

Supplementary Material

On the Catalytic Effects of the Thiazolium Salt in the Oxa-Diel-Alder Reaction between Benzaldehyde and Danishefsky's Diene: A Molecular Electron Density Theory Study

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1.- ELF topological analysis of the C–C and C–O single bond formation along the most favorable para/endo reaction paths associated with the ODA reaction between benzaldehyde 1 and Danishefsky diene 2.

Several theoretical studies have shown that the ELF topological analysis of electron density changes $\rho(\mathbf{r})$, along a reaction path can be used as a valuable tool to understand the bonding changes along with the reaction and establish its molecular mechanism. Herein, to understand the molecular mechanism of the ODA reactions between benzaldehyde **1** and Danishefsky diene **2**, an ELF topological analysis of the stationary points and the most relevant structures involved in the formation of the C–C and C–O single bonds along the *para/endo* isomeric reaction channels was performed. The populations of the most significant valence basins of the selected points along with the reaction path associated with the *para/endo* isomeric reaction channel of the O-DA reaction between benzaldehyde **1** and Danishefsky diene **2** are displayed in Table S1. The attractor positions of the ELF valence basins are shown in Figure S1.

The *para/endo* pathway of this ODA reaction begins at the molecular complex, **MC1**, which is a minimum in the PES connecting the separated reagents, benzaldehyde **1** and the Danishefsky diene **2**, with **TS1-pm**. The ELF picture of **MC1** exhibits the topological characteristics of the separated reagents. Thus, the diene framework at **MC** is characterized by the presence of four $V(C1,C2)$, $V'(C1,C2)$, $V(C3,C4)$ and $V'(C3,C4)$ disynaptic basins, integrating 1.83e, 1.82e, 1.89e and 1.72e, which belong to the C1–C2 and C3–C4 double bonds, as well as one $V(C2,C3)$ disynaptic basin, with a population of 2.25e, related to the C2–C3 single bond. On the other hand, one $V(O5,C6)$ disynaptic basin, integrating 2.36e, describes the O5–O6 bonding region of the benzaldehyde moiety. The presence of one $V(O5,C6)$ disynaptic basin instead of two $V(O5,C6)$ and $V'(O5,C6)$ disynaptic basins emphasizes the single bond character of the O5–C6 bonding region, which is very polarised toward the electronegative O5 oxygen. This is evidenced by the total population of the two $V(O5)$ and $V'(O5)$ monosynaptic basins associated with the O5 oxygen lone pairs, 5.25e. At **MC1**, the GEDT is null, 0.01e.

At **S1-1**, several significant topological changes are observed. The two pairs of disynaptic basins $V(C1,C2)$ and $V'(C1,C2)$, and $V(C3,C4)$ and $V'(C3,C4)$, present in **MC1**, have merged into one $V(C1,C2)$ and $V(C3,C4)$ disynaptic basins, integrating 2.71e and 2.90e, respectively. A strong depopulation of the two C–C double bond regions present in the reagents is observed. Together with the depopulation of these regions, two

new V(C1) and V(C3) monosynaptic basins, integrating 0.79e and 0.31e, have been created at the C1 and C3 carbons. In addition, while the total population of the V(O5) and V'(O5) monosynaptic basins have increased by 0.49e, a new V(C6) monosynaptic basin is also observed at the C6 carbon with a population of 0.10e. At **S1-1**, the GEDT has strongly increased to 0.32e.

At **TS1-pn**, the first most relevant topological change and the ODA reaction between benzaldehyde **1** and the Danishefsky diene **2** are observed. A new V(C1,C6) disynaptic basin, integrating 0.99e, has appeared from the merger of the two V(C1) and V(C6) monosynaptic basins present at **S1-1**. This relevant topological change indicates that the first C1–C6 single bond formation has already begun at a C–C distance of *ca.* 1.96 Å through the C-to-C coupling of the two C1 and C6 *pseudoradical* centers. The high GEDT at **TS1-pm**, 0.33e, emphasizes the polar nature of this ODA reaction.

At **S1-2**, while the population of the V(C3,C4) disynaptic basin has decreased to 2.26e, the V(C3) monosynaptic basin presents at the previous **S1-2** structure, and **TS1-pn** has disappeared, its electron density being distributed into the C2–C3 bonding region. As the increase of the total population in this region by 0.90e, the V(C2,C3) disynaptic basin present at **TS1-pm** has split into two new V(C2,C3) and V'(C2,C3) disynaptic basins integrating 1.86e and 1.74e, respectively, as a consequence of the increase of the population in the C2–C3 bonding region by *ca.* 0.90e. The V(C1,C6) disynaptic basin associated with the recently formed C1–C6 single bond region increases its population in 0.77e due to an electron rearrangement of the C1–C2–C3–C4 skeleton of the diene framework. In addition, together with the depopulation of the V(O5,C6) disynaptic basin to 1.33e, the two V(O5) and V'(O5) monosynaptic basins acquire populations of 3.35e and 2.86e. At **S1-2**, the GEDT reaches the maximum value along the cycloaddition, 0.38e.

At **S1-3**, the second most relevant topological change along the reaction path is observed. While the V(O5) and V'(O5) monosynaptic basins have decreased their populations by 0.63e and 0.05e, a new V(C4,O5) disynaptic basin has appeared with a population of 0.66e. This significant topological change indicates that the formation of the second C4–O5 single bond has already started at the short distance of *ca.* 1.76 Å through the donation of the electron density of mainly one of the O5 oxygen lone pairs the C4 carbon. At **S1-3**, the GEDT scarcely varies.

Finally, at dihydropyranone **14**, the two C1–C6 and C4–O5 single bonds formed along the O-DA reaction between benzaldehyde **1** and the Danishefsky diene **2** have

reached populations of 1.90e and 1.32e. The low populations of the V(C4,O5) and V(O5,C6) disynaptic basins compared to the expected 2e of the population are indicative of a high polarisation of the C4–O5 and O5–C6 bonds toward the O5 oxygen so that the total population of the V(O5) and V'(O5) monosynaptic basins is 4.98e. Finally, in agreement with the Lewis formula of dihydropyranone **14**, the C1–C2 and C3–C4 single bonds and the C2–C3 double bond of this pyranone are characterized by two V(C1,C2) and V(C3,C4) disynaptic basins integrating 2.08e and 2.05e, respectively, and two V(C2,C3) and V'(C2,C3) disynaptic basins integrating 1.92e and 1.89e. At dihydropyranone **14**, the GEDT has slightly decreased to 0.31e, but remains unexpectedly high due to the polarisation towards the O5 oxygen.

Table S1. ELF valence basin populations at some selected points of the IRC involved in forming the C1–C6 and C4–O5 single bonds along the most favorable *paralendo* reaction path associated with the ODA reaction between benzaldehyde **1** and diene **2**. The stationary points **MC1**, **TS1-pn**, and dihydropyranone **14** are also included. Distances are given in Angstroms, Å, while GEDT values and electron populations are given the in electrons, e.

Structures	MC1	S1-1	TS1-pn	S1-2	S1-3	14
d(C1–C6)	3.234	1.994	1.963	1.600	1.597	1.534
d(C4–O5)	2.935	2.193	2.176	1.767	1.756	1.418
GEDT	0.01	0.32	0.33	0.38	0.37	0.31
V(C1,C2)	1.83	2.71	2.66	2.17	2.16	2.08
V'(C1,C2)	1.82					
V(C2,C3)	2.25	2.64	2.70	1.86	1.87	1.92
V'(C2,C3)				1.74	1.75	1.89
V(C3,C4)	1.89	2.90	2.84	2.26	2.26	2.05
V'(C3,C4)	1.72					
V(C3)		0.31	0.33			
V(O5,C6)	2.36	1.92	1.87	1.33	1.32	1.29
V(C1)		0.79				
V(C6)		0.10				
V(C1,C6)			0.99	1.76	1.77	1.90
V(O5)	2.63	2.83	2.83	3.35	2.72	2.38
V'(O5)	2.62	2.91	2.93	2.86	2.81	2.60
V(C4,O5)					0.66	1.32

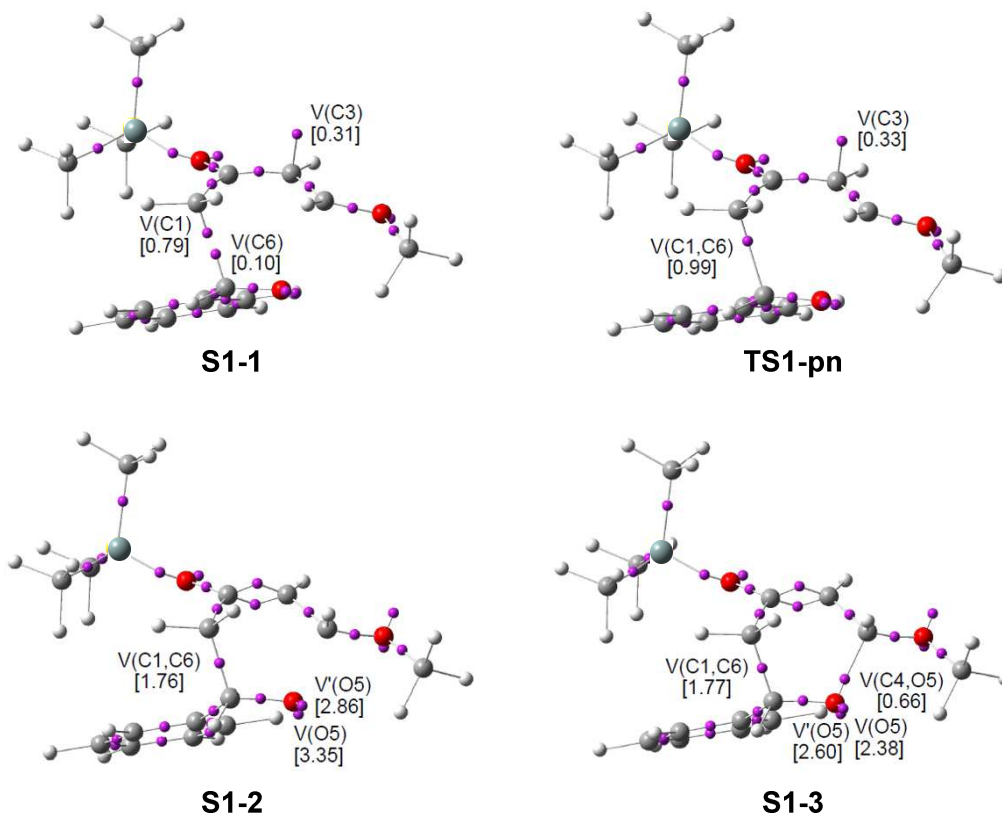


Figure S1. ELF attractor positions of **TS1-pn** and the selected points of the IRC involved in the formation of the C1–C6 and C4–O5 single bonds along the most favorable *para/endo* reaction path associated with the ODA reaction between benzaldehyde **1** and diene **2**. The electron populations, expressed in electrons, e, are given in brackets.

2. ELF topological analysis of the C–C and C–O single bond formation along the most favorable para/endo reaction path associated with the ODA reaction between benzaldehyde 1 and Danishefsky diene 2 in the presence of thiazolium 3.

The populations of the most significant valence basins of the selected points along the reaction path associated with the *para/endo* isomeric reaction path of the ODA reaction between benzaldehyde **1** and the Danishefsky diene **2** in the presence of thiazolium **3**, are displayed in Table S2. The attractor positions of the ELF valence basins are represented in Figure S2. Since thiazolium **3** participates in this ODA reaction, the ELF topological analysis along the reacting path has been focused only on the most relevant bonding changes comprising the two interaction frameworks, *i.e.*, complex **15** and the Danishefsky diene.

