Supporting Information

A DFT and Experimental Exploration of the Mechanism of $InCl_3$ Catalyzed Type-II Cycloisomerization of 1,6-Enynes: Identifying $InCl_2^+$ as the Catalytic Species and Answering Why NonConjugated Dienes are Generated

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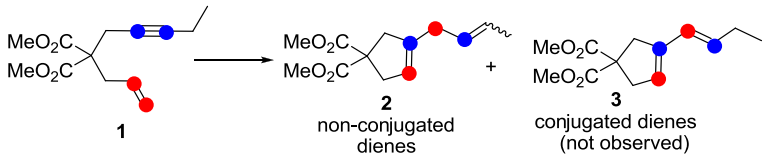
1.1. Additional details of $InCl_3$ and InI_3 catalyzed cycloisomerizations of 1

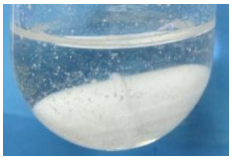
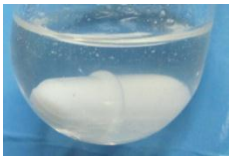
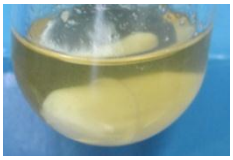
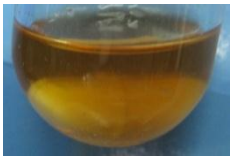
Cycloisomerization of 1 under different reaction conditions (Scheme 3 in text)



Reaction Conditions	Results
a, 10 mol% $InCl_3$, DCE, 80 °C, 2h	74%, **2**-*E* : **2**-*Z* = 4:1[a]
b, 20 mol% $InCl_3$, CH_3CN, 90 °C, 2h	conversion: 10%[b], **2**-*E* : **2**-*Z*= 3:1[a]
c, 150 mol% $InCl_3$, CH_3CN, 90 °C, 1h	conversion: 54%[b], **2**-*E* : **2**-*Z*= 3:1[a]
d, 400 mol% $InCl_3$, CH_3CN, 90 °C, 1h	conversion: 100%[b], **2**-*E* : **2**-*Z*= 3:1[a]
e, 10 mol%(AgX + $InCl_3$),DCE, 80 °C, 3h X = SbF_6, BF_4, OTf, $OCOCF_3$	brsm[c] : 63% ~ 74%, **2**-*E* : **2**-*Z* = 3:1[a] conversion: 55% ~ 83%,
f, 10 mol% InI_3, DCE, 80 °C, 2h	75%, **2**-*E*:**2**-*Z* = 4:1[a]

[a] the *E*/*Z* ratio was determined by GC.
[b] the products cannot be isolated in silica gel and conversion was determined by GC
[c] see expermental part for details.

Condition a: Reaction under the standard reaction conditions used by Chatani.

0 min	10 min	1 h	2 h
			

Reaction time	**Area%**			Ratio
	4.5 min*	5.2 min*	5.3 min*	
30 min	1.37816	1.22569	0.29790	4.4:4:1
1.5h	0.27199	3.27969	0.77760	0.3:4:1
2h	0.08064	1.84758	0.45107	0:4:1

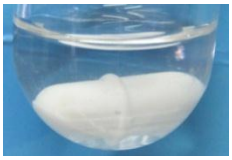
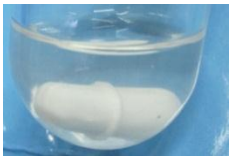
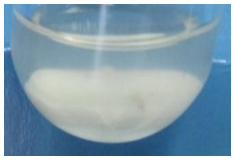
* GC retention Time, 4.5 min (**1**), 5.2 min (**2**-*E*), 5.3 min (**2**-*Z*)

Conditions b, c and d: Reactions catalyzed by $InCl_3$ in CH_3CN.

Condition b: To a mixture of anhydrous CH_3CN (2.5 mL) and $InCl_3$ (22 mg, 0.10 mmol) under argon, **1** (119 mg, 0.50 mmol) was added. The resulting mixture was stirred at 90 ℃. After 2 h, the ratio of **1**:(**2**-*E* +**2**-*Z*) was found to be about 10:1. No improved result was obtained even extending the reaction time to 5 h.

We carried out this reaction by cooling the reaction to room temperature in 2 h, the reaction mixture was directly concentrated in vacuum. The residue was subjected to flash column chromatography on silica gel (eluted with PE/EA 30:1 to 20:1) to give a mixture of **1**, **2**-*Z* and **2**-*E* (99 mg). The ratio of **1**:(**2**-*E* +**2**-*Z*) is >100:1, as determined by GC. This indicates that the generated diene products stay in the silica

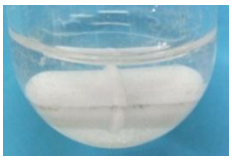
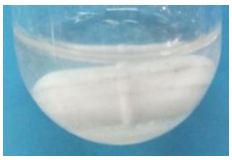
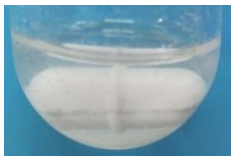
gel during the column chromatography.

0 min	10 min	1 h	2 h
			

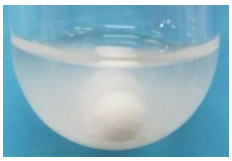
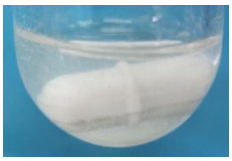
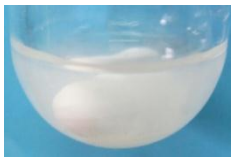
Reaction time	**Area%**			Ratio
	4.5 min*	5.2 min*	5.3 min*	
2h	1.17365	0.07577	0.02155	54:3.5:1
5h	1.08225	0.06504	0.01780	60:3.6:1
Isolated mixture	1.43259	0.01410	0.00137	>1000:10:1

* GC retention Time, 4.5 min (**1**), 5.2 min (**2**-*E*), 5.3 min (**2**-*Z*)

Condition c (reaction process is shown below**)**:

0 min	10 min	1 h
		

Condition d: To a mixture of anhydrous CH_3CN (2.5 mL) and $InCl_3$ (265 mg, 1.2 mmol) under argon, **1** (71 mg, 0.30 mmol) was added. The resulting mixture was stirred at 90 ℃ until GC indicated the disappearance of the starting material (here 1 h was used). The reaction mixture was directly used for ESI-HRMS analysis.
[(**2**+**$InCl_2$**)$^+$]: HRMS (ESI) calcd for $C_{13}H_{18}Cl_2InO_4$: 422.96147. Found: 422.96135.

0 min	10 min	1 h
		

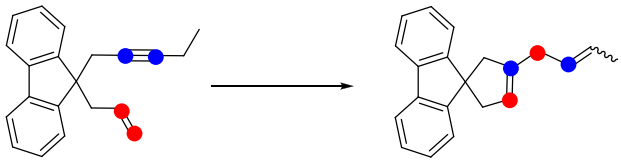
Condition e: Reactions with $InCl_3$/AgX (results).

AgX	Mixture of **1**, **2**-*E* and **2**-*Z*		Conversion	yield	brsm.
	Weight	Ratio (by GC) **1**:**2**-*E*:**2**-*Z*			
$AgSbF_6$	84 mg	1.4:3.3:1.0	83%	52%	63%
AgOTf	91 mg	2.6:3.5:1.0	73%	49%	69%
$AgBF_4$	95 mg	3.5:4.0:1.0	67%	47%	73%
$Ag(OCOCF_3)$	102 mg	5.0:3.9:1.0	55%	43%	74%

Condition f: Reaction catalyzed by InI_3 in DCE

To a mixture of anhydrous DCE (2.5 mL) and InI_3 (25.0 mg, 0.05 mmol) under argon, **1** (119 mg, 0.50 mmol) was added. The resulting mixture was stirred at 80 ℃ for additional 2 h. The reaction was cooled to room temperature and the reaction mixture was directly concentrated in vacuum. The residue was subjected to flash column chromatography on silica gel to give a mixture of **2**-*E* and **2**-*Z* (89 mg), 75%. The ratio of **2**-*E*:**2**-*Z* is 4:1, as determined by GC.

1.2. $InCl_3$ catalyzed cycloisomerization of 1′ in CH_3CN



1' **2'** non-conjugated dienes

Reaction Conditions	Results
a, 5 mol% $InCl_3$, DCE, 80 °C, 2h	74%, **2'**-*E* : **2'**-*Z* = 2.6:1[a]
b, 20 mol% $InCl_3$, CH_3CN, 90 °C, 2h	conversion: 10%[b], **2'**-*E* : **2'**-*Z*= 3:1[a]
c, 400 mol% $InCl_3$, CH_3CN, 90 °C, 1h	conversion: 90%[b], **2'**-*E* : **2'**-*Z*= 3:1[a]

[a] the *E*/*Z* ratio was determined by GC.
[b] the products cannot be isolated in silica gel and conversion was determined by GC.

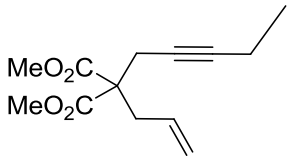
Condition b. Stoichiometric reaction of 1′ in CH_3CN (20 mol% $InCl_3$)

To a mixture of anhydrous CH_3CN (2.5 mL) and $InCl_3$ (22mg, 0.10 mmol) under argon, **1′** (136 mg, 0.50 mmol) was added. The resulting mixture was stirred at 90 ℃. After 2 h, the ratio of **1′**:(**2′**-*E* +**2′**-*Z*) was found to be about 10:1. No improved result was obtained even extending the reaction time to 5 h. Some insoluble species was found in the resulting reaction mixture.

Condition c. Stoichiometric reaction of 1′ in CH_3CN (400 mol% $InCl_3$)

To a mixture of anhydrous CH_3CN (2.5 mL) and $InCl_3$ (442 mg, 2.0 mmol) under argon, **1′** (136 mg, 0.50 mmol) was added. The resulting mixture was stirred at 90 ℃. After 1 h, the ratio of **1′**:(**2′**-*E* +**2′**-*Z*) was found to be about 1:10. No improved result was obtained even extending the reaction time to 5 h. Some insoluble species was found in the resulting reaction mixture.

1.3. ^{1}H and ^{13}C NMR spectra of new compounds



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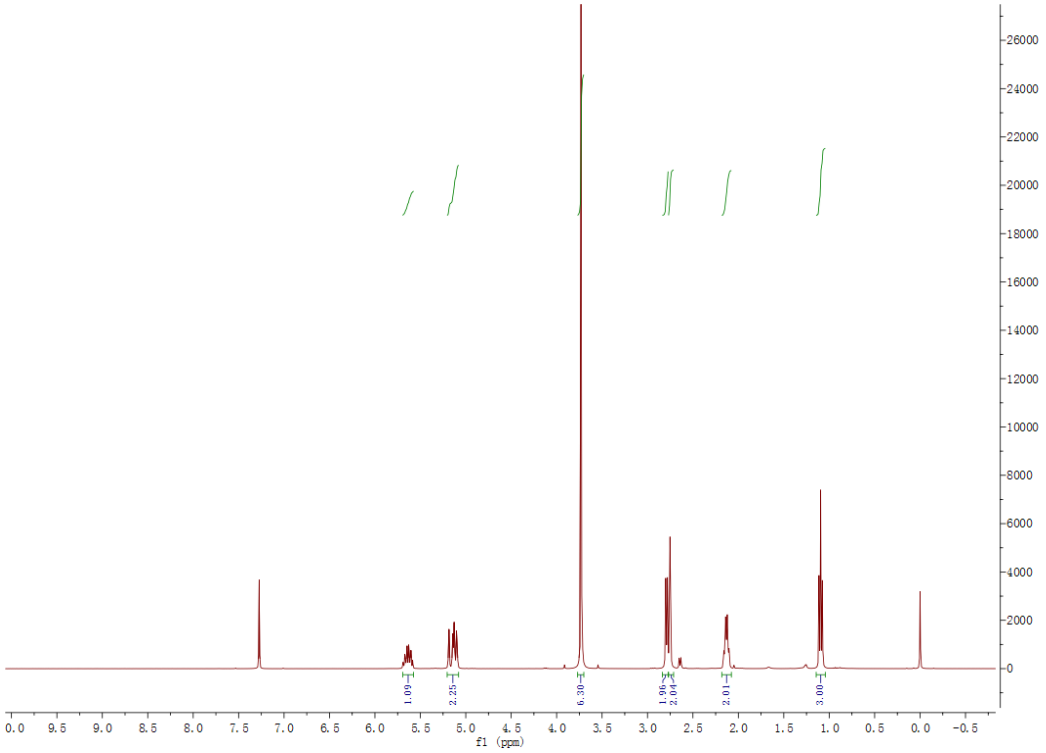

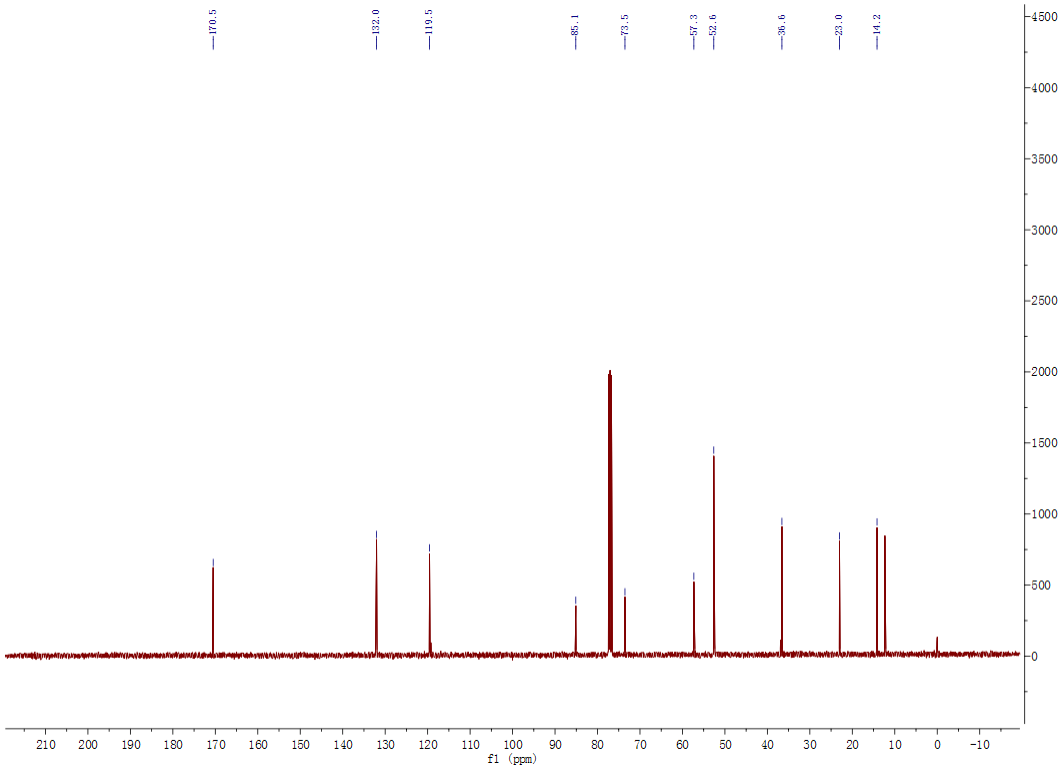

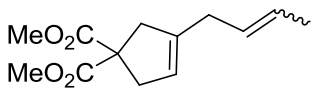
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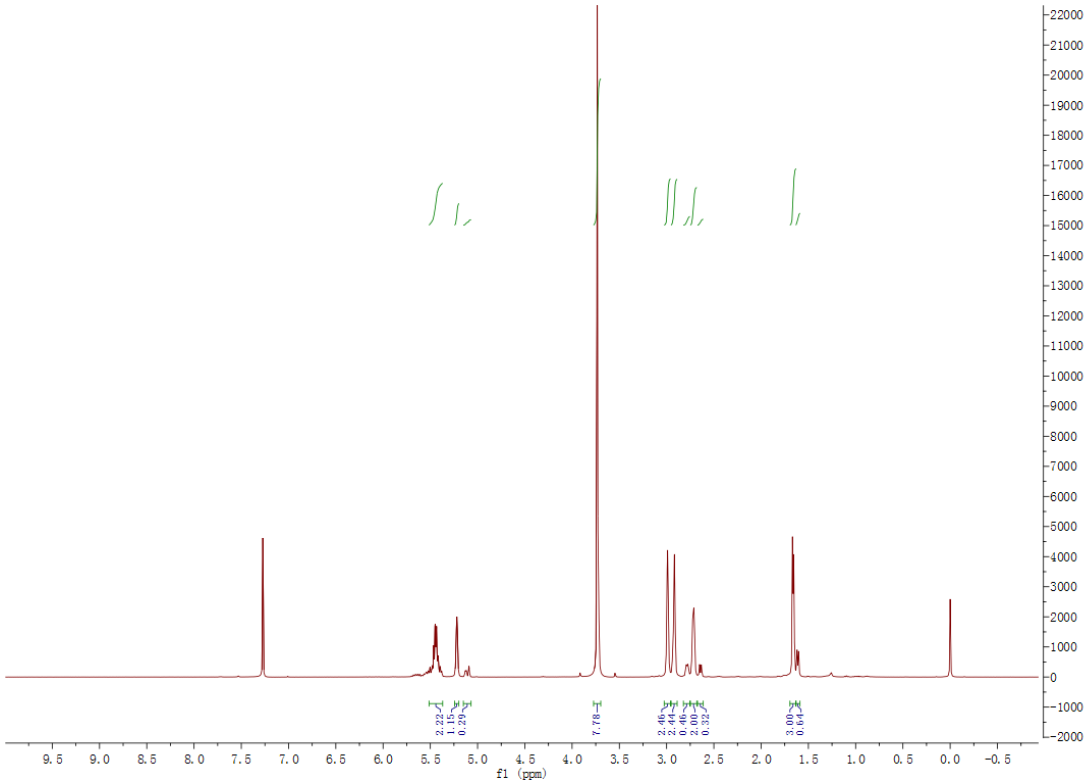
MeO2C

