1.637689	-0.713797	-0.095564
O	-2.848934	-0.129702	-0.112044
C	-3.415720	0.172369	1.160263
H	2.074383	-2.178308	-0.361847
H	0.621279	-2.053801	0.707793
H	0.768980	-1.563489	-2.318819

H	-1.501660	-0.704329	-2.199516
H	-1.298620	-1.088360	0.864451
H	-3.476565	-0.725005	1.789378
H	-4.420340	0.551232	0.968098
H	-2.824285	0.941493	1.671712
C	0.498320	0.835558	0.749875
C	1.670107	0.055672	0.540866
C	2.680267	0.512777	-0.510383
H	2.194976	0.751765	-1.454619
H	3.455694	-0.246927	-0.663464
H	3.176392	1.427134	-0.158335
C	2.341722	-0.435619	1.824602
H	1.610281	-0.778925	2.565009
H	3.044754	-1.253346	1.631584
H	2.911548	0.386004	2.277519
H	0.040095	0.806960	1.737976
C	-0.064147	1.797960	-0.164917
O	0.306286	2.044470	-1.314386
H	-0.929790	2.359329	0.261786

TS-9aZ: (one imaginary frequency, -383.43 cm^{-1})

H	-3.246173	-0.894563	0.638080
C	-3.169924	-0.496608	-0.377848
H	-3.044488	-1.322667	-1.074025
O	-2.003137	0.326949	-0.517546
C	-1.680240	1.109501	0.506068
H	-2.368660	1.094004	1.352394
C	-0.674390	2.064301	0.455705
C	0.412022	2.077561	-0.419988
C	0.840343	0.933517	-1.137573
H	-4.060979	0.094304	-0.621306
C	1.657288	-0.267422	0.056256
C	2.080826	-1.355131	-0.942882
C	0.715209	-0.664395	1.067698
C	-0.327740	-1.623151	0.930126
O	-0.714432	-2.174536	-0.114998
C	2.862500	0.492835	0.616467
H	0.803579	-0.206429	2.051090
H	-0.857491	-1.849253	1.886521
H	0.071897	0.266406	-1.515119
H	1.644302	1.106744	-1.852248
H	1.094513	2.921995	-0.342276
H	-0.716820	2.809333	1.247753
H	2.554110	1.294548	1.295642
H	3.506540	-0.193529	1.181170
H	3.468978	0.933391	-0.183468
H	2.669655	-0.932821	-1.765210
H	2.713623	-2.085975	-0.423339
H	1.212612	-1.880833	-1.339483

Compound 9a: (No imaginary frequency)

C	-0.693909	-1.355033	-1.152250

C	-1.146964	-0.596268	0.067009
C	-0.095305	0.491697	0.443565
C	1.327781	-0.134065	0.541608
C	1.717243	-0.703892	-0.845855
C	0.583282	-1.411871	-1.542920
O	-2.442198	-0.060099	-0.207078
C	-3.208098	0.235629	0.945259
C	-0.236506	1.661456	-0.526900
O	0.649248	2.163801	-1.186921
C	2.360897	0.911916	1.003692
C	1.326763	-1.280019	1.580215
H	-0.372599	0.901278	1.429583
H	-1.268946	2.058840	-0.594936
H	2.566833	-1.392737	-0.729303
H	2.073035	0.108621	-1.492669
H	0.839327	-1.987738	-2.431444
H	-1.475795	-1.879900	-1.696477
H	2.418589	1.756111	0.314969
H	2.109589	1.292301	2.002435
H	3.354944	0.452215	1.069485
H	2.354542	-1.618359	1.756710
H	0.920063	-0.946678	2.543596
H	0.751786	-2.149771	1.247692
H	-4.202467	0.526316	0.596688
H	-3.302090	-0.642835	1.602878
H	-2.787570	1.065408	1.533581
H	-1.246743	-1.289990	0.918676

TS-9bE: (one imaginary frequency, -412.94 cm^{-1})

C	-0.610613	0.757971	0.887973
C	-1.756614	0.101367	0.357119
C	-1.123068	-1.009912	-1.173858
C	-0.314480	-2.041130	-0.677036
C	0.982170	-1.865713	-0.169842
C	1.663028	-0.670049	-0.237082
H	1.356358	0.154209	-0.872440
O	2.860221	-0.561783	0.356190
C	3.528273	0.694689	0.213990
H	4.535581	0.550846	0.606802
H	3.578865	0.995540	-0.838607
H	3.010242	1.470013	0.789546
H	1.463626	-2.680782	0.365603
H	-0.769529	-3.017436	-0.520645
H	-2.067242	-1.312528	-1.620862
C	-2.422900	-0.888329	1.306297
H	-2.971914	-0.342013	2.085129
H	-3.142499	-1.527911	0.783127
H	-1.687243	-1.528971	1.802831
C	-2.766674	0.945675	-0.425644
H	-3.488505	0.318118	-0.959246
H	-3.331344	1.560713	0.287712
H	-2.266937	1.611539	-1.128854

H	-0.661603	-0.162221	-1.676425
H	-0.229354	0.434599	1.854013
C	0.062670	1.871181	0.290222
O	-0.057153	2.277860	-0.875711
H	0.796206	2.373164	0.965665

TS-9bZ: (one imaginary frequency, -444.41 cm^{-1})

C	3.073630	-0.671927	-0.971464
O	2.247443	-0.513104	0.178518
C	1.750970	0.726187	0.378581
C	0.896409	1.045395	1.422206
C	-0.050616	0.190679	1.983315
C	-0.371003	-1.060204	1.413990
H	2.282262	1.522333	-0.144576
C	-1.270614	-0.725682	-0.279930
C	-2.634387	-0.201488	0.176822
C	-1.349183	-2.167450	-0.794918
C	-0.465850	0.132740	-1.095591
C	-0.599985	1.558663	-1.250274
O	-1.328669	2.322266	-0.612007
H	3.521907	-1.663636	-0.895920
H	3.865322	0.088079	-0.992446
H	2.478655	-0.603175	-1.889981
H	0.221825	-0.343568	-1.792658
H	0.054078	1.973765	-2.055386
H	0.447222	-1.652230	1.022191
H	-1.122157	-1.653023	1.932873
H	-0.729045	0.620537	2.716784
H	0.845682	2.102720	1.665604
H	-2.554662	0.789621	0.619945
H	-3.299533	-0.116282	-0.692510
H	-3.101364	-0.895957	0.885031
H	-1.755241	-2.847534	-0.037879
H	-2.013793	-2.212217	-1.667150
H	-0.367573	-2.544203	-1.102438

Compound 9b: (No imaginary frequency)

C	-1.525341	-0.900125	0.893035
C	-0.438255	-0.908416	1.934766
C	0.770898	-0.367975	1.763547
C	1.197092	0.349246	0.510756
C	-0.003796	0.595767	-0.459438
C	-1.001199	-0.595338	-0.530841
O	2.257710	-0.400852	-0.087200
C	3.133903	0.362365	-0.891208
C	-0.595402	1.945340	-0.078441
O	-1.704182	2.169628	0.354949
C	-2.179365	-0.269354	-1.469469
H	1.614277	1.330785	0.801656
C	-0.279537	-1.839556	-1.097006
H	0.432710	0.756309	-1.458676
H	0.124552	2.788114	-0.213165

H	-2.033846	-1.874540	0.890885
H	-2.285982	-0.160491	1.175315
H	-0.672456	-1.384928	2.886111
H	1.522444	-0.427796	2.547816
H	-2.763135	0.582333	-1.114552
H	-1.820651	-0.046732	-2.482883
H	-2.848228	-1.135503	-1.543671
H	3.910921	-0.319278	-1.246439
H	2.630585	0.803188	-1.766114
H	3.605734	1.176210	-0.317581
H	-0.994828	-2.665239	-1.196646
H	0.129599	-1.633878	-2.093833
H	0.546093	-2.170496	-0.464424

TS-10aE: (one imaginary frequency, -504.10 cm^{-1})

C	1.187492	1.681381	-0.844397
C	0.489467	2.143563	0.269065
C	-0.767037	1.636867	0.602901
C	-1.362339	0.600063	-0.115755
C	0.201350	-1.017220	0.075390
C	1.382926	-0.493233	-0.508335
C	2.642081	-0.287376	0.229215
O	3.748693	-0.357557	-0.279861
H	2.535090	-0.052936	1.309587
C	0.103645	-1.221351	1.576418
H	-0.941662	-1.357598	1.872198
H	0.507866	-0.377547	2.141599
H	0.655485	-2.122667	1.881677
C	-0.556664	-2.055043	-0.732735
H	-1.602254	-2.120090	-0.413787
H	-0.523116	-1.845226	-1.808105
H	-0.111971	-3.049351	-0.581860
O	-2.516977	0.047115	0.382049
H	-1.242966	0.512483	-1.193648
H	-1.222520	1.899766	1.554723
H	1.003779	2.771601	0.993506
H	0.649223	1.396002	-1.742319
H	2.205297	2.013624	-1.027344
H	1.558772	-0.731634	-1.556972
C	-3.597858	-0.032605	-0.541353
H	-4.392292	-0.594905	-0.045952
H	-3.967351	0.968146	-0.802225
H	-3.303496	-0.556399	-1.461066

TS-10aZ: (one imaginary frequency, -516.67 cm^{-1})

C	-0.158510	-1.877823	0.895081
C	0.733659	-1.273352	1.763256
C	1.536474	-0.190638	1.383252
C	1.450440	0.422429	0.125481
O	1.320008	-0.329459	-1.040684
C	2.577143	-0.707752	-1.593469
H	2.023327	1.342094	-0.029100

C	-1.401531	0.089022	0.271868
C	-0.532129	1.201531	0.135602
C	-0.429970	1.931311	-1.202196
C	-0.491635	2.140329	1.333185
C	-2.049889	-0.602514	-0.844299
O	-3.033306	-1.320195	-0.723521
H	0.046238	-1.925960	-0.162815
H	-0.923689	-2.551928	1.269794
H	0.658151	-1.492148	2.827511
H	2.014059	0.390150	2.169757
H	2.360346	-1.253035	-2.515221
H	3.138723	-1.352941	-0.905026
H	3.188677	0.175305	-1.831296
H	-0.250097	1.256895	-2.039762
H	0.383923	2.664794	-1.180358
H	-1.358269	2.484906	-1.395691
H	0.377894	2.807177	1.300655
H	-0.468167	1.587132	2.276987
H	-1.389506	2.774116	1.343306
H	-1.909901	-0.051023	1.221537
H	-1.589641	-0.453558	-1.843197

Compound 10a: (No imaginary frequency)

C	1.239460	1.773282	0.040142
C	-0.158901	2.326126	-0.024895
C	-1.237216	1.561382	-0.206418
C	-1.177354	0.057999	-0.363424
C	0.120028	-0.556010	0.230871
C	1.304759	0.282765	-0.361752
O	-2.299290	-0.564700	0.266181
C	-3.470724	-0.589413	-0.523478
C	0.076639	-0.506145	1.772048
C	2.657833	-0.287488	0.018247
O	3.410137	-0.845632	-0.750473
H	1.244368	0.206979	-1.454916
C	0.231681	-2.021191	-0.229584
H	-0.020188	0.515948	2.150007
H	1.902861	2.352865	-0.616762
H	1.640030	1.917065	1.056492
H	-0.268596	3.403114	0.095984
H	-2.226243	2.013960	-0.243862
H	2.947705	-0.149208	1.085458
H	-1.203312	-0.195503	-1.439082
H	-0.785480	-1.073349	2.132015
H	0.977751	-0.951629	2.207663
H	-4.230997	-1.121442	0.054670
H	-3.848112	0.418902	-0.752421
H	-3.306245	-1.120502	-1.474487
H	-0.666169	-2.573249	0.063794
H	0.339530	-2.090703	-1.318913

H	1.099089	-2.518442	0.218152

TS-10bE: (one imaginary frequency, -519.31 cm^{-1})

C	1.221543	1.777289	-0.542536
C	0.239711	2.312484	0.287353
C	-1.018774	1.720839	0.405980
C	-1.340899	0.533990	-0.250603
C	0.266784	-0.868241	0.531921
C	1.509237	-0.203211	0.352729
H	1.966625	0.234774	1.235622
C	-0.243951	-0.980457	1.955598
H	-1.326956	-1.141704	1.979062
H	-0.011224	-0.082249	2.536035
H	0.230343	-1.834395	2.462670
C	-0.131176	-2.041614	-0.348635
H	-1.204382	-2.235371	-0.253864
H	0.096974	-1.891665	-1.408462
H	0.388689	-2.956267	-0.029191
O	-2.533907	-0.075069	0.052488
H	-0.953878	0.310448	-1.242381
H	-1.708517	2.062136	1.174356
H	0.518963	3.079815	1.006566
H	0.940683	1.321932	-1.487729
H	2.229890	2.180909	-0.528910
C	2.511985	-0.613314	-0.644514
C	-3.344172	-0.414892	-1.067982
H	-4.186374	-0.992936	-0.681631
H	-3.720105	0.486699	-1.569876
H	-2.790286	-1.024368	-1.795084
O	3.707069	-0.388659	-0.544103
H	2.122524	-1.145176	-1.540129

TS-10bZ: (one imaginary frequency, -516.67 cm^{-1})

C	-0.332415	-1.993940	-0.248073
C	0.152063	-1.858552	1.041148
C	1.023249	-0.828397	1.416903
C	1.436278	0.186327	0.542647
C	-0.384193	1.188573	0.111741
C	-1.159441	0.268065	-0.634351
C	-2.458971	-0.270895	-0.226176
O	-3.299072	-0.695893	-1.007728
H	-2.670105	-0.252356	0.864409
C	-0.850959	1.608058	1.499591
H	-0.065683	2.168389	2.019521
H	-1.127380	0.755905	2.125286
H	-1.727354	2.266349	1.426679
C	0.238549	2.326976	-0.691877
H	1.014290	2.851156	-0.121454
H	0.679177	1.963600	-1.622479
H	-0.534936	3.065389	-0.941840
H	2.013278	1.012999	0.968966
O	1.791251	-0.089543	-0.776452

C	3.167017	-0.430801	-0.912736
H	3.816312	0.383598	-0.558217
H	3.343568	-0.591657	-1.979000
H	3.409160	-1.345434	-0.355465
H	1.149539	-0.629746	2.479153
H	-0.311923	-2.439389	1.836795
H	0.240614	-1.658475	-1.098373
H	-1.158395	-2.668141	-0.454561
H	-0.994667	0.228813	-1.708891

Compound 10b: (No imaginary frequency)

C	0.820846	1.803327	-0.445951
C	-0.592962	2.209000	-0.134083
C	-1.529927	1.355206	0.285067
C	-1.272309	-0.128307	0.453824
C	0.230646	-0.451855	0.663664
C	1.017819	0.272185	-0.484312
O	-1.723774	-0.872441	-0.683889
C	-3.121566	-0.853720	-0.887502
C	0.653827	0.037009	2.065907
C	2.498206	-0.051641	-0.463603
O	3.053030	-0.803052	-1.235532
H	-1.823082	-0.490307	1.340695
H	0.622911	-0.120147	-1.427144
C	0.449951	-1.974213	0.583204
H	0.494211	1.110192	2.205514
H	1.124396	2.234077	-1.410160
H	1.494941	2.259332	0.297851
H	-0.832315	3.266248	-0.245264
H	-2.531944	1.719420	0.503157
H	3.085572	0.467727	0.330295
H	-3.331729	-1.562890	-1.692639
H	-3.667641	-1.170605	0.016236
H	-3.489260	0.138139	-1.187876
H	0.072795	-0.485807	2.835113
H	1.710023	-0.180199	2.258592
H	-0.196119	-2.489005	1.304795
H	0.218456	-2.360528	-0.411289
H	1.487540	-2.233655	0.820208

TS-11aE: (one imaginary frequency, -427.16 cm^{-1})

H	4.311898	1.170238	-0.263752
C	3.521756	0.540362	-0.674697
H	2.953198	1.108842	-1.420546
O	2.697088	0.195824	0.434489
C	1.621723	-0.615580	0.271522
C	1.655436	-1.565886	-0.892985
C	0.829811	-0.692721	1.413826
C	-0.457303	-1.211174	1.565452
C	-1.349188	-1.585403	0.538524
H	3.974027	-0.338866	-1.146433
C	-1.912548	0.019415	-0.412433

C	-2.781606	-0.644857	-1.486215
C	-0.744738	0.662685	-0.924888
C	-0.088264	1.823330	-0.387420
O	-0.332570	2.420688	0.664058
C	-2.746378	0.758196	0.632530
H	-0.380855	0.333401	-1.897752
H	0.726684	2.205924	-1.052066
H	-0.971789	-2.106287	-0.333916
H	-2.300804	-1.996580	0.872607
H	-0.885353	-1.084935	2.557936
H	1.235468	-0.140652	2.258607
H	-2.126613	1.142134	1.440721
H	-3.234083	1.622652	0.163695
H	-3.532676	0.107526	1.033761
H	-3.516348	-1.331538	-1.051069
H	-3.336508	0.127176	-2.034024
H	-2.180151	-1.199937	-2.215030
H	1.674591	-1.060553	-1.862361
H	2.570554	-2.172140	-0.820577
H	0.810405	-2.248718	-0.877481

TS-11aZ: (one imaginary frequency, -359.45 cm^{-1})