Like the previous reaction, the *para/endo* reaction pathway of this ODA begins at **MC2**, a minimum in the PES connecting the separated reagents, the Danishefsky diene

2, and complex 15 **TS2-pn**. As expected, the two C1–C2 and C3–C4 double bond regions of the diene framework at **MC2-pm** are characterized by the presence of two V(C1,C2) and V'(C1,C2) disynaptic basins integrating 1.84e and 1.82e, and two V(C3,C4) and V'(C3,C4) disynaptic basins integrating 1.87e and 1.77e. The V(C2,C3) disynaptic basin presenting an electron population of 2.23e defines the C2–C3 single bond region. At the benzaldehyde moiety, the V(O5,C6) disynaptic basin associated with the O5–C6 bonding region presents a population of 2.33e, while the two V(O5) and V'(O5) monosynaptic basins related to the two O5 oxygen lone pairs integrate 2.59e and 2.69e. A comparative analysis of the valence basin populations of **MC1** and **MC2** indicates that their electronic structures are very similar, the most noticeable feature at both structures being the polarisation of the O5–C6 single bond toward the O5 oxygen. At **MC2**, the GEDT is negligible.

At **S2-1**, two V(C1) and V(C6) monosynaptic basins, with populations of 0.69e and 0.11e, respectively, have been created at the C1 and C6 carbons as a consequence of the depopulation of the C1–C2 and O5–C6 bonding regions by 0.90e and 0.39e, respectively. Thus, the C1–C2 bonding region is now characterized by one V(C1,C2) disynaptic basin integrating 2.76e. At the same time, the population of the V(C2,C3) disynaptic basin, as well as the total population of the V(O5) and V'(O5) monosynaptic basins, have increased to 2.46e and 5.73e, respectively. The small amount of electron density loss by the V(C3,C4) and V'(C3,C4) disynaptic basins reaching up to 1.75e and 1.67e, respectively, also contributes to the increase of the population of the V(C2,C3) disynaptic basin. Here, the first difference between the ODA reactions in the absence and in the presence of thiazolium **3** is observed; unlike **S1-1**, **S2-1** does not present any V(C3) monosynaptic basin located at the C3 carbon of the Danishefsky diene framework. This fact may be due to the electrophilic activation of the benzaldehyde moiety by the HB formed with thiazolium **3**. At **S2-1**, the GEDT strongly increases to 0.39e.

At **TS2-pn**, the two V(C1) and V(C6) monosynaptic basins present at **S2-1** have merged into a new V(C1,C6) disynaptic basin, integrating 0.96e. This relevant topological change indicates that, as along the ODA reaction between complex **17** and diene **2**, the first C1–C6 single bond formation has already begun at a C–C distance of *ca.* 1.98 Å through the C-to-C coupling of the two C1 and C6 *pseudoradical* centers. In addition, while the population of the V(O5,C6) disynaptic basin has slightly decreased to 1.84e, the total population of the V(O5) and V'(O5) monosynaptic basins has increased

to 5.81e. The high GEDT at **TS2-pn**, 0.42e, emphasizes the strong polar nature of this ODA reaction, which is in complete agreement with the acceleration observed in the thiazolium-catalyzed process. Interestingly, the increase of the polar character of the reaction goes accompanied by an increase of the geometrical asynchronicity.

At **S2-2**, the V(C2,C3) disynaptic basin present at **TS2-pn** has split into two new V(C2,C3) and V'(C2,C3) disynaptic basins, integrating 1.88e and 1.76e, respectively, as a consequence of the slight depopulation of the C1-C2 bonding region [see V(C1,C2) in Table S2] as well as of the strong depopulation of the C3-C4 bonding region, which is described by one V(C3,C4) disynaptic basin, with a population of 2.31e. The V(C1,C6) disynaptic basin associated with the recently formed C1-C6 single bond has reached a population of 1.85e, and the V(O5) and V'(O5) monosynaptic basins have continued to increase their populations to 3.09e and 3.08e, as the V(O5,C6) disynaptic basin has been depopulated to 1.25e. At **S2-2**, the GEDT reaches the maximum value along the reaction path, 0.51e.

At **S2-3**, a new V(C4,O5) disynaptic basin is created with a population of 0.58e at the expense of the depopulation of the V(O5) and V'(O5) monosynaptic basins to 2.65e and 3.01e. This significant topological change indicates that the formation of the second C4-O5 single bond region has already started at the distance of *ca.* 1.80 Å through the donation of the electron density of mainly one of the O5 oxygen lone pairs to the C4 carbon. At **S2-3**, the GEDT scarcely varies.

Finally, the ELF of dihydropyranone **21** is topologically very similar to that of dihydropyranone **14**, as expected. The two C1-C6 and C4-O5 single bond regions formed along the ODA reaction between the Danishefsky diene **2** and complex **15** have reached populations of 1.91e and 1.32e, and a high polarisation within the pyranone framework towards the O5 oxygen is also characterized. The most notable difference between both ODA reactions is that the total electron population of the V(O5) and V'(O5) monosynaptic basins associated with the O5 oxygen lone pairs is 0.18e higher at dihydropyranone **21** than at **14**, as the consequence of the HB interaction between the O6 oxygen atom of **21** and the thiazolium H-N hydrogen of thiazolium **3**. At **21**, the GEDT is also high, 0.38e.

Table S2. ELF valence basin populations at some selected IRC points involved forming the C1–C6 and C4–O5 single bonds along the *para/endo* reaction path associated with the ODA reaction between complex **15** and the Danishefsky diene **2** in the presence of thiazolium **3**. The stationary points **MC2**, **TS2-pn** and dihydropyranone **21** are also included. Distances are given in Angstroms, Å, while GEDT values and electron populations are given in electrons, e.

Structures	MC2	S2-1	TS2-pn	S2-2	S2-3	21
d(C1–C6)	3.146	2.022	1.982	1.565	1.563	1.540
d(C4–O5)	2.874	2.565	2.558	1.815	1.795	1.444
GEDT	0.05	0.39	0.42	0.51	0.50	0.38
V(C1,C2)	1.84	2.76	2.68	2.14	2.14	2.10
V'(C1,C2)	1.82					
V(C2,C3)	2.23	2.46	2.49	1.88	1.88	1.91
V'(C2,C3)				1.76	1.75	1.86
V(C3,C4)	1.87	1.75	1.76	2.31	2.29	2.12
V'(C3,C4)	1.77	1.67	1.63			
V(O5,C6)	2.33	1.94	1.84	1.25	1.26	1.26
V(C1)		0.69				
V(C6)		0.11				
V(C1,C6)			0.96	1.85	1.86	1.91
V(O5)	2.59	2.74	2.77	3.09	2.65	2.37
V'(O5)	2.69	2.99	3.04	3.08	3.01	2.79
V(C4,O5)					0.58	1.26

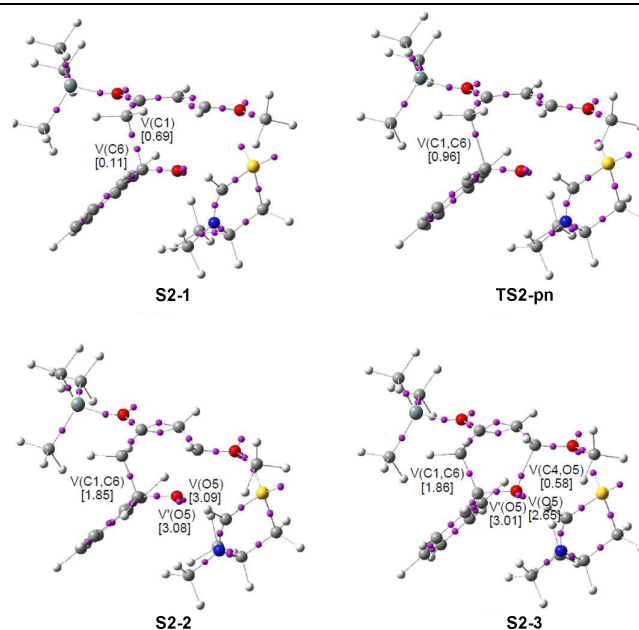


Figure S2. ELF attractor positions of **TS2-pn** and the selected points of the IRC involved in the formation of the C1–C6 and C4–O5 single bonds along the *para/endo* reaction path associated to the ODA reaction between benzaldehyde **1** and the Danishefsky diene **2** in presence of thiazolium **3**. The electron populations, expressed in electrons, e, are given in brackets.

Table S3. M06-2X/6-311G(d,p) Total energies, in a.u., in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2**.

	gas phase	solution
1	-345.510764	-345.516937
2	-754.353336	-754.359673
MC1	-1099.873084	-1099.882117
TS1-pn	-1099.845967	-1099.856559
TS1-px	-1099.839801	-1099.852071
TS1-mn	-1099.818761	-1099.830371
TS1-mx	-1099.822761	-1099.831415
14	-1099.910478	-1099.918037
18	-1099.911487	-1099.920483
19	-1099.897211	-1099.906699
20	-1099.898723	-1099.906798

Table S4. M06-2X/6-311G(d,p) enthalpies (H, in a.u.), entropies (S, in cal·mol⁻¹·K) and Gibbs free energies (G, in a.u.), and relative enthalpies (ΔH , in kcal·mol⁻¹), entropies (ΔS , in cal/mol·K) and Gibbs free energies (ΔG , in kcal·mol⁻¹), computed at 25 °C and 1 atm in solution, for the stationary points involved in the *para* regioisomeric reaction paths of the ODA reaction between benzaldehyde **1** and Danishefsky diene **2**.

	H	ΔH	S	ΔS	G	ΔG
1	-345.398967		79.5		-345.436741	
2	-754.117621		128.1		-754.178486	
MC1	-1099.52041	-2.4	170.0	-37.7	-1099.60117	8.8
TS1-pn	-1099.49529	13.4	157.7	-49.9	-1099.57023	28.2
TS1-px	-1099.49082	16.2	159.5	-48.1	-1099.56661	30.5
14	-1099.55240	-22.5	150.2	-57.4	-1099.62377	-5.4
18	-1099.55481	-24.0	155.8	-51.8	-1099.62885	-8.5

Table S5. M06-2X/6-311G(d,p) Total energies, in a.u., in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2** in the presence of thiazolium **3**.

	gas phase	solution
15	-1343.653856	-1343.714624
2	-754.353336	-754.359673
MC2	-2098.033583	-2098.089505
TS2-pn	-2098.015362	-2098.070006
TS2-px	-2098.009508	-2098.065075
21	-2098.063953	-2098.120652
22	-2098.066246	-2098.125459

Table S6. M06-2X/6-311G(d,p) Total energies, in a.u., in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2** in the presence of [thiazolium][Cl] salt.

	gas phase	solution
16	-1804.077689	-754.359673
2	-754.353336	-1804.104505
MC3	-2558.443808	-2558.477753
TS3-pn	-2558.421692	-2558.456951
TS3-px	-2558.413413	-2558.452455
23	-2558.478400	-2558.510092
24	-2558.486953	-2558.516477

Table S7. M06-2X/6-311G(d,p) enthalpies (H, in a.u.), entropies (S, in cal/mol.K) and Gibbs free energies (G, in a.u.), computed at 25 °C and 1 atm in solution, for the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2** in the presence of [thiazolium][Cl] salt.

	H	S	G
16	-1803.648454	181.9	-1803.734901
2	-754.117621	128.1	-754.178486
MC3	-2557.776872	264.2	-2557.902409
TS3-pn	-2557.756456	255.6	-2557.877912
TS3-px	-2557.752182	259.1	-2557.875298
23	-2557.805196	252.5	-2557.925150
24	-2557.812752	247.3	-2557.930243

Table S8. M06-2X/6-311G(d,p) relative energies, ΔE in kcal·mol⁻¹, in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2**. Single Point in B3LYP and MPW1K at the same basis set.