2-*E* and ***2***-*Z*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0.46
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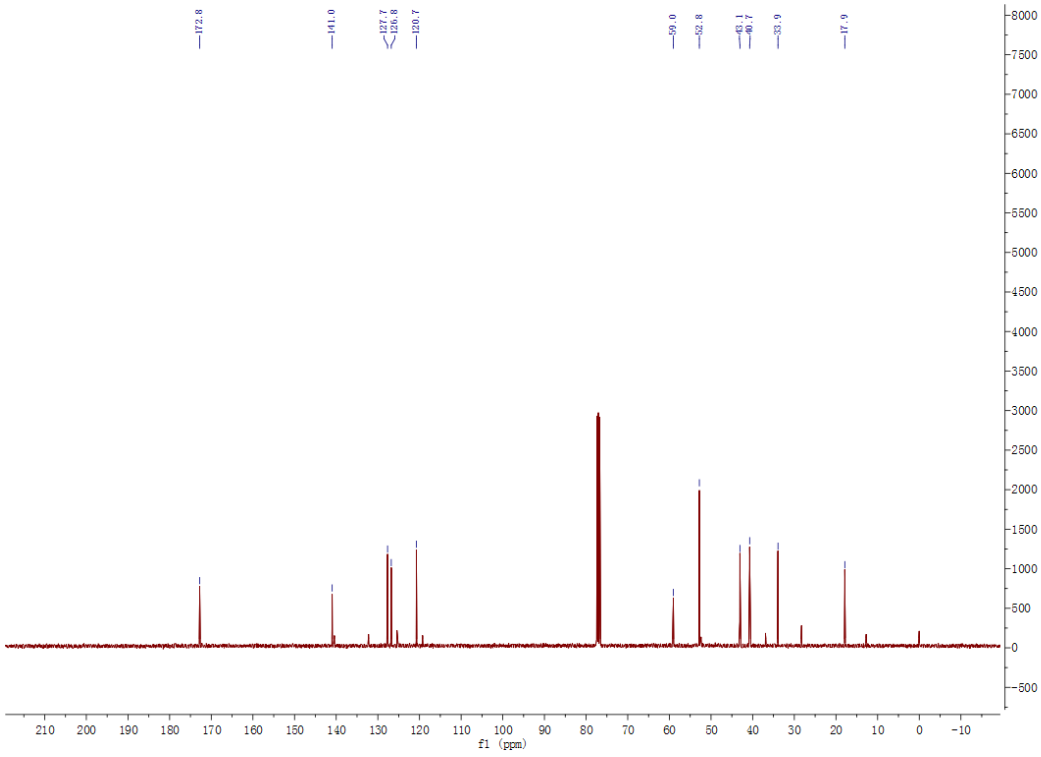
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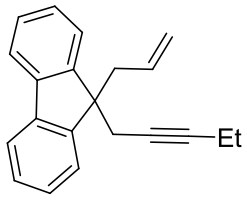
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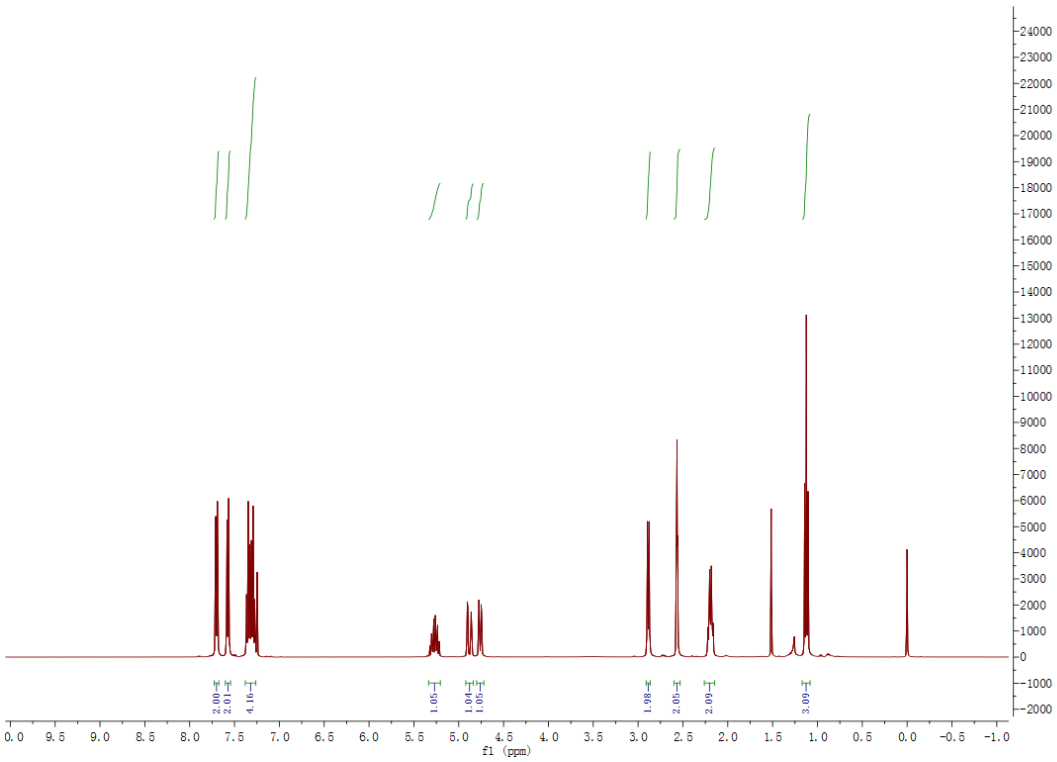
1'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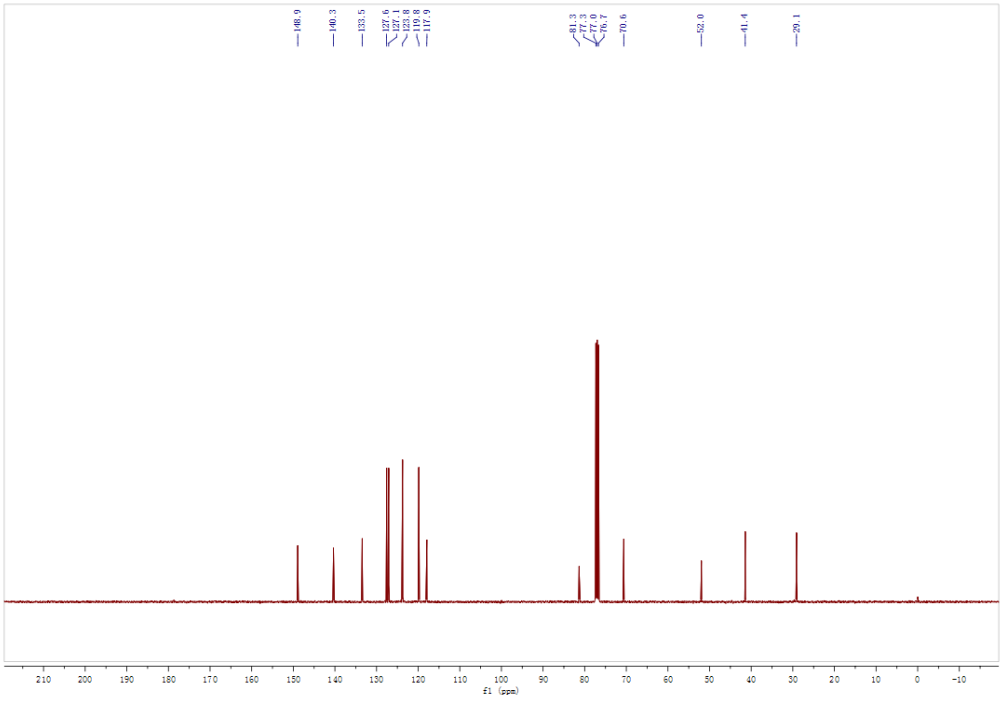
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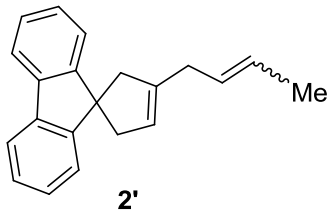
f1 (ppm)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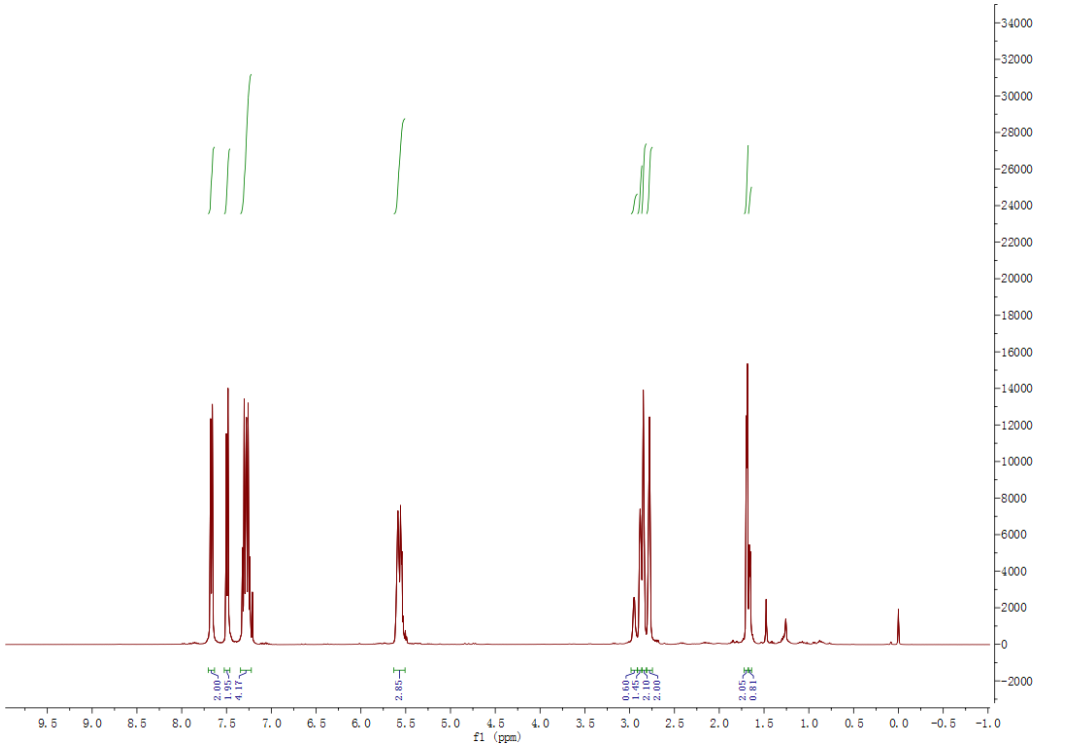
2'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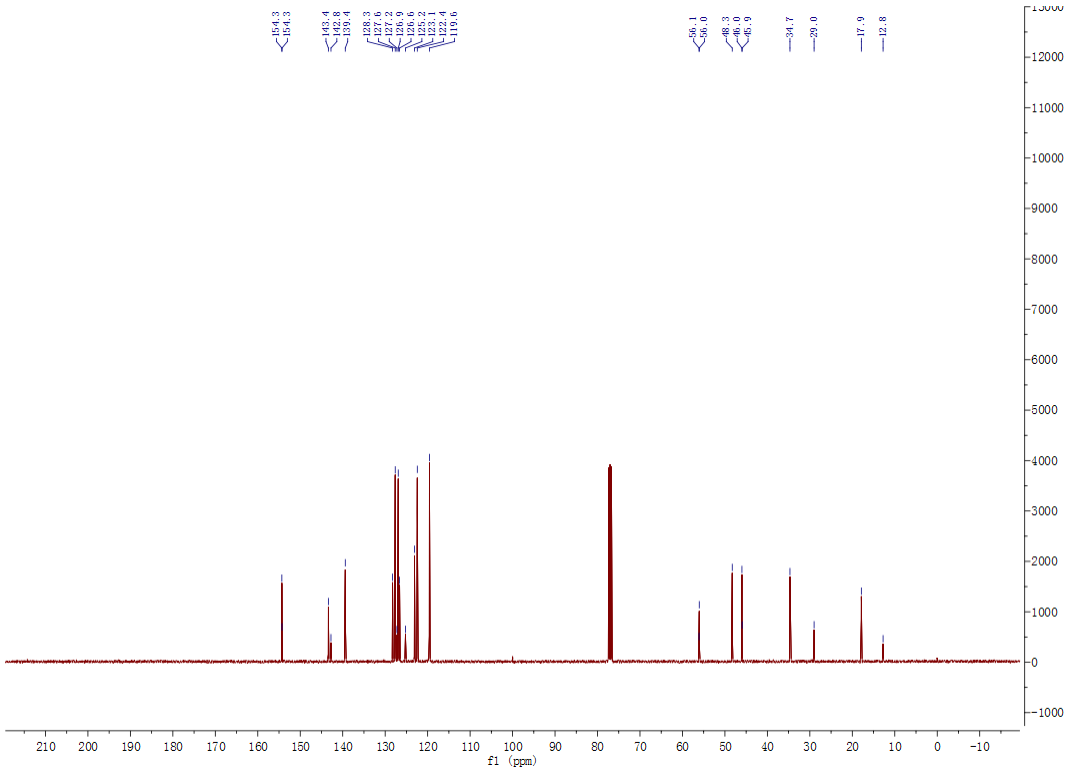
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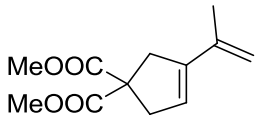
12.8
f1 (ppm)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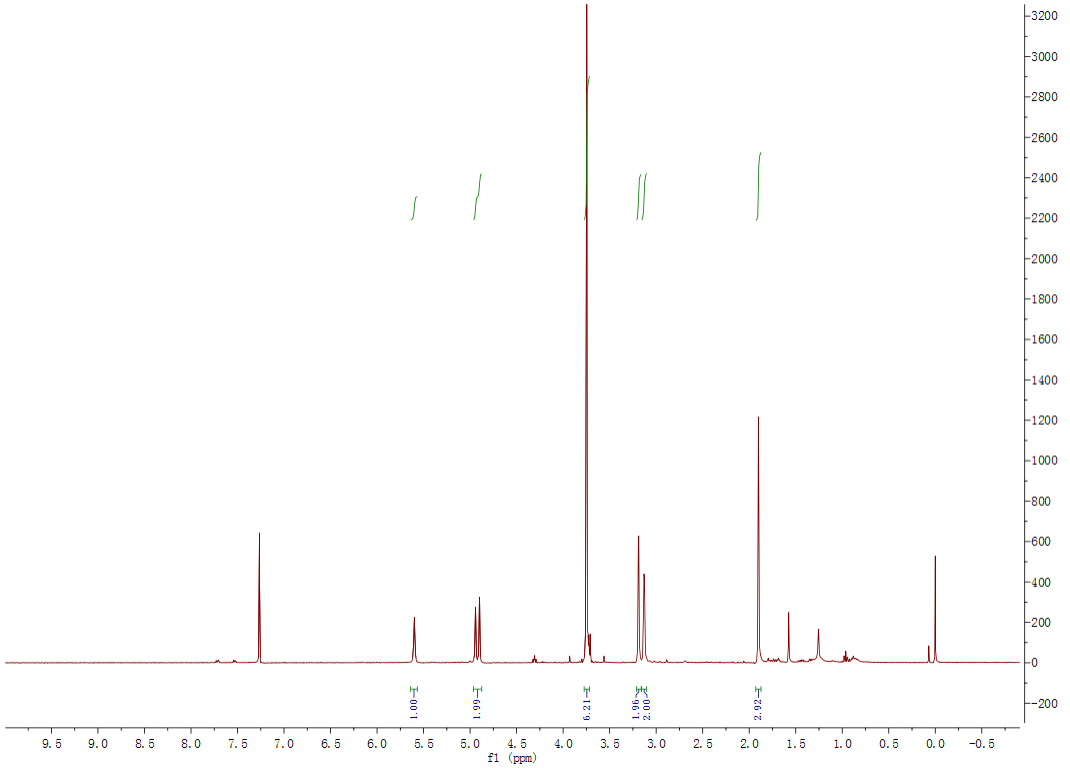
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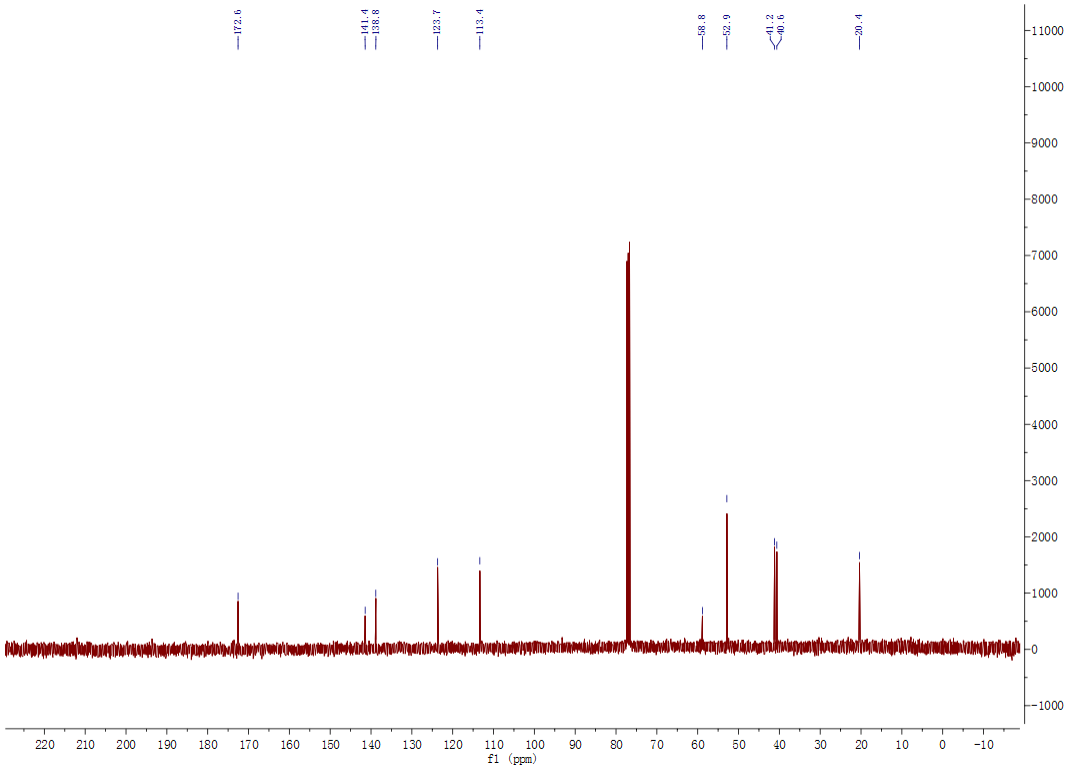
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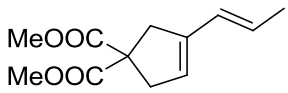
f1 (ppm)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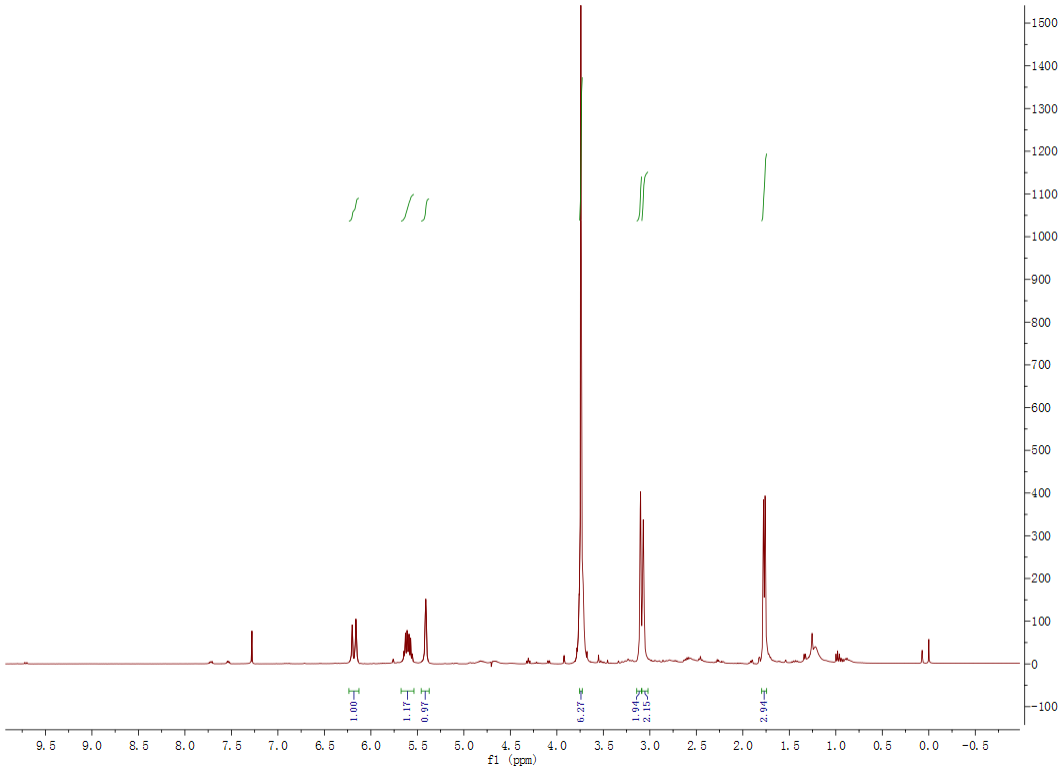
MeOOC

21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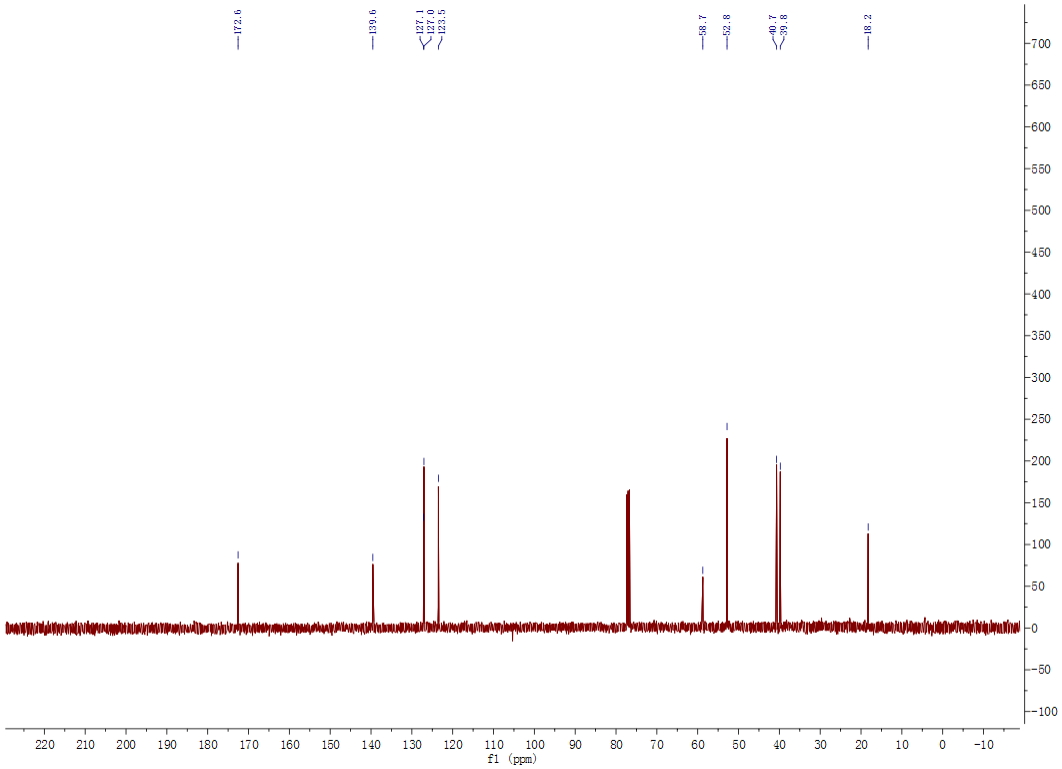
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139.6
127.1
127.0
123.5
58.7
52.8
40.7
39.8
18.2
f1 (ppm)

2. Calculation Details and Results

2.1. Computational Methods

All calculations were performed with the Gaussian 03 program.[1]All gas phase stationary points were optimized using B3LYP[2] functional with the LANL2DZ[3] basis set and pseudo potential for In and 6-31G(d)[4] for all other atoms. Key word "5D" was used in all calculations. Full Hessian matrixes in Gaussian 03 were calculated to verify the nature of all stationary points as minima or first-order saddle points. The first-order saddle points were further characterized by intrinsic reaction coordinate (IRC)[5] calculations to confirm that the stationary points are correctly connected to the corresponding reactants and products. Solvation corrections to free energies were performed using UAHF radii and a CPCM[6] dielectric continuum solvent model in 1,2-dicloroethane was used. Solvation calculations were carried out on the gas-phase optimized structures. All of the energies discussed in the paper and the Supporting Information are Gibbs free energies in the gas phase (ΔG_{gas}). Gibbs energies in solution (ΔG_{sol}) and the gas phase enthalpies (ΔH_{gas}) are also provided for reference.