H	2.340267	1.865184	-1.616099
C	2.691399	1.162065	-0.863640
H	3.677208	0.766870	-1.135703
O	1.723089	0.104110	-0.861497
C	1.714338	-0.831872	0.088929
C	2.801991	-0.839750	1.127973
C	0.803606	-1.885066	-0.006948
C	-0.368865	-1.928068	-0.763683
C	-1.056761	-0.788884	-1.251401
H	2.730510	1.677011	0.096972
C	-1.936545	0.054149	0.164792
C	-2.645084	1.172686	-0.616718
C	-0.977376	0.483743	1.147875
C	-0.090480	1.584153	1.032622
O	0.104994	2.302642	0.032928
C	-2.930360	-0.980837	0.699269
H	-0.886534	-0.102290	2.060860
H	0.513056	1.773597	1.953961
H	-0.455877	0.053092	-1.579499
H	-1.887551	-1.008357	-1.921748
H	-0.904052	-2.876569	-0.758464
H	1.029188	-2.741079	0.624991
H	-2.422235	-1.794322	1.227776
H	-3.620086	-0.503121	1.406961
H	-3.531726	-1.416896	-0.107066
H	-3.231596	0.769222	-1.450415
H	-3.338598	1.689274	0.058864
H	-1.925853	1.902494	-0.988600
H	2.683890	-1.699267	1.790297
H	3.797876	-0.889490	0.668738

H	2.772267	0.066705	1.742318

Compound 11a: (No imaginary frequency)

C	1.038485	-0.535642	0.076801
C	-0.054344	0.363429	-0.612864
C	-1.528266	-0.127924	-0.418491
C	-1.836111	-0.295113	1.088394
C	-0.709902	-0.932981	1.855745
C	0.547775	-1.025412	1.419336
C	-2.503284	0.887996	-1.051101
C	-1.763396	-1.481802	-1.127186
C	0.179730	1.798285	-0.121273
O	-0.416682	2.349016	0.777581
C	1.499719	-1.723849	-0.786036
O	2.186375	0.291750	0.418278
C	3.118397	0.601972	-0.603527
H	0.154566	0.382242	-1.693149
H	0.962541	2.353246	-0.681062
H	-2.750915	-0.894234	1.204699
H	-2.047716	0.683424	1.535930
H	-0.947964	-1.311678	2.849100
H	1.320982	-1.469099	2.043610
H	-2.424181	1.876125	-0.592706
H	-2.319858	0.989235	-2.128919
H	-3.536497	0.542082	-0.926274
H	-2.839289	-1.688821	-1.169498
H	-1.388973	-1.473157	-2.158137
H	-1.296456	-2.315498	-0.596395
H	0.702093	-2.454468	-0.920043
H	1.831287	-1.405089	-1.780295
H	2.336255	-2.227199	-0.288157
H	3.795928	1.344551	-0.173018
H	3.708538	-0.270355	-0.913483
H	2.649301	1.038809	-1.497863

TS-11bE: (one imaginary frequency, -399.44 cm^{-1})

C	1.246864	-1.070944	1.075233
C	0.397603	-2.028066	0.477409
C	-0.863448	-1.778337	-0.067952
C	-1.696582	-0.690306	0.191703
O	-2.703046	-0.553093	-0.696286
C	-3.605728	0.550465	-0.604964
C	-1.704760	0.123743	1.445836
C	2.003429	0.060815	-0.305429
C	2.887761	0.942628	0.582375
C	0.929005	0.701622	-0.999461
C	0.180252	1.829503	-0.575273
O	0.196204	2.383478	0.544708
C	2.819050	-0.900021	-1.169391
H	-4.174902	0.534171	-1.535540
H	-4.295077	0.439231	0.239579
H	-3.064625	1.497960	-0.519216

H	-2.733783	0.295796	1.777781
H	-1.212545	1.104459	1.329657
H	-1.183103	-0.417489	2.237263
H	-1.228016	-2.454044	-0.839943
H	0.849569	-2.978836	0.198460
H	2.146523	-1.468839	1.542893
H	3.441942	-0.329340	-1.870772
H	3.488966	-1.520946	-0.563503
H	2.174558	-1.560542	-1.758231
H	3.544415	0.340873	1.220743
H	3.528649	1.558172	-0.062389
H	2.286143	1.613397	1.195949
H	0.811538	-0.249181	1.633036
H	0.636546	0.289367	-1.963522
H	-0.522745	2.216103	-1.350126

TS-11bZ: (one imaginary frequency, -374.27 cm^{-1})

C	2.464976	-1.704173	-0.767119
O	1.822922	-1.082269	0.342610
C	1.762467	0.269699	0.412750
C	0.925759	0.864620	1.351322
C	-0.243144	0.332372	1.894296
C	-0.864903	-0.854124	1.428747
C	2.821928	1.066170	-0.298242
C	-1.656124	-0.546871	-0.249399
C	-2.925316	0.235428	0.117602
C	-1.986345	-1.986997	-0.663940
C	-0.731117	0.099808	-1.141208
C	-0.531901	1.510055	-1.267230
O	-1.048617	2.405057	-0.582969
H	2.380287	-2.777688	-0.591157
H	3.523934	-1.432774	-0.832859
H	1.958417	-1.446555	-1.704936
H	-0.167035	-0.526095	-1.831324
H	0.183744	1.790777	-2.077883
H	-0.200867	-1.667415	1.161681
H	-1.725675	-1.187259	2.007287
H	-0.811367	0.990933	2.546992
H	1.133377	1.911096	1.551541
H	-2.684660	1.235358	0.474795
H	-3.550815	0.346296	-0.777527
H	-3.513344	-0.304750	0.869262
H	-2.511259	-2.526503	0.132615
H	-2.640713	-1.978805	-1.544415
H	-1.083607	-2.552367	-0.921358
H	2.672895	2.131730	-0.116443
H	3.826492	0.788664	0.052593
H	2.798075	0.907126	-1.381465

Compound 11b: (No imaginary frequency)

C	-1.259603	-0.715452	-0.202775
C	-1.723302	-0.262155	1.201089

C	-0.580237	0.067812	2.119584
C	0.669533	0.300322	1.715252
C	1.129091	0.284766	0.274337
C	-0.109836	0.216723	-0.704957
O	1.927134	-0.913247	0.162715
C	2.751004	-1.069131	-0.977277
C	-0.559720	1.633308	-1.042173
O	-1.469901	2.244013	-0.522703
C	-2.447623	-0.670132	-1.186026
C	-0.770763	-2.180428	-0.136400
C	2.012625	1.526795	0.031625
H	0.271299	-0.187932	-1.653993
H	0.040881	2.123733	-1.841745
H	-2.337375	-1.054553	1.652442
H	-2.372045	0.618141	1.113126
H	-0.805907	0.126546	3.183902
H	1.450612	0.518698	2.441550
H	-2.884955	0.328350	-1.262200
H	-2.139421	-0.991416	-2.189611
H	-3.235006	-1.356528	-0.851837
H	3.151375	-2.084959	-0.921194
H	2.197193	-0.969762	-1.923016
H	3.592331	-0.362590	-0.991369
H	-1.613442	-2.833308	0.122875
H	-0.385008	-2.510329	-1.109157
H	0.021499	-2.323369	0.599332
H	2.335368	1.621444	-1.010635
H	1.481276	2.442924	0.307058
H	2.906446	1.454211	0.660696

TS-12aE: (one imaginary frequency, -495.99 cm^{-1})

C	1.291074	-1.831519	0.458663
C	0.414019	-2.047061	-0.603777
C	-0.803872	-1.387676	-0.750259
C	-1.329514	-0.402881	0.106857
C	0.433916	1.055662	-0.050861
C	1.569334	0.379594	0.472244
C	2.823061	0.193967	-0.279940
O	3.926521	0.139349	0.238719
H	2.715474	0.108096	-1.382001
C	0.346064	1.342471	-1.539301
H	-0.676355	1.617498	-1.813905
H	0.645000	0.486390	-2.149411
H	1.001857	2.184790	-1.804136
C	-0.169643	2.152444	0.808250
H	-1.222538	2.321653	0.559812
H	-0.081203	1.940765	1.878415
H	0.365151	3.094943	0.621281
O	-2.335042	0.366369	-0.481097
C	-1.452925	-0.518450	1.613707
H	-1.281281	-1.437375	-1.727143
H	0.793472	-2.575852	-1.476581

H	0.934011	-1.698769	1.469639
H	2.296305	-2.240822	0.406819
H	1.752329	0.488286	1.541081
C	-3.681138	-0.006221	-0.199095
H	-4.312136	0.654345	-0.798191
H	-3.870956	-1.049373	-0.488711
H	-3.937634	0.122720	0.860174
H	-1.873306	0.401065	2.029081
H	-2.121446	-1.346844	1.883639
H	-0.500828	-0.699240	2.110234

TS-12aZ: (one imaginary frequency, -527.54 cm^{-1})

C	-0.723001	-1.711338	0.754796
C	0.276870	-1.394362	1.680180
C	1.311620	-0.512392	1.376394
C	1.512846	0.087384	0.125651
O	1.238060	-0.610830	-1.054988
C	2.068925	-1.753587	-1.272068
C	2.583093	1.135648	-0.055940
C	-1.553414	0.206882	0.333716
C	-0.585510	1.206882	0.034366
C	-0.432691	1.723505	-1.385611
C	-0.358169	2.246395	1.115076
C	-2.479788	-0.317441	-0.689620
O	-3.592194	-0.750817	-0.441775
H	-0.466107	-1.856230	-0.285080
H	-1.604199	-2.252793	1.089379
H	0.101764	-1.619234	2.730756
H	1.878954	-0.094135	2.205904
H	1.787699	-2.153140	-2.249562
H	1.910358	-2.517793	-0.501824
H	3.131778	-1.478178	-1.290974
H	3.526199	0.675599	-0.384600
H	2.304484	1.861830	-0.825409
H	2.781084	1.672772	0.876037
H	-0.254846	0.924628	-2.108054
H	0.400867	2.429362	-1.457116
H	-1.332963	2.274030	-1.694652
H	0.569997	2.807266	0.960394
H	-0.329927	1.791675	2.110571
H	-1.178872	2.980285	1.114548
H	-2.019730	0.261312	1.314635
H	-2.098153	-0.319528	-1.732481

Compound 12a: (No imaginary frequency)

C	1.428653	0.316682	-0.285096
C	1.329867	1.807688	0.099251
C	-0.080529	2.324599	0.025883
C	-1.147372	1.537768	-0.125517
C	-1.093758	0.026544	-0.273329
C	0.256117	-0.536547	0.315237
O	-2.116009	-0.583978	0.545531

C	-3.469461	-0.438164	0.163416
C	0.233156	-0.434545	1.858820
C	0.440568	-2.019125	-0.065756
C	2.792423	-0.221984	0.107142
O	3.541694	-0.803443	-0.647360
H	1.390726	0.226439	-1.375810
H	0.028691	0.582414	2.204874
H	1.980977	2.398292	-0.560157
H	1.722309	1.970231	1.116021
H	-0.213274	3.401956	0.119134
H	-2.136450	1.988706	-0.176771
H	3.095898	-0.034459	1.162723
C	-1.312339	-0.342093	-1.755916
H	-0.547295	-1.081474	2.263082
H	1.190463	-0.757383	2.282701
H	-4.056412	-0.898760	0.963013
H	-3.780847	0.612581	0.072974
H	-3.702191	-0.952611	-0.779018
H	-0.459963	-2.586120	0.188889
H	0.649921	-2.153898	-1.131944
H	1.280212	-2.457928	0.484144
H	-1.486829	-1.415860	-1.874918
H	-2.176167	0.192262	-2.164806
H	-0.449196	-0.059952	-2.364304

TS-12bE: (one imaginary frequency, -521.77 cm^{-1})

C	1.281077	1.908656	-0.054671
C	0.158952	2.166193	0.732502
C	-1.022787	1.434898	0.645012
C	-1.263800	0.353260	-0.221716
C	0.454300	-0.980120	0.512785
C	1.655329	-0.220696	0.412384
H	2.107288	0.104100	1.345670
C	-0.048804	-1.219165	1.925153
H	-1.107591	-1.494002	1.931953
H	0.089314	-0.335378	2.555473
H	0.516259	-2.043505	2.385499
C	0.175145	-2.151062	-0.415903
H	-0.892064	-2.393172	-0.412430
H	0.488115	-1.985224	-1.448968
H	0.711880	-3.039431	-0.052842
O	-2.357827	-0.433745	0.145632
C	-0.988287	0.350459	-1.714692
H	-1.729661	1.527235	1.467623
H	0.293877	2.773895	1.626000
H	1.184336	1.691099	-1.108765
H	2.236207	2.354546	0.210024
C	2.653943	-0.404319	-0.651556
C	-3.609925	-0.089429	-0.440270
H	-4.348627	-0.768912	-0.008722
H	-3.886137	0.947109	-0.200285
H	-3.606709	-0.213325	-1.531044

H	-1.356253	-0.578623	-2.157735
H	-1.498273	1.188020	-2.208532
H	0.070885	0.430213	-1.958678
O	3.829794	-0.094382	-0.545614
H	2.280562	-0.831679	-1.608536

TS-12bZ: (one imaginary frequency, -509.67 cm^{-1})

C	-0.662851	-1.879830	-0.032463
C	-0.048285	-1.669100	1.204951
C	0.946453	-0.709470	1.382083
C	1.468817	0.105311	0.366711
C	-0.567044	1.137592	-0.205500
C	-1.423613	0.067227	-0.582099
C	-2.705807	-0.203919	0.097413
O	-3.695001	-0.643669	-0.463915
H	-2.728513	0.013599	1.186716
C	-0.830321	1.902081	1.079339
H	0.002155	2.573485	1.314149
H	-0.984176	1.240499	1.936374
H	-1.728747	2.530156	0.983270
C	-0.033207	1.974253	-1.353350
H	0.748041	2.670581	-1.031903
H	0.370738	1.345877	-2.151600
H	-0.842420	2.586027	-1.777929
C	2.450931	1.200231	0.708779
H	2.275558	1.598833	1.712161
H	2.398116	2.022636	-0.010024
H	3.482073	0.820026	0.676163
O	1.645079	-0.387065	-0.931456
C	2.611910	-1.433939	-1.038294
H	3.595706	-1.112022	-0.671728
H	2.689405	-1.669163	-2.102680
H	2.299055	-2.327771	-0.485147
H	1.187504	-0.415425	2.402026
H	-0.510992	-2.086816	2.097148
H	-0.086355	-1.810530	-0.943133
H	-1.538342	-2.521175	-0.089689
H	-1.471324	-0.155564	-1.646625

Compound 12b: (No imaginary frequency)

C	1.204905	0.403153	-0.321579
C	1.053092	1.843659	0.207393
C	-0.378816	2.197921	0.488097
C	-1.369623	1.303775	0.489636
C	-1.185840	-0.182531	0.216423
C	0.307655	-0.618180	0.466224
O	-1.421596	-0.494748	-1.178831
C	-2.530918	0.108607	-1.815802
C	0.634200	-0.612519	1.975995
C	0.564597	-2.035519	-0.086635
C	2.673292	0.026763	-0.322902
O	3.282968	-0.370404	-1.292118

C	-2.193940	-0.972119	1.071029
H	0.875493	0.366210	-1.364010
H	0.377604	0.335666	2.458431
H	1.473318	2.548993	-0.523032
H	1.648125	1.987282	1.124094
H	-0.593109	3.242374	0.713259
H	-2.384268	1.633581	0.709472
H	3.201676	0.160476	0.650432
H	-2.553915	-0.300006	-2.829770
H	-3.486924	-0.130127	-1.326215
H	-2.431953	1.201073	-1.876141
H	0.089129	-1.408459	2.492911
H	1.699793	-0.801843	2.143777
H	-0.099747	-2.770553	0.379428
H	0.413214	-2.076807	-1.166896
H	1.592968	-2.348192	0.126754
H	-2.086963	-2.049293	0.918745
H	-2.080607	-0.752115	2.136681
H	-3.216443	-0.695102	0.792402

TS-11aE(ac): (one imaginary frequency, -446.06 cm^{-1})

C	-2.884770	0.156305	0.389100
O	-2.148249	-0.354219	-0.646756
C	-0.907666	-0.962034	-0.439452
C	-0.098207	-0.878951	-1.564082
C	1.265522	-1.169613	-1.629484
C	2.087765	-1.400531	-0.505592
C	2.240774	0.234603	0.526412
C	0.925257	0.718861	0.806033
C	0.232098	1.757795	0.080871
O	0.567371	2.267675	-0.990912
H	-0.698275	2.101729	0.584031
H	0.453596	0.412101	1.736298
C	2.970515	-0.316044	1.757200
H	2.313547	-0.932056	2.380917
H	3.328922	0.517567	2.373983
H	3.843642	-0.916643	1.478416
C	3.158812	1.084701	-0.355635
H	3.416540	2.010996	0.173858
H	2.672152	1.369098	-1.286511
H	4.093641	0.552001	-0.565924
H	3.131982	-1.624071	-0.718598
H	1.702293	-1.998272	0.311612
H	1.753698	-0.953538	-2.576757
H	-0.545452	-0.378097	-2.418984
C	-0.879772	-2.011420	0.641707
H	-0.097217	-2.745181	0.445243
H	-1.840643	-2.542103	0.618673
H	-0.765821	-1.605662	1.646917
C	-4.192983	0.693158	-0.134142
H	-4.729395	-0.081456	-0.691153
H	-4.799048	1.044659	0.701232

H	-4.000805	1.520305	-0.825990
O	-2.511300	0.187500	1.537058

TS-11aZ(ac): (one imaginary frequency, -372.11 cm^{-1})