	M06-2X		B3LYP		MPW1K	
	gas phase	solution	gas phase	solution	gas phase	solution
MC1	-5.6	-3.5	3.4	5.7	-3.5	-0.9
TS1-pn	11.4	12.6	19.6	21.4	12.4	14.3
TS1-px	15.2	15.4	19.8	20.7	14.9	15.8
TS1-mn	28.5	29.0	34.8	35.6	30.3	31.2
TS1-mx	25.9	28.4	34.8	37.3	28.7	31.4
14	-29.1	-26.0	-11.4	-8.2	-29.6	-26.2
18	-29.7	-27.5	-16.4	-14.0	-31.7	-29.1
19	-20.8	-18.9	-5.4	-3.3	-21.6	-19.4
20	-21.7	-18.9	-7.0	-4.1	-22.7	-19.6

Table S9. M06-2X/6-311G(d,p) relative energies, ΔE in kcal·mol⁻¹, in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2** in the presence of thiazolium **3**. Single Point in B3LYP and MPW1K at the same basis set.

	M06-2X		B3LYP		MPW1K	
	gas phase	solution	gas phase	solution	gas phase	solution
MC2	-16.6	-9.5	1.2	8.2	-9.7	-2.4
TS2-pn	-5.1	2.7	10.2	17.7	-1.1	6.8
TS2-px	-1.5	5.8	7.6	14.6	1.3	8.7
21	-35.6	-29.1	-12.6	-6.2	-33.6	-26.8
22	-37.1	-32.1	-16.1	-11.2	-36.1	-30.9

Table S10. M06-2X/6-311G(d,p) relative energies, ΔE in kcal·mol⁻¹, in gas phase and in solution, of the stationary points involved in the ODA reaction between benzaldehyde **1** and Danishefsky diene **2** in the presence of [thiazolium][Cl] salt. Single Point in B3LYP and MPW1K at the same basis set.

	M06-2X		B3LYP		MPW1K	
	gas phase	solution	gas phase	solution	gas phase	solution
MC3	-8.0	-8.5	5.6	8.5	-2.7	0.4
TS3-pn	5.9	4.5	16.1	6.8	12.3	3.0
TS3-px	11.1	7.4	15.3	6.0	12.7	3.5
23	-29.7	-28.8	-7.7	-4.9	-28.3	-25.2
24	-35.1	-32.8	-12.3	-9.0	-33.2	-29.6

1

C	-0.35939200	1.28791100	-0.00006100
C	-1.72965200	1.05568900	0.00002400
C	-2.20555800	-0.25080500	0.00006400
C	-1.31780400	-1.32640700	0.00001400
C	0.04838200	-1.09540800	-0.00007400
C	0.52783500	0.21500600	-0.00011400
H	0.02620300	2.30259000	-0.00009200
H	-2.42364300	1.88704400	0.00006300
H	-3.27341500	-0.43445000	0.00013200
H	-1.69772700	-2.34071300	0.00004200
H	0.76459800	-1.90860700	-0.00012000
C	1.99009400	0.46800100	-0.00023300
O	2.82539900	-0.39610900	0.00024800
H	2.27736200	1.53908800	0.00027100

2

C	-0.29994900	-1.72647200	-0.11728800
C	-0.40947300	-0.39750400	-0.24164000
H	-1.15437700	-2.35700200	-0.31385300
H	0.62847100	-2.20663300	0.16014600
C	-1.66681900	0.30168400	-0.53416900
C	-2.83712900	-0.09358100	-0.03678800
H	-1.61641000	1.19228300	-1.14972100
H	-2.91284400	-0.93515400	0.65115800
O	-3.99903600	0.51142300	-0.36702400
C	-5.07551200	0.24779200	0.51341500
H	-5.95401300	0.72586300	0.08644800
H	-5.25586500	-0.82891200	0.59865600
H	-4.88134300	0.66359200	1.50648000
O	0.62705000	0.47563400	-0.11897600
Si	2.27277300	0.17912200	0.07193400
C	2.59880900	-0.63027500	1.72763800
H	2.16701100	-0.03224300	2.53376200
H	2.18392900	-1.63701000	1.79977600
H	3.67605600	-0.69902500	1.90325600
C	3.03778100	1.87794000	0.02450800
H	4.12257300	1.82351600	0.14606700
H	2.82784000	2.37176600	-0.92664500
H	2.63839800	2.50498400	0.82452000
C	2.90853200	-0.87062800	-1.33958000
H	2.68819500	-0.39399800	-2.29778900
H	3.99381300	-0.98118700	-1.26288500
H	2.46819100	-1.86874000	-1.35503300

MC1

C	-0.22301000	-1.31850900	2.30854700
C	-0.67488000	-0.87050900	1.13105600
C	0.08484000	-0.92035700	-0.12411200
C	1.00832500	-1.84535300	-0.38658200

O	3.34453800	-0.74758300	1.34199000
C	2.66655900	0.19694900	1.66524300
H	-0.05165300	-0.10820900	-0.83253900
H	-0.85625500	-1.27031300	3.18378400
H	2.38554900	0.35689300	2.72373400
H	0.77016900	-1.73664300	2.39641100
C	2.11818400	1.18663800	0.71167900
C	1.09945400	2.04024900	1.12859600
C	2.54501000	1.18925500	-0.61620300
C	0.48750000	2.88476900	0.21063500
H	0.76072300	2.00644700	2.15905400
C	1.94622500	2.04559500	-1.52756200
H	3.32360500	0.49842200	-0.91661600
C	0.91161700	2.88522800	-1.11531600
H	-0.31910500	3.53623500	0.52410900
H	2.26895600	2.05113800	-2.56148900
H	0.43233200	3.54171400	-1.83247400
O	1.76753300	-1.79352100	-1.49971100
O	-1.88880800	-0.25056700	1.07563800
Si	-2.99172700	-0.14875400	-0.19054100
C	-2.55068100	1.26275500	-1.34119700
H	-1.64214100	1.07335600	-1.91691200
H	-2.40388600	2.18661700	-0.77622300
H	-3.36640500	1.42998100	-2.05079800
C	-3.06046900	-1.77071000	-1.11699300
H	-2.13759200	-1.96051700	-1.66853300
H	-3.88992200	-1.76546600	-1.82956200
H	-3.21595500	-2.60262200	-0.42541500
C	-4.61266700	0.22047600	0.65505300
H	-5.41746100	0.34749100	-0.07346800
H	-4.54094300	1.13833800	1.24296000
H	-4.89102200	-0.59024600	1.33170400
C	2.92597600	-2.61568000	-1.45796600
H	3.59236600	-2.28719500	-0.65658300
H	3.41691400	-2.50884000	-2.42272000
H	2.65068500	-3.66449500	-1.30839300
H	1.19721900	-2.68093800	0.28495200

TS1-pn

C	-0.82980400	-0.26649900	-2.15366400
C	-0.24540800	-0.93042600	-1.06339500
C	-1.00643500	-1.41079900	0.01544100
C	-2.37505200	-1.30467600	-0.02465300
O	-2.67613900	0.82243500	-0.61441700
C	-1.66121700	1.25664500	-1.24259400
H	-0.54224900	-1.61231200	0.97223600
H	-0.13016700	0.07778000	-2.90681800
H	-1.82520800	1.75068500	-2.21379100
H	-1.77601500	-0.62573300	-2.53653500
C	-0.54569200	1.88578700	-0.44719300
C	0.55602800	2.47683700	-1.06543900

C	-0.64355900	1.90649400	0.94171100
C	1.54172600	3.09314100	-0.30585200
H	0.63676700	2.45475500	-2.14826300
C	0.33820000	2.53262000	1.70418900
H	-1.51542200	1.44903400	1.39548400
C	1.43013500	3.12947400	1.08341900
H	2.39158600	3.55656700	-0.79354200
H	0.24996300	2.55727200	2.78453500
H	2.19183700	3.62281000	1.67614700
O	-3.08061100	-1.43039100	1.08641100
O	1.08752100	-0.84701300	-0.97865300
Si	2.20928700	-1.43440200	0.14832600
C	2.06060800	-0.54297600	1.77901800
H	1.08645000	-0.66115600	2.25694200
H	2.22764000	0.52655900	1.63392200
H	2.82335600	-0.91835600	2.46791000
C	1.95843300	-3.27840200	0.33116400
H	0.99244700	-3.52749400	0.77464900
H	2.73907900	-3.70085200	0.96974400
H	2.01827500	-3.77271100	-0.64145300
C	3.84441400	-1.04469600	-0.65175800
H	4.67767400	-1.35934800	-0.01858300
H	3.93241700	0.03144800	-0.81867700
H	3.94051200	-1.54692600	-1.61652800
C	-4.47520100	-1.16320800	0.92948600
H	-4.60026200	-0.17947700	0.47647200
H	-4.90600400	-1.18767200	1.92670500
H	-4.93917500	-1.93479700	0.30917800
H	-2.93274400	-1.31458800	-0.95230600

TS1-px

C	-0.13133700	0.07820300	0.68313100
C	-1.07872900	1.06568800	0.34232900
C	-0.72037000	2.40528100	0.18040600
C	0.59154600	2.77472300	0.36040600
O	1.60345500	1.29554000	-0.91380900
C	1.09274400	0.13409700	-0.83187400
H	-1.39110600	3.06657900	-0.35152700
H	-0.47686600	-0.94441400	0.78189800
H	0.36344400	-0.17224900	-1.60351900
H	0.61869500	0.34035900	1.41954400
C	1.97600800	-1.01307800	-0.39891800
C	1.62624500	-2.33029800	-0.68839400
C	3.16129700	-0.75573000	0.28490100
C	2.44231700	-3.38108300	-0.28491200
H	0.71476800	-2.52874400	-1.24528200
C	3.97541700	-1.80473800	0.69443100
H	3.43555900	0.27697800	0.46805500
C	3.61732200	-3.12032700	0.41338900
H	2.16636400	-4.40247100	-0.52003900
H	4.89776500	-1.59787400	1.22498700

H	4.25563500	-3.93735600	0.72782100
O	1.01925000	3.93730600	-0.09534000
O	-2.30013500	0.73537500	-0.11076800
Si	-3.19544100	-0.69424700	0.04168000
C	-4.83522000	-0.25024900	-0.71789100
H	-4.71571200	0.02048300	-1.76917100
H	-5.53271900	-1.08964700	-0.66141200
H	-5.28396400	0.59997100	-0.20008800
C	-3.36739800	-1.11824600	1.85253900
H	-3.97486400	-2.01938500	1.97280900
H	-2.40085900	-1.30134300	2.32659500
H	-3.85995400	-0.30713200	2.39375800
C	-2.37935100	-2.08224400	-0.91355900
H	-3.11819700	-2.85419300	-1.14636500
H	-1.97591500	-1.71396900	-1.86055900
H	-1.56806900	-2.55820500	-0.35902100
C	2.43301400	4.11808300	-0.01814900
H	2.64095800	5.09516600	-0.44550800
H	2.76127200	4.09489200	1.02493800
H	2.92292200	3.33016900	-0.59030100
H	1.25540500	2.25559300	1.04119700