2.2. Discussions of considering either $InCl_3$ or $(InCl_3)_2$ as the possible catalytic species of the enyne cycloisomerization

We found that, if $InCl_3$ monomer or $(InCl_3)_2$ dimer was proposed as the catalytic species, the cycloisomerization of enyne gave the wrong reaction products (conjugated diene), as suggested by B3LYP calculations (Figure S1 and S2). To check whether this discrepancy between experiments and calculations was caused by computational methods, we computed the single point energies of the competing transition states using MP2 method, and MPW1K[7], M06[8] (Gaussian 09 program), M06-2X[8] (Gaussian 09 program) functionals (Table S1). All these calculations indicated that generations of conjugated-dienes are favored. This further supported $InCl_3$ monomer and $(InCl_3)_2$ dimer are not the real catalytic species.

a. $InCl_3$ monomer catalyzed reaction of 4

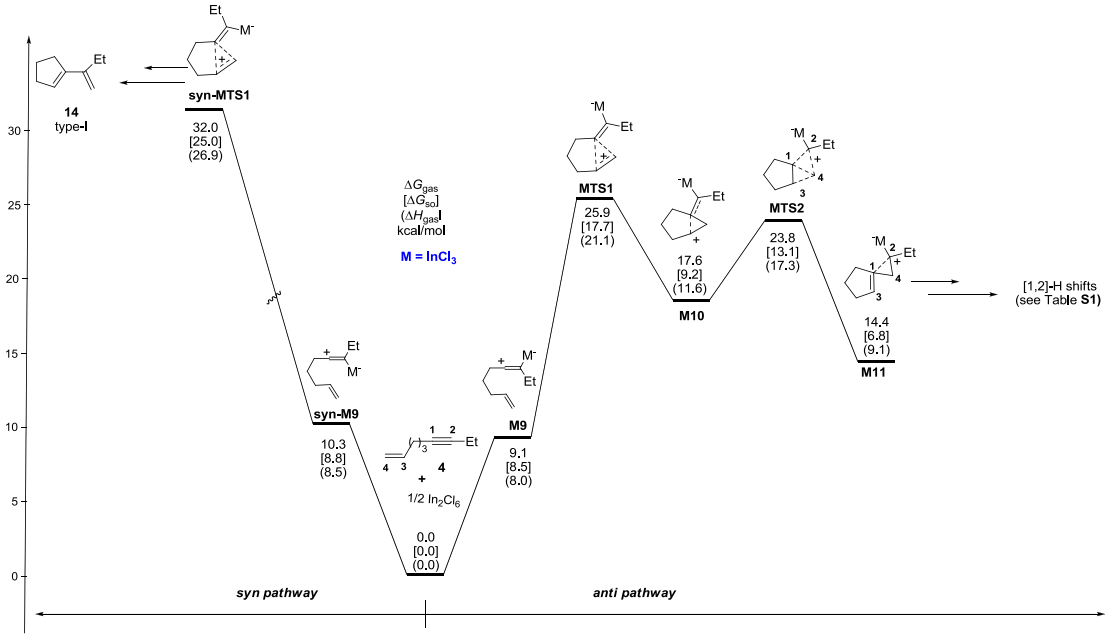
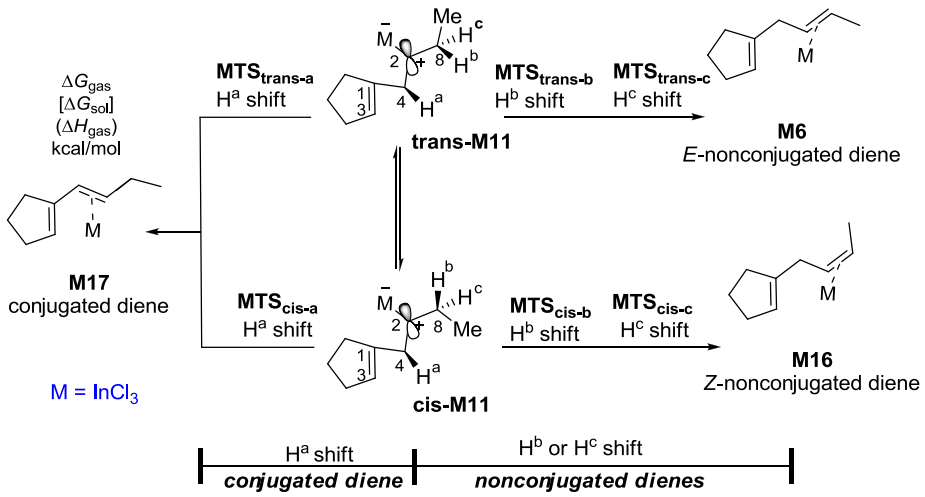
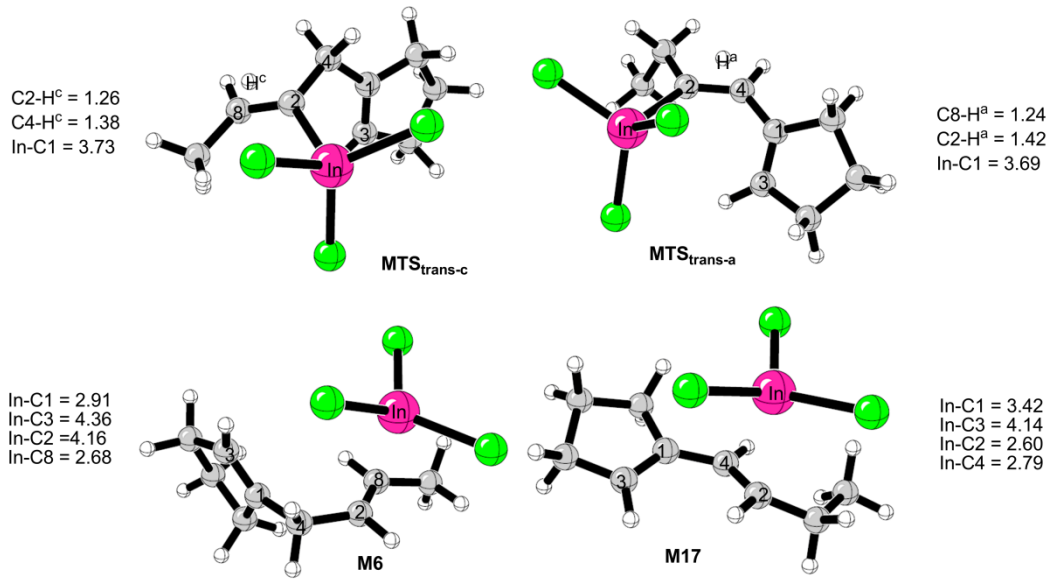


Figure S1. $InCl_3$ monomer catalyzed reaction of **4** (nonclassical cyclopropanation and homoallylic cation rearrangement).

Table S1. Computed energies of the [1,2]-H shifts taking $InCl_3$ as the possible catalytic specie and selected computed structures (distances in Å).





a) B3LYP results

	$\triangle H^a$	$\triangle G^a$	$\triangle G_{sol}{}^a$
MTS_{cis-a}	17.7	22.7	15.9
$MTS_{trans-a}$	17.1	21.6	14.8
MTS_{cis-b}	21.1	25.0	19.1
$MTS_{trans-b}$	19.2	23.6	16.3
MTS_{cis-c}	19.7	23.7	17.3
$MTS_{trans-c}$	20.7	25.0	18.6
M6	-18.8	-14.3	-17.1
M16	-18.4	-15.0	-18.8
M17	-21.3	-17.2	-20.2

[a] The energies reported are relative to the sum of the energies of **4** and 1/2**$(InCl_3)_2$** (Figure S1).

b) Single point energy calculations with various computational methods

	$\triangle E_{B3LYP}{}^a$	$\triangle E_{MP2}{}^b$	$\triangle E_{M06}{}^b$	$\triangle E_{M06\text{-}2X}{}^b$	$\triangle E_{MPW1K}{}^b$	$\triangle E_{M06(sol)}{}^b$
MTS_{cis-a}	0.0	0.0	0.0	0.0	0.0	0.0
MTS_{cis-b}	2.8	2.8	3.7	3.1	3.1	4.2
MTS_{cis-c}	1.6	1.0	1.5	1.0	1.6	1.0
$MTS_{trans-a}$	**-0.6**	**-1.7**	**-1.1**	**-0.9**	**-0.7**	**-0.8**
$MTS_{trans-b}$	**1.1**	**0.6**	**0.4**	**0.2**	**1.0**	**0.0**
$MTS_{trans-c}$	2.5	2.2	2.2	1.7	2.5	3.0

[a] LANL2DZ for In, and 6-31+G(d,p)for all other atoms.

[b] LANL2DZ for In, and 6-31G(d) for all other atoms.

b. $(InCl_3)_2$ dimer catalyzed reaction of 4

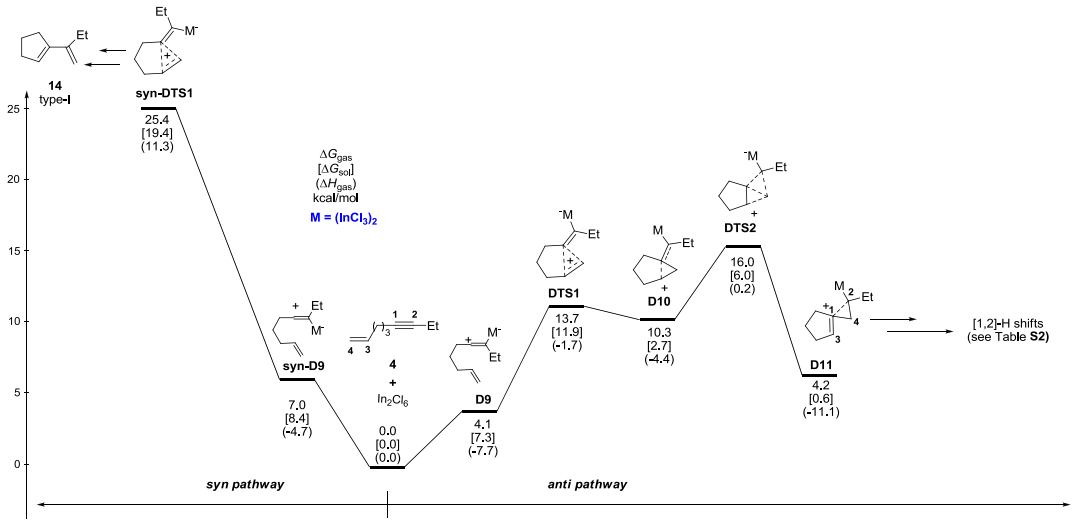
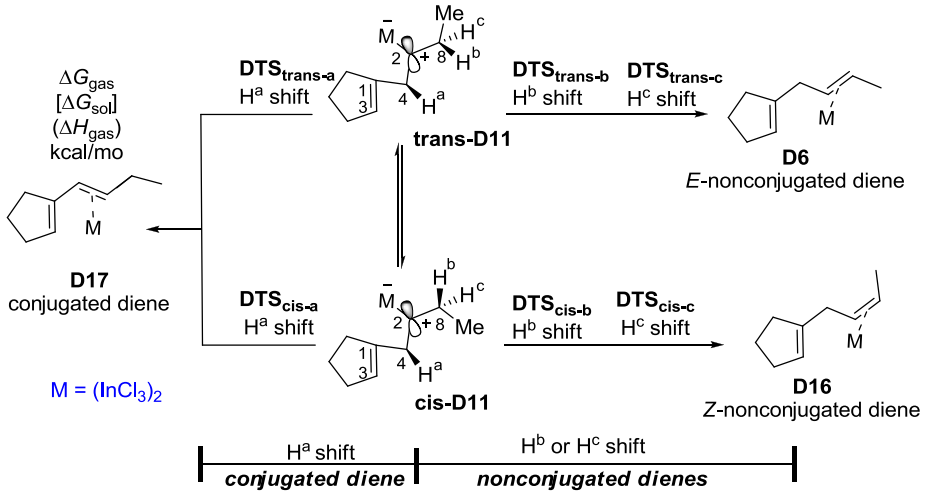
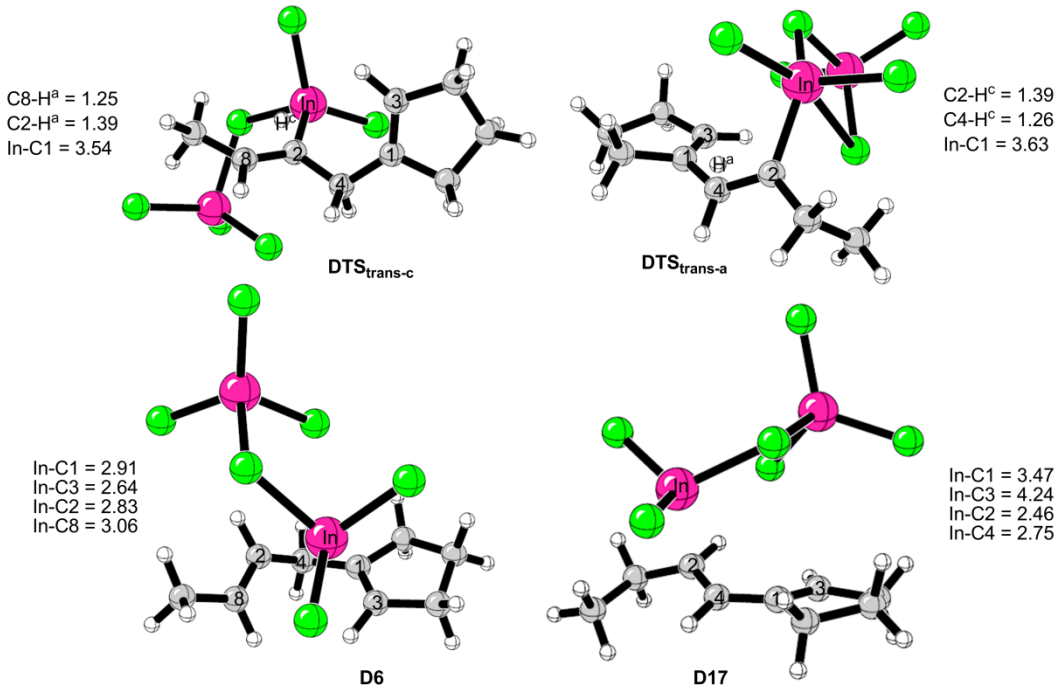


Figure S2. $(InCl_3)_2$ dimer catalyzed reaction of **4** (nonclassical cyclopropanation and homoallylic cation rearrangement).

Table S2. Computed energies of the [1,2]-H shifts taking $(InCl_3)_2$ as the possible catalytic specie and selected computed structures (distances in Å).





a) B3LYP results

	$\triangle H^a$	$\triangle G^a$	$\triangle G_{sol}{}^a$
DTS$_{cis-a}$	-4.9	10.6	9.4
DTS$_{trans-a}$	-4.8	10.5	9.8
DTS$_{cis-b}$	-2.2	12.0	10.8
DTS$_{trans-b}$	-4.6	10.2	8.1
DTS$_{cis-c}$	-3.8	10.5	10.2
DTS$_{trans-c}$	-2.1	13.8	11.4
D6	-33.9	-30.0	-34.2
D16	-33.0	-30.2	-30.5
D17	-39.6	-36.7	-36.1

[a] The energies reported are relative to the sum of the energies of **4** and 1/2**(InCl$_3$)$_2$** (Figure S2).

b) Single point energy calculations with various computational methods

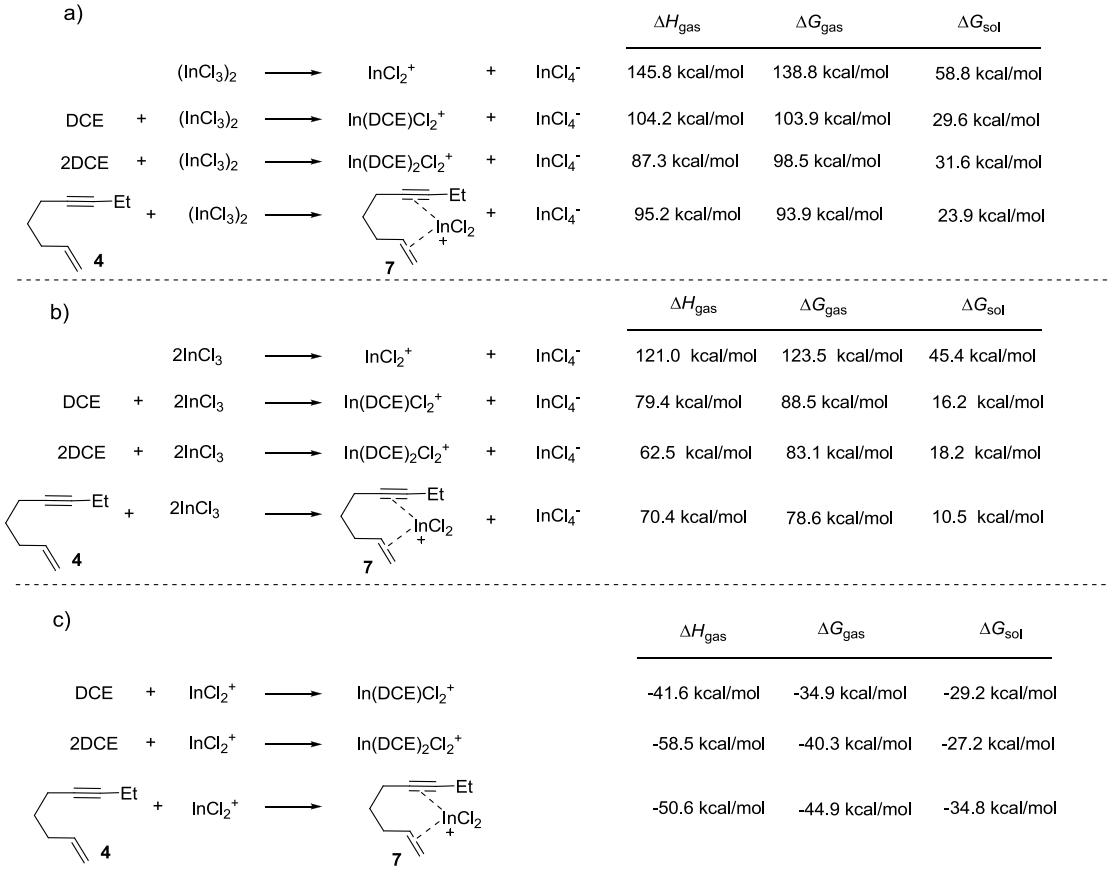
	$\triangle E_{B3LYP}{}^a$	$\Delta E_{MP2}{}^b$	$\Delta E_{M06}{}^b$	$\Delta E_{M06\text{-}2X}{}^b$	$\Delta E_{MPW1K}{}^b$	$\Delta E_{M06(sol)}{}^b$
DTS$_{cis-a}$	0.0	0.0	**0.0**	**0.0**	**0.0**	**0.0**
DTS$_{trans-a}$	**-0.5**	**-1.0**	0.8	2.0	1.0	1.5
DTS$_{cis-b}$	2.0	2.0	3.3	2.9	2.7	2.4
DTS$_{trans-b}$	2.3	2.7	2.6	1.9	2.9	**1.2**
DTS$_{cis-c}$	0.3	0.9	2.2	1.4	0.8	3.1
DTS$_{trans-c}$	0.0	**0.6**	**0.9**	**0.3**	**0.1**	**1.2**

[a] LANL2DZ for In, and 6-31+G(d,p) for all other atoms.