C	2.664671	-1.579481	1.336565
C	2.439983	-0.558796	0.256959
O	3.030881	-0.461998	-0.785351
O	1.436311	0.325326	0.666086
C	1.050409	1.437722	-0.016059
C	1.959057	2.063807	-1.036757
C	-0.063712	2.121161	0.458211
C	-1.114195	1.634975	1.242745
C	-1.461545	0.268969	1.377971
C	-2.262224	-0.316242	-0.203589
C	-2.728940	-1.707272	0.260276
C	-1.274336	-0.297776	-1.248934
C	-0.169027	-1.182294	-1.354772
O	0.203277	-2.003780	-0.492252
C	-3.445630	0.618440	-0.462896
H	-1.353407	0.465736	-2.020280
H	0.433364	-1.071438	-2.281851
H	-0.657862	-0.460611	1.405871
H	-2.246724	0.069949	2.106826
H	-1.847866	2.373953	1.560690
H	-0.140197	3.149665	0.111131
H	-3.114990	1.617356	-0.765453
H	-4.067669	0.213136	-1.271152
H	-4.080723	0.719462	0.424802
H	-3.364170	-1.637749	1.150507
H	-3.326707	-2.160910	-0.540083
H	-1.878610	-2.357728	0.463249
H	1.559458	3.040891	-1.320178
H	2.972047	2.193439	-0.639031
H	2.055322	1.441760	-1.928332
H	3.547968	-2.168765	1.087646
H	2.792646	-1.094118	2.308965
H	1.787304	-2.229691	1.380492

Compound 11a(ac): (No imaginary frequency)

C	-0.217946	-1.316256	1.371226
C	0.412587	-0.824927	0.091715
C	-0.422125	0.343276	-0.538875
C	-1.974153	0.149000	-0.423846
C	-2.379383	-0.075000	1.051350
C	-1.447550	-1.000867	1.782636
C	0.695474	-1.995312	-0.864207
O	1.736013	-0.327375	0.566025
C	2.664558	0.148224	-0.292896
C	0.053731	1.665478	0.076935
O	-0.405665	2.191830	1.067458
C	-2.689603	1.395163	-0.987830
C	-2.447406	-1.061818	-1.260826

H	-0.155606	0.397309	-1.600514
H	0.890556	2.147060	-0.469571
H	-3.403289	-0.473820	1.088167
H	-2.400066	0.883320	1.584131
H	-1.804120	-1.415145	2.724840
H	0.412505	-1.976044	1.964038
H	-2.439303	2.303289	-0.434170
H	-2.432868	1.551178	-2.043507
H	-3.776192	1.259250	-0.931107
H	-3.540341	-1.041017	-1.346174
H	-2.036293	-1.038998	-2.277125
H	-2.179300	-2.016616	-0.800696
H	-0.224702	-2.519654	-1.123082
H	1.176865	-1.648752	-1.780134
H	1.359465	-2.709684	-0.364880
C	3.958105	0.427795	0.439625
O	2.482192	0.346949	-1.476500
H	4.686598	0.844471	-0.256769
H	3.779892	1.129785	1.260675
H	4.348149	-0.495699	0.879971

TS-11bE(ac): (one imaginary frequency, -389.76 cm^{-1})

C	-1.830062	-1.174204	-0.953152
C	-0.835332	-2.028555	-0.413455
C	0.414519	-1.583595	0.023324
C	1.032912	-0.396847	-0.339067
C	0.936214	0.330053	-1.638936
O	2.033698	0.037386	0.530016
C	3.363990	-0.076733	0.184587
C	-2.513895	-0.077693	0.410517
C	-3.106079	-1.048276	1.436259
C	-3.606104	0.660338	-0.377705
C	-1.441462	0.722703	0.933465
C	-0.927192	1.938763	0.394939
O	-1.179213	2.430487	-0.719774
C	4.219494	0.611810	1.216753
O	3.749494	-0.654521	-0.799488
H	1.942923	0.589814	-1.977512
H	0.346769	1.257323	-1.571199
H	0.479408	-0.310904	-2.396755
H	0.918311	-2.156938	0.800232
H	-1.147014	-3.013211	-0.071223
H	-2.727275	-1.677914	-1.312057
H	-3.693901	-0.492188	2.177432
H	-3.774150	-1.776555	0.962190
H	-2.325044	-1.595763	1.973421
H	-4.283986	-0.045898	-0.869737
H	-4.202892	1.259325	0.321520
H	-3.174609	1.336229	-1.115547
H	-1.520439	-0.368488	-1.611202
H	-0.986480	0.405627	1.869565
H	-0.191643	2.448953	1.055023

H	5.270856	0.418952	1.001704
H	4.029157	1.690392	1.192340
H	3.966155	0.257837	2.220589

TS-11bZ(ac): (one imaginary frequency, -431.05 cm^{-1})

C	-2.440883	0.542745	-0.324251
O	-1.672960	0.015617	0.681805
C	-0.952589	-1.171871	0.560140
C	0.104982	-1.369011	1.439184
C	0.954591	-0.394976	1.961876
C	0.960278	0.948557	1.517547
C	-1.655802	-2.316819	-0.110616
C	1.612956	1.023499	-0.275551
C	3.121057	0.826548	-0.076427
C	1.272695	2.478125	-0.624381
C	0.915160	0.067384	-1.085152
C	1.337269	-1.285859	-1.342647
O	2.280186	-1.881993	-0.813186
C	-3.252993	1.695965	0.212033
O	-2.442682	0.148314	-1.464819
H	0.050959	0.402942	-1.651709
H	0.711311	-1.812892	-2.098083
H	-0.003079	1.411471	1.341983
H	1.659072	1.613479	2.023067
H	1.799545	-0.751830	2.545696
H	0.393461	-2.406941	1.578389
H	3.350621	-0.174672	0.282980
H	3.634011	0.955597	-1.037979
H	3.520380	1.577047	0.615879
H	1.603701	3.170625	0.157838
H	1.781230	2.763367	-1.553596
H	0.197332	2.621003	-0.778356
H	-1.067890	-3.230067	0.005156
H	-2.644115	-2.474066	0.345364
H	-1.815910	-2.127531	-1.173054
H	-3.866251	2.107436	-0.590056
H	-3.889785	1.360204	1.036858
H	-2.591259	2.473602	0.608695

Compound 11b(ac): (No imaginary frequency)

C	0.499520	-0.213427	-0.647393
C	1.322342	1.039049	-0.208524
C	2.156755	0.705718	1.049263
C	1.380430	-0.069491	2.075863
C	0.236381	-0.712462	1.832223
C	-0.430131	-0.792962	0.479506
C	2.252466	1.490719	-1.353621
C	0.373656	2.218710	0.105444
O	-1.643700	0.041998	0.636973
C	-2.548894	0.182039	-0.356856
C	-0.891230	-2.241441	0.233828
C	1.346972	-1.357445	-1.201654

O	2.506758	-1.589714	-0.933687
H	-0.164225	0.064757	-1.473729
H	0.805173	-2.015472	-1.915072
H	2.526630	1.637874	1.499833
H	3.044906	0.126983	0.767016
H	1.796699	-0.109461	3.081889
H	-0.275739	-1.245003	2.631712
H	2.990465	0.728053	-1.612103
H	1.674693	1.734360	-2.254497
H	2.794955	2.396853	-1.058021
C	-3.686012	1.070708	0.098024
H	0.965445	3.121049	0.301215
H	-0.282689	2.434939	-0.746920
H	-0.254087	2.027360	0.978008
H	-1.368205	-2.357962	-0.740260
H	-0.043747	-2.930173	0.310044
H	-1.612662	-2.515546	1.010962
O	-2.462386	-0.314774	-1.461267
H	-4.447128	1.112119	-0.682016
H	-4.119038	0.691271	1.028677
H	-3.310351	2.079627	0.300494

TS-12aE(ac): (one imaginary frequency, -498.49 cm^{-1})

C	1.752918	-1.868230	0.277721
C	0.816672	-1.966697	-0.753576
C	-0.369667	-1.238915	-0.776851
C	-0.794302	-0.352731	0.223551
C	1.013603	1.078176	0.087313
C	2.147079	0.296451	0.442665
C	3.325297	0.144274	-0.434964
O	4.462191	-0.007584	-0.022210
H	3.121048	0.178343	-1.525606
C	0.823069	1.529352	-1.348852
H	-0.200585	1.881045	-1.506957
H	1.030617	0.735636	-2.070893
H	1.499186	2.366743	-1.574154
C	0.518237	2.087135	1.108074
H	-0.534260	2.340872	0.947501
H	0.653592	1.742586	2.137901
H	1.095194	3.017097	1.002374
O	-1.815493	0.535678	-0.173547
C	-0.796478	-0.620316	1.717383
H	-0.888720	-1.159333	-1.729939
H	1.131023	-2.426214	-1.688586
H	1.444486	-1.815021	1.312319
H	2.735657	-2.311755	0.142771
H	2.427589	0.294684	1.495684
C	-3.156318	0.225887	-0.249976
O	-3.916574	1.097013	-0.584495
C	-3.584018	-1.182920	0.102341
H	-1.381850	0.152085	2.222192
H	-1.245524	-1.596074	1.941478

H	0.199099	-0.611877	2.161685
H	-4.607381	-1.320951	-0.248034
H	-2.930011	-1.940670	-0.336375
H	-3.566714	-1.316845	1.189686

TS-12aZ(ac): (one imaginary frequency, -530.34 cm^{-1})

C	-0.691113	-1.097234	1.624583
C	-0.116657	0.003253	2.263345
C	0.610002	0.971215	1.574737
C	0.888766	0.954173	0.205081
O	1.149119	-0.289367	-0.432859
C	2.391031	-0.849958	-0.258808
C	1.595583	2.106173	-0.456955
C	-1.974146	-0.134684	0.166514
C	-1.350420	0.933657	-0.536868
C	-1.050092	0.802945	-2.020874
C	-1.759347	2.327443	-0.099849
C	-2.344437	-1.404904	-0.484223
O	-3.250450	-2.126336	-0.102101
H	-0.158881	-1.609524	0.836623
H	-1.409712	-1.711408	2.160899
H	-0.456480	0.254871	3.266100
H	0.790147	1.919486	2.077014
C	2.472853	-2.161452	-1.003952
O	3.274246	-0.353449	0.395170
H	2.678679	2.009606	-0.315253
H	1.402817	2.130052	-1.533470
H	1.276827	3.059213	-0.025562
H	-0.483741	-0.097697	-2.265512
H	-0.482599	1.665410	-2.383735
H	-1.986173	0.780805	-2.596944
H	-1.078230	3.096169	-0.479946
H	-1.804036	2.408226	0.991022
H	-2.761623	2.565907	-0.486564
H	-2.671549	0.141333	0.953498
H	-1.726658	-1.701779	-1.358618
H	3.488797	-2.551495	-0.935213
H	1.774329	-2.885249	-0.569464
H	2.192618	-2.024471	-2.052936

Compound 12a(ac): (No imaginary frequency)

C	-0.722039	-0.570088	-0.170784
C	-1.987249	0.296759	0.165559
C	-1.945855	1.682061	-0.512118
C	-0.579340	2.305358	-0.455721
C	0.522818	1.654038	-0.079094
C	0.529494	0.210640	0.383998
C	-3.281470	-0.411466	-0.194718
O	-4.036002	-0.909305	0.611892
O	1.671860	-0.508060	-0.216451
C	2.954985	-0.130105	-0.023698
C	0.675966	0.146591	1.915286

C	-0.588334	-0.775214	-1.698783
C	-0.846085	-1.955227	0.494370
H	-2.026183	0.428838	1.251943
H	-0.406574	0.163134	-2.230059
H	-2.679321	2.344393	-0.032036
H	-2.268228	1.605951	-1.563151
H	-0.505788	3.352088	-0.747868
H	1.477452	2.166889	-0.034461
H	-3.525928	-0.438078	-1.281409
H	0.244373	-1.446734	-1.917840
H	-1.496518	-1.231745	-2.106705
C	3.886144	-1.077129	-0.750849
H	0.101333	-2.498566	0.421593
H	-1.128976	-1.886619	1.549161
H	-1.612870	-2.555438	-0.006802
H	0.882673	-0.875629	2.245587
H	1.499141	0.786400	2.236192
H	-0.238177	0.492834	2.405319
O	3.319643	0.826480	0.626219
H	4.919338	-0.786860	-0.557037
H	3.717624	-2.106541	-0.418816
H	3.688409	-1.044542	-1.827585

TS-12bE(ac): (one imaginary frequency, -520.92 cm^{-1})

C	1.762757	1.887360	0.215195
C	0.659903	2.004565	1.063420
C	-0.509846	1.270510	0.890592
C	-0.737007	0.349447	-0.143825
C	1.021856	-1.062871	0.365715
C	2.196001	-0.255275	0.359755
H	2.657738	-0.064550	1.324936
C	0.545960	-1.517658	1.731885
H	-0.505003	-1.820975	1.711495
H	0.676042	-0.734824	2.485466
H	1.137002	-2.386745	2.056510
C	0.747626	-2.083730	-0.726663
H	-0.308325	-2.369740	-0.728200
H	1.015671	-1.747630	-1.730404
H	1.329080	-2.994533	-0.524269
O	-1.810409	-0.538117	0.081221
C	-0.469862	0.585671	-1.618710
H	-1.190940	1.209359	1.737160
H	0.808657	2.471693	2.035110
H	1.634770	1.831535	-0.857113
H	2.716626	2.312168	0.516187
C	3.186459	-0.266528	-0.731516
C	-3.144479	-0.232517	-0.081073
O	-3.950817	-1.098150	0.140607
C	-3.505593	1.163713	-0.541696
H	-0.967935	-0.189966	-2.205718
H	-0.856992	1.561959	-1.936401
H	0.588786	0.558683	-1.879427

O	4.353833	0.057242	-0.591876
H	2.812685	-0.570317	-1.733909
H	-4.574694	1.305131	-0.380317
H	-2.939266	1.936983	-0.016814
H	-3.297404	1.267864	-1.612375

TS-12bZ(ac): (one imaginary frequency, -510.73 cm^{-1})

C	0.686868	-1.757457	-0.726975
C	0.357046	-0.974238	-1.834370
C	-0.357454	0.215698	-1.723996
C	-0.854895	0.758309	-0.535118
C	1.199238	0.952462	0.564975
C	1.724283	-0.367401	0.610941
C	3.020479	-0.735939	0.009654
O	3.762195	-1.590692	0.463775
H	3.299635	-0.180489	-0.910897
C	1.852133	1.992086	-0.328907
H	1.247523	2.903564	-0.377553
H	2.004464	1.629992	-1.349442
H	2.835998	2.282618	0.067822
C	0.669995	1.491146	1.881679
H	0.080811	2.404133	1.750433
H	0.056010	0.752101	2.403454
H	1.511346	1.752117	2.539829
C	-1.529151	2.104574	-0.528169
H	-1.033779	2.792649	-1.218927
H	-1.525944	2.550953	0.470357
H	-2.574618	1.997106	-0.840711
O	-1.360247	-0.111878	0.470199
C	-2.612671	-0.642671	0.284730
O	-3.309432	-0.421369	-0.674547
C	-2.972158	-1.531467	1.452241
H	-0.348487	0.890528	-2.577393
H	0.864048	-1.168000	-2.777429
H	-0.004912	-1.868271	0.094301
H	1.387984	-2.579082	-0.845885
H	1.515588	-0.937671	1.514572
H	-4.003363	-1.868900	1.343816
H	-2.305569	-2.400650	1.481902
H	-2.849159	-0.991795	2.396236

Compound 12b(ac): (No imaginary frequency)

C	-0.878695	-0.272309	0.738305
C	-1.498166	0.345980	-0.567356
C	-1.546578	-0.668555	-1.725634
C	-0.286301	-1.478510	-1.825185
C	0.671856	-1.480699	-0.896157
C	0.601360	-0.681430	0.391867
C	-2.881633	0.926838	-0.343426
O	-3.126661	2.111423	-0.272235
O	1.287409	0.622357	0.217952
C	2.558992	0.697774	-0.231488

C	1.305959	-1.444669	1.522310
C	-1.674517	-1.513432	1.203092
C	-0.921667	0.783122	1.863126
H	-0.859212	1.188115	-0.851078
H	-1.588348	-2.351838	0.505668
H	-1.721811	-0.136954	-2.671280
H	-2.407754	-1.346981	-1.611942
H	-0.170431	-2.099241	-2.712781
H	1.567134	-2.076636	-1.038030
H	-3.706390	0.180517	-0.263031
C	2.993819	2.145461	-0.318648
H	-1.324861	-1.854820	2.182176
H	-2.736495	-1.271066	1.314888
H	-0.414701	0.425021	2.764591
H	-0.454207	1.721272	1.556944
H	-1.958793	0.999927	2.140090
H	1.292866	-0.878777	2.457941
H	0.824276	-2.411520	1.692664
H	2.344552	-1.628591	1.241691
O	3.259732	-0.249638	-0.517275
H	3.998197	2.195724	-0.740552
H	2.295972	2.716687	-0.938888
H	2.989581	2.598596	0.678563

TS-11aE(si): (one imaginary frequency, -407.43 cm^{-1})