TS1-mn

C	0.84274000	-1.21968800	1.60335600
C	0.93743300	-0.65960400	0.33394500
C	-0.02512100	-0.97170900	-0.61661200
C	-1.09859800	-1.80543400	-0.32001500
C	-1.83437400	-0.70097100	1.32543500
O	-0.90529400	-0.70813100	2.20126300
H	-0.10004700	-0.35608600	-1.50712200
H	1.44250100	-0.79641600	2.39885700
H	-2.62595900	-1.45364800	1.42888500
H	0.57904400	-2.26109200	1.71804400
C	-2.23632500	0.56718900	0.67124200
C	-3.42530700	0.64241300	-0.05426200
C	-1.40601000	1.68633100	0.75313900
C	-3.78017400	1.82156300	-0.69789600
H	-4.07298900	-0.22687200	-0.11227600
C	-1.75942300	2.86094800	0.10352300
H	-0.48583700	1.61369700	1.32084300
C	-2.94591600	2.93241700	-0.62302000
H	-4.70625800	1.87529400	-1.25803800
H	-1.11006400	3.72641200	0.16510300
H	-3.22126100	3.85222400	-1.12524200
O	-2.06012700	-1.94023900	-1.27466900
O	1.73909500	0.43910300	0.12851000
Si	3.35390500	0.29215600	-0.32038000
C	3.97386400	2.04270300	-0.45390200
H	3.88129500	2.56121500	0.50280600
H	5.02522200	2.06543700	-0.75115900
H	3.39957500	2.60067600	-1.19650600
C	3.44089200	-0.60830600	-1.95659300

H	2.99005300	-1.60124600	-1.88009000
H	2.90811800	-0.05741700	-2.73540800
H	4.47710600	-0.73467100	-2.28092300
C	4.28032400	-0.66739500	0.99263500
H	5.33746300	-0.75691400	0.72814500
H	4.21898800	-0.17000900	1.96371900
H	3.87912200	-1.67815900	1.10321800
C	-3.00043000	-2.96631900	-1.03369700
H	-3.55214300	-2.79194800	-0.10383400
H	-3.69693800	-2.95586500	-1.86916100
H	-2.50957600	-3.94396700	-0.98338400
H	-0.98293000	-2.65151200	0.35433900

TS1-mx

C	0.84491300	-0.69037800	-1.62373800
C	1.45583600	0.48058400	-1.18877100
C	0.66490400	1.48504300	-0.64511700
C	-0.71530800	1.33001900	-0.53945400
C	-0.77690300	-0.46746900	0.56010300
O	0.03827400	-1.29066400	0.01330500
H	1.13459200	2.28673400	-0.08424700
H	1.46693200	-1.54382200	-1.86194400
H	-0.46434900	0.04008000	1.47883400
H	-0.10852800	-0.65438300	-2.13245500
C	-2.24156100	-0.67883600	0.42686000
C	-3.12401500	-0.01062600	1.27769700
C	-2.74960900	-1.52163500	-0.56434200
C	-4.49677900	-0.16513600	1.12483900
H	-2.72583400	0.63925100	2.04950600
C	-4.12193400	-1.66649500	-0.72119400
H	-2.05385400	-2.07052300	-1.18892800
C	-4.99979800	-0.98536300	0.11906600
H	-5.17593300	0.35382700	1.79120900
H	-4.51066100	-2.32116800	-1.49246200
H	-6.06983000	-1.10496900	-0.00088000
O	-1.43225400	2.25430000	0.15995800
O	2.81431300	0.52394000	-1.01606200
Si	3.57975000	-0.20997700	0.29909100
C	5.36155300	0.31271600	0.14800500
H	5.96354500	-0.11451200	0.95385900
H	5.78327900	-0.02170300	-0.80232800
H	5.45452600	1.39977300	0.19430200
C	3.38422400	-2.06526400	0.19588900
H	2.33067100	-2.33977500	0.29791100
H	3.76336900	-2.45968200	-0.75022800
H	3.93849500	-2.54945700	1.00481400
C	2.79107700	0.40597600	1.87816200
H	3.29790800	-0.01949200	2.74850400
H	2.83170700	1.49430000	1.96297100
H	1.74486800	0.09179300	1.92020200
C	-2.61655600	2.68679000	-0.49334200

H	-3.17052300	3.28783300	0.22518300
H	-2.36995400	3.29510500	-1.36926700
H	-3.22895000	1.83094400	-0.79508000
H	-1.27089900	0.81934300	-1.32232800

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C	0.26361600	-0.39164500	2.14498600
C	-0.54079600	-1.02012500	1.04535200
C	0.07610000	-1.76066200	0.12649900
C	1.54883600	-2.01582400	0.21022500
O	2.27615500	-1.07355400	0.98505400
C	1.60941300	0.04394100	1.55210300
H	-0.43908500	-2.22546300	-0.70411000
H	-0.28343300	0.46064200	2.54731800
H	2.26911200	0.36117600	2.36382100
H	0.43746000	-1.10329000	2.95743500
C	1.44427700	1.21720600	0.59740300
C	0.97727700	2.43278000	1.10364500
C	1.74966200	1.12580200	-0.75714800
C	0.80030600	3.53028800	0.27079500
H	0.75635500	2.52598000	2.16280800
C	1.57350800	2.22627700	-1.59227500
H	2.10228600	0.18571900	-1.16155900
C	1.09643500	3.42833700	-1.08564600
H	0.43717300	4.46556800	0.68042800
H	1.80671300	2.13795400	-2.64704200
H	0.95877800	4.28159900	-1.73896900
O	2.04057700	-2.05648900	-1.10131400
O	-1.86074600	-0.72613200	1.05896500
Si	-2.80052500	-0.29842200	-0.28308200
C	-1.78668800	0.82026000	-1.37902700
H	-0.96309700	0.28370300	-1.85497200
H	-1.34813600	1.64196500	-0.80364300
H	-2.41228300	1.25153800	-2.16550500
C	-3.36795300	-1.82970600	-1.19714100
H	-2.55104700	-2.33225800	-1.71889000
H	-4.12024700	-1.56146900	-1.94435200
H	-3.82257600	-2.54575000	-0.50839200
C	-4.26591300	0.57877400	0.46366200
H	-4.97902100	0.87827500	-0.30843900
H	-3.94907000	1.47626600	0.99907400
H	-4.78729100	-0.07028600	1.17085500
C	3.39683200	-2.45427400	-1.16830400
H	4.04538600	-1.71956100	-0.68504500
H	3.65118300	-2.53580600	-2.22345600
H	3.53828600	-3.42932500	-0.68622400
H	1.76253700	-2.98844300	0.67957400

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C	0.09886000	0.39491200	0.56236000
C	1.22146900	-0.59285600	0.72334000
C	1.00657700	-1.90372000	0.66443800
C	-0.37728600	-2.46122700	0.50557200
O	-1.38206300	-1.48587300	0.65887900
C	-1.10810100	-0.29939200	-0.07043900
H	1.82741700	-2.60351700	0.75388600
H	0.41538100	1.22868400	-0.07223400
H	-0.85513300	-0.57169000	-1.10357000
H	-0.17412100	0.81533600	1.53633100
C	-2.33129200	0.58094300	-0.06611900
C	-2.46235000	1.57699900	-1.03277900
C	-3.31027500	0.44943600	0.91561000
C	-3.55297200	2.43764400	-1.01633400
H	-1.70896200	1.67214700	-1.80919000
C	-4.40468400	1.30814300	0.92892100
H	-3.20978000	-0.33420100	1.65569900
C	-4.52796000	2.30466300	-0.03276300
H	-3.64662500	3.20581900	-1.77473700
H	-5.16477000	1.19690600	1.69330100
H	-5.38192100	2.97121700	-0.02016800
O	-0.45345900	-3.08061500	-0.74990700
O	2.45859600	-0.08266900	0.96853300
Si	3.37213900	0.87233800	-0.07639600
C	5.14734700	0.44622400	0.29388700
H	5.34892400	-0.60532000	0.07955800
H	5.83060900	1.05361700	-0.30502300
H	5.37354100	0.62444600	1.34758400
C	3.05927000	2.68350000	0.27281000
H	3.72490300	3.30632600	-0.33140500
H	2.03267400	2.98203000	0.04956000
H	3.25312300	2.91115700	1.32374100
C	2.89936800	0.43119200	-1.83138300
H	3.53954000	0.95445800	-2.54633100
H	3.00615000	-0.64283800	-2.00212700
H	1.86321500	0.69803100	-2.05652600
C	-1.65582400	-3.80422200	-0.93222400
H	-1.59822700	-4.27342900	-1.91248500
H	-1.76149600	-4.58202200	-0.16569500
H	-2.52502100	-3.14278900	-0.88972100
H	-0.59683600	-3.19727300	1.28967600

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C	0.71741000	1.67997000	0.22119100
C	1.43392700	0.45240200	0.71291900
C	0.79684000	-0.68406600	0.97737500
C	-0.68894000	-0.79420000	0.78891800
C	-1.31399600	0.61357300	0.69692300
O	-0.58736600	1.40432000	-0.22364800
H	1.34498500	-1.55932700	1.30722900
H	1.26520600	2.09448900	-0.62771700

H	-1.25577400	1.06904200	1.69813100
H	0.71009400	2.43742500	1.02078100
C	-2.75017400	0.54991500	0.25418000
C	-3.76458000	0.39699300	1.19582500
C	-3.06612600	0.55269000	-1.10287200
C	-5.08435100	0.23090400	0.78906300
H	-3.52044200	0.40437600	2.25379600
C	-4.38518100	0.39159200	-1.50885100
H	-2.26764900	0.67281500	-1.82333200
C	-5.39595800	0.22418400	-0.56605900
H	-5.86762800	0.11345700	1.52849200
H	-4.62673100	0.39273100	-2.56530300
H	-6.42309000	0.09684700	-0.88662800
O	-0.93530700	-1.55535500	-0.38182200
O	2.77342400	0.63816400	0.87858900
Si	3.90534700	-0.01295200	-0.19411400
C	5.53437200	0.70723900	0.34755000
H	5.76351800	0.41821000	1.37554400
H	6.34837000	0.35606700	-0.29144500
H	5.51301100	1.79798300	0.30060700
C	3.42595200	0.51213500	-1.92324600
H	2.40379900	0.19334900	-2.14931300
H	3.48204700	1.59633000	-2.04654700
H	4.08595300	0.05597400	-2.66559400
C	3.90448600	-1.87805700	-0.07613800
H	4.71027100	-2.29441000	-0.68715300
H	4.05769700	-2.21181100	0.95295000
H	2.96145000	-2.29520300	-0.43709300
C	-1.95820900	-2.52139300	-0.25259400
H	-2.92822400	-2.06813100	-0.02268800
H	-2.02679700	-3.03558800	-1.21049600
H	-1.70893300	-3.25277000	0.52663400
H	-1.13482200	-1.30083600	1.65670600

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C	0.67094000	-1.79847800	-0.24614500
C	1.42239900	-0.56116200	-0.65505400
C	0.80429600	0.59291800	-0.88997900
C	-0.67903000	0.72738700	-0.68199900
C	-1.18797600	-0.43140500	0.19035500
O	-0.72511700	-1.65162300	-0.35523700
H	1.35082100	1.46841700	-1.22210800
H	0.95510600	-2.06571900	0.78430100
H	-0.76914400	-0.28277200	1.19687500
H	0.96514000	-2.62146700	-0.89989500
C	-2.69176400	-0.45079900	0.26357100
C	-3.35242800	0.40239100	1.14729900
C	-3.43553600	-1.26804000	-0.58484100
C	-4.74139600	0.44536900	1.17497500
H	-2.77001100	1.03936800	1.80394200
C	-4.82545200	-1.22752500	-0.55190400
H	-2.91603300	-1.94007400	-1.25634900

C	-5.48156100	-0.36962000	0.32393500
H	-5.24635700	1.11024800	1.86584000
H	-5.39757800	-1.87005700	-1.21087200
H	-6.56439300	-0.34047300	0.34850700
O	-0.95390500	1.95175000	-0.02032200
O	2.76391000	-0.76946300	-0.75691500
Si	3.90114700	-0.01173200	0.23575200
C	5.51209500	-0.84145100	-0.19119800
H	5.76129300	-0.68636200	-1.24321400
H	6.33052300	-0.44108300	0.41220700
H	5.45451900	-1.91732100	-0.01359400
C	3.39162300	-0.31003700	2.00965200
H	2.38440100	0.07752100	2.18846200
H	3.39671300	-1.37517500	2.25303800
H	4.06820000	0.19656600	2.70263100
C	3.97134500	1.82386800	-0.11110200
H	4.82192200	2.27028100	0.41179700
H	4.09485100	2.02106300	-1.17874700
H	3.06638800	2.33100100	0.23074800
C	-1.84845700	2.79440700	-0.71619100
H	-1.99568700	3.67999300	-0.09890900
H	-1.43374900	3.09961700	-1.68432000
H	-2.81542200	2.30428500	-0.87699000
H	-1.21124700	0.69413400	-1.64233500