[b] LANL2DZ for In, and 6-31G(d) for all other atoms.

2.3. Additional discussion of generation of $InCl_2^+$

Table S3.



The above results show that generation of $InCl_2^+$ is very reasonable. Similar phenomenon has been found by the generation of $AlMe_2^+$ catalyst from $AlMe_2Cl$, which was used as the catalyst for the Diels-Alder reaction.[9]

2.4. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ without any solvent coordinated to $InCl_2^+$.

In(III) prefers to be tetracoordinated. Therefore, DCE can stabilize the cyclopropanation and homoallylic cation rearrangement processes (from **9** to **11** in text) through a chlorine atom coordination to the In center. Without the solvent stabilization, the Gibbs energies of **TS1′**, **10′** and **TS2′** are 15.5, 4.6 and 11.9 kcal/mol, respectively, see details in Figure S3.

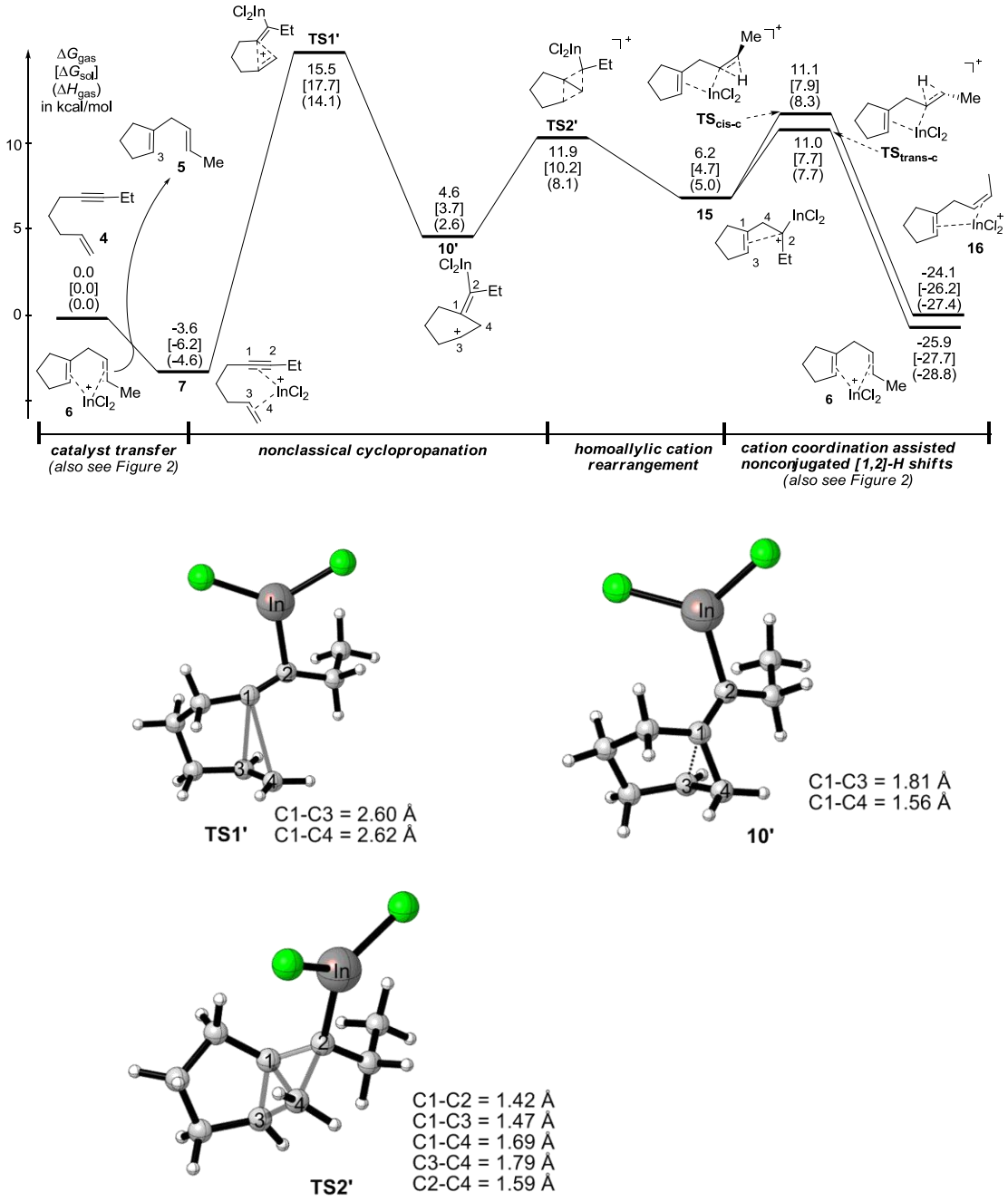


Figure S3. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ without any solvent coordinated to $InCl_2^+$ and selected computed structures (distances in Å).

2.5. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in toluene solution.

Toluene was also used as the reaction solvent in Chatani's experiments. Therefore, we calculated the catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in toluene solution. Similar energy surface for the cycloisomerization of **4**, which is shown below, was obtained and the DFT calculations showed that nonconjugated dienes are preferred, similar to that from the reactions in DCE solution. This is consistent with Chatani's experimental results.

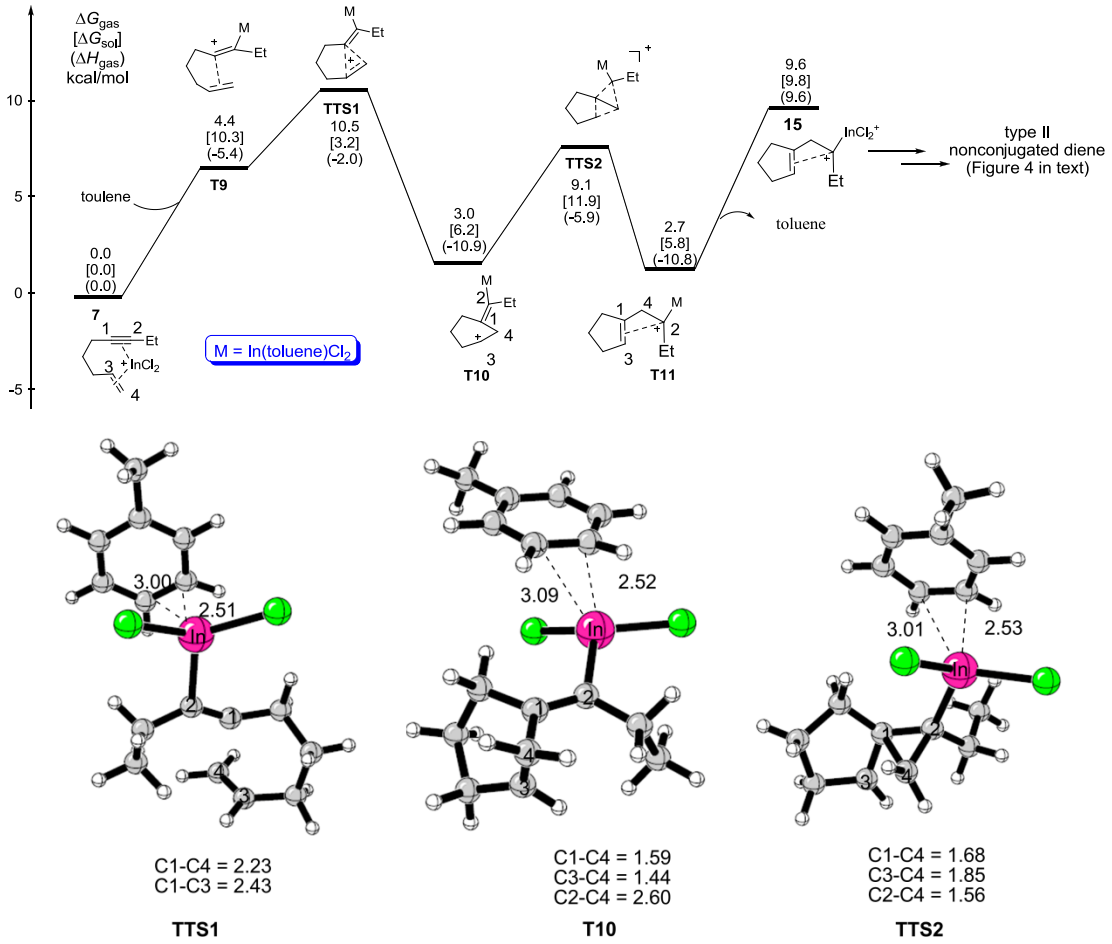


Figure S4. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in toluene solution and selected computed structures (distances in Å). (Solvation corrections to free energies were performed using UAHF radii and a CPCM dielectric continuum solvent model in toluene)

2.6. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in CH_3CN solution.

CH_3CN was also used as the reaction solvent in our reactions (Schemew 3 and 4). Therefore, we calculated the possible catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in CH_3CN solution. The energy surface for the cycloisomerization of **4** is similar to that from the reaction in DCE solution. In particular, due to the strong coordination ability of CH_3CN, all species in this energy surface have the CH_3CN as a coordination ligand (without this coordination, the active free energy of cycloisomerization is 15.4 kcal/mol, about 5 kcal/mol higher than that in Figure S5). Calculations support that a catalytic cycle is possible. However, due to the low solubility of the product-$InCl_2^+$ in CH_3CN solution, the reaction can only be stoichiometric.

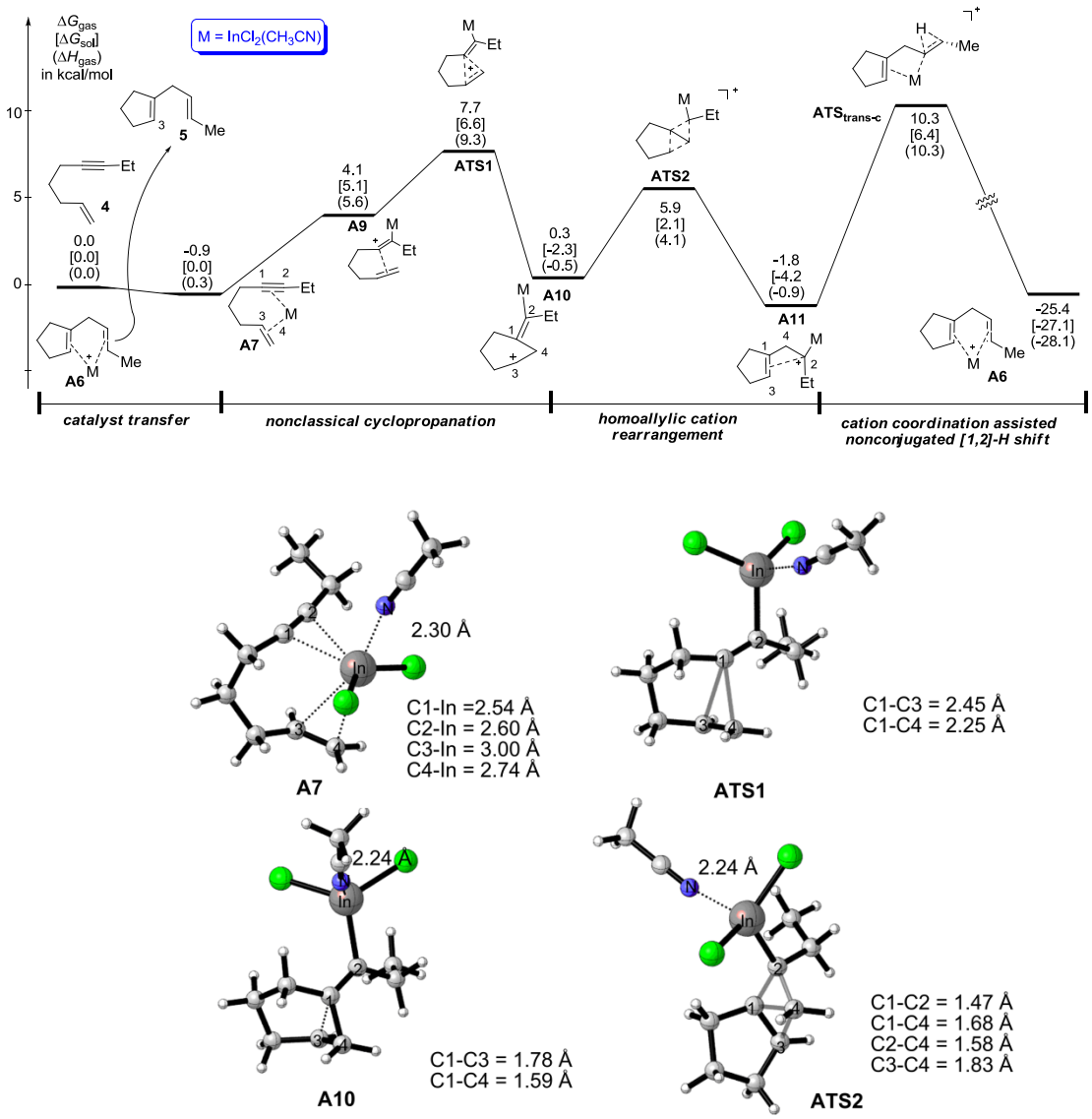
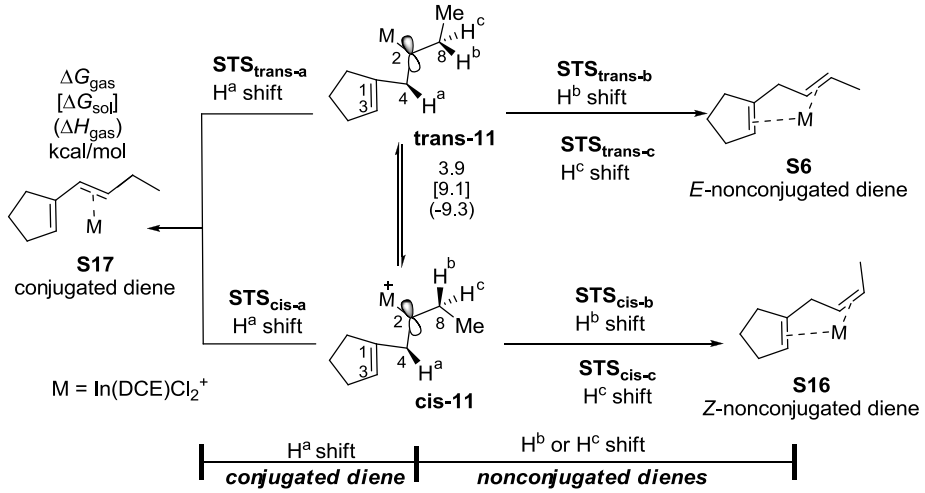


Figure S5. Catalytic cycle of enyne cycloisomerization by $InCl_2^+$ in CH_3CN solution and selected computed structures (distances in Å). (Solvation corrections to free energies were performed using UAHF radii and a CPCM dielectric continuum solvent model in CH_3CN)

2.7. Additional discussion of the [1,2]-H shift processes catalyzed by $InCl_2^+$

In Table S4, we give the results of [1,2]-H shift processes using **11** (in Figure 2) as the precursor, which has a DCE coordinated to the In center. These pathways are disfavored than the pathway without DCE solvent shown in Figure 2. Furthermore, we calculated the singe-point energies of all the transition states catalyzed by $InCl_2^+$, showing that the nonconjugated [1,2]-H-shifts are favored than the conjugated [1,2]-H-shifts. This indicates that, with DCE coordination to In metal, the nonconjugated [1,2]-H shifts are also favored. This selectivity is still attributed to the coordination of the cationic In species to the C1=C3 bond, that is, the cation-coordination assisted nonconjugated [1,2]-H shifts are preferred.

Table S4. Computational results of the [1,2]-H shift processes taking **11** as the precursor.



	$\triangle H^a$	$\triangle G^a$	$\triangle G_{sol}{}^a$
STS$_{cis-a}$	-5.2	6.4	13.6
STS$_{trans-a}$	-5.7	6.2	13.1
STS$_{cis-b}$	-4.3	7.4	13.9
STS$_{trans-b}$	-4.3	8.0	13.3
STS$_{cis-c}$	-4.7	7.3	13.5
STS$_{trans-c}$	-3.9	8.5	13.7

[a] The energies reported are relative to that of **15** (Figure 2).

Here in Table S5 we list the energies of the competing [1,2]-H shifts computed by other calculations methods, showing that the same trend as that obtained by B3LYP is hold.

We also optimized stationary points of H-shift transition states and **7** using M06 functional (Table S5, last column). Similar energy barriers were found compared with the B3LYP results. In this case, the nonconjugated TSs are still lower in energy than the conjugated TSs.

Table S5. Computed relative energies of the [1,2]-H shift transition states catalyzed by $InCl_2^+$ (transition states in Figure 5)

	$\triangle E_{B3LYP}{}^a$	$\Delta E_{MP2}{}^b$	$\Delta E_{M06}{}^b$	$\Delta E_{M06\text{-}2X}{}^b$	$\Delta E_{MPW1K}{}^b$	$\Delta E_{M06(sol)}{}^b$	$\Delta G_{M06(gas)}{}^c$
TS$_{cis-a}$	0.0	0.0	0.0	0.0	0.0	0.0	15.3
TS$_{trans-a}$	**-0.6**	**-1.6**	**-1.2**	**-1.4**	**-1.2**	**-1.2**	**15.2**
TS$_{cis-b}$	-3.0	-5.6	-4.8	-5.7	-5.4	-4.6	11.4
TS$_{trans-b}$	-2.9	-5.7	-5.3	-5.4	-5.2	-4.5	11.8
TS$_{cis-c}$	-3.4	-5.9	-5.3	-6.0	-5.8	-5.4	**10.4**
TS$_{trans-c}$	**-3.8**	**-6.5**	**-6.2**	**-6.9**	**-6.5**	**-5.9**	**10.9**

[a] LANL2DZ for In, and 6-31+G(d,p) for all other atoms.

[b] LANL2DZ for In, and 6-31G(d) for all other atoms.

[c] Stationary points were optimized using M06 functional (LANL2DZ for In, and 6-31G(d) for all other atoms). The energies are relative to that of **7**.