C	-3.679681	1.644616	-0.732636
Si	-2.995137	0.130207	0.135688
C	-2.663134	0.503786	1.953295
O	-1.549192	-0.176512	-0.710432
C	-0.403001	-0.860769	-0.541310
C	-0.405488	-1.875511	0.570198
C	0.496533	-0.757743	-1.599973
C	1.846354	-1.111869	-1.655329
C	2.681330	-1.451317	-0.565630
C	-4.140426	-1.353835	-0.058298
C	2.990832	0.098101	0.515883
C	3.752928	-0.557345	1.674359
C	1.728707	0.653947	0.900183
C	1.048473	1.745745	0.266557
O	1.370450	2.345347	-0.765245
C	3.910768	0.947947	-0.363727
H	1.273969	0.285543	1.818845
H	0.126699	2.065282	0.812089
H	2.281881	-2.077485	0.224460
H	3.694379	-1.748973	-0.834996
H	2.342607	-0.874429	-2.594078
H	0.104138	-0.203480	-2.449057
H	3.386356	1.328117	-1.238361
H	4.257873	1.817650	0.208755
H	4.794303	0.374542	-0.669502
H	4.570555	-1.193235	1.316003
H	4.193507	0.220883	2.309813

H	3.094387	-1.166358	2.304068
H	-0.513985	-1.413591	1.555081
H	-1.267184	-2.542179	0.423230
H	0.489255	-2.493843	0.572943
H	-3.566355	0.929861	2.408720
H	-2.393555	-0.384275	2.534933
H	-1.860649	1.241927	2.064772
H	-5.124836	-1.136448	0.375282
H	-4.291450	-1.600054	-1.115543
H	-3.752374	-2.248248	0.442516
H	-4.633954	1.957293	-0.291513
H	-2.979922	2.484180	-0.656731
H	-3.848972	1.449225	-1.797372

TS-11aZ(si): (one imaginary frequency, -367.96 cm^{-1})

C	-2.034331	-1.828592	-1.490636
Si	-2.401482	-0.411793	-0.323989
C	-3.738291	0.720413	-1.032824
O	-0.941748	0.504274	-0.341152
C	-0.443541	1.565247	0.271181
C	-1.210630	2.134267	1.435129
C	0.675651	2.226741	-0.238389
C	1.605305	1.740482	-1.160212
C	1.823767	0.368691	-1.434945
C	-2.870604	-1.015993	1.391359
C	2.762757	-0.411734	-0.003945
C	2.885685	-1.845291	-0.540197
C	2.014658	-0.251811	1.213513
C	0.870615	-0.980959	1.616058
O	0.229899	-1.832819	0.962877
C	4.114573	0.307027	0.014969
H	2.328379	0.534533	1.897922
H	0.504398	-0.712171	2.634290
H	0.957143	-0.282996	-1.415374
H	2.497368	0.164468	-2.266942
H	2.363255	2.448781	-1.492400
H	0.848892	3.217074	0.177271
H	4.016984	1.344173	0.352775
H	4.797844	-0.204898	0.704785
H	4.584170	0.310359	-0.975687
H	3.300677	-1.860828	-1.554619
H	3.571235	-2.406083	0.108055
H	1.919443	-2.349257	-0.525863
H	-0.720637	3.024455	1.835371
H	-2.232498	2.402814	1.136576
H	-1.289254	1.393032	2.237400
H	-2.903963	-2.489025	-1.594289
H	-1.765320	-1.467347	-2.489720
H	-1.198856	-2.411565	-1.092447
H	-3.766999	-1.645968	1.318831
H	-2.051766	-1.624746	1.786561
H	-3.096718	-0.207447	2.094893

H	-4.663260	0.151387	-1.191883
H	-3.982899	1.557831	-0.368873
H	-3.435765	1.135938	-2.000949

Compound 11a(si): (No imaginary frequency)

C	-0.373493	-0.997818	1.247725
C	-0.099543	-0.584197	-0.181759
C	-1.274757	0.294393	-0.746608
C	-2.699886	-0.099894	-0.237968
C	-2.721543	-0.107988	1.308322
C	-1.518696	-0.788297	1.901820
C	0.193586	-1.806851	-1.066496
O	1.058481	0.281088	-0.203244
Si	2.718007	0.108828	-0.017230
C	-0.913684	1.764648	-0.485083
O	-1.309602	2.437607	0.442039
C	-3.745502	0.897618	-0.779862
C	-3.103979	-1.501911	-0.749727
H	-1.259472	0.186004	-1.841297
H	-0.245808	2.210253	-1.249480
H	-3.638239	-0.605929	1.655647
H	-2.764345	0.921827	1.683060
H	-1.595662	-1.109147	2.940250
H	0.454773	-1.492471	1.750844
H	-3.559625	1.917477	-0.436569
H	-3.755325	0.897423	-1.877823
H	-4.748381	0.607756	-0.443754
H	-4.167134	-1.674059	-0.543620
H	-2.959867	-1.594835	-1.833194
H	-2.545691	-2.302355	-0.256864
H	-0.672237	-2.465175	-1.156399
H	0.490795	-1.482826	-2.069692
H	1.012938	-2.394184	-0.636445
C	3.190248	-0.995411	1.443977
H	4.281277	-0.999964	1.565300
H	2.755773	-0.629474	2.381146
H	2.876397	-2.037620	1.310641
C	3.513674	-0.572993	-1.591161
H	4.607669	-0.553668	-1.503816
H	3.218462	-1.608140	-1.795799
H	3.242837	0.030293	-2.465816
C	3.319412	1.865299	0.287295
H	4.409271	1.897493	0.408514
H	3.057376	2.523507	-0.549055
H	2.866079	2.285083	1.192228

TS-11bE(si): (one imaginary frequency, -322.77 cm^{-1})

C	-2.604540	-0.974291	-0.857484
C	-1.737779	-2.060981	-0.383967
C	-0.400196	-1.984686	-0.107249
C	0.512019	-0.958370	-0.494144
C	0.347529	-0.065362	-1.656004

O	1.641671	-0.939071	0.204515
Si	3.034870	0.083436	0.223901
C	-3.072753	0.052005	0.337435
C	-3.845331	-0.757650	1.396118
C	-4.036219	1.032564	-0.374856
C	-1.939508	0.776538	0.978217
C	-1.185184	1.812538	0.435893
O	-1.149213	2.196359	-0.780217
C	3.950241	-0.537898	1.738477
C	4.051634	-0.222302	-1.332498
C	2.508163	1.875754	0.408915
H	1.304686	0.284639	-2.045494
H	-0.243652	0.827652	-1.310239
H	-0.223422	-0.543474	-2.454488
H	0.049929	-2.763156	0.506605
H	-2.241551	-2.960531	-0.033332
H	-3.532047	-1.384449	-1.271085
H	-4.279409	-0.083874	2.144055
H	-4.665805	-1.327817	0.942256
H	-3.190946	-1.460649	1.924079
H	-4.828563	0.489980	-0.906898
H	-4.510665	1.687068	0.364733
H	-3.487959	1.659152	-1.081498
H	-2.149446	-0.328272	-1.606141
H	-1.725231	0.531853	2.017582
H	-0.491475	2.301005	1.152563
H	5.034823	0.253614	-1.225617
H	4.221078	-1.293652	-1.490440
H	3.590410	0.183697	-2.238824
H	4.877131	0.027828	1.892737
H	3.338207	-0.429339	2.640650
H	4.216730	-1.596016	1.638418
H	3.384623	2.530970	0.324080
H	1.775055	2.193104	-0.340278
H	2.061205	2.047113	1.394454

TS-11bZ(si): (one imaginary frequency, -373.53 cm^{-1})

Si	2.582163	0.392361	0.128867
O	1.106922	-0.113916	-0.556084
C	0.380375	-1.248078	-0.584760
C	-0.709581	-1.377217	-1.443773
C	-1.501055	-0.355751	-1.962444
C	-1.471577	0.978714	-1.479532
C	0.953967	-2.458650	0.101265
C	-2.229655	1.027561	0.228240
C	-3.725928	0.821565	-0.038315
C	-1.925752	2.483399	0.613157
C	-1.582615	0.073499	1.090496
C	-2.014152	-1.262419	1.368388
O	-2.955882	-1.879357	0.851892
C	2.738507	2.156706	-0.494862
C	3.999990	-0.667149	-0.518824

C	2.511184	0.357880	2.011493
H	-0.711227	0.411057	1.648545
H	-1.397110	-1.770360	2.149461
H	-0.492962	1.385208	-1.251155
H	-2.100612	1.684754	-2.021541
H	-2.347601	-0.663589	-2.572402
H	-1.052680	-2.396565	-1.595258
H	-3.933492	-0.192414	-0.376134
H	-4.286457	0.974998	0.892556
H	-4.093214	1.548576	-0.772975
H	-2.238282	3.182865	-0.170725
H	-2.470843	2.745649	1.528260
H	-0.857804	2.639100	0.804359
H	0.228926	-3.274760	0.114982
H	1.859920	-2.807890	-0.414048
H	1.228465	-2.232956	1.136765
H	3.412457	0.832301	2.420784
H	1.646094	0.913713	2.389878
H	2.463061	-0.656864	2.420914
H	4.960348	-0.213067	-0.242953
H	3.991664	-1.684212	-0.112838
H	3.972342	-0.738658	-1.612274
H	3.666453	2.619343	-0.137341
H	2.748449	2.189267	-1.590064
H	1.903252	2.777277	-0.150575

Compound 11b(si): (No imaginary frequency)

C	1.057808	-0.174470	-0.655640
C	1.948998	1.001780	-0.141347
C	2.778091	0.531740	1.076538
C	1.967398	-0.259342	2.064856
C	0.789708	-0.823161	1.791511
C	0.096047	-0.778217	0.445978
C	2.892109	1.484969	-1.262758
C	1.068142	2.202727	0.271122
O	-1.044213	0.077714	0.599805
Si	-2.554090	0.219471	-0.116821
C	-0.373697	-2.205509	0.097618
C	1.844222	-1.303609	-1.313898
O	2.970123	-1.658751	-1.035261
H	0.393846	0.208205	-1.442275
H	1.287846	-1.836380	-2.118465
H	3.210985	1.408855	1.578422
H	3.623731	-0.079674	0.738459
H	2.384976	-0.374503	3.064628
H	0.248846	-1.367475	2.564457
H	3.585406	0.705138	-1.587547
H	2.320720	1.826954	-2.135748
H	3.487166	2.335896	-0.909585
C	-3.201624	1.868316	0.518737
H	1.711436	3.048801	0.543279
H	0.429769	2.526638	-0.560170

H	0.420164	1.971698	1.117519
H	-0.873788	-2.246877	-0.876788
H	0.463589	-2.910656	0.084529
H	-1.082327	-2.542733	0.860299
H	-4.210289	2.072976	0.138978
H	-3.248785	1.873840	1.613698
H	-2.552502	2.696005	0.211536
C	-2.461786	0.250774	-2.008117
C	-3.726960	-1.161863	0.423269
H	-3.467470	0.383789	-2.427377
H	-1.844147	1.080817	-2.371204
H	-2.057109	-0.676888	-2.429890
H	-4.745556	-0.949500	0.073501
H	-3.441965	-2.141965	0.025507
H	-3.765283	-1.242067	1.516172

TS-12aE(si): (one imaginary frequency, -499.50 cm^{-1})

C	-2.492937	1.791973	0.423623
C	-1.529000	2.027625	-0.560018
C	-0.293416	1.389982	-0.616899
C	0.202313	0.426690	0.282575
C	-1.567902	-1.061042	0.004165
C	-2.750148	-0.381510	0.409059
C	-3.929122	-0.229228	-0.464545
O	-5.079197	-0.195533	-0.058828
H	-3.713342	-0.145063	-1.550852
C	-1.332611	-1.368861	-1.462711
H	-0.281318	-1.622087	-1.631847
H	-1.590231	-0.530720	-2.115249
H	-1.937184	-2.232862	-1.776762
C	-1.039106	-2.135986	0.934349
H	0.035807	-2.296572	0.795366
H	-1.234747	-1.910507	1.987448
H	-1.538466	-3.090644	0.711937
O	1.270787	-0.316386	-0.184510
C	0.204543	0.553453	1.791263
H	0.248370	1.454189	-1.558387
H	-1.845054	2.552826	-1.459890
H	-2.224583	1.680785	1.464843
H	-3.491041	2.199372	0.284637
H	-3.037023	-0.491371	1.454783
Si	2.940018	-0.033800	-0.133068
C	3.640871	-1.180261	-1.447313
C	3.294490	1.775051	-0.531673
C	3.646043	-0.480780	1.559735
H	0.509089	-0.389627	2.249941
H	0.934094	1.319284	2.091396
H	-0.756647	0.843508	2.211550
H	4.741108	-0.407776	1.547539
H	3.281887	0.181519	2.352990
H	3.388062	-1.509284	1.838358
H	4.734535	-1.109473	-1.491276

H	3.383334	-2.224949	-1.238282
H	3.248298	-0.932860	-2.440024
H	4.370107	1.978698	-0.459765
H	2.974473	2.033674	-1.547384
H	2.783394	2.455858	0.158924

TS-12aZ(si): (one imaginary frequency, -539.01 cm^{-1})

C	1.154715	1.122490	1.541648
C	0.833001	-0.028020	2.278285
C	0.214197	-1.123430	1.685971
C	-0.240566	-1.176825	0.357949
O	-0.780320	-0.057731	-0.247629
Si	-2.380997	0.504206	-0.189366
C	-0.736994	-2.482867	-0.213318
C	2.427944	0.367243	0.074524
C	1.948735	-0.809259	-0.577724
C	1.480413	-0.749841	-2.018961
C	2.633080	-2.101918	-0.181094
C	2.558227	1.651120	-0.646087
O	3.391472	2.500199	-0.380395
H	0.446961	1.502693	0.818956
H	1.785496	1.880481	2.000121
H	1.319844	-0.183939	3.239291
H	0.275105	-2.079890	2.202369
C	-2.238682	2.360873	-0.455091
C	-3.159978	0.102774	1.479085
C	-3.375162	-0.267386	-1.595692
H	-1.808372	-2.619244	-0.005053
H	-0.619254	-2.509397	-1.300706
H	-0.205749	-3.336162	0.217373
H	0.702222	0.000789	-2.176352
H	1.081709	-1.717817	-2.340016
H	2.316584	-0.518740	-2.695197
H	2.065250	-2.983894	-0.497607
H	2.788170	-2.157174	0.901389
H	3.624779	-2.174443	-0.655111
H	3.241828	0.222941	0.781937
H	1.819126	1.828044	-1.456354
H	-3.229942	2.824409	-0.530151
H	-1.705815	2.845770	0.370611
H	-1.696969	2.587800	-1.380689
H	-4.382443	0.166066	-1.640034
H	-2.893791	-0.083928	-2.563463
H	-3.488080	-1.351213	-1.480268
H	-4.169563	0.528327	1.538907
H	-3.247523	-0.977009	1.645954
H	-2.568409	0.517177	2.302432

Compound 12a(si): (No imaginary frequency)

C	1.260806	-0.501602	0.269671
C	2.573249	0.203088	-0.227753
C	2.658045	1.677850	0.218110

C	1.340299	2.390680	0.091299
C	0.186227	1.767263	-0.151318
C	0.034794	0.269474	-0.361720
C	3.824373	-0.534435	0.213515
O	4.521192	-1.202080	-0.519655
O	-1.130137	-0.180459	0.342401
Si	-2.786649	-0.156014	0.094032
C	-0.138159	-0.002964	-1.870264
C	1.161299	-0.458331	1.811409
C	1.264087	-1.978168	-0.172429
H	2.587103	0.159129	-1.322024
H	1.084672	0.563434	2.193663
H	3.422440	2.195010	-0.378470
H	3.009607	1.745366	1.260262
H	1.351842	3.472256	0.221011
H	-0.732767	2.342931	-0.236125
H	4.095360	-0.415349	1.287817
H	0.272865	-0.999972	2.141422
H	2.034782	-0.934258	2.270783
C	-3.498997	-0.628089	1.771635
H	0.280933	-2.426992	0.001088
H	1.521040	-2.097453	-1.229869
H	1.998151	-2.552668	0.402773
H	-0.410924	-1.045610	-2.053227
H	-0.931391	0.634922	-2.275858
H	0.773530	0.224113	-2.429948
H	-4.594869	-0.669568	1.742305
H	-3.136453	-1.612237	2.090075
H	-3.210937	0.096474	2.541793
C	-3.426474	1.549241	-0.419137
H	-4.518875	1.522387	-0.522960
H	-3.186899	2.313942	0.328951
H	-3.018014	1.879735	-1.381443
C	-3.319852	-1.429033	-1.198733
H	-4.414465	-1.506219	-1.226132
H	-2.983906	-1.170141	-2.208929
H	-2.926362	-2.424561	-0.961097

TS-12bE(si): (one imaginary frequency, -528.68 cm^{-1})

C	-2.437748	-1.862078	-0.012295
C	-1.266735	-2.125226	0.705073
C	-0.079010	-1.418074	0.547383
C	0.155233	-0.358873	-0.350605
C	-1.579625	0.991495	0.462340
C	-2.776068	0.213999	0.448128
H	-3.176373	-0.074435	1.416770
C	-0.988988	1.258842	1.832669
H	0.070257	1.527866	1.764239
H	-1.089984	0.391591	2.492522
H	-1.513494	2.099785	2.311783
C	-1.366074	2.143248	-0.503628
H	-0.301699	2.390065	-0.577032