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C	-1.59256300	-2.82003400	-0.76334400
C	-2.01193600	-1.80933600	0.08389600
C	-3.37210100	-1.65566800	0.36858600
C	-4.30871300	-2.52059800	-0.19421200
C	-3.88831300	-3.53099300	-1.05180400
C	-2.53500200	-3.67846700	-1.33410700
H	-0.53874600	-2.95846200	-0.97624100
H	-1.30403900	-1.13829200	0.55802400
H	-5.36183500	-2.40091900	0.03807300
H	-4.61122300	-4.20447800	-1.49412300
H	-2.20760900	-4.47107900	-1.99590700
C	-3.81725800	-0.57609500	1.26642800
O	-3.07811800	0.27632900	1.71141700
H	-4.89159700	-0.56858000	1.52080400
H	6.48412100	-1.72812900	-1.34705500
C	5.46586600	-1.47402900	-1.08050200
C	4.93935100	-1.89277800	0.13541200
C	4.67923300	-0.73565600	-1.95969500
C	3.62943700	-1.56862600	0.47530900
H	5.54430800	-2.47724600	0.81752100
C	3.37150100	-0.41387600	-1.61958700
H	5.08297300	-0.41757200	-2.91294200
C	2.83664000	-0.82543300	-0.39800700
H	3.21645000	-1.91091900	1.41953800
H	2.75744600	0.14798500	-2.31754700

C	1.42754600	-0.43963700	-0.01984900
C	1.34280100	1.04990600	0.35580800
H	1.08520900	-1.03846800	0.83048500
H	0.74734800	-0.63274600	-0.85467900
C	2.11488400	1.40138500	1.62728200
N	-0.07229100	1.39341100	0.65629100
H	1.67841100	1.66937200	-0.47757100
S	0.91746100	1.16974900	3.00638800
H	2.97302700	0.74796500	1.77332900
H	2.43274500	2.44260500	1.64776800
C	-0.37461900	1.37744400	1.91229200
C	-1.04128000	1.64765600	-0.42534400
H	-1.40642800	1.46387800	2.23856100
C	-0.93926400	3.08102900	-0.93920200
H	-2.03254500	1.43485000	-0.02334600
H	-0.83477000	0.92703700	-1.22067100
C	-1.92872600	3.32851300	-2.07828200
H	-1.14143600	3.77111200	-0.11376600
H	0.07864700	3.28455900	-1.28870100
C	-1.85273200	4.76260200	-2.59514400
H	-1.72422900	2.62859700	-2.89475300
H	-2.94302000	3.11428000	-1.72730500
H	-2.56399500	4.92378500	-3.40535200
H	-2.08169600	5.47696700	-1.80140700
H	-0.85441000	4.98955900	-2.97593700

MC2

C	-1.07453500	1.17731600	-2.83555000
C	-0.61871600	1.57931500	-1.58961000
C	-0.84357200	2.88837700	-1.15784100
C	-1.55764900	3.77911700	-1.95828600
C	-2.00999800	3.37556300	-3.20996800
C	-1.75934500	2.08002100	-3.65019300
H	-0.90741400	0.16360100	-3.18188300
H	-0.12476200	0.89259200	-0.91234400
H	-1.74142900	4.79007000	-1.60916300
H	-2.55363700	4.06764000	-3.84052600
H	-2.10994500	1.76595000	-4.62588000
C	-0.25706300	3.35844400	0.11313300
O	0.66084700	2.80103400	0.67799500
H	-0.67088600	4.30073900	0.51374500
C	-2.73937500	2.18556200	1.69904200
H	-3.46151900	2.43551700	0.93373200
H	-2.65176900	2.84410500	2.55182600
C	-2.00170100	1.06824200	1.63839100
C	-0.94271800	0.71329100	2.59012500
H	-0.76996600	-0.34328700	2.75816300
C	-0.16294000	1.61544800	3.18673300
H	-0.28071600	2.68466300	3.03234600
O	-2.11452100	0.12996000	0.65816900
Si	-3.53912900	-0.34926800	-0.14567000
C	-4.73900600	-0.95091700	1.14792400

H	-5.68237200	-1.25367000	0.68604900
H	-4.34019100	-1.81047500	1.69134800
H	-4.96204400	-0.16390700	1.87258700
C	-4.27358200	1.05784700	-1.13971600
H	-3.51213600	1.77925400	-1.44383000
H	-4.74207400	0.67050100	-2.04867300
H	-5.04362200	1.58954800	-0.57564600
C	-2.94210200	-1.72925300	-1.24719500
H	-2.55086200	-2.56497000	-0.66249300
H	-3.75867400	-2.10990900	-1.86597600
H	-2.15114900	-1.38675300	-1.91881500
O	0.88996100	1.24764100	3.95628100
C	1.38499900	2.26302200	4.82625200
H	0.64685600	2.49900300	5.59512700
H	2.28187800	1.86403600	5.29312000
H	1.63253500	3.16548300	4.25959000
H	-0.50291400	-7.01136200	-0.84299000
C	-0.26971500	-5.95588100	-0.77840700
C	-0.62520200	-5.23168100	0.35473000
C	0.37791800	-5.31991400	-1.83215100
C	-0.32904800	-3.87521400	0.43295600
H	-1.13866300	-5.72092400	1.17339300
C	0.67200500	-3.96333200	-1.75197800
H	0.64738100	-5.87903000	-2.71975500
C	0.32265000	-3.22999900	-0.61898400
H	-0.62326200	-3.30352900	1.30935400
H	1.16379100	-3.46868700	-2.58432900
C	0.66232900	-1.76551500	-0.51336600
C	2.13843200	-1.54147300	-0.12268900
H	0.01002400	-1.27467400	0.21890000
H	0.48782300	-1.27396300	-1.47591100
C	2.55844300	-2.20256500	1.18541300
N	2.32313900	-0.08680300	0.12247600
H	2.80018200	-1.84666700	-0.93546300
S	2.07462300	-1.01146100	2.49757800
H	2.04993900	-3.15079200	1.34651900
H	3.63727600	-2.34330600	1.24400400
C	2.16451700	0.26113900	1.35822600
C	2.61522300	0.84198800	-0.98275000
H	2.09220900	1.30505700	1.64529800
C	4.11483100	0.90685400	-1.25844400
H	2.20825900	1.81522500	-0.70657300
H	2.07097900	0.48285900	-1.85974200
C	4.41876300	1.82111200	-2.44502700
H	4.62614300	1.27542100	-0.36304900
H	4.50291700	-0.09792000	-1.45939100
C	5.91705100	1.92069900	-2.71851100
H	3.90365700	1.44339600	-3.33402100
H	4.01029300	2.81688500	-2.24632900
H	6.11739000	2.57449800	-3.56762300
H	6.44646800	2.32447300	-1.85268400
H	6.34022100	0.93927200	-2.94434200

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C	-0.40308800	-1.25016700	-1.65811000
C	-1.02062500	-0.33540700	-0.81274200
C	-1.66708800	0.78778500	-1.33703800
C	-1.66451400	0.98630100	-2.71621700
C	-1.02038000	0.08765100	-3.56335400
C	-0.38984600	-1.03453700	-3.03609300
H	0.06652800	-2.13678900	-1.24714600
H	-1.02307000	-0.50624800	0.25874800
H	-2.15973800	1.85902800	-3.13052200
H	-1.01821500	0.25953800	-4.63298500
H	0.09802300	-1.74421400	-3.69337100
C	-2.25854600	1.85188400	-0.44234100
O	-1.55643500	2.28469200	0.52860100
H	-2.83626400	2.59274900	-1.01733800
C	-3.91970000	1.08657000	0.25874500
H	-4.54939100	0.89283200	-0.60223700
H	-4.18768100	1.98187900	0.80567000
C	-3.50384100	-0.02444700	1.01132900
C	-2.72056700	0.09369100	2.19356800
H	-2.27735500	-0.80753100	2.59993800
C	-2.37464700	1.30474900	2.69482200
H	-2.85847900	2.22784900	2.40002700
O	-3.61392800	-1.26168300	0.55913600
Si	-4.65672000	-1.98299400	-0.60611200
C	-6.40368000	-1.52512700	-0.14576900
H	-7.10687800	-2.03739900	-0.80788900
H	-6.62955600	-1.83234500	0.87792700
H	-6.59663900	-0.45360400	-0.22795300
C	-4.19767600	-1.42149400	-2.32298200
H	-3.13558200	-1.58817300	-2.51998900
H	-4.76697400	-2.01275700	-3.04667000
H	-4.41603600	-0.36958200	-2.51590800
C	-4.30466600	-3.79177300	-0.38013000
H	-4.51902500	-4.11064300	0.64178700
H	-4.91537700	-4.39412200	-1.05690100
H	-3.25543200	-4.00978100	-0.59246600
O	-1.41533200	1.41456300	3.60560600
C	-1.19458100	2.73874700	4.10576100
H	-2.03761900	3.05261300	4.72284400
H	-0.29394600	2.69088800	4.71173300
H	-1.05630800	3.42864100	3.26982900
H	7.35881000	-3.86788800	0.34452300
C	6.45275500	-3.28289200	0.24758900
C	5.31311600	-3.64046700	0.95769500
C	6.42468800	-2.17606400	-0.59575800
C	4.14847500	-2.88972700	0.82890800
H	5.32711400	-4.50684300	1.60748000
C	5.26076800	-1.42892600	-0.72353600
H	7.30788700	-1.90043200	-1.15878600
C	4.11242200	-1.77762500	-0.01085400
H	3.25587500	-3.18047200	1.37473600

H	5.23964200	-0.57585000	-1.39584400
C	2.86558200	-0.93720900	-0.12984200
C	3.01814100	0.39340600	0.62434100
H	2.00022400	-1.46994400	0.27686000
H	2.65151700	-0.72567000	-1.18155700
C	3.13598100	0.22899300	2.14141400
N	1.79562500	1.20847600	0.41495700
H	3.87670200	0.94610400	0.24246600
S	1.42181200	0.35100200	2.79856800
H	3.56763000	-0.73330600	2.41021700
H	3.71550500	1.02999600	2.59724000
C	0.93327000	1.16301800	1.37694300
C	1.49328900	1.83484000	-0.89032000
H	-0.07276500	1.59568700	1.23413800
C	2.62937900	2.70966800	-1.40042100
H	0.58152700	2.41575600	-0.74092500
H	1.26291200	1.03463700	-1.60090800
C	2.19200000	3.46382900	-2.65736000
H	2.92833400	3.42160300	-0.62374600
H	3.50632300	2.09842000	-1.64027200
C	3.31809700	4.31485600	-3.23690100
H	1.84522100	2.74295000	-3.40539200
H	1.33384800	4.09760200	-2.41328900
H	2.98720300	4.85110200	-4.12668300
H	3.66299700	5.05366500	-2.50995500
H	4.17266600	3.69525300	-3.51845900