2.8. The energy surface for cycloisomerization of Me-7 to give both type-I and type-II products.

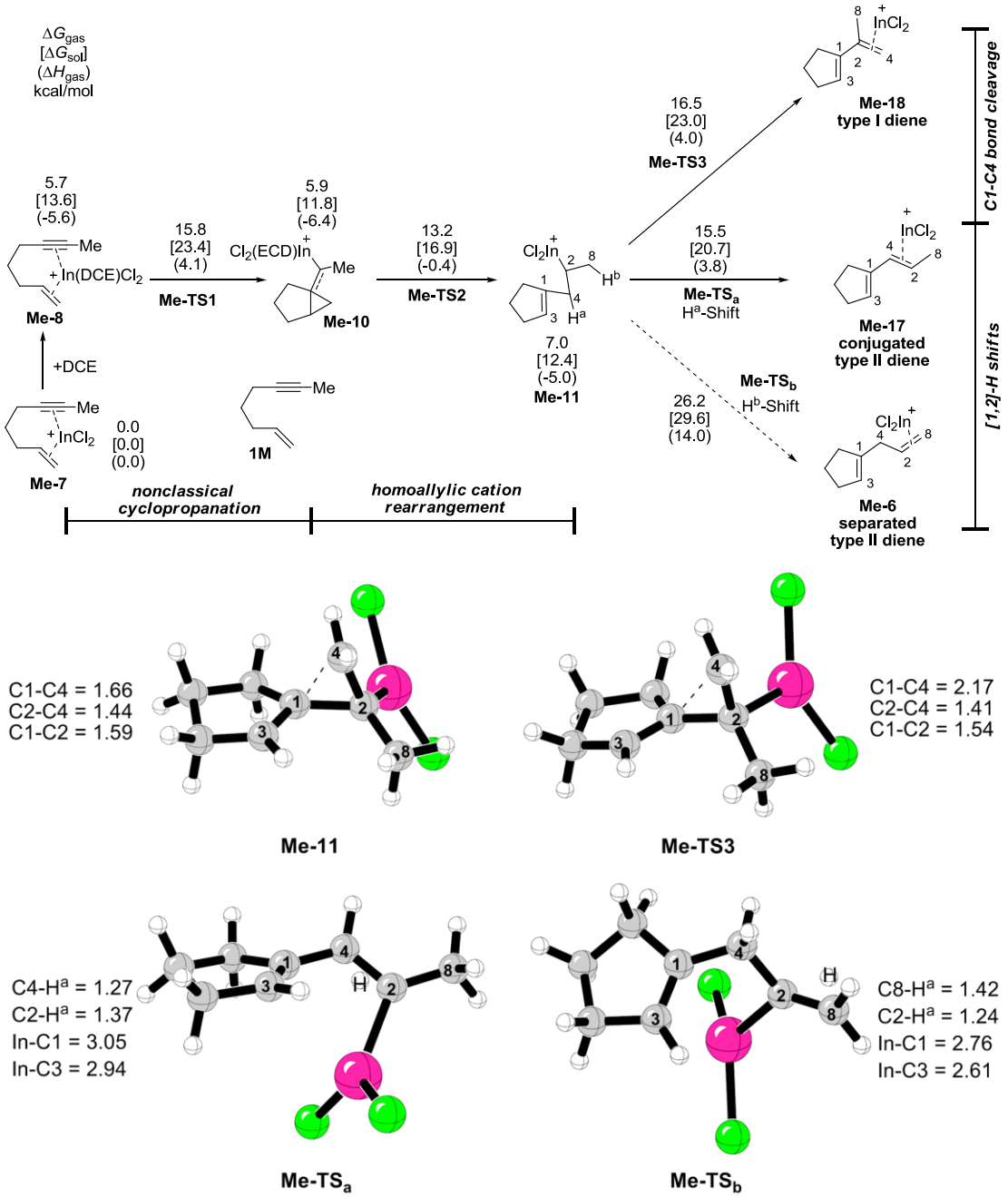


Figure S6. The energy surface for Me-enyne isomerization to give both type-I and type-II products, and the selected computed structures (distances in Å).

The cycloisomerization starts from $InCl_2$ cation coordinated complex **Me-7**, which has the In coordinated to both the double and triple bond of enyne **1M**, similar to the reaction of **4**. Coordinating solvent can assist the release of double bond from the catalyst and lower the activation energy of cyclopropanation. The anti cyclopropanation from **Me-8** to form intermediate **Me-10** has an activation free

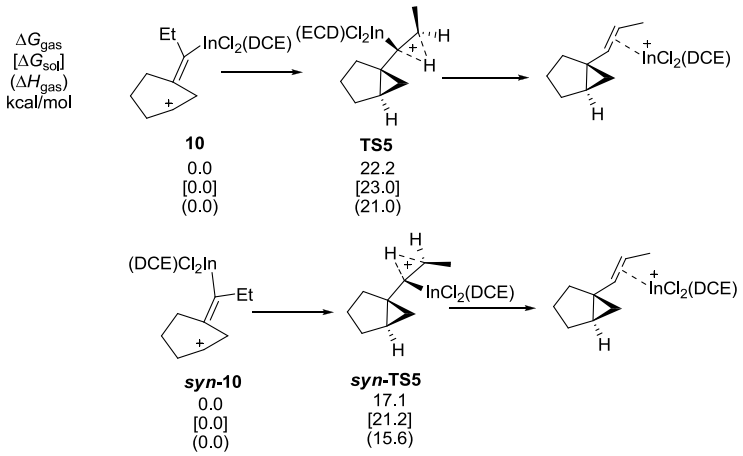
energy of 15.8 kcal/mol. The followed rearrangement via **Me-TS2** is facile with an activation free energy of 7.3 kcal/mol, giving **Me-11**.

The subsequent reaction of **Me-11** has three plausible mechanistic pathways: the first one is the C1-C4 bond cleavage and C1-C2 bond formation to form type-I diene product (via **Me-TS3**), the second is [1,2]-hydrogen shift from internal carbon C4 to from conjugated type-II diene (via **Me-TSa**), and the last is the [1,2]-hydrogen shift from terminal carbon C8 to form separated type II diene (via **Me-TS$_b$**). We located all the plausible transition states in these three pathways, finding that that [1,2]-H shift from C4 requires an activation free energy of 15.5 kcal/mol, much lower than [1,2]-H shift from C8-H (26.2 kcal/mol). Calculations found that the C1-C4 bond cleavage transition state **Me-TS3** is 1.0 kcal/mol higher in free energy than [1,2]-H shift transition state **Me-TS$_a$**, suggesting that type-I and type-II will be generated together. This is well consistent with the experimental observation (the ratio of conjugated type II and type I products of **20** and **21** is 1:1.1, see Scheme 7).

2.9. Two disfavored [1,2]-H shift processes from 10 and *syn*-10

10 and ***syn*-10** could undergo [1,2]-H-shift processes, giving vinylcyclopropane products (Scheme S1). However, these transformations are disfavored compared to the processes shown in Figures 2 and 6, respectively.

Scheme S1. Two disfavored [1,2]-H shift processes from **10** and ***syn*-10**.



2.10. Computed Energies of All Stationary Points

Thermal enthalpy corrections (*H*, in Hartree)
Thermal free energy corrections (*G*, in Hartree)
Thermal correction to Gibbs free energy (*TCGFE*, in Hartree)
Total free energy in solution (E_{sol}, in hartree),
Thermal corrected Gibbs free energy in dichloroethane solution (G_{sol}, which equals to E_{sol} + TCGFE, in Hartree). For the stationary points in Figures S4 and S5, free energies in toluene and CH_3CN were used, respectively.
Single point energies were calculated by MP2, and MPW1K, M06 (Gaussian 09 program), M06-2X (Gaussian 09 program) functionals with LANL2DZ basis set and pseudo potential for metal In, and 6-31G(d) for all other atoms (E_{MP2}, E_{M06}, $E_{M06\text{-}2x}$, E_{MPW1K} in Hartree).

	H	*G*	G_{sol}	*TCGFE*	$E_{sol(B3LYP)}$
4	-351.086525	-351.137344	-351.136808	0.166568	-351.303376
5	-351.131279	-351.177873	-351.179961	0.171450	-351.351411
6	-1273.272772	-1273.333871	-1273.389937	0.166230	-1273.556167
7	-1273.234223	-1273.298296	-1273.355564	0.162730	-1273.518294
8	-2272.188817	-2272.269548	-2272.313237	0.212411	-2272.525648
9	-2272.176889	-2272.260330	-2272.300898	0.209024	-2272.509922
TS1	-2272.172235	-2272.252992	-2272.296711	0.211084	-2272.507795
10	-2272.189314	-2272.268436	-2272.313573	0.214718	-2272.528291
TS2	-2272.181089	-2272.257696	-2272.305899	0.215878	-2272.521777
11	-2272.188008	-2272.267479	-2272.313975	0.213301	-2272.527276
15	-1273.218897	-1273.282651	-1273.338292	0.162651	-1273.500943
16	-1273.270526	-1273.330985	-1273.387591	0.167211	-1273.554802
17	-1273.254182	-1273.318805	-1273.370367	0.162851	-1273.533218
$TS_{trans\text{-}a}$	-1273.208486	-1273.270188	-1273.326469	0.161251	-1273.487720
$TS_{trans\text{-}b}$	-1273.212834	-1273.274292	-1273.332571	0.161269	-1273.493840
$TS_{trans\text{-}c}$	-1273.214580	-1273.275059	-1273.333416	0.161971	-1273.495387
$TS_{cis\text{-}a}$	-1273.207324	-1273.269611	-1273.325860	0.160367	-1273.486227
$TS_{cis\text{-}c}$	-1273.213673	-1273.274895	-1273.333107	0.161302	-1273.494409
$TS_{cis\text{-}b}$	-1273.213012	-1273.274480	-1273.331717	0.161205	-1273.492922
syn-TS1	-2272.158692	-2272.239047	-2272.284356	0.210711	-2272.495067
syn-10	-2272.187420	-2272.262991	-2272.312642	0.217748	-2272.530390
syn-TS2	-2272.205684	-2272.183956	-2272.260038	0.216891	-2272.527215
18	-2272.189002	-2272.167196	-2272.243459	0.216450	-2272.308729
$TS_{rotation}$	-2272.177963	-2272.156816	-2272.233456	0.214370	-2272.276105
TS3	-1273.202371	-1273.264115	-1273.318403	0.163256	-1273.48166
TS4	-2272.177986	-2272.155939	-2272.233035	0.212436	-2272.48946
cyclobutene	-351.11472	-351.104821	-351.148783	0.17456	-351.325788
TS5	-351.062666	-351.107061	-351.108858	0.17147	-351.280332
***Syn*-TS5**	-2272.159017	-2272.235844	-2272.280442	0.212319	-2272.49276
TS1′	-1273.204448	-1273.267793	-1273.317543	0.161917	-1273.47946
10′	-1273.222699	-1273.28513	-1273.339911	0.165001	-1273.50491

TS2′	-1273.213936	-1273.273517	-1273.329564	0.166856	-1273.49642
^{M06}**7**	-1272.875858	-1272.938579			
^{M06}**TS$_{trans-a}$**	-1272.853782	-1272.914311			
^{M06}**TS$_{trans-b}$**	-1272.860056	-1272.919712			
^{M06}**TS$_{trans-c}$**	-1272.861801	-1272.921121			
^{M06}**TS$_{cis-a}$**	-1272.852259	-1272.914159			
^{M06}**TS$_{cis-c}$**	-1272.859446	-1272.920429			
^{M06}**TS$_{cis-b}$**	-1272.86058	-1272.92198			
^{M06} Stationary points were optimized at M06/6-31G(d) level					
STS$_{trans-a}$	-2272.174392	-2272.253986	-2272.300002	0.209948	-2272.509950
STS$_{trans-b}$	-2272.172080	-2272.251106	-2272.299681	0.209920	-2272.509601
STS$_{trans-c}$	-2272.171527	-2272.250372	-2272.299183	0.209877	-2272.509060
STS$_{cis-a}$	-2272.173512	-2272.253605	-2272.299358	0.208971	-2272.508329
STS$_{cis-c}$	-2272.172721	-2272.252251	-2272.299511	0.209280	-2272.508791
STS$_{cis-b}$	-2272.172067	-2272.252098	-2272.298830	0.208870	-2272.507700
Me-4	-311.803659	-311.852040	-311.850730	0.138780	-311.989510
Me-6	-1233.976978	-1234.034210	-1234.093148	0.140532	-1234.233680
Me-7	-1233.949500	-1234.010080	-1234.065984	0.135860	-1234.201844
Me-TS1	-1233.919630	-1233.980485	-1234.031743	0.134164	-1234.165907
Me-10	-1233.937484	-1233.995813	-1234.052311	0.139207	-1234.191518
Me-TS2	-1233.929262	-1233.985433	-1234.044063	0.140225	-1234.184288
Me-11	-1233.935320	-1233.994045	-1234.054295	0.137697	-1234.191992
Me-TS3	-1233.918760	-1233.978086	-1234.034045	0.135696	-1234.169741
Me-18	-1233.980625	-1234.042102	-1234.097602	0.135537	-1234.233139
Me-TS$_a$	-1233.922199	-1233.981110	-1234.040331	0.133720	-1234.174051
Me-TS$_b$	-1233.913165	-1233.970666	-1234.033590	0.135361	-1234.168951
Me-17	-1233.969071	-1234.030085	-1234.084832	0.136340	-1234.221172
7 ^{a}	-1273.234223	-1273.298296	-1273.331134	0.162730	-1273.493864
T9 ^{a}	-1544.668380	-1544.754517	-1544.775852	0.277974	-1545.053826
TTS1 ^{a}	-1544.662969	-1544.744873	-1544.787058	0.281611	-1545.068669
T10 ^{a}	-1544.677154	-1544.756867	-1544.782410	0.285950	-1545.068360
TTS2 ^{a}	-1544.669165	-1544.747086	-1544.773224	0.286226	-1545.059450
T11 ^{a}	-1544.676993	-1544.757345	-1544.782950	0.284180	-1545.067130
15 ^{a}	-1273.218897	-1273.282651	-1273.315817	0.162651	-1273.478468
^{a} Solvation corrections to free energies were performed in toluene (Figure S4)					
M9	-1733.716188	-1733.788787	-1733.782086	0.156953	-1733.939039
MTS1	-1733.695186	-1733.761965	-1733.767435	0.161946	-1733.929381
M10	-1733.710385	-1733.775252	-1733.780899	0.165923	-1733.946822
MTS2	-1733.701251	-1733.765343	-1733.774818	0.164899	-1733.939717
M11	-1733.714359	-1733.780271	-1733.784814	0.163842	-1733.948656
MTS$_{cis-a}$	-1733.700621	-1733.767079	-1733.770363	0.159458	-1733.929821
MTS$_{cis-b}$	-1733.695262	-1733.763501	-1733.765192	0.157782	-1733.922974

MTS_{cis-c}	-1733.697547	-1733.765586	-1733.768121	0.157574	-1733.925695
$MTS_{trans-a}$	-1733.701541	-1733.768867	-1733.772057	0.158948	-1733.931005
$MTS_{trans-b}$	-1733.698301	-1733.765695	-1733.769687	0.158231	-1733.927918
$MTS_{trans-c}$	-1733.695905	-1733.763515	-1733.765947	0.158210	-1733.924157
M6	-1733.758858	-1733.826023	-1733.822938	0.163551	-1733.986489
M16	-1733.758858	-1733.826023	-1733.8229	0.16355	-1733.986489
M17	-1733.758115	-1733.827133	-1733.8256	0.16178	-1733.987387
***syn*-M9**	-1733.715329	-1733.786853	-1733.781617	0.158044	-1733.939661
***syn*-MTS1**	*-1733.685936*	*-1733.752330*	-1733.755742	*0.161849*	*-1733.917591*
$(InCl_3)_2$	-2765.245192	-2765.307429	-2765.296314	-0.040021	-2765.256293
***syn*-D9**	-3116.339198	-3116.433618	-3116.419787	0.147255	-3116.567042
***syn*-DTS1**	-3116.313684	-3116.404206	-3116.402171	0.149619	-3116.551790
D9	-3116.343941	-3116.438247	-3116.421536	0.147249	-3116.568785
DTS1	-3116.334462	-3116.422903	-3116.414213	0.152466	-3116.566679
D10	-3116.338743	-3116.428398	-3116.428819	0.153153	-3116.581972
DTS2	-3116.331445	-3116.419231	-3116.423572	0.153509	-3116.577081
D11	-3116.349391	-3116.438087	-3116.432137	0.153117	-3116.585254
DTS_{cis-a}	-3116.339488	-3116.427827	-3116.418099	0.149557	-3116.567656
DTS_{cis-b}	-3116.335253	-3116.425605	-3116.415908	0.147257	-3116.563165
DTS_{cis-c}	-3116.337843	-3116.428020	-3116.416794	0.147761	-3116.564555
$DTS_{trans-a}$	-3116.339396	-3116.428044	-3116.417498	0.149868	-3116.567366
$DTS_{trans-b}$	-3116.339095	-3116.428480	-3116.420185	0.148031	-3116.568216
$DTS_{trans-c}$	-3116.335124	-3116.422758	-3116.414982	0.149801	-3116.564783
D6	-3116.381638	-3116.470361	-3116.464552	0.154218	-3116.61877
D16	-3116.380175	-3116.470543	-3116.458597	0.15248	-3116.611077
D17	-3116.390773	-3116.481045	-3116.467535	0.152762	-3116.620297
CH_3CN [b]	-132.701306	-132.728821	-132.729705	0.022665	-132.752370
4 [b]	-351.086525	-351.137344	-351.130592	0.166568	-351.297160
5 [b]	-351.131279	-351.177873	-351.173806	0.171450	-351.345256
A6 [b]	-1406.019207	-1406.090398	-1406.131681	0.207618	-1406.339299
A7 [b]	-1405.974034	-1406.051323	-1406.088441	0.201897	-1406.290338
A9 [b]	-1405.965574	-1406.043304	-1406.080309	0.199856	-1406.280165
ATS1 [b]	-1405.959611	-1406.037561	-1406.077952	0.200025	-1406.277977
A10 [b]	-1405.97521	-1406.049354	-1406.092072	0.20587	-1406.297942
ATS2 [b]	-1405.967883	-1406.040425	-1406.085184	0.206032	-1406.291216
A11 [b]	-1405.975859	-1406.052726	-1406.095134	0.201966	-1406.2971
$ATS_{trans-c}$ [b]	-1405.95798	-1406.033503	-1406.078249	0.199406	-1406.277655
[b] Solvation corrections to free energies were performed in CH_3CN (Figure S5)					
$InCl_3$	-1382.602849	-1382.641478	-1382.637486	-0.02847	-1382.609016
$InCl_2^+$	-922.030757	-922.058847	-922.125618	-0.020921	-922.104697
$InCl_4^-$	-1842.982081	-1843.027355	-1843.077052	-0.032239	-1843.044813
DCE	-998.946347	-998.981202	-998.982684	0.029629	-999.012313
DCE+$InCl_2$	-1921.043401	-1921.095722	-1921.154775	0.021022	-1921.175797
$InCl_2^+$+2DCE	-2920.016726	-2920.085528	-2920.134305	0.070802	-2920.205107

$(InCl_2+2)^+$	-1728.96	-1729.042746		0.237435	

	$E_{B3LYP/6-31+G**}$	E_{MP2}	E_{M06}	E_{M06-2X}	E_{MPW1K}	$E_{sol(M06)}$
TS_{cis-a}	-1273.462211	-1269.514012	-1273.071801	-1273.183945	-1273.368204	-1273.176204
TS_{cis-b}	-1273.467035	-1269.522907	-1273.079409	-1273.193020	-1273.376808	-1273.183577
TS_{cis-c}	-1273.467688	-1269.523354	-1273.080216	-1273.193465	-1273.377470	-1273.184773
$TS_{trans-a}$	-1273.463153	-1269.516635	-1273.073770	-1273.186115	-1273.370071	-1273.178130
$TS_{trans-b}$	-1273.466882	-1269.523156	-1273.080212	-1273.192570	-1273.376462	-1273.183436
$TS_{trans-c}$	-1273.46827	-1269.524415	-1273.081610	-1273.195019	-1273.378611	-1273.185618
DTS_{cis-a}	-3116.620695	-3109.708624	-3116.101842	-3116.210344	-3116.552045	-3116.137912
DTS_{cis-b}	-3116.617535	-3109.705371	-3116.096521	-3116.205755	-3116.547675	-3116.134155
DTS_{cis-c}	-3116.620158	-3109.707197	-3116.098313	-3116.208079	-3116.550826	-3116.132927
$DTS_{trans-a}$	-3116.621456	-3109.710286	-3116.100522	-3116.207145	-3116.550427	-3116.135490
$DTS_{trans-b}$	-3116.617088	-3109.704282	-3116.097716	-3116.207250	-3116.547501	-3116.135987
$DTS_{trans-c}$	-3116.620763	-3109.707622	-3116.100336	-3116.209908	-3116.551843	-3116.136042
MTS_{cis-a}	-1733.962828	-1729.282360	-1733.539949	-1733.653475	-1733.875756	-1733.579157
MTS_{cis-b}	-1733.958412	-1729.277961	-1733.534080	-1733.648494	-1733.870748	-1733.572517
MTS_{cis-c}	-1733.960308	-1729.280771	-1733.537561	-1733.651825	-1733.873148	-1733.577579
$MTS_{trans-a}$	-1733.963821	-1729.285011	-1733.541661	-1733.654953	-1733.876830	-1733.580423
$MTS_{trans-b}$	-1733.961125	-1729.281412	-1733.539354	-1733.653221	-1733.874182	-1733.579135
$MTS_{trans-c}$	-1733.95882	-1729.278917	-1733.536380	-1733.650753	-1733.871733	-1733.574354

3. References:

(1) Full citation of Gaussian 03: Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A. Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision C.02; Gaussian Inc.: Wallingford CT, 2004.