H	-1.744638	1.956765	-1.510893
H	-1.878946	3.040380	-0.126113
O	1.270383	0.424998	-0.117819
C	-0.195749	-0.361725	-1.823979
H	0.652616	-1.520517	1.345752
H	-1.356073	-2.721330	1.612051
H	-2.407827	-1.683501	-1.078748
H	-3.369701	-2.315428	0.316177
C	-3.845646	0.398433	-0.548774
Si	2.919891	0.055680	-0.034631
C	3.769662	1.715364	-0.269401
C	3.370933	-0.669509	1.649103
C	3.376211	-1.164752	-1.398365
H	-0.001367	0.623930	-2.251792
H	0.447710	-1.082011	-2.347409
H	-1.228759	-0.631140	-2.037149
O	-5.017779	0.124986	-0.350043
H	-3.529344	0.785114	-1.542580
H	4.860254	1.613068	-0.214042
H	3.521810	2.154752	-1.242189
H	3.462557	2.427364	0.505291
H	4.461517	-0.738405	1.752360
H	3.001188	-0.040262	2.467082
H	2.966485	-1.678000	1.791681
H	4.438440	-1.432310	-1.335478
H	2.799852	-2.093957	-1.315305
H	3.197854	-0.745644	-2.395132

TS-12bZ(si): (one imaginary frequency, -520.12 cm^{-1})

C	-1.119813	-1.712830	0.637490
C	-0.919964	-0.974999	1.813991
C	-0.308082	0.273766	1.800101
C	0.268620	0.881591	0.672731
C	-1.779964	0.952008	-0.540342
C	-2.172170	-0.414360	-0.652320
C	-3.485133	-0.895361	-0.173127
O	-4.132197	-1.771572	-0.720418
H	-3.866593	-0.410393	0.751131
C	-2.580409	1.898571	0.334850
H	-2.061231	2.855432	0.455065
H	-2.768859	1.487926	1.330789
H	-3.558549	2.123492	-0.117554
C	-1.204570	1.570604	-1.798165
H	-0.770129	2.558279	-1.610557
H	-0.434545	0.931294	-2.239884
H	-1.994921	1.713007	-2.549991
C	0.761861	2.305876	0.764397
H	0.140414	2.903222	1.437533
H	0.775035	2.784678	-0.218849
H	1.791914	2.335304	1.148433
O	0.922673	0.124118	-0.280613
Si	2.526433	-0.430220	-0.268583

C	3.638518	0.832366	-1.123616
C	2.490009	-2.023542	-1.268641
C	3.106413	-0.739302	1.498158
H	-0.461370	0.922161	2.660980
H	-1.484135	-1.248755	2.703723
H	-0.346533	-1.737667	-0.115967
H	-1.741231	-2.604313	0.676565
H	-1.873008	-0.917461	-1.570730
H	3.501144	-2.428633	-1.397694
H	1.883299	-2.792728	-0.777567
H	2.071293	-1.854823	-2.267581
H	4.657947	0.439779	-1.229142
H	3.268419	1.065090	-2.128980
H	3.705008	1.774185	-0.567158
H	4.125311	-1.146499	1.497200
H	3.120432	0.179610	2.095642
H	2.455122	-1.455810	2.009946

Compound 12b(si): (No imaginary frequency)

C	-1.458195	0.557078	-0.608374
C	-1.810309	-0.629703	0.356867
C	-1.902762	-0.175148	1.827367
C	-0.776378	0.744656	2.202552
C	0.056444	1.285709	1.310345
C	-0.021956	1.062926	-0.192745
C	-3.088351	-1.349028	-0.025470
O	-3.138730	-2.476818	-0.466558
O	0.909307	0.049003	-0.612576
Si	2.388504	-0.512735	-0.055359
C	0.377175	2.369015	-0.902876
C	-2.493817	1.699071	-0.494669
C	-1.456561	0.036979	-2.059420
H	-1.006249	-1.365820	0.259682
H	-2.465714	2.195401	0.480338
H	-1.896145	-1.055285	2.485145
H	-2.865136	0.325518	2.021606
H	-0.654527	0.970131	3.261614
H	0.854978	1.943624	1.651754
H	-4.029517	-0.775893	0.146969
C	3.053926	-1.519574	-1.500851
H	-2.318184	2.459807	-1.261580
H	-3.509798	1.322138	-0.653640
H	-1.124392	0.810548	-2.759279
H	-0.800000	-0.827815	-2.173313
H	-2.467573	-0.260285	-2.360310
H	0.340845	2.254295	-1.989685
H	-0.265534	3.205837	-0.613274
H	1.404526	2.628015	-0.627772
H	4.016217	-1.983965	-1.252153
H	2.357913	-2.320680	-1.774861
H	3.202727	-0.892114	-2.387075
C	3.596822	0.886210	0.352088

H	4.580522	0.466260	0.599078
H	3.734353	1.562478	-0.499747
H	3.276897	1.486495	1.211563
C	2.187508	-1.626557	1.456957
H	3.148947	-2.078897	1.732466
H	1.814805	-1.075092	2.326438
H	1.485098	-2.443703	1.253504

TS-11aE(N): (one imaginary frequency, -408.28 cm^{-1})

C	-2.824143	0.523428	-1.016094
N	-1.914669	0.611005	0.139188
C	-0.723104	1.245438	0.112681
C	0.086722	1.244028	1.264719
C	1.465522	1.433585	1.377013
C	2.464832	1.427227	0.384045
C	2.652911	-0.475442	-0.247806
C	1.539991	-0.719697	-1.102396
C	0.387910	-1.528720	-0.882454
O	0.008125	-2.133753	0.136219
H	-0.233635	-1.622580	-1.809807
H	1.609675	-0.310510	-2.111699
C	3.986812	-0.294660	-0.975159
H	3.895967	0.382748	-1.831607
H	4.321024	-1.267767	-1.358545
H	4.771195	0.086785	-0.312319
C	2.778463	-1.300587	1.023505
H	3.053336	-2.329908	0.756599
H	1.831776	-1.355149	1.559666
H	3.561930	-0.902208	1.678985
H	3.465949	1.674303	0.734009
H	2.260875	1.823885	-0.603318
H	1.833263	1.359462	2.400331
H	-0.405553	0.939431	2.183755
C	-0.445659	2.105064	-1.098387
H	0.485292	2.654380	-0.977729
H	-1.251647	2.843267	-1.206875
H	-0.398151	1.530984	-2.027161
H	-3.132385	1.517048	-1.357755
C	-3.999062	-0.320621	-0.505207
C	-3.342192	-1.238187	0.536591
C	-2.315239	-0.325871	1.213026
H	-2.311981	0.022044	-1.850206
H	-4.746792	0.325116	-0.028798
H	-4.492956	-0.863711	-1.316151
H	-4.056644	-1.660719	1.249119
H	-2.806385	-2.060912	0.051776
H	-2.756433	0.236564	2.049168
H	-1.442620	-0.879466	1.560026

TS-11aZ(N): (one imaginary frequency, -405.29 cm^{-1})

C	2.744873	-1.464568	1.115550
C	1.865843	-0.252391	1.433390

N	1.695621	0.420868	0.131730
C	2.644884	-0.121730	-0.869955
C	3.618762	-0.970304	-0.044693
C	0.889682	1.474094	-0.094381
C	1.219485	2.342950	-1.291769
C	-0.138753	1.919229	0.768035
C	-1.034046	1.211665	1.575905
C	-1.413144	-0.138156	1.463670
C	-2.612431	-0.355599	-0.137347
C	-1.819551	-0.032474	-1.273356
C	-0.683907	-0.755706	-1.714115
O	-0.120105	-1.715649	-1.143720
C	-3.787919	0.575709	0.123855
C	-2.952299	-1.829160	0.091583
H	3.148633	0.684139	-1.409349
H	-2.019979	0.901708	-1.795086
H	-0.232699	-0.361031	-2.655861
H	-0.724943	-0.869566	1.051996
H	-2.058440	-0.521741	2.251926
H	-1.672833	1.837688	2.199819
H	-0.323826	2.990762	0.697817
H	-3.492625	1.626720	0.042964
H	-4.581226	0.391692	-0.613951
H	-4.219504	0.413507	1.118084
H	-2.080511	-2.462123	-0.077572
H	-3.348580	-2.008099	1.097605
H	-3.731846	-2.120610	-0.625617
H	0.525944	3.184038	-1.345495
H	2.243688	2.736275	-1.243887
H	1.125780	1.779137	-2.225588
H	4.441073	-0.349570	0.332560
H	4.051913	-1.781615	-0.636424
H	2.087210	-0.741014	-1.579806
H	2.110829	-2.291277	0.778643
H	3.320660	-1.795859	1.984802
H	0.914194	-0.533681	1.879248
H	2.359713	0.448293	2.122582

Compound 11a(N): (No imaginary frequency)

C	-0.100263	-1.165761	1.223241
C	0.328216	-0.507655	-0.073403
C	-0.840899	0.393698	-0.625831
C	-2.295176	-0.120372	-0.371625
C	-2.492104	-0.389803	1.138157
C	-1.331446	-1.131437	1.740210
C	0.738707	-1.636986	-1.054549
N	1.456437	0.460833	0.175228
C	2.244466	0.899933	-0.987762
C	-0.596894	1.806385	-0.054055
O	-1.094639	2.254156	0.958705
C	-3.313262	0.931696	-0.861021
C	-2.576702	-1.422804	-1.154366

H	-0.708361	0.485818	-1.714536
H	0.033295	2.460383	-0.693207
H	-3.415911	-0.966633	1.288139
H	-2.621991	0.559665	1.670166
H	-1.519808	-1.676820	2.664493
H	0.653368	-1.775314	1.717577
H	-3.207699	1.882853	-0.334486
H	-3.199818	1.117062	-1.937369
H	-4.335538	0.569127	-0.697774
H	-3.650376	-1.644448	-1.123752
H	-2.288850	-1.332973	-2.209066
H	-2.057167	-2.284467	-0.727513
H	-0.078300	-2.339701	-1.226574
H	1.044754	-1.243218	-2.029344
H	1.578475	-2.204383	-0.638412
C	3.579156	0.100762	-0.975323
H	4.423451	0.742654	-1.247593
H	3.554534	-0.722924	-1.695719
C	3.690966	-0.431249	0.478660
C	2.479432	0.210420	1.199003
H	2.458808	1.971506	-0.867039
H	1.684110	0.792734	-1.919554
H	3.620494	-1.524705	0.500578
H	4.638749	-0.159615	0.955308
H	2.094031	-0.373593	2.033479
H	2.776628	1.186934	1.607960

TS-11bE(N): (one imaginary frequency, -399.20 cm^{-1})

C	-2.589617	-1.136096	-0.803398
N	-2.090885	-0.375393	0.352574
C	-2.917608	0.820648	0.607946
C	-3.753776	0.966279	-0.669768
C	-3.939053	-0.485003	-1.135044
C	-0.880311	-0.592948	0.918168
C	-0.105516	-1.706497	0.532809
C	1.254866	-1.919100	0.768535
C	2.238207	-0.952653	1.058652
C	-0.501362	0.303354	2.064984
C	2.690559	0.034207	-0.608538
C	3.725803	0.985868	-0.006422
C	1.495276	0.609742	-1.131025
C	0.812865	1.755381	-0.651458
O	1.051667	2.430766	0.373791
C	3.318145	-1.039269	-1.492557
H	-2.285893	1.691626	0.795535
H	-3.558259	0.664577	1.488074
H	-1.386237	0.567942	2.652126
H	-0.023923	1.234129	1.716402
H	0.197938	-0.211995	2.724621
H	-0.612222	-2.477467	-0.041541
H	1.621352	-2.903328	0.476025
H	3.217002	-1.339835	1.337675

H	3.783565	-0.571932	-2.371152
H	4.099780	-1.596340	-0.963196
H	2.570194	-1.753371	-1.852795
H	4.485096	0.448819	0.573268
H	4.242713	1.503718	-0.825930
H	3.245387	1.740193	0.617193
H	1.963532	-0.053739	1.597546
H	1.012842	0.098868	-1.963276
H	-0.064641	2.043755	-1.280645
H	-4.697527	1.488735	-0.489559
H	-3.188484	1.535455	-1.416685
H	-4.740630	-0.967874	-0.563432
H	-4.187187	-0.572043	-2.196557
H	-2.691850	-2.199116	-0.558148
H	-1.870549	-1.052639	-1.631189

TS-11bZ(N): (one imaginary frequency, -414.09 cm^{-1})

C	2.643871	0.527796	-1.061348
N	1.825939	0.278694	0.140096
C	0.851812	1.119489	0.573601
C	-0.069711	0.801679	1.593839
C	-0.738284	-0.394124	1.841283
C	-0.901985	-1.472032	0.936018
C	0.911154	2.555097	0.096134
C	-2.172721	-0.960756	-0.420943
C	-3.467090	-0.740139	0.359239
C	-2.193878	-2.272240	-1.215848
C	-1.636360	0.144674	-1.152146
C	-1.977612	1.526429	-1.020210
O	-2.729991	2.070111	-0.198508
C	3.871071	-0.375761	-0.884000
H	2.918010	1.582446	-1.145275
H	-0.942416	-0.084861	-1.961837
H	-1.487302	2.163561	-1.798622
H	-0.092932	-1.713656	0.255090
H	-1.375005	-2.363193	1.347084
H	-1.419638	-0.373899	2.690495
H	-0.424387	1.663363	2.154902
H	-3.417844	0.165268	0.962026
H	-4.297807	-0.610402	-0.346610
H	-3.696927	-1.607030	0.991138
H	-2.390328	-3.139406	-0.574690
H	-2.991640	-2.228662	-1.967842
H	-1.249588	-2.442672	-1.745758
H	0.047168	3.106536	0.468921
H	1.832594	3.049292	0.437874
H	0.886775	2.620285	-0.995096
H	4.651578	0.159191	-0.329947
C	3.332514	-1.542147	-0.043872
H	4.295478	-0.688350	-1.842302
C	2.350112	-0.862979	0.915063
H	2.067980	0.260351	-1.959905

H	2.797515	-2.255001	-0.683418
H	4.115096	-2.091501	0.487250
H	1.560096	-1.534913	1.249559
H	2.854521	-0.478413	1.813492

Compound 11b(N): (No imaginary frequency)

C	-0.919087	0.194858	-0.734971
C	-1.598319	-1.088736	-0.150713
C	-2.187177	-0.780719	1.244019
C	-1.274124	0.051923	2.097369
C	-0.224728	0.738975	1.640892
C	0.208148	0.825026	0.187447
C	-2.720176	-1.566311	-1.097516
C	-0.580552	-2.245037	-0.034547
N	1.463512	0.056632	-0.018478
C	2.217573	0.268370	-1.256003
C	0.422096	2.334794	-0.122110
C	-1.916379	1.282490	-1.123649
O	-2.962703	1.534386	-0.563549
H	-0.428688	-0.085020	-1.676456
H	-1.611184	1.889499	-2.006511
H	-2.417342	-1.724474	1.759250
H	-3.139976	-0.247162	1.136452
H	-1.517182	0.114602	3.157857
H	0.357322	1.342216	2.336206
H	-3.513559	-0.823591	-1.212381
H	-2.319873	-1.802685	-2.092165
H	-3.175865	-2.482952	-0.703720
C	3.416415	-0.676345	-1.086599
H	-1.105832	-3.159514	0.269763
H	-0.095139	-2.443917	-0.997338
H	0.206334	-2.036502	0.690594
H	0.640100	2.517812	-1.179428
H	-0.457923	2.924883	0.152366
H	1.266956	2.715577	0.462837
H	1.614297	0.032276	-2.138987
H	4.283471	-0.344991	-1.666720
C	3.675835	-0.675951	0.444035
H	3.151090	-1.681277	-1.429017
C	2.470507	0.082456	1.048315
H	2.575280	1.309275	-1.368765
H	3.730485	-1.697819	0.830931
H	4.617206	-0.181167	0.702829
H	2.082348	-0.393185	1.952896
H	2.774516	1.111850	1.321434

TS-12aE(N): (one imaginary frequency, -464.21 cm^{-1})

C	-2.355704	1.622491	0.164841
C	-1.371305	1.923203	-0.813414
C	-0.039337	1.533134	-0.774291
C	0.684677	0.922022	0.279971
C	-1.201539	-0.969043	0.413392

C	-2.461649	-0.280679	0.392733
C	-3.437317	-0.564084	-0.698639
O	-4.623531	-0.761840	-0.518236
H	-3.016639	-0.564150	-1.728074
C	-0.671716	-1.678698	-0.809738
H	0.407731	-1.853198	-0.712742
H	-0.843379	-1.118165	-1.733244
H	-1.135549	-2.672631	-0.939307
C	-0.788783	-1.602879	1.720307
H	0.296624	-1.759366	1.773825
H	-1.092239	-1.006163	2.588286
H	-1.247368	-2.599251	1.845455
N	1.892482	0.317510	-0.015701
C	0.521611	1.313798	1.729792
H	0.486571	1.609400	-1.723076
H	-1.728585	2.273067	-1.780532
H	-2.136634	1.810311	1.210748
H	-3.371391	1.941896	-0.070930
H	-2.982231	-0.287148	1.352490
C	2.914238	-0.042595	0.983935
H	2.590533	-0.906285	1.580043
C	4.159948	-0.383420	0.149023
H	0.720811	0.489095	2.418945
H	1.231704	2.118889	1.969070
H	-0.473218	1.694044	1.939912
H	4.785023	-1.141028	0.630871
C	3.577932	-0.834938	-1.197757
H	4.773541	0.514395	0.008066
C	2.389396	0.112881	-1.381080
H	3.109801	0.780205	1.680637
H	4.294407	-0.771966	-2.022196
H	3.224161	-1.871025	-1.133934
H	2.717588	1.065450	-1.830724
H	1.606901	-0.301391	-2.022246