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C	-3.07861700	4.11838500	0.84617200
C	-2.60187500	2.82254300	0.99432400
C	-2.62015000	1.94295100	-0.08697300
C	-3.10765500	2.37386300	-1.31858300
C	-3.57373700	3.67655900	-1.47068300
C	-3.56139600	4.54927400	-0.38793300
H	-3.06640700	4.79997500	1.68867900
H	-2.19336800	2.48173600	1.93961400
H	-3.10071700	1.69621200	-2.16687300
H	-3.94104200	4.01117600	-2.43331000
H	-3.92542700	5.56276500	-0.50402400
C	-2.02460300	0.56688900	0.05595800
O	-1.07991600	0.41294900	0.89762600
H	-1.95234900	0.04945500	-0.91928800
C	-3.60121700	-0.38468300	0.70187000
H	-4.42404700	-0.05758600	0.07784600
H	-3.59807800	0.06418000	1.68691900
C	-3.18390300	-1.71881400	0.57792100
C	-2.18004100	-2.30457400	1.40111200
H	-1.79000100	-3.27335500	1.11596700
C	-1.60963700	-1.61223100	2.41383700
H	-2.00766800	-0.67377600	2.78285400
O	-3.53331400	-2.46372700	-0.45882900
Si	-4.86880500	-2.37428300	-1.54008100

C	-6.42638400	-2.29565900	-0.52214000
H	-7.29863700	-2.31016000	-1.18122100
H	-6.49950900	-3.16048300	0.14125900
H	-6.49026600	-1.39305200	0.08863400
C	-4.65873900	-0.88120800	-2.64258400
H	-3.63864400	-0.82487500	-3.03209300
H	-5.33072500	-0.96857400	-3.50102600
H	-4.89174300	0.05995200	-2.14035700
C	-4.71974100	-3.95447200	-2.50082200
H	-4.77391000	-4.82082500	-1.83855200
H	-5.52670100	-4.03942800	-3.23265900
H	-3.77141900	-3.99871400	-3.04054600
O	-0.51607300	-2.05877400	3.02172900
C	-0.11183300	-1.31365500	4.17387100
H	-0.86419600	-1.39535200	4.95982900
H	0.82178500	-1.75341200	4.51291500
H	0.04152300	-0.26541500	3.90312600
H	9.38299800	-0.91643200	-1.51359800
C	8.30534600	-0.83288200	-1.44851700
C	7.53362000	-1.95921700	-1.18977400
C	7.68954400	0.40118300	-1.63433300
C	6.14863900	-1.85093200	-1.11141500
H	8.00746600	-2.92390100	-1.05618400
C	6.30670200	0.50691600	-1.55654200
H	8.28688800	1.27900600	-1.84785100
C	5.52394400	-0.61782100	-1.29198700
H	5.54768400	-2.73600500	-0.92529000
H	5.83118300	1.46969600	-1.71988600
C	4.02534200	-0.48807800	-1.17289400
C	3.62897000	0.18843300	0.15079100
H	3.55158700	-1.47325400	-1.21922000
H	3.63220700	0.10364400	-2.00383700
C	3.98372800	-0.63969300	1.38627300
N	2.15292600	0.33703400	0.19404300
H	4.07460300	1.18324900	0.21570500
S	2.50291300	-1.67977200	1.72453700
H	4.84935300	-1.27582800	1.21182200
H	4.15266900	-0.01917000	2.26481800
C	1.52538900	-0.57583700	0.85790400
C	1.47736100	1.43522100	-0.53006800
H	0.42358600	-0.57991200	0.86514400
C	1.22083100	2.62332400	0.39051500
H	0.53755700	1.04868400	-0.92256900
H	2.12628700	1.70845500	-1.36470600
C	0.57030100	3.78445900	-0.36171100
H	0.55480100	2.28630600	1.19077700
H	2.16442100	2.95349400	0.84089100
C	0.36297000	4.99191200	0.54862300
H	1.19385800	4.06906900	-1.21604000
H	-0.39488000	3.45764400	-0.76231300
H	-0.16356200	5.79098300	0.02519000
H	-0.23384000	4.71610900	1.42100500

H	1.31835900	5.38827100	0.90121000
21			
C	1.47987000	-0.86666400	4.17051900
C	1.11690300	0.45422800	4.41245000
C	2.09785300	1.44486300	4.53199200
C	3.43993100	1.07963700	4.42807400
C	3.80386800	-0.24525000	4.19914100
C	2.82280200	-1.22130500	4.06391800
H	0.71102800	-1.62028300	4.04147400
H	0.06896300	0.72615800	4.48103200
H	4.20923700	1.83957600	4.52179300
H	4.85094100	-0.51053600	4.11650600
H	3.10145400	-2.24921800	3.86465700
C	1.73604200	2.90701400	4.71902800
O	0.83582500	3.04775200	5.81484000
H	2.64707000	3.45222600	4.98179200
C	1.17366800	3.51087800	3.41766300
H	1.81948700	3.20945700	2.59369300
H	1.21263600	4.60384500	3.47978900
C	-0.25771200	3.07363300	3.22085700
C	-1.05812400	3.13786700	4.28801300
H	-2.10659100	2.87419500	4.25996000
C	-0.46335300	3.62871600	5.56547000
H	-0.33270600	4.72183400	5.57931900
O	-0.68853100	2.63764600	2.03122300
Si	0.10160600	2.25430800	0.57648100
C	0.93807600	3.77964300	-0.10651800
H	1.26757000	3.58564500	-1.13113900
H	0.23863400	4.61847800	-0.14220600
H	1.81570600	4.09404100	0.46169600
C	1.32203200	0.86899000	0.88117400
H	0.81077400	-0.01351300	1.27365900
H	1.79203300	0.58539900	-0.06502600
H	2.12137400	1.12599500	1.58175100
C	-1.28276500	1.69842800	-0.52945200
H	-2.00797600	2.50097100	-0.67891300
H	-0.90266700	1.40106100	-1.50982600
H	-1.80885500	0.84430800	-0.09818200
O	-1.26695400	3.24616000	6.63372300
C	-1.01065700	3.97806600	7.82630300
H	-1.19385100	5.04430000	7.66734100
H	-1.70142700	3.60542700	8.58001700
H	0.02075600	3.83466800	8.16206200
H	-3.26586300	-6.91840900	8.04866600
C	-2.69243000	-6.03576000	7.79438900
C	-3.28937100	-4.99548800	7.09248800
C	-1.35319000	-5.94515600	8.16166100
C	-2.54999900	-3.86376000	6.76291100
H	-4.32837000	-5.06615000	6.79506200
C	-0.61659100	-4.81480000	7.83092400
H	-0.88164700	-6.75874500	8.69897300

C	-1.20901600	-3.76300300	7.13069400
H	-3.01582100	-3.05911000	6.20179300
H	0.43256700	-4.75705600	8.10609300
C	-0.41190800	-2.52321400	6.80835100
C	-0.20886800	-1.65197800	8.05984800
H	-0.92351300	-1.92538600	6.04735100
H	0.56636600	-2.79719500	6.40421900
C	-1.50797000	-1.05820700	8.60178600
N	0.62177000	-0.47568900	7.69594400
H	0.31108400	-2.21772000	8.83519200
S	-1.72932800	0.53907900	7.71386300
H	-2.35978600	-1.70833300	8.41142000
H	-1.44662600	-0.83429800	9.66588900
C	-0.04878600	0.59334600	7.41799300
C	2.08282200	-0.58981200	7.55723100
H	0.41789300	1.48252000	6.98953900
C	2.79250400	-0.43548600	8.89799000
H	2.40744700	0.17343700	6.84786800
H	2.29067800	-1.56437800	7.11004000
C	4.30548400	-0.57611100	8.72903300
H	2.55418600	0.54706700	9.31833900
H	2.42959600	-1.18679500	9.60773700
C	5.04826400	-0.39743900	10.05013900
H	4.53171200	-1.56017900	8.30579400
H	4.65470300	0.16402500	8.00148700
H	6.12477500	-0.50099400	9.91207300
H	4.85833600	0.59082100	10.47476000
H	4.73141200	-1.14439400	10.78149200

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C	-2.02974600	3.57350900	-0.44533400
C	-2.24048100	2.33599400	0.15649500
C	-1.63150500	1.19270200	-0.36215000
C	-0.81930500	1.30195300	-1.49078600
C	-0.61390000	2.53817400	-2.09623000
C	-1.21548900	3.67794800	-1.56988000
H	-2.51000900	4.45663700	-0.04114100
H	-2.86962700	2.24801900	1.03413700
H	-0.35948700	0.41041300	-1.90781900
H	0.00436500	2.61009700	-2.98387500
H	-1.06257100	4.64063500	-2.04236500
C	-1.87073300	-0.15841300	0.26254900
O	-2.02867500	0.02825200	1.66662600
H	-0.99850800	-0.80405100	0.08078100
C	-3.09534500	-0.87125000	-0.29756600
H	-2.93084000	-1.08401000	-1.35789400
H	-3.97445000	-0.22242500	-0.22074000
C	-3.29717400	-2.15179800	0.47074600
C	-2.76258100	-2.29845300	1.68479400
H	-2.88031000	-3.22827000	2.22534900
C	-2.09257600	-1.17800400	2.40804300
H	-2.65322400	-0.91303900	3.31110200

O	-4.00413400	-3.14399600	-0.09061200
Si	-4.81466200	-3.33324500	-1.56703600
C	-5.90811100	-1.85049400	-1.88792300
H	-6.61024300	-2.08532900	-2.69282300
H	-6.49924600	-1.59810700	-1.00392300
H	-5.34935500	-0.96330100	-2.19298600
C	-3.55761900	-3.54880600	-2.93486500
H	-2.86450400	-4.35974500	-2.69958700
H	-4.06700600	-3.80943100	-3.86677100
H	-2.97358800	-2.64572700	-3.12733200
C	-5.81354900	-4.87862200	-1.31967900
H	-6.53335900	-4.75140200	-0.50849700
H	-6.36728700	-5.13588500	-2.22582600
H	-5.16777800	-5.72234200	-1.06769600
O	-0.78574700	-1.56435800	2.79218700
C	-0.38318700	-1.01028000	4.03515500
H	-1.03700100	-1.35122000	4.84237900
H	0.62945900	-1.35849000	4.23145200
H	-0.39584300	0.08721800	4.01175600
H	7.43160700	-0.57104500	-3.77736600
C	6.50000400	-0.32101700	-3.28532500
C	5.53385100	-1.29937600	-3.08479500
C	6.26420700	0.98326900	-2.86098200
C	4.33547100	-0.97571700	-2.45589800
H	5.70845400	-2.31325800	-3.42312700
C	5.06706100	1.30438300	-2.23410100
H	7.01038600	1.75078300	-3.02550800
C	4.09298500	0.32726600	-2.02394700
H	3.57671600	-1.73974100	-2.31509000
H	4.88236300	2.32761500	-1.91981900
C	2.81165700	0.67828000	-1.30844700
C	3.05479900	0.85529300	0.19991400
H	2.06599100	-0.10976900	-1.45115800
H	2.39027200	1.60261500	-1.71305500
C	3.41801800	-0.44837500	0.90927200
N	1.79319500	1.30168000	0.84425500
H	3.81743100	1.61685300	0.37309500
S	1.81715800	-1.19249700	1.43518600
H	3.94305100	-1.13458000	0.24729300
H	4.00974100	-0.28011300	1.80795600
C	1.09625800	0.35515800	1.37840900
C	1.36348000	2.70823200	0.77622800
H	0.08907400	0.52355900	1.75892000
C	1.97489500	3.53936000	1.89915800
H	0.27360200	2.72380800	0.82110900
H	1.65932500	3.08838700	-0.20363700
C	1.53098800	4.99856700	1.79301800
H	1.66221500	3.12413500	2.86310400
H	3.06817800	3.48184300	1.86226600
C	2.09789800	5.85285500	2.92337800
H	1.84852900	5.40292000	0.82641600
H	0.43694700	5.04136500	1.80494800