(2) (a) Becke, A. D. *J. Chem. Phys.***1993**, *98*, 5648. (b) Lee, C.; Yang, W.;Parr, R. G.*Phys. Rev. B***1988**, *37*, 785.

(3) (a) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, *82*, 299.(b) Dunning, T. H., Jr.; Hay, P. J. In *Modern Theoretical Chemistry*; Schaefer, H.F., III. Ed.; Plenum Press: New York, 1977; pp 1-28.
(4) Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. A. *Ab Initio Molecular Orbital Theory*; Wiley: New York, 1986.
(5) (a) Fukui, K. *J. Phys. Chem.* **1970**, *74*, 4161. (b) Gonzalez, C.; Schlegel,H. B. *J. Chem. Phys.* **1989**, *90*, 2154. (c) Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523.
(6) (a) Barone, V.; Cossi, M.*J. Phys. Chem. A* **1998**, *102*, 1995. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669. (c)Takano, Y.; Houk, K. N. *J. Chem. Theory Comput.* **2005**, *1*, 70.
(7) Lynch, B. J.; Fast, P. L.; Harris, M.; Truhlar, D. G. *J. Phys. Chem. A.* **2000**, *104*, 4811.
(8) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.
(9) $AlMe_2Cl$ was found to use $AlMe_2^+$ as the catalyst for Diels-Alder reactions, see: (a) Evans, D. A.; Chapman, K. T.; Bisaha, J. *J. Am. Chem. Soc.* **1988**, *110*, 1238. (b) Tietze, L. F.; Schuffenhauer, A.; Schreiner, P. R. *J. Am. Chem. Soc.* **1998**, *120*, 7952. (c) Lam, Y.-h.; Cheong, P. H.-Y.; Blasco Mata, J. M.; Stanway, S. J.; Gouverneur, V. r.; Houk, K. N. *J. Am. Chem. Soc.* **2009**, *131*, 1947.

4 Coordinates of All Stationary Points

In_2Cl_6:

In	-1.84953300	-0.00009700	-0.00000700
Cl	0.00015600	0.00012300	-1.71859700
Cl	-2.89613200	2.03114300	0.00009500
Cl	-2.89616200	-2.03129200	-0.00019800
Cl	2.89672600	-2.03094400	-0.00014300
In	1.84962900	-0.00001300	0.00001900
Cl	2.89510500	2.03175700	0.00006700
Cl	0.00003200	-0.00047200	1.71874300

$InCl_3$

In	0.00000000	0.00000000	0.00000000
Cl	0.00000000	2.28896900	0.00000000
Cl	1.98230500	-1.14448500	0.00000000
Cl	-1.98230500	-1.14448500	0.00000000

$InCl_2^+$

In	0.00000000	0.00018500	0.00000000
Cl	2.20504100	-0.01647100	0.00000000
Cl	-2.20504100	0.01593800	0.00000000

$InCl_4^-$

In	0.00000000	0.00017500	0.00000000
Cl	1.94006500	1.36889200	-0.00414700
Cl	-0.00378200	-1.37337400	-1.93652400
Cl	0.00116100	-1.36862800	1.93988300
Cl	-1.93744500	1.37260400	0.00078900

$In(butene)_2Cl_2^+$

In	0.01016700	0.00062100	-0.14570100
C	-0.43527300	1.74615300	1.75955700
C	-0.01743500	2.54815900	0.74751000
H	0.25197500	1.43175200	2.54382900
H	-0.72046300	2.95677900	0.02202100
H	-0.83678200	-1.45002800	2.33946100
C	0.09668300	-1.69582100	1.83407700
C	0.11139300	-2.54712900	0.77708100
H	1.04762600	-2.88190100	0.33261600
Cl	-2.06062300	-0.14557000	-1.08099800

Cl	2.14776900	0.11952700	-0.92084900
C	-1.19193158	-3.12507619	0.19491085
H	-1.82598525	-2.32434850	-0.12401096
H	-0.96188270	-3.75238760	-0.64082708
H	-1.69348312	-3.70005302	0.94507597
C	1.40921354	-1.24107797	2.49896223
H	2.02091903	-0.74239203	1.77644668
H	1.18811126	-0.57043130	3.30285702
H	1.93056298	-2.09445293	2.87954852
C	1.45603405	2.97609822	0.61576413
H	1.57396781	3.58515091	-0.25604230
H	1.74427399	3.53389004	1.48218551
H	2.07363390	2.10658792	0.52961148
C	-1.93078871	1.43609032	1.95677235
H	-2.05203233	0.78292992	2.79556998
H	-2.46353082	2.34694432	2.13405979
H	-2.31589463	0.96296365	1.07771343

Butene

C	0.54531000	-0.38566400	0.00008700
H	1.52610400	0.09460800	0.00008700
C	-0.54531000	0.38566400	0.00008700
H	-1.52610400	-0.09460800	0.00008700
C	-0.54531000	1.88838300	-0.00006400
H	0.47391900	2.29008500	-0.00056600
H	-1.06725400	2.28836000	-0.88033300
H	-1.06640900	2.28847400	0.88067000
C	0.54531000	-1.88838300	-0.00006400
H	-0.47391900	-2.29008500	-0.00056600
H	1.06725400	-2.28836000	-0.88033300
H	1.06640900	-2.28847400	0.88067000

4:

C	1.09383600	1.03785400	-0.15245600
C	2.08968600	0.38394100	-0.36913000
C	3.30013900	-0.40698300	-0.60861500
C	3.68554100	-1.30112600	0.58521000
C	-0.11983700	1.81514000	0.11432400
C	-1.29516000	0.96870300	0.65333800
C	-1.78376800	-0.10015800	-0.34051100
C	-2.88806700	-0.95309300	0.22122600
C	-4.11916000	-1.05416700	-0.28246400

H	3.15982500	-1.03182900	-1.50172600
H	4.13552900	0.26772700	-0.84280400
H	4.59465800	-1.86951400	0.35934400
H	3.86913800	-0.69792800	1.48015300
H	2.88398600	-2.01048000	0.81529100
H	0.10700800	2.60988600	0.83846900
H	-0.43722100	2.32682800	-0.80617200
H	-2.12476000	1.64309400	0.90086400
H	-0.98702100	0.48731300	1.59053400
H	-0.92717500	-0.73426200	-0.61132500
H	-2.12321900	0.38451700	-1.26600500
H	-2.63748700	-1.51896500	1.12092800
H	-4.87549600	-1.68773100	0.17348800
H	-4.41702300	-0.50932100	-1.17656500

Cyclobutene

C	1.13702200	0.95582800	−0.44806700
C	0.13239600	−0.16760800	−0.44362300
C	0.76779300	−1.52063800	−0.28693800
C	2.21534500	−1.11664200	0.18767400
C	2.17481300	0.40462600	0.54423700
C	−0.91981000	0.60794300	−0.10500700
C	−0.06828000	1.87906100	−0.04298800
C	−2.36239000	0.38957900	0.22890800
H	0.02621200	2.30239000	0.96611600
H	−0.31063600	2.69467000	−0.73801200
H	1.59103400	1.20785800	−1.41659200
H	1.81000700	0.53517600	1.57172200
H	3.16668300	0.86717500	0.48200600
H	2.55842900	−1.72844300	1.02871900
H	2.92425400	−1.27869700	−0.63316300
H	0.24927500	−2.14635000	0.44785800
H	0.81294300	−2.09476500	−1.22139100
H	−2.55572400	0.75836000	1.24866200
H	−2.97969900	1.02703600	−0.42396100
C	−2.82239400	−1.06819000	0.10860500
H	−3.89280500	−1.16188500	0.32245600
H	−2.64381800	−1.45263800	−0.90196500
H	−2.28312800	−1.71363700	0.81073400

7:

C	-1.76901800	-1.33728900	-1.16503400
C	-1.90215400	0.17293300	-0.97042100
C	-2.90474100	0.45631500	-0.08077200
C	-3.57094700	-0.77525700	0.42812600
C	-3.05872500	-1.90146400	-0.50629600
C	-1.10744300	1.19651300	-1.80413200
C	-0.46187100	1.27564400	-0.50400500
H	-1.67531700	2.06770600	-2.13578800
H	-0.58703600	0.69708800	-2.62135800
H	-3.19029100	1.45506100	0.23509200
H	-3.27831200	-0.93003200	1.47961100
H	-4.66257800	-0.66592500	0.44301600
H	-2.87403600	-2.83482900	0.02836600
H	-3.80459500	-2.10620900	-1.27932000
H	-1.68591300	-1.59811500	-2.22439200
H	-0.87789200	-1.74768500	-0.66515900
In	1.15532900	-0.09429800	0.07141000
Cl	2.97196200	-0.17912300	-1.30272300
Cl	0.88651000	-1.37901300	1.94306300
C	-0.66440900	2.50809900	0.33632600
C	-0.61999700	2.34417300	1.85806600
H	-1.56323600	3.05615100	0.02301800
H	0.17454200	3.15322600	0.01269700
H	-0.65691000	3.32257600	2.34443500
H	-1.46583400	1.75232700	2.22396000
H	0.29810300	1.84955100	2.19981900

8:

C	2.13711900	-1.81133800	1.21785900
C	0.91720500	-2.40581400	1.28687300
C	2.21280200	0.88695400	-0.61127000
C	3.17655800	-0.00499700	-1.29123800
C	3.98035100	-0.93857500	-0.36081800
C	3.19211700	-2.13587700	0.20148600
C	1.60461800	1.83760800	-0.12743200
In	0.00939500	-0.29235000	0.09388300
Cl	-0.05795600	-1.38072400	-1.95745100
Cl	-0.63175300	0.57869900	2.16239000
H	2.76411700	-2.73798400	-0.60868800
H	3.90991600	-2.78831000	0.72334200
H	4.42153700	-0.35592100	0.45643200
H	4.81487100	-1.33474900	-0.94829200
H	2.66232100	-0.58180000	-2.06807500

H	3.87111300	0.66650500	-1.81271500
C	1.06543700	3.09077600	0.42425700
H	2.41080100	-1.10272400	2.00280900
H	0.27410900	-2.25890400	2.15212700
H	0.63209700	-3.17740300	0.57343000
H	0.12504200	3.34490900	-0.07863900
H	0.82838400	2.94574600	1.48352800
C	2.08413500	4.23978600	0.24885900
H	2.30541600	4.41728500	-0.80703400
H	1.65734200	5.15406000	0.67096400
H	3.01870200	4.02169800	0.77291000
Cl	-2.05898200	1.54870600	-1.05819000
C	-3.69752700	0.73959300	-0.89660400
C	-3.83369000	-0.07507200	0.37043000
H	-3.82531200	0.14216900	-1.79907900
H	-4.41123800	1.56616600	-0.88551400
H	-3.54667900	0.47780400	1.26540100
H	-4.86539500	-0.42324400	0.46164500
Cl	-2.81261700	-1.58129300	0.32800200

9:

C	1.58660200	2.23247100	0.02106000
C	1.46657800	0.73122900	0.03631600
In	-0.62417300	-0.06759800	-0.60610900
Cl	-0.65143100	-2.27258300	-1.22500600
C	2.03890300	-0.35738200	0.23435900
C	2.55506300	-1.70624700	0.39947000
C	3.96437100	-1.92980300	-0.21365500
C	5.07952100	-1.21548600	0.57123400
C	4.95579300	0.28248200	0.55037100
C	4.76447200	1.05003300	1.63129400
Cl	-1.66216300	1.74262000	-1.56152200
H	5.08985500	-1.57646400	1.60735400
H	6.04015800	-1.50733300	0.12584900
H	3.95906900	-1.60911400	-1.26163500
H	4.14270300	-3.01010600	-0.21015700
H	2.55368200	-1.96964600	1.46537100
H	1.84347300	-2.38262100	-0.09797500
H	0.63349100	2.69275500	0.29588100
H	2.31011000	2.47473100	0.80786700
H	5.06230000	0.75786400	-0.42627100
H	4.72997000	2.13422700	1.56390900
H	4.68820000	0.62393100	2.62959700

C	2.06222700	2.77027900	-1.33879900
H	3.02372300	2.33183300	-1.62024700
H	1.33605900	2.56454800	-2.13047700
H	2.18451800	3.85542600	-1.26941300
H	-4.02862100	-0.97268500	2.44352100
C	-4.11441600	-0.20551000	1.67299300
C	-3.15799800	0.94194400	1.89559100
H	-5.13158400	0.19760000	1.67403500
Cl	-3.85587900	-1.00238600	0.07586600
H	-3.17926000	1.68695800	1.09998100
H	-3.31049000	1.40800100	2.87080400
Cl	-1.39344500	0.35872000	1.96771700

TS1:

C	-1.79943000	1.99767900	-1.19230900
C	-1.55456900	0.66491300	-0.51526400
In	0.47329600	0.49634200	0.41778000
Cl	0.74517800	-1.09161400	2.07896500
C	-2.24983100	-0.39864300	-0.32125000
C	-2.45920300	-1.68210200	0.37823500
C	-3.73192100	-1.66798100	1.24177800
C	-4.97785600	-1.43432100	0.34358300
C	-4.70128200	-0.28819500	-0.57628600
C	-4.06192500	-0.44219400	-1.76705700
Cl	1.51162300	2.53753500	0.33499300
H	-5.17542400	-2.34216300	-0.23734200
H	-5.85288000	-1.23659900	0.96983900
H	-3.65227500	-0.87740200	1.99557700
H	-3.82888600	-2.62067600	1.77092800
H	-2.48123700	-2.51285100	-0.33811400
H	-1.58304500	-1.83397000	1.02491700
H	-0.88053600	2.34524600	-1.67470800
H	-2.53979800	1.86024900	-1.98710000
H	-4.96020200	0.71520900	-0.24123600
H	-3.88796400	0.39570900	-2.43286700
H	-3.86221300	-1.42988900	-2.17545400
C	-2.28393000	3.06857000	-0.19728000
H	-3.21418500	2.76524400	0.29337900
H	-1.53458700	3.26886100	0.57452500
H	-2.46634400	4.00484700	-0.73311900
Cl	4.20543400	-0.07945700	0.09577000
C	4.11762200	-1.47421000	-1.03535900

C	2.77582700	-2.16630200	-0.98917400
H	4.87476000	-2.20079300	-0.72401800
H	4.35973100	-1.11319600	-2.03601100
H	2.74653200	-3.02722200	-1.65951400
H	2.46716200	-2.44567800	0.01839100
Cl	1.41063800	-1.07816900	-1.63308200

10:

C	-1.69494400	0.62948200	-0.54263100
In	0.30168500	0.52289800	0.40933200
Cl	1.58890200	2.40678500	0.03367400
C	-2.42999800	-0.50888600	-0.79909000
C	-2.10752900	-1.91536800	-0.30245200
C	-3.09598000	-2.19860800	0.84433500
C	-4.45882600	-1.56435600	0.43788600
C	-4.16796500	-0.34461100	-0.40030400
C	-3.70161800	-0.47244200	-1.75259100
Cl	0.39334600	-0.74090000	2.33401100
H	-5.03950700	-2.27406900	-0.16386900
H	-5.05194900	-1.29886200	1.31606100
H	-2.73174400	-1.71210300	1.75514800
H	-3.20204700	-3.26622600	1.05399800
H	-2.22078700	-2.64019100	-1.11673600
H	-1.07658400	-1.99403600	0.05384400
H	-4.40711700	0.64435200	-0.02101600
H	-3.74936600	0.38645900	-2.41469800
H	-3.82833200	-1.42970700	-2.25322200
C	-2.13960900	2.02202500	-0.87060000
C	-2.26791000	2.91346100	0.39035300
H	-3.08040600	2.05431800	-1.43147500
H	-1.36873800	2.46816600	-1.51700100
H	-2.60784200	3.90891900	0.09201000
H	-2.99110200	2.50408100	1.10306700
H	-1.30875700	3.03970400	0.90378400
H	4.07042500	-2.27868700	-1.25638200
C	4.15094400	-1.21362200	-1.03388100
C	3.19135300	-0.38666200	-1.85669600
H	5.16401000	-0.87480700	-1.27339800
Cl	3.90653700	-0.99387800	0.73333000
H	3.18477900	0.66946100	-1.58615500
H	3.36416800	-0.51651900	-2.92644400
Cl	1.43067400	-0.95287300	-1.63400100

TS2:

C	-1.75678300	0.85843000	0.18866500
In	0.29802600	0.52190700	-0.51449000
C	-2.65225400	-0.25703800	0.51197700
C	-2.41003700	-1.74643300	0.36184600
C	-3.72101800	-2.31438700	-0.23325500
C	-4.80946400	-1.27329900	0.12380300
C	-4.04037100	0.00328600	0.35316300
C	-2.89124000	0.62807100	-0.89990900
Cl	1.50659300	2.46515500	-0.70252400
Cl	0.47889100	-1.23336000	-2.03538600
H	-5.58960600	-1.16724300	-0.63596300
H	-5.32019500	-1.51721600	1.06588400
H	-3.95388000	-3.30881500	0.15215100
H	-3.62481400	-2.40489100	-1.31987500
H	-1.52035500	-1.98776600	-0.22420100
H	-2.23762400	-2.10991900	1.38574200
H	-4.53246700	0.90461400	0.70182300
H	-3.42817100	1.55273600	-1.09222100
H	-2.72398900	-0.00362700	-1.76751200
C	-1.91929800	2.19957700	0.92538300
C	-1.19287600	2.21285600	2.27598800
H	-2.98071900	2.43327400	1.08683800
H	-1.52256000	2.99643200	0.28569600
H	-1.34955300	3.17245700	2.77731000
H	-1.56082100	1.42236800	2.94004900
H	-0.10944900	2.09011600	2.15825600
H	4.20683800	-1.20782700	2.03803400
C	3.93224600	-1.56983300	1.04604000
C	2.53299000	-2.13864500	1.01692100
H	4.61777400	-2.37327000	0.75767500
Cl	4.14879700	-0.22165500	-0.12088600
H	2.19702500	-2.41297000	0.01657400
H	2.42720500	-2.97543300	1.70962900
Cl	1.27576300	-0.90966700	1.63234900

11:

C	-2.97785100	-1.46897900	0.17652400
C	-2.99052800	-0.13437100	-0.57738600
C	-3.98204700	0.67299800	-0.08329700
C	-4.76132100	0.00779300	0.99837700
C	-4.36486000	-1.48451000	0.87072100
C	-2.27742000	0.10438100	-1.94985900

C	-1.49431100	0.80670100	-0.96116900
H	-2.85921700	0.68181300	-2.66973700
H	-1.91748300	-0.84890400	-2.33643500
H	-4.18902900	1.68185200	-0.42791300
H	-4.46152100	0.44123900	1.96765900
H	-5.83645500	0.20422400	0.90830000
H	-4.34166000	-1.99862400	1.83350100
H	-5.09114700	-2.00095600	0.23554300
H	-2.81892900	-2.32461000	-0.48442200
H	-2.18353200	-1.49104900	0.93554600
In	0.18935600	-0.27490400	-0.01550100
Cl	0.51006500	-2.27670000	-1.11468400
Cl	0.53993300	0.03274600	2.25027900
C	-1.55190500	2.31498500	-0.90977900
C	-1.49514100	2.96293900	0.47683100
H	-2.40707600	2.69636900	-1.48507600
H	-0.66619900	2.62774000	-1.48927700
H	-1.43125500	4.05080200	0.38440100
H	-2.39241400	2.72852800	1.06153600
H	-0.63118300	2.62266800	1.05701800
H	2.99035900	1.31893300	1.34192000
C	3.49334100	1.47618800	0.38753800
C	4.56807600	0.45577400	0.09654600
H	3.87326600	2.49611300	0.30673200
Cl	2.13689900	1.42495400	-0.89246100
H	4.98534200	0.57315200	-0.90473900
H	5.36410500	0.60106600	0.83409500
Cl	3.97424300	-1.23237900	0.25925500