TS-12aZ(N): (one imaginary frequency, -437.28 cm^{-1})

C	-1.107444	-1.374963	1.061339
C	-0.619598	-0.562311	2.123451
C	0.130292	0.585125	1.899439
C	0.837840	0.933947	0.725892
N	1.571790	-0.008992	0.021523
C	2.157774	-1.178893	0.712204
C	1.178618	2.390925	0.505832
C	-2.270362	-0.264165	0.094708
C	-1.639928	0.872487	-0.516950
C	-1.017629	0.775097	-1.886744
C	-2.126031	2.242262	-0.115026
C	-2.872551	-1.288222	-0.810714
O	-3.959948	-1.801334	-0.630797
H	-0.430468	-1.635302	0.251863
H	-1.736228	-2.217141	1.350177
H	-1.133275	-0.634582	3.080268

H	0.075424	1.367694	2.656070
C	3.201477	-1.724033	-0.270516
H	1.405726	-1.927842	0.974962
H	2.253369	2.580107	0.642287
H	0.916644	2.741470	-0.499938
H	0.629319	3.013402	1.215507
H	-0.476851	-0.165215	-2.034824
H	-0.310778	1.597565	-2.056342
H	-1.766882	0.850338	-2.693709
H	-1.380620	3.022721	-0.312139
H	-2.395750	2.282063	0.945711
H	-3.026690	2.529358	-0.686785
H	-2.992252	-0.006758	0.869761
H	-2.253048	-1.580973	-1.686547
H	4.016023	-2.242829	0.243735
H	2.735987	-2.437126	-0.962285
C	3.655749	-0.472650	-1.032396
C	2.344616	0.304174	-1.197289
H	2.618632	-0.849531	1.654694
H	4.363433	0.105422	-0.425121
H	4.134736	-0.693349	-1.991477
H	2.503634	1.379080	-1.306072
H	1.810031	-0.037631	-2.093455

Compound 12a(N): (No imaginary frequency)

C	-0.823191	-0.477422	-0.208074
C	-2.234642	0.121888	0.135044
C	-2.345749	1.614243	-0.239565
C	-1.107551	2.388219	0.118427
C	0.046390	1.821934	0.477967
C	0.284387	0.324413	0.615673
C	-3.363054	-0.654471	-0.518160
O	-4.087055	-1.434208	0.062776
N	1.629083	-0.054679	0.096116
C	2.390623	0.868431	-0.746242
C	0.196081	0.031158	2.136898
C	-0.546313	-0.359975	-1.723128
C	-0.789700	-1.972937	0.161171
H	-2.398109	0.009019	1.211608
H	-0.541563	0.678014	-2.069594
H	-3.215481	2.052917	0.269470
H	-2.555159	1.728262	-1.315487
H	-1.181024	3.474598	0.080212
H	0.881920	2.460347	0.757521
H	-3.512022	-0.457382	-1.605202
H	0.427253	-0.799977	-1.951562
H	-1.300269	-0.905237	-2.301839
C	3.564632	0.001239	-1.217314
H	0.230803	-2.358423	0.068148
H	-1.146124	-2.161219	1.178883
H	-1.425847	-2.556871	-0.512690
H	0.418257	-1.010070	2.381621

H	0.903034	0.664070	2.682875
H	-0.801247	0.263125	2.517366
H	4.436910	0.600471	-1.497651
H	3.265056	-0.582876	-2.093572
C	3.835675	-0.935257	-0.010783
C	2.623371	-0.732129	0.932975
H	1.781280	1.251327	-1.568802
H	2.779595	1.742464	-0.187458
H	3.917497	-1.977680	-0.332995
H	4.768921	-0.681857	0.502136
H	2.240588	-1.682755	1.315102
H	2.932843	-0.129856	1.807551

TS-12bE(N): (one imaginary frequency, -382.88 cm^{-1})

C	2.600730	0.487583	-1.209521
N	1.975467	0.361398	0.114971
C	2.861831	-0.330286	1.056251
C	3.749316	-1.178784	0.140945
C	3.937961	-0.271389	-1.085541
C	0.782931	0.956720	0.450595
C	0.482040	1.021893	1.929764
C	0.117989	1.770938	-0.490027
C	-1.213563	2.174840	-0.482587
C	-2.270033	1.533027	0.231684
C	-2.366989	-0.169227	-0.460837
C	-3.731491	-0.573270	0.006735
O	-4.706876	-0.648948	-0.714595
C	-1.280139	-1.021106	-0.059895
C	-1.277366	-1.696390	1.287474
C	-0.399843	-1.662071	-1.094443
H	-2.407418	0.013616	-1.534816
H	0.658744	-1.662692	-0.785970
H	-0.471878	-1.153405	-2.061351
H	-0.668432	-2.720968	-1.260086
H	-0.254989	-1.958897	1.593608
H	-1.709961	-1.077888	2.083379
H	-1.839336	-2.646419	1.285612
H	0.689576	2.060869	-1.369112
H	-1.516066	2.810691	-1.312746
H	-2.129833	1.280792	1.280921
H	-3.254424	1.979323	0.077068
H	2.288166	-0.930815	1.765667
H	0.273591	0.052959	2.393772
H	1.350029	1.446326	2.452927
H	-0.361091	1.684078	2.118879
H	-3.813974	-0.812511	1.089962
H	3.220270	-2.097428	-0.137281
H	4.693672	-1.460304	0.616483
H	3.472342	0.382421	1.636940
H	4.753794	0.437582	-0.903354
H	4.182875	-0.826068	-1.995765
H	2.769341	1.541649	-1.469605

H	1.941502	0.064020	-1.976753

TS-12bZ(N): (one imaginary frequency, -474.78 cm^{-1})

C	2.437244	0.683575	-0.912033
N	1.613251	-0.006191	0.091572
C	2.291354	-1.236646	0.558116
C	3.616594	-1.271892	-0.222260
C	3.320216	-0.432436	-1.473620
C	0.731085	0.685191	0.920657
C	1.044264	2.144467	1.173535
C	-0.056608	-0.009929	1.870380
C	-0.739389	-1.198270	1.659260
C	-0.943124	-1.728228	0.356151
C	-1.905701	-0.430935	-0.681726
C	-3.281453	-0.838445	-0.277582
O	-4.010117	-1.536728	-0.956008
C	-1.488057	0.930765	-0.495768
C	-0.909119	1.632728	-1.701016
C	-2.237004	1.835341	0.458223
H	-3.613228	-0.481429	0.721631
H	-1.676544	2.757498	0.649169
H	-2.437038	1.356090	1.420921
H	-3.210172	2.145603	0.039639
H	-0.268505	2.480685	-1.425828
H	-0.333096	0.949820	-2.334637
H	-1.711090	2.053553	-2.331865
H	0.337913	2.569457	1.889792
H	0.994061	2.749338	0.260932
H	2.058829	2.267651	1.580232
H	1.687480	-2.129837	0.352806
H	-0.258336	0.525199	2.797642
H	-1.373491	-1.560061	2.466341
H	-0.105287	-1.740038	-0.329901
H	-1.546963	-2.631490	0.276551
H	-1.685558	-0.829861	-1.673466
H	3.936309	-2.293078	-0.451253
H	4.414173	-0.797146	0.362065
H	2.438188	-1.200931	1.643840
H	4.220184	-0.048087	-1.963292
H	2.759031	-1.022928	-2.207936
H	3.065506	1.467273	-0.457231
H	1.814004	1.158146	-1.672988

Compound 12b(N): (No imaginary frequency)

C	2.344557	0.424748	1.008627
N	1.363999	0.028143	-0.012759
C	2.192754	-0.221800	-1.201990
C	3.176490	0.965849	-1.214232
C	3.231556	1.436670	0.264654
C	0.290954	-0.954883	0.345906
C	-1.029317	-0.169011	0.764416
C	-1.574393	0.504911	-0.544921

C	-2.023935	-0.539006	-1.585344
C	-1.039572	-1.666029	-1.701370
C	-0.014252	-1.832105	-0.863908
C	-2.077381	-1.126379	1.379104
C	-0.742908	0.937654	1.798548
C	-2.707495	1.477186	-0.288386
O	-2.613124	2.683842	-0.359422
C	0.760324	-1.920416	1.462703
H	-0.744957	1.093820	-0.950527
H	-2.256423	-2.010657	0.760605
H	-2.151472	-0.054494	-2.563776
H	-3.017521	-0.940644	-1.328257
H	-1.186879	-2.371635	-2.518390
H	0.668340	-2.666002	-1.022306
H	-3.689325	1.010387	-0.036371
H	-1.757955	-1.469765	2.368327
H	-3.034983	-0.612990	1.520008
H	-0.250771	0.536609	2.691297
H	-0.120539	1.730240	1.376139
H	-1.679186	1.398815	2.132744
H	0.913421	-1.413454	2.419846
H	0.036521	-2.725059	1.617505
H	1.709337	-2.386935	1.175328
H	2.758527	-1.171711	-1.127559
H	2.805156	1.766556	-1.860821
H	4.156652	0.663803	-1.596394
H	1.580121	-0.275716	-2.103564
H	4.248526	1.455142	0.669451
H	2.818945	2.445632	0.361697
H	2.962405	-0.427830	1.347476
H	1.864773	0.853808	1.889389

Cartesian coordinates and imaginary frequncies of compounds pathway B

Compound 13: (No imaginary frequency)

C	-0.087822	-0.364950	0.374802
O	1.247470	-0.635530	0.416441
H	-0.393201	0.551556	0.882613
C	-0.958032	-1.145924	-0.264940
H	-0.641993	-2.055708	-0.764520
H	-2.005237	-0.870731	-0.304738
C	1.993968	0.130376	1.350277
H	1.712874	-0.109441	2.384853
H	1.860397	1.208754	1.184252
H	3.043875	-0.126499	1.196258

Compound 14a: (No imaginary frequency)

C	0.049766	-0.267432	0.217572
C	1.513914	-0.086986	-0.059222
C	-0.777468	-0.992079	-0.584983
C	2.473130	-0.779409	0.880817
C	1.933180	0.676034	-1.074586
C	-0.435719	0.388609	1.453526
C	-0.285318	-1.717790	-1.812940
C	-2.260724	-1.186087	-0.362777
H	2.992445	0.826302	-1.269625
H	1.237330	1.189870	-1.732509
H	2.324818	-0.420558	1.904449
H	3.512670	-0.593309	0.593135
H	2.305321	-1.864760	0.885784
H	-1.514372	0.287212	1.679632
O	0.277023	1.018631	2.217712
H	-0.617750	-2.764514	-1.789290
H	0.799160	-1.688139	-1.916775
H	-0.725979	-1.276586	-2.718109
H	-2.806677	-0.912422	-1.275379
H	-2.685845	-0.615871	0.462400
H	-2.474504	-2.248713	-0.184531

Compound 14s: (No imaginary frequency)

C	-0.016310	-0.179894	0.268832
C	1.481286	-0.078364	0.262162
C	-0.716205	-1.053342	-0.506250
C	2.063489	1.101841	-0.481387
C	2.246846	-0.957445	0.918658
C	-0.682035	0.770095	1.190543
C	-0.040804	-1.995628	-1.468041
C	-2.224071	-1.151175	-0.486256
H	3.330703	-0.866918	0.934613
H	1.817345	-1.794610	1.462213
H	1.804743	1.056164	-1.547618
H	3.153593	1.141480	-0.390194
H	1.653253	2.048707	-0.104343
H	0.028942	1.392492	1.778327

O	-1.883947	0.908275	1.357300
H	-0.263200	-3.036619	-1.194775
H	1.042721	-1.874748	-1.500511
H	-0.449988	-1.852661	-2.477672
H	-2.687129	-0.220451	-0.832399
H	-2.605154	-1.304241	0.527506
H	-2.564678	-1.971554	-1.126106

Compound 19: (No imaginary frequency)

O	-1.316353	0.749507	1.421072
C	-0.151011	0.735437	1.072451
C	0.404629	-0.169541	0.035030
C	-0.367564	-1.052728	-0.608333
H	-1.427600	-1.118066	-0.377715
H	0.027319	-1.721563	-1.367251
H	1.468546	-0.081668	-0.177216
H	0.583463	1.429415	1.535507

TS-15a1: (one imaginary frequency, 456.01 cm^{-1})

C	-0.241581	-1.040444	1.604679
C	0.563286	-1.077732	0.486282
C	0.900893	0.105785	-0.261751
C	0.532291	1.411574	0.210957
C	-1.554543	1.392144	0.230734
C	-2.137512	0.133843	0.365231
O	-2.296724	-0.599868	-0.748110
C	-2.772920	-1.930190	-0.561049
H	-2.887861	-2.361109	-1.556340
H	-3.742161	-1.929604	-0.045934
H	-2.046709	-2.509880	0.020238
H	-2.645748	-0.210013	1.260860
H	-1.744994	2.091378	1.038997
H	-1.619784	1.815286	-0.766115
H	1.219316	0.945135	2.252347
H	0.113529	2.333404	2.183032
H	1.763421	2.485274	1.596931
H	1.786792	2.885167	-0.791322
H	0.236074	3.503264	-0.225468
C	0.722910	2.636810	-0.687673
C	0.907692	1.798333	1.650794
C	1.486174	-0.008311	-1.599997
H	1.556187	0.945376	-2.157607
O	1.934314	-1.019776	-2.133300
C	0.947794	-2.454589	-0.025458
H	0.557676	-2.645372	-1.029021
H	2.032909	-2.559147	-0.110437
H	0.576379	-3.225074	0.659524
H	-0.525819	-1.973899	2.085314
H	-0.447425	-0.154139	2.182084
H	0.303858	2.518472	-1.689474

TS-15a2: (one imaginary frequency, 470.17 cm^{-1})

C	-0.174505	-1.339701	1.290159

C	0.693737	-1.190049	0.231389
C	1.174212	-2.470126	-0.432147
C	1.030739	0.096986	-0.320813
C	1.837609	0.185977	-1.540625
O	2.446250	-0.724580	-2.097213
C	0.463403	1.311226	0.204486
C	0.504295	1.569149	1.721447
C	0.680086	2.630568	-0.544489
C	-1.543065	1.093752	-0.189994
C	-2.189364	0.053520	0.472326
O	-2.777402	0.302520	1.665491
C	-3.435188	-0.805878	2.274412
H	-3.881445	-0.432613	3.197232
H	-2.719803	-1.604773	2.501939
H	-4.223604	-1.198458	1.619787
H	-2.423549	-0.895118	0.001439
H	-1.451961	0.981115	-1.263988
H	-1.808990	2.092378	0.145474
H	1.090227	0.807961	2.241590
H	-0.482923	1.620907	2.191787
H	0.991651	2.535357	1.901272
H	1.725005	2.956632	-0.469561
H	0.068453	3.414360	-0.085292
H	1.932380	1.203876	-1.964109
H	0.926679	-2.507628	-1.496322
H	2.263007	-2.559027	-0.382228
H	0.730577	-3.336822	0.069561
H	-0.453639	-2.344342	1.600308
H	-0.426213	-0.558472	1.986268
H	0.414522	2.584090	-1.603575

Compound 15: (No imaginary frequency)

C	1.105538	0.295084	0.198491
C	0.975619	-1.053451	0.067639
C	-0.348991	-1.755126	0.274835
C	-1.414584	-0.898648	0.961987
C	-1.421548	0.486704	0.335029
C	-0.078626	1.235714	0.496948
C	2.435925	0.936156	0.098633
C	2.114247	-1.980533	-0.289514
H	-0.162822	-2.681633	0.834452
H	-0.741790	-2.074915	-0.703746
H	-1.181222	-0.824426	2.037499
O	-2.723004	-1.438885	0.811604
H	-2.232934	1.081759	0.769989
H	-1.651805	0.368302	-0.732483
C	-0.102862	2.420104	-0.501770
C	0.042889	1.800446	1.933986
H	2.441575	2.025295	0.311146
O	3.495565	0.387762	-0.167277
H	2.882288	-1.989955	0.492341
H	2.629702	-1.658880	-1.197936

H	1.744597	-3.002000	-0.427835
H	0.982957	2.345988	2.073558
H	0.012564	1.005054	2.686151
H	-0.778228	2.497594	2.141806
H	0.748023	3.097200	-0.377787
H	-1.013376	3.011906	-0.348699
H	-0.103863	2.062456	-1.537670
C	-2.984893	-2.580505	1.602711
H	-2.785227	-2.389054	2.669380
H	-2.396550	-3.456984	1.292303
H	-4.045860	-2.814227	1.479020

TS-15s1: (one imaginary frequency, 447.05 cm^{-1})

C	-0.222977	-1.053720	1.585433
C	0.578220	-1.056476	0.464601
C	0.972004	-2.431548	-0.066126
C	0.908004	0.135559	-0.270499
C	1.497128	-0.031563	-1.600696
O	1.683022	0.829329	-2.457186
C	0.519509	1.434987	0.213218
C	0.865502	1.789763	1.671558
C	0.733541	2.667766	-0.660149
C	-1.535822	1.391392	0.172653
C	-2.135454	0.144757	0.346911
O	-2.308839	-0.622741	-0.741458
C	-2.812088	-1.934857	-0.510674
H	-2.961884	-2.387402	-1.491816
H	-3.768407	-1.899612	0.026826
H	-2.086733	-2.517319	0.069949
H	-2.641021	-0.167863	1.255646
H	-1.743418	2.124596	0.945956
H	-1.582711	1.770814	-0.842663
H	1.224109	0.934839	2.244744
H	0.038519	2.255488	2.218926
H	1.677811	2.527738	1.647591
H	1.806594	2.864828	-0.769033
H	0.279253	3.539595	-0.172354
H	1.834269	-1.062920	-1.822257
H	0.528250	-2.650181	-1.044268
H	2.057687	-2.531862	-0.175242
H	0.643566	-3.210146	0.629120
H	-0.492182	-1.998249	2.052730
H	-0.442880	-0.179264	2.175032
H	0.333077	2.561515	-1.666029