H	1.77280600	6.88943100	2.83187300
H	1.76749500	5.48286200	3.89647100
H	3.19012300	5.84250300	2.91220300

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C	0.05877800	-1.75852400	0.21835600
C	2.37925800	-1.35995300	1.04307100
C	1.85934300	-0.16774900	0.23568600
N	0.47955100	-0.50318800	-0.11617400
H	-0.73923900	-2.15691600	-0.40091400
H	3.45353000	-1.49769600	0.93489200
C	-0.46132900	0.52482300	-0.53071100
H	0.00201200	1.11361800	-1.33037800
H	-1.31814700	0.01405900	-0.97656800
C	-0.93890400	1.46274100	0.57986300
H	-0.08120700	1.97076800	1.03561200
H	-1.41667200	0.87548600	1.36786800
C	-1.91671600	2.50276700	0.03568800
H	-1.42174000	3.10412600	-0.73540800
H	-2.75041500	1.99024000	-0.45651200
C	-2.45814800	3.41612400	1.13175100
H	-1.65167900	3.98251600	1.60479000
H	-3.18449000	4.12891400	0.73566400
H	-2.95294700	2.82844800	1.90933100
C	2.68456400	0.09143500	-1.03904300
H	2.71329600	-0.83561600	-1.61758400
H	2.16705700	0.83907700	-1.64601400
C	4.07801700	0.57217800	-0.72662900
C	5.17923300	-0.27374700	-0.85678100
C	4.28718600	1.87304300	-0.26360600
C	6.45843700	0.16614000	-0.53085200
H	5.03138400	-1.28447700	-1.22427300
C	5.56228500	2.31639400	0.06391400
H	3.44055200	2.54646600	-0.16768300
C	6.65274500	1.46211400	-0.06809400
H	7.30296900	-0.50357300	-0.64179000
H	5.70699100	3.33002700	0.41850000
H	7.64797200	1.80688200	0.18498400
S	1.49397500	-2.81077100	0.37624300
H	2.11973500	-1.26592100	2.09707800
H	1.88206500	0.72555000	0.86963700
C	-5.06373500	0.54984000	-1.47812400
C	-5.61214700	1.35723200	-0.48813000
C	-5.23671500	1.17195100	0.83952800
C	-4.31526400	0.18268900	1.18327400
C	-3.76136700	-0.61720400	0.19600400
C	-4.13106100	-0.42870700	-1.13719000
H	-5.34879400	0.68332800	-2.51706400
H	-6.33002500	2.12549100	-0.74765600
H	-5.66504300	1.80103800	1.61129600
H	-4.02410400	0.03583100	2.21702100
H	-3.04319800	-1.38823700	0.44932800

C	-3.50572000	-1.25151400	-2.19711500
O	-2.55638400	-1.97420000	-2.02175000
H	-3.95944900	-1.15323100	-3.20297600
Cl	-0.89307300	-1.78119800	1.99594100

MC3

C	1.43622100	-0.26598600	-2.76598500
C	0.94282200	-1.08139100	-1.75626000
C	1.23030700	-2.44678200	-1.77824800
C	2.02973700	-2.98443300	-2.78587400
C	2.51248700	-2.16686400	-3.80122400
C	2.20863400	-0.80911400	-3.79216300
H	1.21991900	0.79623500	-2.76508100
H	0.34790000	-0.68677800	-0.93819800
H	2.25532600	-4.04629400	-2.78219400
H	3.12138100	-2.58344700	-4.59404100
H	2.58276000	-0.16782400	-4.58146900
C	0.62026600	-3.35158300	-0.77629600
O	-0.34449600	-3.06818500	-0.10790500
H	1.08258200	-4.35479900	-0.70422400
C	2.97388300	-2.63472900	1.23000200
H	3.72434500	-2.66412800	0.45097100
H	2.83519200	-3.51279300	1.84484600
C	2.24398100	-1.53256700	1.46420100
C	1.13029200	-1.43122600	2.40476700
H	0.92388500	-0.45314300	2.82071000
C	0.29645100	-2.44205200	2.65958200
H	0.40781500	-3.41826300	2.19471400
O	2.42799400	-0.35682100	0.80024000
Si	3.86846800	0.34014900	0.26703300
C	5.01239700	0.50345400	1.73591700
H	5.97576800	0.92344300	1.43480400
H	4.58213000	1.15408400	2.50052200
H	5.19812000	-0.47391600	2.18848300
C	4.67952100	-0.68658500	-1.07510300
H	3.93317500	-1.23410000	-1.65488600
H	5.23095200	-0.04342900	-1.76662700
H	5.38595700	-1.40786600	-0.65697700
C	3.31569400	2.00063300	-0.37533000
H	2.87360100	2.60139600	0.42323700
H	4.15229300	2.56350200	-0.79701900
H	2.55885300	1.88546300	-1.15482400
O	-0.76855000	-2.28924000	3.46949300
C	-1.71987200	-3.34738600	3.41309800
H	-1.30974300	-4.25211300	3.87162000
H	-2.59116900	-3.00926700	3.96816900
H	-2.01123000	-3.55042300	2.37877600
H	0.37263000	7.25279400	0.29294000
C	0.20913800	6.18676800	0.19129900
C	0.57062000	5.32280700	1.21948600
C	-0.35981200	5.67446700	-0.96988400
C	0.36191900	3.95452100	1.08516500

H	1.01758600	5.71422200	2.12571700
C	-0.56541500	4.30562400	-1.09995600
H	-0.64003600	6.34161300	-1.77652200
C	-0.20795900	3.42778800	-0.07560200
H	0.64714700	3.27786000	1.88573400
H	-1.00315600	3.90921900	-2.01135400
C	-0.46554300	1.95051300	-0.20006000
C	-1.93145600	1.55796600	0.09052000
H	0.18470100	1.38458800	0.47554400
H	-0.23711200	1.62246200	-1.21936900
C	-2.38316200	1.87374400	1.51170600
N	-2.07297600	0.11044400	-0.04532700
H	-2.58805800	2.07193200	-0.61962600
S	-1.78222300	0.46657100	2.50103600
H	-1.96021200	2.80062900	1.89484900
H	-3.47133000	1.90650600	1.57405600
C	-2.18066100	-0.61375200	1.12700400
C	-2.34986300	-0.49230200	-1.33921700
H	-1.62447300	-1.54497200	1.13180300
C	-3.75565200	-0.22860500	-1.88512000
H	-2.17271500	-1.56738800	-1.24176600
H	-1.61319500	-0.11945000	-2.06170400
C	-3.95671500	-0.90199200	-3.24142100
H	-4.49780400	-0.59270600	-1.17203800
H	-3.91372000	0.85083800	-1.99253400
C	-5.34246400	-0.63314400	-3.82277900
H	-3.18864200	-0.55424400	-3.94157600
H	-3.80788400	-1.98118500	-3.12990300
H	-5.47527300	-1.12600000	-4.78767400
H	-6.12131900	-0.99663300	-3.14833400
H	-5.50227600	0.43841900	-3.96778400
Cl	-3.99242200	-1.33453900	1.39544100

TS3-pn

C	-3.95759600	-1.34407700	0.70413100
C	-3.78312400	-1.10307700	-0.67684500
C	-2.74740500	-1.68565700	-1.43035700
C	-1.86429100	-2.56432200	-0.86518900
O	-1.35050100	-1.14016800	1.08026700
C	-2.40286700	-0.58968100	1.54425600
C	-2.23983000	2.90587700	0.05754400
C	-2.14577200	1.52605100	0.19133400
C	-2.56856400	0.90088800	1.36559300
C	-3.07212300	1.67877400	2.40535900
C	-3.15110200	3.06263900	2.28153100
C	-2.73647900	3.67879800	1.10589500
H	-1.91696200	3.38292100	-0.86060200
H	-1.75126400	0.92007800	-0.61769900
H	-3.38858100	1.19698000	3.32581900
H	-3.53162100	3.65905300	3.10234300
H	-2.79547300	4.75607700	1.00617200
H	-2.74580900	-0.91182400	2.54292500

H	-4.81507200	-0.87669300	1.17715900
H	-3.78069000	-2.35911800	1.03944700
H	-2.55947000	-1.30524000	-2.42664200
H	-2.04560500	-3.05329300	0.08440600
O	-4.44613600	-0.13424200	-1.30515100
Si	-5.97635500	0.56606100	-1.03255500
C	-7.20944400	-0.82166000	-0.82620000
H	-8.21876000	-0.41443100	-0.72252300
H	-7.20239100	-1.48034000	-1.69778900
H	-7.00458500	-1.42993200	0.05732000
C	-5.93951400	1.70179000	0.44298400
H	-5.09475200	2.39210800	0.37523900
H	-6.85902000	2.29466300	0.46164200
H	-5.86308700	1.17630600	1.39650000
C	-6.26629800	1.53133600	-2.59593800
H	-6.24111600	0.87827800	-3.47057100
H	-7.23712800	2.03233100	-2.57252300
H	-5.49554900	2.29534600	-2.72101800
O	-0.76031200	-2.89206200	-1.48911600
C	0.14209000	-3.76375300	-0.76866200
H	-0.30604900	-4.75500400	-0.68279500
H	1.07026600	-3.79701900	-1.33023600
H	0.35184500	-3.33606200	0.21318800
H	8.84592100	2.03032100	-1.91199500
C	7.83908500	1.91936700	-1.52800800
C	6.92233500	2.95539800	-1.65950900
C	7.45407800	0.73594700	-0.90679800
C	5.62905000	2.80586400	-1.17048600
H	7.21048400	3.87913300	-2.14711300
C	6.16251500	0.58806800	-0.41475200
H	8.15874500	-0.08072300	-0.80689700
C	5.23571400	1.62660000	-0.53922200
H	4.91488200	3.61570000	-1.27889300
H	5.88157100	-0.34889300	0.05649700
C	3.82920600	1.49085500	0.00538700
C	3.25007800	0.10770500	-0.28099300
H	3.18637100	2.25954700	-0.43611700
H	3.84305900	1.65922400	1.08758600
C	3.22395900	-0.24456400	-1.78133800
N	1.86413500	-0.01361500	0.21927900
H	3.79869200	-0.68379400	0.23440700
S	1.52097300	-0.79148700	-2.19390600
H	3.47675500	0.60920900	-2.40979900
H	3.88111800	-1.09088900	-1.97348300
C	0.99570400	-0.48466300	-0.60718700
C	1.55604900	0.20454400	1.64340100
H	-0.02431800	-0.67891100	-0.26437300
C	2.43387700	-0.65668900	2.54669000
H	0.50369000	-0.05516900	1.76969700
H	1.68149200	1.27073800	1.85416300
C	1.89526600	-0.65375600	3.97590700
H	2.46739100	-1.67467700	2.14474200

H	3.46631500	-0.28824000	2.54231100
C	2.77915600	-1.47121800	4.91421300
H	1.81527200	0.37600500	4.34332800
H	0.88010600	-1.06426600	3.96998100
H	2.37343800	-1.49147600	5.92729400
H	2.86625900	-2.50029100	4.55925100
H	3.78697300	-1.05176800	4.96262300
Cl	3.38671600	-3.05966200	-0.05671200