12

C	-1.72075700	0.82310000	0.28752200
In	0.30172700	0.50693100	-0.52462400
C	-2.62204300	-0.24349400	0.53905700
C	-2.39029600	-1.73587000	0.41775200
C	-3.68336400	-2.31189600	-0.20412200
C	-4.78769800	-1.27628400	0.11770100
C	-4.04414500	0.04092000	0.27969100
C	-3.08446700	0.53466800	-0.87873700
Cl	1.48279600	2.46150100	-0.74841000
Cl	0.47229500	-1.26247100	-2.02032500
H	-5.56516100	-1.22450700	-0.64980700
H	-5.28526200	-1.50223800	1.06787100
H	-3.91995000	-3.30392000	0.18591000

H	-3.55729800	-2.41832800	-1.28628000
H	-1.48161800	-1.99984500	-0.12867400
H	-2.26010900	-2.07631900	1.45601700
H	-4.55559400	0.87968100	0.74240300
H	-3.25422800	1.58344100	-1.09726800
H	-2.89349400	-0.09832500	-1.73949900
C	-1.93172600	2.20235300	0.90935400
C	-1.17717400	2.28576300	2.24841100
H	-2.99351400	2.41210800	1.08579000
H	-1.55423700	2.97565000	0.23111300
H	-1.34045800	3.26907300	2.69913000
H	-1.52821800	1.52623300	2.95518700
H	-0.09520200	2.16997000	2.11778700
H	4.22380900	-1.16231700	2.03973300
C	3.94529100	-1.54053300	1.05494100
C	2.54892100	-2.11659900	1.04232100
H	4.63350900	-2.34430800	0.77410000
Cl	4.14775600	-0.20828500	-0.13308800
H	2.20958400	-2.41043800	0.04867800
H	2.44962700	-2.94126900	1.75033500
Cl	1.28938600	-0.88173100	1.64127600

13

C	-1.75784800	0.86895400	0.17592400
In	0.29994200	0.52349700	-0.51160600
C	-2.66212600	-0.25358500	0.49036200
C	-2.41581100	-1.74440900	0.34240900
C	-3.73256100	-2.31376000	-0.23776600
C	-4.81809300	-1.27594300	0.13789800
C	-4.04913300	-0.00467400	0.37244900
C	-2.85325000	0.64719700	-0.91847300
Cl	1.51206200	2.46517300	-0.69524300
Cl	0.48016200	-1.22826300	-2.03782000
H	-5.60742800	-1.16127600	-0.61141800
H	-5.32140900	-1.52631000	1.08329700
H	-3.95896000	-3.31030900	0.14593700
H	-3.65196300	-2.39799800	-1.32623900
H	-1.53448200	-1.98326700	-0.25696800
H	-2.22882600	-2.10994900	1.36249200
H	-4.53656300	0.90959900	0.69275300
H	-3.44615900	1.53787600	-1.10426000
H	-2.68477200	0.01116100	-1.78306900
C	-1.91708000	2.20174500	0.92789900

C	-1.19706900	2.20304600	2.28158700
H	-2.97881900	2.43814800	1.08513700
H	-1.51577900	3.00311000	0.29661200
H	-1.35520400	3.15793400	2.79134600
H	-1.56739300	1.40658700	2.93721100
H	-0.11317000	2.08096800	2.16689600
H	4.20333300	-1.21752200	2.03915300
C	3.92921900	-1.57668900	1.04599800
C	2.52918300	-2.14347800	1.01404300
H	4.61392300	-2.38033400	0.75626800
Cl	4.14887300	-0.22590700	-0.11730400
H	2.19381900	-2.41465000	0.01263600
H	2.42173000	-2.98207600	1.70430000
Cl	1.27292500	-0.91473800	1.63169800

TS3

C	1.87920800	-0.96009500	-0.95889900
C	1.89270800	0.07483300	0.14238100
C	3.16512000	0.37587100	0.52664400
C	4.18241700	-0.34342600	-0.30242000
C	3.35144900	-0.98478600	-1.45049200
C	0.90241000	0.05136400	2.06174600
C	0.68542400	0.72248600	0.83602900
H	1.04308900	0.58138900	3.00869900
H	0.94761000	-1.03452400	2.11257500
H	3.42630400	1.09203400	1.30104900
H	4.97941800	0.32025100	-0.65635200
H	4.67849600	-1.10444000	0.32041200
H	3.44701200	-0.37735900	-2.35482600
H	3.68736800	-1.99423100	-1.69424900
H	1.55361100	-1.94092300	-0.58590800
H	1.17022700	-0.67974900	-1.75693300
In	-1.21954800	-0.21863700	0.02177400
Cl	-1.32240300	-2.48284500	0.32586400
Cl	-2.87157200	1.11551000	-0.78767800
C	0.57473600	2.26036700	0.84564200
H	1.41057300	2.65793000	1.43758100
H	-0.33684100	2.54276800	1.38694000
C	0.58275500	2.90828600	-0.54256200
H	0.52947800	3.99591700	-0.44347200
H	1.49890800	2.66943900	-1.09238000
H	-0.27719900	2.60000200	-1.14766200

15:

C	-1.76901800	-1.33728900	-1.16503400
C	-1.90215400	0.17293300	-0.97042100
C	-2.90474100	0.45631500	-0.08077200
C	-3.57094700	-0.77525700	0.42812600
C	-3.05872500	-1.90146400	-0.50629600
C	-1.10744300	1.19651300	-1.80413200
C	-0.46187100	1.27564400	-0.50400500
H	-1.67531700	2.06770600	-2.13578800
H	-0.58703600	0.69708800	-2.62135800
H	-3.19029100	1.45506100	0.23509200
H	-3.27831200	-0.93003200	1.47961100
H	-4.66257800	-0.66592500	0.44301600
H	-2.87403600	-2.83482900	0.02836600
H	-3.80459500	-2.10620900	-1.27932000
H	-1.68591300	-1.59811500	-2.22439200
H	-0.87789200	-1.74768500	-0.66515900
In	1.15532900	-0.09429800	0.07141000
Cl	2.97196200	-0.17912300	-1.30272300
Cl	0.88651000	-1.37901300	1.94306300
C	-0.66440900	2.50809900	0.33632600
C	-0.61999700	2.34417300	1.85806600
H	-1.56323600	3.05615100	0.02301800
H	0.17454200	3.15322600	0.01269700
H	-0.65691000	3.32257600	2.34443500
H	-1.46583400	1.75232700	2.22396000
H	0.29810300	1.84955100	2.19981900

$TS_{trans\text{-}a}$:

C	-4.08440200	-0.76855000	-1.24751700
C	-3.16817700	0.05441600	-0.35879600
C	-3.07489100	-0.46655800	0.88368200
C	-3.88517500	-1.72747800	1.01916200
C	-4.23795400	-2.08913900	-0.44709300
C	-2.58173000	1.35131200	-0.74714600
C	-1.23807100	1.71332300	-0.47796600
H	-3.27777300	2.13792600	-1.06899700
H	-1.83139000	1.21188500	-1.70958200
H	-2.57401200	0.00552600	1.72668300
H	-3.33938500	-2.52101100	1.54216800
H	-4.77831600	-1.51794300	1.62596200
H	-3.52036400	-2.82442000	-0.82399200

H	-5.23605400	-2.52138200	-0.54565200
H	-5.04499800	-0.24908400	-1.37817700
H	-3.67254500	-0.93039200	-2.25023500
In	0.08363600	0.02877800	0.15966300
Cl	0.10660500	-1.67909700	-1.40043300
Cl	0.41525400	-0.08036800	2.42941500
C	-0.80858100	3.13873000	-0.60121000
C	-0.67961800	3.70828700	0.84119500
H	-1.53796200	3.73649300	-1.16244400
H	0.16183500	3.21493700	-1.10270000
H	-0.34389700	4.74649600	0.77122300
H	-1.64082300	3.69224000	1.36288600
H	0.04922400	3.15510800	1.44187500
Cl	2.39068300	1.23081700	-0.75005100
C	3.48007300	-0.07527900	-1.51426100
C	4.43590100	-0.66234100	-0.50301900
H	4.00923500	0.46862600	-2.29862800
H	2.79177600	-0.80618800	-1.93869400
H	5.09600500	-1.35160200	-1.03950000
H	5.04147000	0.10388100	-0.01666200
Cl	3.59366600	-1.60203300	0.77746900

$TS_{trans\text{-}b}$:

C	-3.77432600	-1.24174900	-0.89856600
C	-3.06661600	0.00912500	-0.42044000
C	-2.96562800	0.03262500	0.93006900
C	-3.59559800	-1.18376400	1.56454200
C	-3.80923100	-2.14218800	0.36275500
C	-2.58092200	1.09015400	-1.36914500
C	-1.34001000	1.68533000	-0.74011300
H	-3.36514000	1.83400500	-1.57009700
H	-2.31942900	0.61989600	-2.32557200
H	-2.59961300	0.87016500	1.52223200
H	-2.97913700	-1.61809200	2.35895400
H	-4.54483000	-0.88990300	2.03561600
H	-2.98543200	-2.86155900	0.31487300
H	-4.73778400	-2.71179500	0.44256800
H	-4.78375700	-0.96965400	-1.24188400
H	-3.26760100	-1.71534600	-1.74637200
In	-0.10481500	-0.00796300	0.02862500
Cl	-0.09619700	-1.84401700	-1.35424600
Cl	0.54736300	0.16852500	2.24137600
C	-1.28212500	3.05489500	-0.44653100

C	-0.22015400	3.75574900	0.34563900
H	-2.14200500	3.66904300	-0.73864000
H	-0.76552500	2.56519900	-1.54080100
H	0.07550300	4.69655300	-0.12838700
H	-0.66458700	4.01236700	1.31704400
H	0.65722200	3.13214000	0.52436800
Cl	3.55848300	-1.99109400	0.07074800
C	4.51132100	-0.47519300	-0.07891300
C	3.71913800	0.75154300	0.31002700
H	4.88810600	-0.41169700	-1.10094500
H	5.35963300	-0.54846400	0.60920500
H	3.22724000	0.65726100	1.27825600
H	4.33635400	1.65080900	0.26969300
Cl	2.35338800	1.10129800	-0.90133100

$TS_{trans\text{-}c}$:

C	-3.81969800	-1.09030600	-0.94999300
C	-3.07292000	0.02624200	-0.25136800
C	-2.86086300	-0.26980200	1.05240200
C	-3.43325000	-1.61659100	1.42888500
C	-3.73596300	-2.26826900	0.05386500
C	-2.67958800	1.30929600	-0.94909500
C	-1.37817000	1.86500800	-0.40189900
H	-3.50017500	2.04248100	-0.94163100
H	-2.47722900	1.09366900	-2.00951200
H	-2.46030300	0.41135700	1.80285500
H	-2.75433100	-2.21086900	2.04959500
H	-4.34498200	-1.46378900	2.02415100
H	-2.90898200	-2.92619800	-0.23163300
H	-4.64590300	-2.87228500	0.06785700
H	-4.85817100	-0.77099300	-1.12517500
H	-3.39314400	-1.33266600	-1.92965700
In	-0.14082200	0.04298000	0.05873500
Cl	0.56961400	-0.15994500	2.25545700
Cl	-0.14456300	-1.43540900	-1.70440700
C	-1.18088600	3.24710000	-0.32467900
C	0.06465700	3.95565900	0.09229500
H	-1.57785500	2.43833800	0.70918500
H	-2.01722500	3.89212100	-0.62115900
H	0.81687200	3.28708100	0.51398500
H	0.48211500	4.41671100	-0.81499400
H	-0.15621600	4.77353400	0.78550000
Cl	2.40905000	1.15542100	-0.67841500

C	3.73563000	0.54293700	0.46508800
C	4.45904800	-0.65605300	-0.10399400
H	3.23042100	0.33188400	1.40753400
H	4.40805500	1.39695300	0.56501200
H	4.84545300	-0.46317100	-1.10596100
H	5.29674100	-0.88174100	0.56350800
Cl	3.42043800	-2.12122900	-0.18184200

$TS_{cis\text{-}a}$:

C	-3.95403400	-0.72125900	-1.32988900
C	-3.10785700	-0.11147700	-0.22838300
C	-2.91275000	-0.97058200	0.79420900
C	-3.57822500	-2.29783200	0.54533600
C	-4.48829200	-2.02927600	-0.68504200
C	-2.62504700	1.28372200	-0.23811700
C	-1.30231000	1.65504300	0.10987200
H	-3.38899200	2.06447300	-0.32279300
H	-1.88939000	1.48031900	-1.20507400
H	-2.38959300	-0.73902700	1.72018100
H	-2.81352400	-3.06117700	0.33967800
H	-4.13372800	-2.64868700	1.42170200
H	-4.49203400	-2.86327000	-1.39012200
H	-5.51938000	-1.87925500	-0.35108500
H	-4.75831400	-0.05204800	-1.65981400
H	-3.32921300	-0.92027800	-2.21226200
In	0.14305400	-0.04453100	0.24144300
Cl	0.20248700	-1.28684900	-1.71049500
Cl	0.56207600	-0.70377000	2.40027100
C	-0.92692200	3.07979600	0.37596500
C	-1.96073800	4.18441400	0.13338900
H	0.01780700	3.30587100	-0.13583100
H	-0.64769500	3.05188000	1.44676600
H	-1.52489600	5.15093800	0.40027000
H	-2.25653500	4.23995400	-0.92049300
H	-2.85979900	4.05044000	0.74335100
Cl	3.76729800	-1.56945600	0.35857300
C	4.50951000	-0.28016400	-0.65029100
C	3.48733800	0.48159300	-1.46024400
H	5.19130100	-0.76410800	-1.35715500
H	5.08433800	0.37441800	0.00657100
H	3.95716200	1.23789700	-2.09134200
H	2.82633300	-0.16091300	-2.04185300
Cl	2.35475500	1.48188100	-0.36730300

$TS_{cis\text{-}b}$:

C	-3.56018000	-1.09281200	-1.36489000
C	-2.96177200	-0.13950800	-0.35194100
C	-2.82405500	-0.73332200	0.85701400
C	-3.31180500	-2.16323500	0.84388600
C	-3.45765200	-2.47428500	-0.66914300
C	-2.63447300	1.30366800	-0.67271300
C	-1.34636100	1.74038200	-0.01476600
H	-3.48946300	1.96110500	-0.46340500
H	-2.44139400	1.40463000	-1.75328200
H	-2.54052900	-0.23022100	1.78108200
H	-2.63730900	-2.85126500	1.36438800
H	-4.27483400	-2.21452700	1.37185800
H	-4.60470100	-0.80317700	-1.55540100
H	-3.04306500	-1.06111400	-2.33079700
In	-0.08228600	-0.10106800	0.21461600
Cl	0.46911200	-0.58968200	2.39713900
Cl	0.23623700	-1.33123500	-1.71642500
C	-1.07614500	3.06532200	0.34817300
C	-1.92185800	4.28229900	0.12144900
H	-0.08928900	3.25743900	0.77730700
H	-1.51290300	2.17232000	1.21652800
H	-1.45352400	4.84436600	-0.69919100
H	-2.95016300	4.05628200	-0.16458600
H	-1.91203700	4.93584700	0.99888200
H	-4.31524500	-3.11550200	-0.88417400
H	-2.56157300	-2.99154300	-1.02616700
Cl	2.22941300	1.50467300	-0.37793800
C	3.43891700	0.54856600	-1.41108300
C	4.51230000	-0.09711600	-0.56579300
H	3.86095700	1.30120000	-2.07942600
H	2.83539400	-0.17034100	-1.96505100
H	5.24240200	-0.54487900	-1.24751800
H	5.02066400	0.62669600	0.07307100
Cl	3.87448100	-1.41109400	0.48243400

$TS_{cis\text{-}c}$:

C	-3.67474700	-0.65479100	-0.91874200
C	-2.99337500	-0.14350300	0.33730400
C	-2.72460100	-1.15057500	1.19801300
C	-3.17834700	-2.48753300	0.66687400
C	-3.52402200	-2.19600700	-0.81915300

C	-2.72648600	1.32681700	0.57819100
C	-1.37878200	1.72904300	0.01469100
H	-2.63196700	1.52160600	1.65941000
H	-3.55578400	1.94990600	0.22137800
H	-2.33598100	-1.01880800	2.20552100
H	-2.42590300	-3.27473800	0.78618400
H	-4.05661300	-2.81315000	1.24259700
H	-2.70089500	-2.52382100	-1.45979200
H	-4.42440800	-2.72007700	-1.14713600
H	-4.72831200	-0.33811700	-0.90396300
H	-3.24448300	-0.25021100	-1.84457300
In	-0.08772700	-0.10573700	0.09549300
Cl	0.02410600	-1.29363800	-1.87224900
Cl	0.69263200	-0.61185900	2.21352600
C	-1.08255500	3.02735900	-0.42081100
C	-1.95483900	4.24745800	-0.35668900
H	-1.43602200	2.10226500	-1.26612400
H	-0.05502500	3.20366700	-0.74816900
H	-1.85915600	4.84394100	-1.26875100
H	-3.00611800	4.02707500	-0.16591200
H	-1.57828000	4.86532200	0.47049800
Cl	3.78331600	-1.60714800	-0.43264400
C	4.56999100	-0.02787200	-0.08923400
C	3.65558000	0.93780300	0.62879300
H	4.93499400	0.37916700	-1.03343300
H	5.42331600	-0.22081900	0.56886500
H	3.18682400	0.51042300	1.51496700
H	4.17212600	1.86882900	0.86856600
Cl	2.24661700	1.47849500	-0.45538200

6:

C	2.61823400	1.27017600	0.43398100
C	1.52942300	1.18600500	-0.61098900
C	1.65646100	0.03356000	-1.34986400
C	2.87963800	-0.75957200	-0.93271700
C	3.26396900	-0.13812900	0.43502700
C	0.47777400	2.25933100	-0.82355400
C	-0.70199800	2.02262500	0.11099100
H	0.13880000	2.26144100	-1.86554600
H	0.91179400	3.24384100	-0.61019200
H	1.11910800	-0.14875400	-2.28191400
H	2.71955700	-1.84175000	-0.89501400
H	3.65477000	-0.59122600	-1.69404400

H	2.84306400	-0.73469000	1.25102700
H	4.34437200	-0.09906300	0.58557000
H	3.32136100	2.04617700	0.09172000
H	2.26134100	1.59509300	1.41815200
In	-0.38970200	-0.51121100	0.06251400
Cl	-0.05255400	-0.97829300	2.27362800
Cl	-1.62396300	-1.67143400	-1.47239300
C	-1.97205500	1.75865300	-0.30869800
C	-3.17310600	1.63844700	0.57480900
H	-2.15259100	1.67654400	-1.38285900
H	-0.52450500	2.18301600	1.17657300
H	-3.83571600	2.49106900	0.37067900
H	-3.75429400	0.73932900	0.33889100
H	-2.92094100	1.64712600	1.63882800

17:

C	-3.01456100	0.09284900	1.60218600
C	-2.16865200	0.49412600	0.39612400
C	-2.82413700	0.18826200	-0.76716500
C	-4.13791900	-0.46732600	-0.51607900
C	-4.09433500	-0.83613300	0.98863600
C	-0.92514100	1.18559800	0.49186700
C	0.03561800	1.42479700	-0.51585500
H	-0.66895400	1.56297100	1.48644900
H	-0.27767800	1.18392400	-1.53846000
H	-2.47726700	0.44149800	-1.76583500
H	-4.93947000	0.25291200	-0.75369700
H	-4.30846900	-1.32010400	-1.18564900
H	-5.06528300	-0.72410200	1.47502600
H	-3.79122700	-1.88197700	1.09826100
H	-2.43130000	-0.40263700	2.38569600
H	-3.46029000	0.98783500	2.05656400
In	1.22316400	-0.50502700	-0.08427200
Cl	0.38127300	-2.28720300	-1.22302300
Cl	3.00893000	-0.33319500	1.30306000
C	1.03469000	2.57926400	-0.38721200
C	0.39735400	3.90687000	-0.83989700
H	1.92326000	2.38539500	-0.99950100
H	1.37819300	2.66204600	0.65081600
H	1.13335600	4.71296500	-0.76331200
H	0.06127000	3.85648700	-1.88095000
H	-0.46214200	4.16604100	-0.21232300