TS-15s2: (one imaginary frequency, 458.12 cm^{-1})

C	-0.154553	-1.345182	1.299370
C	0.704925	-1.167507	0.238957
C	1.017348	0.120394	-0.321115
C	0.439771	1.332350	0.209467
C	0.667369	2.650161	-0.528398
C	1.196977	-2.445453	-0.436398

C	1.799842	0.140137	-1.558015
O	1.984298	1.082979	-2.325097
C	0.495356	1.567760	1.731485
C	-1.530195	1.110028	-0.183734
C	-2.185130	0.066819	0.468943
O	-2.781776	0.307125	1.657468
C	-3.445618	-0.805289	2.253049
H	-3.887295	-0.441832	3.181866
H	-2.734015	-1.611331	2.467527
H	-4.237698	-1.183670	1.594684
H	-2.404610	-0.884995	-0.002867
H	-1.437426	1.005436	-1.258670
H	-1.806156	2.105633	0.153312
H	1.088584	0.803009	2.238021
H	-0.488237	1.608980	2.210568
H	0.979652	2.533505	1.917372
H	1.732190	2.908904	-0.510904
H	0.116658	3.450426	-0.020236
H	2.304984	-0.818551	-1.786753
H	0.895115	-2.516419	-1.487373
H	2.289868	-2.527174	-0.409834
H	0.796056	-3.320488	0.083322
H	-0.416179	-2.355884	1.604409
H	-0.425695	-0.570936	1.995884
H	0.374413	2.615379	-1.575967

Compound 15‘: (No imaginary frequency)

C	1.094343	0.348939	0.196464
C	0.985962	-1.001198	0.057337
C	-0.329648	-1.726793	0.249792
C	-1.394550	-0.897636	0.969612
C	-1.439530	0.484947	0.340860
C	-0.111282	1.266127	0.482461
C	2.434767	0.974484	0.127170
C	2.107654	-1.961103	-0.278828
H	-0.132611	-2.670547	0.776627
H	-0.728895	-2.013956	-0.735953
H	-1.134922	-0.820006	2.038466
O	-2.693030	-1.468268	0.848254
H	-2.253908	1.065959	0.788429
H	-1.687295	0.358978	-0.722107
C	-0.159850	2.429326	-0.538512
C	0.001161	1.856811	1.910136
H	3.269381	0.300944	-0.143156
O	2.688331	2.145463	0.366818
H	2.392508	-2.539605	0.610852
H	3.009049	-1.501115	-0.682167
H	1.748728	-2.689493	-1.017178
H	0.926417	2.425843	2.020999
H	-0.013530	1.073115	2.676411
H	-0.842635	2.530962	2.102124
H	0.697326	3.094844	-0.430788

H	-1.076598	3.011487	-0.383842
H	-0.177734	2.046937	-1.566225
C	-2.918840	-2.601708	1.661430
H	-2.720938	-2.384699	2.723640
H	-2.306882	-3.467166	1.364990
H	-3.973047	-2.868171	1.546478

TS-16a1: (one imaginary frequency, 542.74 cm^{-1})

C	-0.136592	0.167704	0.047821
C	-0.133010	0.191652	1.438481
C	1.145934	0.655803	2.110608
C	-1.348621	0.023949	2.175214
C	-1.377795	0.365497	3.615771
O	-0.409501	0.457358	4.355967
C	-2.588332	-0.273409	1.551618
C	-2.691912	-1.338095	0.461181
C	-3.907403	-0.133919	2.300021
C	-2.708818	1.681543	0.359212
C	-1.610010	1.772897	-0.479960
H	-1.686298	1.420452	-1.502539
H	-0.870118	2.542281	-0.291583
O	-2.774771	2.521202	1.465173
H	-3.671470	1.330224	-0.016200
H	-1.782457	-1.938965	0.383408
H	-2.923929	-0.934558	-0.532036
H	-3.511197	-2.021858	0.715568
H	-4.048247	-0.943329	3.029638
H	-4.735741	-0.209348	1.585970
H	-2.386620	0.503273	4.045324
H	0.997954	1.542856	2.733374
H	1.542963	-0.112782	2.780396
H	1.904844	0.875629	1.352315
H	0.777018	0.443230	-0.474702
H	-0.797714	-0.454812	-0.529308
H	-4.002127	0.822550	2.815976
C	-3.461347	3.739470	1.207168
H	-3.475121	4.298197	2.146570
H	-2.951262	4.333260	0.435463
H	-4.496960	3.557558	0.881088

TS-16a2: (one imaginary frequency, 541.19 cm^{-1})

C	-0.238392	0.233669	0.004239
C	-0.083280	0.042243	1.391453
C	1.325593	0.143031	1.941498
C	-1.230536	0.065584	2.243043
C	-1.062370	0.335735	3.691398
O	-0.015705	0.326841	4.321935
C	-2.555897	-0.057299	1.767814
C	-2.931653	-1.021217	0.665376
C	-3.759248	0.332805	2.613914
C	-2.413020	2.025155	0.093472
C	-1.047000	2.057672	-0.173868

H	-0.762806	2.164596	-1.218157
H	-0.428222	2.612285	0.522447
H	-2.876225	2.469173	0.967222
O	-3.247299	1.621798	-0.913268
H	-2.114215	-1.704194	0.419729
H	-3.254196	-0.518324	-0.258053
H	-3.782466	-1.629869	1.002787
H	-4.017968	-0.447256	3.346343
H	-4.636982	0.443397	1.967769
H	-2.004464	0.522125	4.242367
H	1.481506	1.039745	2.552227
H	1.563000	-0.698897	2.598889
H	2.047386	0.149462	1.117964
H	0.679252	0.295450	-0.580100
H	-1.047998	-0.213724	-0.554296
H	-3.634613	1.271308	3.160938
C	-4.590371	2.081147	-0.821692
H	-5.139426	1.608443	-1.638374
H	-5.049085	1.798580	0.134193
H	-4.638076	3.172620	-0.933093

Compound 16: (No imaginary frequency)

C	1.168216	-0.035452	0.025405
C	1.153341	-1.395158	0.067560
C	-0.099851	-2.166766	0.409399
C	-1.219054	-1.322126	1.018263
C	-1.366248	-0.035541	0.209891
C	-0.079291	0.843831	0.255570
C	2.434335	0.692484	-0.223479
C	2.351379	-2.270093	-0.218498
H	0.169415	-2.986839	1.089321
H	-0.455474	-2.662776	-0.508433
H	-0.986624	-1.101827	2.067025
O	-2.535856	0.740821	0.497173
H	-1.499983	-0.331695	-0.840912
C	-0.229978	1.893616	-0.875914
C	0.051915	1.587641	1.605153
H	2.343651	1.797628	-0.224093
O	3.537511	0.197359	-0.403416
H	3.107432	-2.176365	0.570052
H	2.858789	-1.986158	-1.143133
H	2.046608	-3.320689	-0.280046
H	0.973868	2.179028	1.633149
H	0.087125	0.896029	2.454064
H	-0.784786	2.278424	1.748205
H	0.531150	2.677979	-0.829444
H	-1.208994	2.373557	-0.785981
H	-0.169935	1.420719	-1.863273
H	-2.157118	-1.888081	1.006521
C	-3.136818	0.642228	1.775971
H	-3.539855	-0.360058	1.975685
H	-3.970746	1.349705	1.765576

H	-2.460719	0.916874	2.596339

TS-16s1: (one imaginary frequency, 569.47 cm^{-1})

C	-0.117714	0.112007	0.064708
C	-0.150273	0.168516	1.460217
C	-1.387785	0.062275	2.165556
C	-2.622264	-0.207756	1.521202
C	-3.941896	0.032975	2.222624
C	1.123987	0.644309	2.148033
C	-1.363045	0.413571	3.605227
O	-2.318308	0.531829	4.358200
C	-2.744781	-1.273378	0.436065
C	-1.409361	1.681117	-0.589900
C	-2.525357	1.812144	0.228974
O	-2.467720	2.728078	1.253341
C	-3.615036	3.555911	1.386514
H	-1.549244	1.256280	-1.577563
H	-0.641049	2.442263	-0.509958
H	-3.519565	1.512987	-0.095265
H	-1.877890	-1.939982	0.411333
H	-2.895199	-0.872606	-0.574392
H	-3.622957	-1.893884	0.653904
H	-4.132655	-0.736150	2.983436
H	-4.758947	-0.018276	1.491445
H	-0.346378	0.529055	4.027591
H	1.013291	1.619476	2.637497
H	1.472547	-0.062577	2.910815
H	1.928351	0.737940	1.412528
H	0.826879	0.326088	-0.431953
H	-0.746510	-0.560726	-0.493135
H	-3.973151	0.989246	2.742335
H	-3.478841	4.134481	2.302760
H	-3.711030	4.241642	0.532426
H	-4.535459	2.962872	1.472582

TS-16s2: (one imaginary frequency, 534.22 cm^{-1})

C	-0.240307	0.242822	0.006992
C	-0.115215	0.030855	1.394932
C	-1.271645	0.071875	2.233063
C	-2.593608	-0.043273	1.749254
C	-3.788102	0.342083	2.598330
C	1.292224	0.132420	1.968162
C	-1.040132	0.356371	3.670454
O	-1.866674	0.703240	4.501796
C	-2.946075	-0.997815	0.629874
C	-1.019196	2.064785	-0.174276
C	-2.389208	2.050852	0.082622
O	-3.216554	1.678146	-0.938029
C	-4.586618	2.032469	-0.782661
H	-0.729305	2.180468	-1.216436
H	-0.403316	2.615986	0.527816
H	-2.851258	2.485750	0.961157

H	-2.127263	-1.685756	0.401256
H	-3.236858	-0.489127	-0.300985
H	-3.810549	-1.600086	0.940407
H	-3.921660	-0.358866	3.434712
H	-4.700653	0.305479	1.992122
H	0.004693	0.199354	4.002186
H	1.485215	1.076632	2.496672
H	1.513958	-0.676938	2.674005
H	2.028152	0.059966	1.161980
H	0.688937	0.295768	-0.560268
H	-1.040653	-0.198533	-0.569912
H	-3.696384	1.329288	3.052853
H	-5.110783	1.639303	-1.655756
H	-5.013230	1.593537	0.126835
H	-4.704701	3.123480	-0.746945

Compound 16‘: (No imaginary frequency)

C	1.157699	0.020215	0.008995
C	1.169587	-1.340135	0.056045
C	-0.065269	-2.138420	0.410645
C	-1.184168	-1.314480	1.045486
C	-1.374839	-0.041724	0.224188
C	-0.109319	0.871471	0.237302
C	2.433456	0.736977	-0.226768
C	2.357456	-2.242337	-0.205393
H	0.226940	-2.964088	1.074753
H	-0.431430	-2.625471	-0.507767
H	-0.928501	-1.078554	2.085385
O	-2.560393	0.705438	0.519582
H	-1.520145	-0.355438	-0.820178
C	-0.288010	1.890632	-0.916158
C	0.017607	1.645300	1.571045
H	3.303015	0.100009	-0.475320
O	2.602996	1.943827	-0.145535
H	2.736895	-2.652125	0.740970
H	3.193319	-1.777003	-0.726460
H	2.031566	-3.102551	-0.804020
H	0.916664	2.264380	1.557032
H	0.083252	0.971551	2.433605
H	-0.845343	2.304077	1.707565
H	0.497390	2.646563	-0.905251
H	-1.260734	2.379989	-0.808678
H	-0.268866	1.385764	-1.890260
H	-2.108723	-1.902113	1.063134
C	-3.128458	0.620800	1.813956
H	-3.489819	-0.389784	2.050308
H	-3.988532	1.296398	1.803177
H	-2.445294	0.942527	2.610712

TS-17s1: (one imaginary frequency, 427.71 cm^{-1})

C	2.148804	0.806057	-0.535426
C	1.404412	-0.150118	0.373655

C	2.054253	-1.073228	1.092904
C	-0.083558	0.013912	0.495973
C	-0.550865	1.031617	1.351305
O	-1.734009	1.470932	1.378908
C	-0.997485	-0.633805	-0.397899
C	-2.298016	-1.183602	0.183315
C	-0.401799	-1.574665	-1.438939
H	3.136334	-1.181202	1.043355
H	1.525937	-1.745043	1.764140
H	1.774643	0.758374	-1.567088
H	3.224213	0.598077	-0.556512
H	2.005170	1.842938	-0.202320
H	0.212823	1.540886	1.971604
H	-0.020561	-2.474840	-0.941530
H	0.433228	-1.128434	-1.986036
H	-1.160421	-1.892200	-2.161907
H	-2.757085	-0.482643	0.876756
H	-2.060616	-2.108884	0.726136
H	-3.017289	-1.438594	-0.602557
C	-2.463314	1.772181	-0.856628
C	-1.755260	0.826486	-1.594801
O	-3.763840	1.597098	-0.628283
H	-2.034126	2.720742	-0.552260
H	-2.356582	0.163132	-2.209882
H	-0.837974	1.176537	-2.055809
C	-4.369672	2.540025	0.268649
H	-5.395869	2.201465	0.416619
H	-3.822275	2.548741	1.212969
H	-4.375589	3.540908	-0.180774

TS-17s2: (one imaginary frequency, 423.34 cm^{-1})

O	-2.046889	1.284350	1.384667
C	-0.814991	1.013514	1.345569
C	-0.229354	0.026161	0.518079
C	-1.087578	-0.763673	-0.320755
C	-1.960961	0.545079	-1.570713
C	-2.422254	1.700167	-0.940565
O	-1.638846	2.779126	-0.950086
C	-2.087889	3.886163	-0.154054
H	-3.055318	4.249411	-0.521353
H	-2.173063	3.562710	0.886582
H	-1.335980	4.667973	-0.266873
H	-3.426267	1.810591	-0.545191
H	-2.733804	-0.120300	-1.942555
H	-1.119419	0.695110	-2.241830
C	-2.324597	-1.408787	0.305803
H	-2.866824	-0.705908	0.934547
H	-1.993113	-2.249466	0.930558
H	-2.995417	-1.815595	-0.459948
C	-0.434247	-1.686615	-1.342411
H	0.440214	-1.229619	-1.814560
H	-0.113910	-2.616383	-0.855256

H	-1.145631	-1.970073	-2.125602
C	1.255943	0.058825	0.377660
C	1.886998	1.185611	0.008231
H	1.333278	2.074842	-0.279359
H	2.973030	1.248975	-0.025519
C	2.044688	-1.172893	0.775770
H	1.844033	-1.434120	1.822886
H	3.121812	-1.010550	0.662881
H	1.774142	-2.050640	0.178466
H	-0.111769	1.641955	1.923498

Compound 17: (No imaginary frequency)

C	2.498407	0.050725	-0.160010
C	1.206978	-0.225965	0.580081
C	1.189387	-0.960446	1.699649
C	-0.046786	0.401870	0.043293
C	-0.379188	1.617978	0.496862
O	-1.471555	2.368453	0.140583
C	-0.937501	-0.333726	-0.965406
C	-1.705484	-1.474831	-0.257048
C	-0.108926	-0.954121	-2.110651
H	2.096429	-1.406944	2.102509
H	0.270890	-1.135881	2.252074
H	2.445665	-0.268627	-1.207043
H	3.347325	-0.456459	0.310624
H	2.706107	1.128831	-0.175494
H	0.229914	2.161234	1.213440
H	0.583723	-1.713122	-1.731667
H	0.471258	-0.194840	-2.647599
H	-0.773144	-1.443929	-2.833503
H	-2.335927	-1.087846	0.545554
H	-1.003392	-2.202671	0.163457
H	-2.348718	-2.001213	-0.974415
C	-2.494532	1.699481	-0.599915
C	-1.908848	0.699622	-1.589297
O	-3.397746	1.044393	0.248153
H	-3.009642	2.519130	-1.122308
H	-2.733406	0.190873	-2.101082
H	-1.368379	1.286421	-2.342650
C	-4.091768	1.910060	1.136395
H	-4.835915	1.297533	1.650528
H	-3.415623	2.360752	1.871522
H	-4.603939	2.714557	0.586390

TS-17s3: (one imaginary frequency, 419.46 cm^{-1})

O	-1.691780	1.574044	1.286093
C	-0.508683	1.142698	1.263474
C	-0.051718	0.044451	0.494241
C	-0.998877	-0.686903	-0.297382
C	-1.779220	0.699004	-1.600141
C	-2.465280	1.707687	-0.930793
O	-3.765536	1.565640	-0.671948

C	-4.349155	2.588434	0.147880
H	-3.787625	2.675882	1.080035
H	-4.354997	3.546551	-0.386691
H	-5.375390	2.273885	0.341325
H	-2.025921	2.676043	-0.716629
H	-0.861485	0.991215	-2.099062
H	-2.398921	-0.009759	-2.141074
C	-2.289470	-1.168315	0.357441
H	-2.730799	-0.403396	0.992642
H	-3.026225	-1.487635	-0.387827
H	-2.047863	-2.041961	0.979103
C	-0.461470	-1.693309	-1.305615
H	-1.222690	-1.951235	-2.048708
H	-0.192624	-2.626276	-0.794373
H	0.426237	-1.323734	-1.827181
H	0.269151	1.708786	1.809246
C	1.426774	-0.107481	0.368245
C	2.205643	0.935912	0.033566
H	3.291269	0.861526	0.029576
H	1.784930	1.897694	-0.246605
C	2.059120	-1.429263	0.761272
H	3.151965	-1.371327	0.723559
H	1.749526	-2.254432	0.110903
H	1.764854	-1.706005	1.781681