TS3-px

C	-3.67202500	-0.01996400	0.64802000
C	-3.57299700	-1.42788300	0.64470500
C	-2.45217700	-2.14036800	1.11720500
C	-1.36166900	-1.51736900	1.64959400
O	-1.31501300	0.21081900	-0.45269000
C	-2.51813800	0.52308800	-0.74543400
C	-2.55081600	4.21937800	0.11850300
C	-2.24438400	2.86521000	0.12184500
C	-2.88217500	1.99337200	-0.75746400
C	-3.82111500	2.49550400	-1.65438800
C	-4.12816400	3.85357900	-1.66356100
C	-3.49682100	4.71706600	-0.77504400
H	-2.04649300	4.88760100	0.80827000
H	-1.50056700	2.46508200	0.80185300
H	-4.29831600	1.82488500	-2.36261000
H	-4.85330600	4.23881300	-2.37080100
H	-3.73463700	5.77392100	-0.78286900
H	-3.01118400	-0.01593500	-1.57678400
H	-4.64176800	0.40053100	0.40679400
H	-3.18073200	0.50118300	1.46089300
H	-2.42913700	-3.21270800	0.97328300
H	-1.32744000	-0.44805100	1.83802100
O	-4.47599200	-2.17744000	0.01725000
Si	-6.09180000	-1.87569400	-0.44198600
C	-7.04408500	-1.34215300	1.07074300
H	-8.09995200	-1.21064500	0.81910300
H	-6.98002100	-2.10079700	1.85417300
H	-6.68118700	-0.39886500	1.48364900
C	-6.14581300	-0.58783800	-1.79431000
H	-5.39539300	-0.79667300	-2.56125200
H	-7.12672800	-0.60878000	-2.27772400
H	-5.98259600	0.42531700	-1.42158800
C	-6.65651600	-3.53065400	-1.07225200
H	-6.56996100	-4.29266000	-0.29502700
H	-7.70057300	-3.48963700	-1.39223900
H	-6.05392200	-3.84870800	-1.92570700
O	-0.30005400	-2.21039800	1.97266500
C	0.80487500	-1.48534200	2.55544300
H	0.51998300	-1.06423100	3.52005400
H	1.60914600	-2.20007800	2.69294700
H	1.13629900	-0.68952900	1.89104100
H	9.54344200	-0.85155400	-0.82116600

C	8.48578700	-0.66582300	-0.96461100
C	7.91991900	-0.78611200	-2.22910300
C	7.68446000	-0.31454000	0.11521600
C	6.56136600	-0.55388600	-2.40579800
H	8.53364300	-1.06621900	-3.07707200
C	6.32472800	-0.07558100	-0.05965600
H	8.11138100	-0.22793800	1.10704900
C	5.75141900	-0.19007800	-1.32928600
H	6.12179600	-0.65465300	-3.39308100
H	5.72699400	0.18248300	0.81091400
C	4.28060100	0.08719700	-1.57222600
C	3.42056500	-0.27184000	-0.36144000
H	3.93878500	-0.48119700	-2.44447800
H	4.15178600	1.14767500	-1.80977100
C	3.47087900	-1.76002600	0.00374500
N	1.99383700	0.03916800	-0.62761400
H	3.70058900	0.29303100	0.53245800
S	1.92901000	-2.51493400	-0.65983100
H	4.32963700	-2.25914000	-0.44060500
H	3.47729500	-1.87393600	1.08893000
C	1.21581000	-0.97128700	-0.82052700
C	1.52548400	1.43828200	-0.61215700
H	0.14846700	-0.81377500	-1.01292300
C	1.29034300	1.92895100	0.81277300
H	0.59834000	1.48036800	-1.18463200
H	2.29319500	2.03453300	-1.10987300
C	1.13112900	3.44785400	0.84772200
H	0.37888100	1.44085000	1.17445100
H	2.10855100	1.62233500	1.47373700
C	0.70431500	3.93330900	2.23073800
H	2.08612200	3.91023800	0.57766100
H	0.40161500	3.76792100	0.09510200
H	0.64406900	5.02266900	2.27081100
H	-0.27713600	3.53159700	2.50078200
H	1.41673600	3.60085900	2.98910900
Cl	3.64460300	0.03071700	2.89504500

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C	3.87679300	1.04577200	1.06695300
C	4.39053600	0.66986600	-0.29402900
C	3.80002700	1.17194700	-1.37436600
C	2.70991000	2.19196900	-1.24945200
O	2.00233900	2.15901200	-0.00900500
C	2.35420500	1.20461600	0.97957600
C	0.40282700	-1.74808200	-0.48035000
C	1.03580200	-0.51104300	-0.38262200
C	1.66751800	-0.14072300	0.80149500
C	1.66155200	-1.03002500	1.87964700
C	1.03778000	-2.26752300	1.77985200
C	0.39864800	-2.62837200	0.59513100
H	-0.08007200	-2.02249000	-1.41092800
H	1.03958900	0.16054500	-1.23340300

H	2.13676800	-0.74300300	2.81410400
H	1.04098600	-2.94466800	2.62600700
H	-0.09408400	-3.58994400	0.51239000
H	1.99310600	1.64246300	1.91498100
H	4.13828300	0.27916400	1.79828900
H	4.32610700	1.98777900	1.39667200
H	4.12929200	0.92720400	-2.37570200
H	3.12549000	3.20846100	-1.31082300
O	5.46021700	-0.16005700	-0.35818800
Si	5.48677200	-1.83127000	-0.12136500
C	5.35046600	-2.23677600	1.70272300
H	5.59288100	-3.29122800	1.86390300
H	6.04382200	-1.64106300	2.30152600
H	4.33555700	-2.07611400	2.07531500
C	4.06199800	-2.60045100	-1.04483900
H	4.02845500	-2.26447300	-2.08408800
H	4.14976500	-3.69047100	-1.04211600
H	3.10871300	-2.34009000	-0.57689500
C	7.14875200	-2.35050800	-0.78250300
H	7.95370200	-1.83564600	-0.25330600
H	7.29882000	-3.42626500	-0.66198700
H	7.23710800	-2.11155000	-1.84425900
O	1.81191800	2.02141300	-2.30435400
C	1.07156200	3.19773600	-2.59994100
H	1.73991300	3.98650700	-2.96236400
H	0.36447200	2.93895600	-3.38556100
H	0.52561800	3.56341000	-1.72519600
H	-7.98470000	-3.37840200	-1.26386000
C	-7.00600000	-2.95035600	-1.08403200
C	-6.08590900	-2.84948700	-2.12049600
C	-6.66173400	-2.50188500	0.18769700
C	-4.82887300	-2.30044400	-1.88624100
H	-6.34447700	-3.20040400	-3.11253300
C	-5.40547100	-1.95518000	0.41655900
H	-7.37233500	-2.58195400	1.00182600
C	-4.47209400	-1.84599500	-0.61688400
H	-4.11007700	-2.22946700	-2.69669800
H	-5.13767400	-1.61409900	1.41240300
C	-3.12915000	-1.21342000	-0.36258000
C	-3.22433600	0.31468900	-0.20991700
H	-2.43690600	-1.42606200	-1.18126100
H	-2.68589600	-1.62743900	0.54862200
C	-3.55389300	1.02833500	-1.52617800
N	-1.94301300	0.85685000	0.23069700
H	-4.01039100	0.55421900	0.51467000
S	-1.94353200	1.48489300	-2.25382300
H	-4.10583200	0.39109000	-2.21521000
H	-4.11125700	1.94679800	-1.34640700
C	-1.35907900	1.78739800	-0.58770800
C	-1.49165500	0.70431500	1.60464500
H	-0.27775100	1.85266900	-0.50792600
C	-2.50047000	1.15304700	2.66072100

H	-0.58326600	1.30430300	1.70337100
H	-1.19848700	-0.33925500	1.77803000
C	-1.87045200	1.15900900	4.05207500
H	-2.86437100	2.15360300	2.40567200
H	-3.36657400	0.48064100	2.66464000
C	-2.87040000	1.52701900	5.14494500
H	-1.44070400	0.17211200	4.25911300
H	-1.03692700	1.86938200	4.06123000
H	-2.40066500	1.54080500	6.13007400
H	-3.29654600	2.51617000	4.96125000
H	-3.69461600	0.80983900	5.17614900
Cl	-1.82594100	3.62670100	-0.04889500

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C	-2.31789700	-1.25549800	1.78951000
C	-3.43648300	-1.30287700	0.78943400
C	-3.36379300	-2.07327800	-0.29229500
C	-2.19440900	-2.97512600	-0.54416000
O	-1.21776000	-2.93974500	0.47298300
C	-1.02796200	-1.67052400	1.08858500
C	2.03201000	-2.95242100	2.96586300
C	0.92394800	-2.91488000	2.12205600
C	0.15968600	-1.75581800	2.01719600
C	0.51419900	-0.63968500	2.77950900
C	1.61413200	-0.67937600	3.62623600
C	2.38165100	-1.83845600	3.71858500
H	2.62067800	-3.85967500	3.03592900
H	0.64492400	-3.78260500	1.53884200
H	-0.06894300	0.27239100	2.70507500
H	1.87427600	0.19430200	4.21260000
H	3.24157200	-1.87160400	4.37681300
H	-0.81455000	-0.92034200	0.31497900
H	-2.23476300	-0.23641800	2.17479000
H	-2.52278400	-1.91794600	2.63652900
H	-4.15792800	-2.09022100	-1.02812600
H	-2.51220100	-4.02517100	-0.57406600
O	-4.49798100	-0.49045400	1.05580900
Si	-4.70605800	0.96227200	0.21955000
C	-6.07575200	1.84037700	1.12346000
H	-6.28829600	2.80966800	0.66579600
H	-6.99373900	1.24903600	1.10257800
H	-5.80750100	2.00930600	2.16837300
C	-3.08579900	1.90247900	0.27991500
H	-2.28647500	1.30399600	-0.17237500
H	-3.17023400	2.82910600	-0.29560300
H	-2.79641600	2.16558200	1.30090100
C	-5.14967100	0.62481400	-1.56316800
H	-6.01383100	-0.03943400	-1.63996100
H	-5.39906500	1.55895700	-2.07422500
H	-4.31300100	0.16577100	-2.09592400
O	-1.65128000	-2.63038100	-1.79137600
C	-0.86701300	-3.66332500	-2.36629000

H	-1.49173300	-4.53139900	-2.60402100
H	-0.42998900	-3.26220700	-3.27869600
H	-0.06197000	-3.97422100	-1.69143400
H	1.56202400	7.27653200	0.01069200
C	1.47683600	6.19934800	0.08720300
C	0.23771400	5.58462900	-0.04661400
C	2.60790600	5.42386900	0.32467600
C	0.13087800	4.20071400	0.05321600
H	-0.64801200	6.18248700	-0.22647000
C	2.49651100	4.04290700	0.42498100
H	3.57636400	5.89712400	0.43547900
C	1.25735100	3.41303100	0.28917700
H	-0.83816600	3.72096300	-0.04429700
H	3.38012100	3.44182400	0.61915500
C	1.15793800	1.91215000	0.35897500
C	1.71476600	1.22382900	-0.89970800
H	0.11608500	1.59738300	0.48381200
H	1.71558800	1.53930200	1.22393300
C	0.86330700	1.46456200	-2.15034800
N	1.73679600	-0.22351400	-0.69416000
H	2.72563300	1.59829100	-1.09216700
S	-0.31828600	0.07506000	-2.21853800
H	0.32029400	2.40772200	-2.10420500
H	1.47468100	1.43709300	-3.05184300
C	0.98638800	-0.97109900	-1.57189400
C	2.81519900	-0.85210600	0.05912900
H	0.61247600	-1.90307400	-1.16002900
C	4.22746500	-0.52798100	-0.42927800
H	2.65232600	-1.93106000	0.00220100
H	2.72067300	-0.58266600	1.11691500
C	5.25651700	-1.40456900	0.28265700
H	4.28593000	-0.67965900	-1.51100300
H	4.46173400	0.52472800	-0.23202300
C	6.69065200	-1.05307400	-0.10371200
H	5.12740500	-1.30570200	1.36671700
H	5.05576000	-2.45375500	0.04178800
H	7.41150700	-1.69804100	0.40204900
H	6.83859100	-1.16277100	-1.18074500
H	6.92299500	-0.01817200	0.16044900
Cl	2.06507800	-1.66909600	-3.05493300