TS-17s4: (one imaginary frequency, 420.95 cm^{-1})

C	1.856899	1.028458	-0.566018
C	1.241661	0.033549	0.396869
C	-0.254162	-0.006115	0.500841
C	-1.078155	-0.706842	-0.443264
C	-0.366917	-1.566308	-1.483852
C	2.002423	-0.727574	1.193177
C	-0.858759	0.878596	1.417872
O	-2.092365	1.150665	1.450514
C	-2.318128	-1.423489	0.101952
C	-1.942954	0.661017	-1.597889
C	-2.414307	1.760460	-0.878735
O	-1.625607	2.828144	-0.777747
C	-2.079761	3.862591	0.109355
H	3.089267	-0.672795	1.170060
H	1.562234	-1.423538	1.902153
H	1.536972	0.848922	-1.600848
H	2.951533	0.995323	-0.541205
H	1.529996	2.046963	-0.319701
H	-0.172171	1.435662	2.084677
H	0.042623	-2.460072	-0.997204
H	0.463899	-1.050421	-1.971451
H	-1.066020	-1.902913	-2.257293
H	-2.884730	-0.785184	0.776653
H	-1.983615	-2.308915	0.659048
H	-2.966131	-1.774332	-0.710127
H	-3.418762	1.834660	-0.476280

H	-1.102898	0.874425	-2.253667
H	-2.710117	0.028346	-2.033824
H	-1.310377	4.635267	0.095668
H	-3.027881	4.279595	-0.250475
H	-2.202737	3.438931	1.109659

Compound 17‘: (No imaginary frequency)

C	-1.917972	0.615303	-1.551905
C	-0.994666	-0.412540	-0.845801
C	-0.047047	0.376356	0.068854
C	-0.344067	1.636314	0.432384
O	-1.438826	2.375033	0.072489
C	-2.477270	1.700686	-0.642579
C	1.250271	-0.178525	0.555743
C	2.396639	0.489496	0.351746
C	-1.840025	-1.446774	-0.063132
C	-0.196701	-1.147143	-1.944997
O	-3.419132	1.145029	0.233759
C	-4.094971	2.101695	1.039462
C	1.253918	-1.479862	1.332130
H	3.341196	0.134689	0.758229
H	2.427043	1.407322	-0.227893
H	0.537251	-1.447693	2.161707
H	2.248121	-1.685252	1.741771
H	0.974232	-2.334605	0.704675
H	0.305588	2.220762	1.075325
H	0.465681	-1.908833	-1.521619
H	0.422950	-0.450670	-2.520678
H	-0.881589	-1.650540	-2.638668
H	-2.405142	-0.968780	0.738583
H	-1.211997	-2.232702	0.366282
H	-2.556930	-1.930975	-0.739022
H	-2.950616	2.502891	-1.227917
H	-2.755882	0.104133	-2.038627
H	-1.345576	1.127185	-2.335390
H	-4.863355	1.556523	1.592204
H	-3.412306	2.589876	1.743914
H	-4.575440	2.873374	0.418378

TS-18s1: (one imaginary frequency, 574.50 cm^{-1})

O	-1.863230	1.486502	0.888398
C	-0.645012	1.147952	1.063331
C	-0.044578	0.048468	0.436712
C	-0.868012	-0.794823	-0.378544
C	-1.746392	0.563591	-1.804210
C	-2.212544	1.670308	-1.090927
H	-3.279358	1.787449	-0.941182
H	-1.619163	2.571987	-1.033540
H	-0.825511	0.651619	-2.381924
O	-2.687247	-0.296113	-2.374687
C	-2.164042	-1.337985	0.211122
H	-2.637944	-0.627385	0.884962

H	-2.869090	-1.628336	-0.570629
H	-1.905636	-2.243433	0.779863
C	-0.222101	-1.772410	-1.342694
H	-0.931535	-2.018179	-2.139061
H	0.025641	-2.709685	-0.828397
H	0.701177	-1.386339	-1.782257
H	-0.006953	1.836072	1.641414
C	1.446465	-0.076184	0.488369
C	2.031029	-1.208022	0.907027
H	3.113028	-1.308691	0.950464
H	1.449870	-2.067893	1.228271
C	2.279866	1.117442	0.071127
H	3.351362	0.910675	0.161151
H	2.054403	2.000637	0.681863
H	2.070651	1.399245	-0.969789
C	-2.990198	0.023013	-3.724710
H	-3.695524	-0.734019	-4.077315
H	-3.449152	1.018625	-3.809879
H	-2.089354	-0.002309	-4.356552

TS-18s2: (one imaginary frequency, 538.11 cm^{-1})

O	-1.811531	1.525017	0.901381
C	-0.596344	1.173458	0.990971
C	-0.061015	0.009164	0.405428
C	-0.933397	-0.845388	-0.336048
C	-1.701295	0.494031	-1.755466
C	-2.448327	1.455101	-1.083383
O	-0.536634	0.904159	-2.403338
C	-0.737508	1.230962	-3.769803
H	-1.420672	2.085199	-3.886345
H	0.241511	1.490698	-4.180762
H	-1.147962	0.377734	-4.332213
H	-2.226544	-0.332049	-2.239568
H	-3.463207	1.238711	-0.776028
H	-2.159005	2.497331	-1.115418
C	-2.236046	-1.318033	0.297633
H	-2.685559	-0.551290	0.925702
H	-2.013374	-2.194073	0.923299
H	-2.960474	-1.641623	-0.459971
C	-0.309061	-1.887605	-1.246483
H	0.535360	-1.477484	-1.804892
H	0.045122	-2.744041	-0.658493
H	-1.046772	-2.279237	-1.955747
C	1.427714	-0.114715	0.384723
C	2.199378	0.839812	-0.155387
H	1.768171	1.686281	-0.680507
H	3.285453	0.786683	-0.110893
C	2.037261	-1.303127	1.099560
H	1.708680	-2.256798	0.670077
H	3.131010	-1.275531	1.055649
H	1.735920	-1.315939	2.155109
H	0.120477	1.882596	1.437420

Compound 18: **(No imaginary frequency)**

C	-1.991447	0.776552	-1.433530
C	-1.008451	-0.292689	-0.896579
C	-0.061978	0.417592	0.084759
C	-0.357247	1.624278	0.593912
O	-1.475107	2.370027	0.347916
C	-2.529453	1.658389	-0.302962
C	1.217692	-0.234196	0.524129
C	1.262320	-0.983343	1.633342
C	-1.760677	-1.437494	-0.177381
C	-0.250754	-0.897389	-2.097076
H	-3.066171	1.042853	0.430611
C	2.461904	0.033719	-0.295705
H	2.185962	-1.450338	1.969669
H	0.379729	-1.150092	2.244132
H	2.338851	-0.274867	-1.339845
H	3.332068	-0.488953	0.115221
H	2.681970	1.109410	-0.313755
H	0.306857	2.148311	1.275144
H	0.437089	-1.685627	-1.774086
H	0.326982	-0.136111	-2.634099
H	-0.967859	-1.339449	-2.796393
H	-2.342561	-1.071510	0.674709
H	-1.042211	-2.170168	0.203941
H	-2.441527	-1.942110	-0.868840
H	-3.215299	2.420531	-0.681483
O	-3.064948	0.134407	-2.111916
H	-1.440848	1.423382	-2.135820
C	-3.653664	0.900757	-3.145656
H	-4.434774	0.279897	-3.592416
H	-4.114372	1.828586	-2.775515
H	-2.918728	1.163994	-3.921887

TS-18s3: **(one imaginary frequency, 564.40 cm^{-1})**

O	-1.852697	1.491101	0.916495
C	-0.641670	1.139305	1.097825
C	-0.047362	0.032503	0.470113
C	-0.872278	-0.805130	-0.346476
C	-1.707963	0.567006	-1.781506
C	-2.194614	1.667820	-1.073717
H	-3.264381	1.773609	-0.936617
H	-1.610464	2.574392	-1.002231
H	-0.771532	0.660405	-2.333271
O	-2.631027	-0.292980	-2.380576
C	-2.179934	-1.336557	0.225189
H	-2.656080	-0.619964	0.891437
H	-2.876794	-1.620030	-0.566608
H	-1.940648	-2.243959	0.799102
C	-0.220108	-1.778159	-1.308753
H	-0.904978	-1.991385	-2.135225
H	-0.019457	-2.734771	-0.807774
H	0.723772	-1.397955	-1.710979

H	0.014402	1.812922	1.673050
C	1.438862	-0.069052	0.527792
C	2.220342	0.984356	0.237150
H	3.300925	0.942492	0.355496
H	1.808261	1.919014	-0.132617
C	2.044521	-1.359710	1.040968
H	3.135495	-1.290040	1.098053
H	1.797066	-2.216194	0.404530
H	1.662046	-1.591637	2.043167
C	-2.912166	0.042763	-3.731608
H	-3.601214	-0.717585	-4.108593
H	-3.381852	1.033860	-3.810403
H	-1.999246	0.038158	-4.346389

TS-18s4: (one imaginary frequency, 542.26 cm^{-1})

O	-1.829383	1.492610	0.973733
C	-0.613495	1.142162	1.078138
C	-0.057096	0.022360	0.437317
C	-0.903546	-0.790685	-0.377690
C	-1.654261	0.602787	-1.737351
C	-2.411078	1.531504	-1.030748
O	-0.485198	1.046447	-2.359476
C	-0.691866	1.489987	-3.692289
H	-1.114956	0.691575	-4.321421
H	0.286711	1.775065	-4.087466
H	-1.366719	2.357400	-3.729779
H	-2.173822	-0.197532	-2.269030
H	-2.119216	2.573369	-1.003744
H	-3.432193	1.303389	-0.754322
C	-2.214549	-1.308194	0.205704
H	-2.681074	-0.584716	0.871272
H	-2.923523	-1.591116	-0.581952
H	-1.994574	-2.219234	0.779879
C	-0.252230	-1.792525	-1.317261
H	0.563218	-1.344598	-1.888858
H	-0.991122	-2.200328	-2.016666
H	0.158182	-2.635152	-0.748712
C	1.437272	-0.104702	0.421774
C	2.036240	-1.140520	1.024287
H	3.118914	-1.245730	1.036039
H	1.466436	-1.912237	1.535555
C	2.232146	0.981408	-0.268015
H	1.915746	1.082759	-1.312344
H	3.307905	0.778035	-0.234948
H	2.053547	1.957328	0.202674
H	0.075140	1.827772	1.600894

Compound 18‘: (No imaginary frequency)

C	-1.985304	0.751916	-1.429242
C	-1.084781	-0.323474	-0.767012
C	-0.066350	0.439210	0.097638
C	-0.305109	1.705120	0.490744

O	-1.407149	2.462133	0.225574
C	-2.488210	1.771121	-0.404348
C	1.245635	-0.157108	0.487062
C	2.394667	0.474052	0.199337
C	-1.944150	-1.306042	0.065419
C	-0.375220	-1.099885	-1.896624
H	-3.096610	1.268277	0.358073
C	1.261844	-1.459266	1.262035
H	3.354517	0.087721	0.534806
H	2.411924	1.392278	-0.380485
H	0.629564	-1.395122	2.156380
H	2.279539	-1.712983	1.575563
H	0.882668	-2.298187	0.666254
H	0.404619	2.267848	1.088075
H	0.248307	-1.907998	-1.502378
H	0.271229	-0.437808	-2.483790
H	-1.120056	-1.542076	-2.566037
H	-2.442308	-0.802793	0.900179
H	-1.326178	-2.103492	0.486933
H	-2.709522	-1.765632	-0.566592
H	-3.101998	2.542979	-0.876346
O	-3.088646	0.121181	-2.069009
H	-1.377970	1.286622	-2.176974
C	-3.594807	0.815162	-3.193798
H	-4.403351	0.203735	-3.603063
H	-4.001038	1.803860	-2.933121
H	-2.821981	0.949365	-3.966057

TS-20-1: (one imaginary frequency, 396.11 cm^{-1})

O	-1.648011	1.110687	1.380095
C	-0.389715	1.083338	1.338672
C	0.318706	0.331901	0.379706
C	-0.448504	-0.416670	-0.534395
C	-1.430629	0.713357	-1.778116
C	-2.054915	1.733157	-1.061821
O	-1.405209	2.879674	-0.899528
C	-1.998969	3.816125	0.014899
H	-2.976340	4.141376	-0.359942
H	-1.320343	4.668462	0.059959
H	-2.101124	3.335110	0.991823
H	-3.048048	1.646990	-0.633106
H	-0.616567	1.029362	-2.425320
H	-2.092845	-0.032404	-2.209526
H	0.075905	-1.039781	-1.257545
H	-1.344181	-0.875644	-0.124464
H	1.385899	0.483917	0.244051
H	0.191568	1.718525	2.036304

TS-20-2: (one imaginary frequency, 410.32 cm^{-1})

O	-1.204419	1.535384	1.307975
C	-0.035981	1.071719	1.281582
C	0.350703	0.032453	0.411994

C	-0.627900	-0.487144	-0.452306
C	-1.251672	0.881109	-1.754170
C	-1.985320	1.812745	-1.027369
O	-3.266443	1.570690	-0.764727
C	-3.895461	2.467872	0.164902
H	-3.314094	2.498644	1.088009
H	-4.892835	2.065164	0.345378
H	-3.978735	3.469452	-0.274436
H	-1.575151	2.755956	-0.682731
H	-1.827169	0.197415	-2.373762
H	-0.321138	1.229408	-2.188902
H	-0.332934	-1.270635	-1.148926
H	-1.629866	-0.608790	-0.046998
H	1.405686	-0.186621	0.269213
H	0.743341	1.542076	1.913039

Compound 20: (No imaginary frequency)

C	-1.884982	0.738153	-1.634589
C	-1.010822	-0.295231	-0.908304
C	-0.106381	0.411640	0.066268
C	-0.366657	1.654214	0.479559
O	-1.448570	2.412503	0.100397
C	-2.472009	1.731638	-0.636890
H	0.778831	-0.087527	0.448729
H	-1.648943	-1.021137	-0.385337
H	-0.422932	-0.865211	-1.638915
O	-3.332512	1.022884	0.210640
C	-4.045325	1.833771	1.134010
H	0.267157	2.212936	1.161327
H	-3.013818	2.548772	-1.134172
H	-2.704978	0.261507	-2.180757
H	-1.280998	1.302579	-2.354588
H	-4.729318	1.170049	1.668017
H	-3.372012	2.319013	1.849696
H	-4.629472	2.609137	0.614732

TS-21-1: (one imaginary frequency, 536.11 cm^{-1})

O	-1.747330	1.598334	0.899464
C	-0.543878	1.233545	1.032452
C	-0.075876	0.042997	0.452267
C	-1.002202	-0.697226	-0.293327
C	-1.609642	0.499079	-1.800892
C	-2.313762	1.532061	-1.193094
O	-0.402185	0.794008	-2.432718
C	-0.560000	1.123029	-3.804274
H	-1.029726	0.300203	-4.366098
H	0.441814	1.300406	-4.203843
H	-1.171367	2.027716	-3.937462
H	-2.177738	-0.313394	-2.264072
H	-3.341624	1.386819	-0.885929
H	-1.940750	2.547492	-1.212803
H	-2.005192	-0.792160	0.111502

H	-0.651723	-1.559690	-0.856312
H	0.992494	-0.128932	0.360116
H	0.174697	1.923793	1.506752

TS-21-2: (one imaginary frequency, 558.04 cm^{-1})

C	-2.121986	1.694924	-1.133629
C	-1.639764	0.591184	-1.831783
O	-2.560013	-0.324056	-2.350073
C	-2.945571	-0.031463	-3.684318
O	-1.880743	1.385278	0.968746
C	-0.674482	1.068442	1.194054
C	-0.059462	0.017798	0.498074
H	1.021790	-0.091122	0.522689
C	-0.851508	-0.653894	-0.442090
H	-0.398374	-1.395431	-1.096175
H	-1.877621	-0.869945	-0.162366
H	-3.185143	1.805610	-0.961032
H	-1.505854	2.573200	-0.997777
H	-0.729372	0.697220	-2.426256
H	-0.068941	1.712302	1.855009
H	-3.621775	-0.830150	-3.999459
H	-3.465321	0.935161	-3.753108
H	-2.076529	-0.009500	-4.360015

Compound 21: (No imaginary frequency)

C	-2.428467	1.799316	-0.442075
C	-1.948065	0.785009	-1.490771
C	-1.047209	-0.250549	-0.817206
C	-0.120809	0.429531	0.160790
C	-0.296131	1.699479	0.541137
O	-1.336248	2.501550	0.161454
O	-3.051472	0.106804	-2.076260
C	-3.643260	0.778547	-3.172243
H	-1.685755	-0.995708	-0.321145
H	-0.477356	-0.795367	-1.580687
H	0.738244	-0.112478	0.543825
H	-2.995118	1.266581	0.334380
H	0.385339	2.234260	1.195687
H	-3.069473	2.568591	-0.879505
H	-1.376411	1.323538	-2.263191
H	-4.454805	0.140093	-3.531208
H	-4.064637	1.756522	-2.895351
H	-2.921126	0.930753	-3.989537

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