16:

C	-2.60180400	1.27927900	-0.47126900
C	-1.28668700	1.46920300	0.24812300
C	-1.25638300	0.72732500	1.40472000
C	-2.56913500	0.00343700	1.63338400
C	-3.27257200	0.08542800	0.25338700
C	-0.18563900	2.39303700	-0.24054700
C	0.72895800	1.62243800	-1.18260000
H	0.37257700	2.80136400	0.60639500
H	-0.62928900	3.23503800	-0.78590900
H	-0.50624000	0.85688100	2.18642000
H	-2.45654000	-1.01825500	2.00962400
H	-3.11843500	0.55593600	2.40918300
H	-3.09816200	-0.83467900	-0.31386400
H	-4.35316700	0.20988800	0.34460200
H	-3.16898600	2.21439400	-0.33794000
H	-2.49691300	1.13966100	-1.55353100
In	0.35044300	-0.61390700	-0.04971500
Cl	-0.55827100	-1.87928600	-1.72001200
Cl	1.84974700	-1.23894000	1.55879200
C	2.07474000	1.42667700	-1.04470100
C	2.98932900	1.92491900	0.02368800
H	0.27261800	1.29705700	-2.12001100
H	2.55941800	0.87261100	-1.85130500
H	3.69706400	2.62773300	-0.43798300
H	2.48300000	2.43791500	0.84347100
H	3.59141900	1.10528500	0.43250700

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C	4.18755800	0.84917500	0.40745200
C	2.87028500	0.16373600	0.19624800
C	3.07753300	-1.25247100	-0.11320300
C	4.57399900	-1.53753600	-0.06814500
C	5.23761700	-0.14078100	-0.16293700
C	2.38823900	-0.55021700	-1.38979900
C	1.66812200	0.60374000	-0.45340400
C	1.59726300	2.05555000	-0.93382500
In	-0.24823100	-0.21937200	0.32305100
Cl	-1.08443200	0.62443200	2.30125000
Cl	-0.39077300	-2.45028700	-0.28394700
H	1.64693200	-1.23321400	-1.80770300
H	3.07390400	-0.14511200	-2.13166100
H	2.39060600	-2.01672000	0.24731500

H	4.80256800	-2.02297900	0.88751900
H	4.89663400	-2.21901500	-0.86021300
H	6.18361100	-0.08824600	0.37978900
H	5.44959700	0.11751000	-1.20569200
H	4.24650900	1.86518500	0.01176300
H	4.28032600	0.92285000	1.50454600
H	0.81522600	2.13800700	-1.69722200
H	2.53627500	2.31844200	-1.44050900
C	1.32390800	3.06297200	0.19306500
H	0.36743200	2.87588100	0.69373200
H	2.10566000	3.03360700	0.96028700
H	1.29301000	4.07872500	-0.21144800
Cl	-1.95212900	1.07135600	-1.36456500
C	-3.53249300	1.42566800	-0.43630800
C	-4.56397600	0.34766500	-0.67009000
H	-3.85112000	2.38560000	-0.84624700
H	-3.23284100	1.52412900	0.60720000
H	-5.48423300	0.66320200	-0.16767400
H	-4.77131500	0.20102900	-1.73121200
Cl	-4.07583200	-1.23459700	0.02747300

$TS_{rotation}$

C	-4.16995600	0.20208200	-0.33153100
C	-3.28096700	-0.52070300	-1.34595600
C	-2.73091300	-0.10936800	-0.00216700
C	-2.71631600	-1.25495400	1.10665600
C	-5.07992400	-0.67493200	0.53283000
C	-1.58854900	0.72481000	0.25374400
In	0.38091800	-0.01387600	-0.52133500
Cl	1.50261400	1.59147100	-1.74891500
Cl	0.30503000	-2.26759600	-0.94733100
H	-5.52540600	-1.47586600	-0.06841500
H	-5.90695500	-0.09591800	0.95276300
H	-2.42546200	-2.18856300	0.61789600
H	-1.99392300	-1.07628100	1.91180600
C	-1.73390200	2.00291200	0.95156500
H	-4.48958400	1.20978700	-0.58367200
H	-2.96471500	0.04598900	-2.21949400
H	-3.45381700	-1.57791400	-1.53408000
H	-2.65814000	2.06100000	1.53753600
H	-0.86546600	2.25216100	1.56961500
C	-1.81026400	3.08273700	-0.20518800
H	-1.92331700	4.05077500	0.29106900

H	-0.89988900	3.09916400	-0.80827100
H	-2.67470900	2.91887200	-0.85183000
Cl	3.90424000	-1.23642900	-0.17890900
C	4.35478900	-0.23078800	1.24230400
C	3.43026400	0.94874900	1.42768300
H	5.35980700	0.16447300	1.06303700
H	4.37721200	-0.87838300	2.11999900
H	3.71622100	1.55467400	2.28919300
H	3.32186500	1.56281700	0.53348200
Cl	1.69777200	0.39948300	1.84874300
C	-4.16653400	-1.23741300	1.64809800
H	-4.45419000	-2.24082300	1.98060800
H	-4.21504200	-0.58263600	2.52494800

syn-TS1

C	3.22691800	-1.58304100	0.84327900
C	2.72566200	-1.99332200	-0.34554900
C	2.71903000	0.60693000	-0.55746500
C	4.17498000	0.71410700	-0.55073800
C	4.83857100	0.32216800	0.77974200
C	4.66255300	-1.19783200	1.02453400
C	1.52299700	1.05359300	-0.62918500
In	-0.21718900	-0.22766100	-0.24068700
Cl	-0.38047800	-0.83942100	1.98761900
Cl	-0.73871500	-1.59566000	-2.00969700
H	5.29122900	-1.74877200	0.31607800
H	5.00583200	-1.44204500	2.03502200
H	4.39206700	0.89916200	1.59659900
H	5.90319800	0.57155600	0.73972600
H	4.61746500	0.17440200	-1.39677100
H	4.33754300	1.79071500	-0.74116700
C	1.26934100	2.54479900	-0.99253000
H	2.55946100	-1.49291600	1.69974600
H	1.69620600	-2.32173300	-0.46179800
H	3.36368800	-2.15658700	-1.21120900
H	2.11498400	2.92310800	-1.57542100
H	0.39425800	2.59456200	-1.64890300
C	1.06106100	3.40391000	0.26100500
H	0.84581900	4.43491500	-0.03849800
H	0.22432700	3.04753200	0.86977200
H	1.95657300	3.41187800	0.88979400
Cl	-2.20673300	1.61092000	-0.26419900
C	-3.39825600	1.19517800	1.11379600

C	-4.54367600	0.34716200	0.61472800
H	-3.73776200	2.17640100	1.44986600
H	-2.79190000	0.70534700	1.87582400
H	-5.24303300	0.22348400	1.44820800
H	-5.06708300	0.81455700	-0.22083700
Cl	-4.01382200	-1.28949300	0.09792000

syn-9

C	2.73186700	-1.25300800	1.03343600
C	2.01946600	-2.02038200	0.04720500
C	2.41360700	-0.65511900	-0.63599300
C	3.80873100	-0.69097100	-1.26275600
C	4.80889100	-0.51651300	-0.10306400
C	4.23724900	-1.29503800	1.11524500
C	1.52049900	0.40174900	-0.66952300
In	-0.43721200	0.52579600	0.38060400
Cl	-1.34288700	2.62699300	0.15621400
Cl	-0.63899900	-0.83668300	2.24668400
H	4.55814300	-2.34338800	1.07432400
H	4.58490600	-0.87250800	2.06081000
H	4.88043200	0.54474200	0.15796300
H	5.81344700	-0.86256900	-0.36120800
H	3.95945000	-1.65098200	-1.76982800
H	3.93810700	0.08756900	-2.01594000
C	1.79942100	1.63408500	-1.48111700
H	2.15547500	-0.73691000	1.79455200
H	0.95599000	-2.17901400	0.19851500
H	2.53197800	-2.85365100	-0.42878700
H	2.47809000	1.43535400	-2.31611100
H	0.86326500	2.01679700	-1.90513200
C	2.40225000	2.75760600	-0.59021000
H	2.56444600	3.64457100	-1.20885600
H	1.72652700	3.03904600	0.22281900
H	3.36194100	2.45312200	-0.16264800
Cl	-3.79016400	-0.02682700	0.40309400
C	-3.77966800	-1.64996400	-0.37810300
C	-3.15061800	-1.60432200	-1.75125100
H	-4.82227800	-1.96044000	-0.49256000
H	-3.26971900	-2.34276700	0.29321800
H	-3.17940200	-2.58337500	-2.23311900
H	-3.58819300	-0.84211700	-2.39494100
Cl	-1.34320700	-1.19914400	-1.69457100

syn-10

C	2.73186700	-1.25300800	1.03343600
C	2.01946600	-2.02038200	0.04720500
C	2.41360700	-0.65511900	-0.63599300
C	3.80873100	-0.69097100	-1.26275600
C	4.80889100	-0.51651300	-0.10306400
C	4.23724900	-1.29503800	1.11524500
C	1.52049900	0.40174900	-0.66952300
In	-0.43721200	0.52579600	0.38060400
Cl	-1.34288700	2.62699300	0.15621400
Cl	-0.63899900	-0.83668300	2.24668400
H	4.55814300	-2.34338800	1.07432400
H	4.58490600	-0.87250800	2.06081000
H	4.88043200	0.54474200	0.15796300
H	5.81344700	-0.86256900	-0.36120800
H	3.95945000	-1.65098200	-1.76982800
H	3.93810700	0.08756900	-2.01594000
C	1.79942100	1.63408500	-1.48111700
H	2.15547500	-0.73691000	1.79455200
H	0.95599000	-2.17901400	0.19851500
H	2.53197800	-2.85365100	-0.42878700
H	2.47809000	1.43535400	-2.31611100
H	0.86326500	2.01679700	-1.90513200
C	2.40225000	2.75760600	-0.59021000
H	2.56444600	3.64457100	-1.20885600
H	1.72652700	3.03904600	0.22281900
H	3.36194100	2.45312200	-0.16264800
Cl	-3.79016400	-0.02682700	0.40309400
C	-3.77966800	-1.64996400	-0.37810300
C	-3.15061800	-1.60432200	-1.75125100
H	-4.82227800	-1.96044000	-0.49256000
H	-3.26971900	-2.34276700	0.29321800
H	-3.17940200	-2.58337500	-2.23311900
H	-3.58819300	-0.84211700	-2.39494100
Cl	-1.34320700	-1.19914400	-1.69457100

Syn-TS2

C	4.23568200	0.89715400	0.10516500
C	2.88268300	0.20208100	0.03730800
C	3.10295000	-1.27614600	-0.00889200
C	4.59392100	-1.53251600	0.18678100

C	5.27777100	-0.20213100	-0.20265600
C	2.61192700	-0.74706400	-1.34734800
C	1.63664000	0.72055200	-0.35071200
C	1.55560200	2.13864800	-0.87085900
In	-0.26196100	-0.22209800	0.31325200
Cl	-1.11042000	0.60850000	2.29228200
Cl	-0.39715200	-2.43749900	-0.32982300
H	1.67521700	-1.16973500	-1.69435000
H	3.29572400	-0.41984400	-2.12464000
H	2.39308100	-1.95939700	0.45299700
H	4.76079900	-1.76907700	1.24346700
H	4.95014200	-2.38422100	-0.39903500
H	6.21195900	-0.04235400	0.34009500
H	5.52744800	-0.19450000	-1.26891400
H	4.32430500	1.77800700	-0.53520300
H	4.32786200	1.24362000	1.14401100
H	0.72329500	2.22791900	-1.57706500
H	2.46587300	2.41009400	-1.41737900
C	1.34055200	3.13830400	0.29062900
H	0.42572300	2.92817500	0.85405100
H	2.17865100	3.12208200	0.99410500
H	1.26007900	4.14971000	-0.11773100
Cl	-1.97955100	1.07018800	-1.36483800
C	-3.56000900	1.41169000	-0.43035800
C	-4.58646600	0.33006600	-0.66901200
H	-3.88387100	2.37269400	-0.83357100
H	-3.25759700	1.50435500	0.61285100
H	-5.50676000	0.63772800	-0.16171000
H	-4.79630400	0.19012800	-1.73054600
Cl	-4.08858700	-1.25450700	0.01584600

TS4

C	4.26085700	0.83911300	-0.48695800
C	2.89572900	0.13816500	-0.53300300
C	3.11122900	-1.28576300	0.04861600
C	4.56225100	-1.38367000	0.49838900
C	5.30068000	-0.28857700	-0.29881200
C	2.82426900	-1.12405800	-1.40162600
C	1.64616000	0.91550100	-0.30082600
C	1.73596000	2.32314700	-0.19645000
In	-0.21330500	-0.13723600	0.41055600
Cl	-1.18505100	0.93819300	2.21224900

Cl	-0.35897400	-2.39827700	0.07875800
H	1.84445300	-1.43723200	-1.75165100
H	3.61432500	-1.26149200	-2.13484800
H	2.34944100	-1.75695600	0.66348900
H	4.62084800	-1.19104800	1.57623500
H	4.97583500	-2.38224200	0.32128000
H	6.19776000	0.06901300	0.21293500
H	5.62439300	-0.67234800	-1.27137900
H	4.46578600	1.44796600	-1.37735500
H	4.29012000	1.50943200	0.38442900
H	1.27238500	1.46154800	-1.31918300
H	2.71572800	2.77083300	-0.38012700
C	0.65541600	3.29612000	0.10812700
H	-0.34930300	2.87233200	0.09931300
H	0.84697000	3.66129400	1.12990400
H	0.71045000	4.16879100	-0.55096400
Cl	-1.93749300	0.84384200	-1.52108800
C	-3.60000500	1.20528600	-0.74625200
C	-4.55674500	0.05065800	-0.92413800
H	-3.93589800	2.09394200	-1.28333700
H	-3.38374200	1.43281800	0.29780900
H	-5.53002800	0.37606500	-0.54170400
H	-4.66559800	-0.23400300	-1.97189500
Cl	-4.06123300	-1.40256400	0.00522300

TS5

C	1.17038400	0.99217600	-0.40851100
C	0.33087600	-0.15987500	-0.42934700
C	1.13838200	-1.42419200	-0.29033600
C	2.35726600	-0.89587900	0.53363300
C	2.52592700	0.61432800	0.17628900
C	-0.95551500	0.30878800	-0.24373700
C	-0.72452400	1.61777700	0.30808000
C	-2.29003400	-0.29355400	-0.59288200
H	-0.26941400	1.70055700	1.28925700
H	-1.36989500	2.47305300	0.06384100
H	1.11596000	1.74429800	-1.18825800
H	2.80333600	1.20919900	1.05557000
H	3.32340200	0.77211900	-0.56487200
H	2.13103200	-0.99656500	1.60127500
H	3.26914500	-1.46963600	0.34000300
H	0.61750300	-2.24325800	0.21703500
H	1.47474300	-1.80258500	-1.26640200

H	-2.81309300	0.38566600	-1.28483600
H	-2.13676500	-1.23053400	-1.14282000
C	-3.19701900	-0.54567300	0.62487100
H	-4.16304700	-0.96422700	0.31838800
H	-2.72970400	-1.24790100	1.32486400
H	-3.38766100	0.38645000	1.16858800

***syn*-TS5**

C	1.74190700	0.99401000	0.45396600
In	-0.21026300	0.45517600	-0.51640000
Cl	-1.69503700	2.18523200	-0.93745500
C	2.69546600	-0.14248600	0.62206800
C	2.19324100	-1.40899700	1.32861200
C	3.08840900	-2.56062700	0.81214000
C	3.50779800	-2.13903200	-0.61334900
C	3.54912100	-0.61906000	-0.57440500
C	4.20450400	0.04828600	0.60115400
Cl	-0.01946500	-1.33308300	-1.93658100
H	4.47350300	-2.56583200	-0.90625500
H	2.76553600	-2.46018500	-1.35132000
H	2.56353400	-3.51911900	0.82523300
H	3.96541300	-2.67259400	1.45775100
H	2.21145400	-1.31679400	2.42117500
H	1.14957000	-1.60108700	1.03851900
H	3.52164400	-0.06609700	-1.51075700
H	4.61526000	1.03955500	0.43201600
H	4.79715300	-0.54386100	1.29327600
C	2.18541800	2.32271800	0.62550200
C	1.43767100	3.58594600	0.39872100
H	3.20982400	2.44880400	0.98854300
H	1.41436200	1.47113800	1.52883100
H	1.57304400	4.27832300	1.23691800
H	1.90987800	4.07098700	-0.47116000
H	0.37824000	3.45005800	0.17481500
H	-3.91930800	-2.01410400	1.75046600
C	-4.06452300	-1.11560900	1.14881800
C	-3.27977100	0.05915600	1.68259100
H	-5.12354400	-0.83866000	1.17164000
Cl	-3.63959400	-1.50783900	-0.55266100
H	-3.33198300	0.94294100	1.04668700
H	-3.55836400	0.29655200	2.71079600
Cl	-1.46165600	-0.33545500	1.81208200

Me-7

C	-1.50704800	-0.44691700	-1.74357300
C	-0.64021800	-1.49952200	-1.79243300
C	-0.80322000	1.58587500	0.60520800
C	-2.20227500	1.21494200	0.95363700
C	-3.10880100	0.90585300	-0.25690100
C	-2.79810500	-0.41830000	-0.98232200
C	0.21408000	2.24618700	0.39419000
In	0.56868500	-0.38755200	0.08799000
Cl	-0.03658000	-1.71350200	1.85432100
Cl	2.62509300	-0.07453300	-0.86402500
H	-2.85993900	-1.27179500	-0.29641000
H	-3.58260100	-0.57482600	-1.74005500
H	-3.07788500	1.74191000	-0.96515500
H	-4.13564900	0.84972200	0.11758200
H	-2.19627600	0.37546200	1.65847200
H	-2.60575000	2.07678300	1.49901900
C	1.41378800	3.05414900	0.19950900
H	-1.28487800	0.42912600	-2.35763200
H	0.18574000	-1.50822200	-2.50236300
H	-0.87054600	-2.43581600	-1.28293800
H	1.12041500	4.11025400	0.26236000
H	2.15898800	2.85855300	0.97722400
H	1.86890700	2.88191000	-0.78055800

Me-8:

C	2.47217000	-1.30108900	1.16108100
C	1.37600700	-2.10389600	1.19631400
C	2.07386900	1.47855300	-0.49197500
C	3.17727500	0.81472300	-1.22088100
C	4.13065600	-0.02752700	-0.34623700
C	3.55989000	-1.37583000	0.13026600
C	1.32792400	2.28748500	0.05045600
In	0.11696300	-0.12541800	0.09890300
Cl	0.27173000	-1.08295800	-2.01100200
Cl	-0.67560900	0.51236700	2.20050000
H	3.23600200	-1.98659900	-0.72072100
H	4.38059000	-1.93052000	0.61207500
H	4.46969300	0.56646500	0.51072300
H	5.01839200	-0.23644900	-0.95191800
H	2.76880700	0.21124000	-2.03875500
H	3.74497900	1.62954100	-1.68840300
H	2.62263900	-0.59847700	1.98394300

H	0.72443200	-2.11792800	2.06760200
H	1.22494500	-2.87598800	0.44342400
Cl	-2.19941900	1.44838000	-0.99831500
C	-3.71758000	0.42928200	-0.84765400
C	-3.69786000	-0.48980900	0.35325600
H	-3.80650000	-0.10992300	-1.79050100
H	-4.52833500	1.15416700	-0.74773800
H	-3.46690800	0.02920400	1.28390600
H	-4.66520000	-0.99125600	0.43524000
Cl	-2.47017000	-1.82131600	0.17193700
C	0.56980000	3.36551900	0.68755100
H	1.16813400	4.28229000	0.61859700
H	-0.38676400	3.54532500	0.18755200
H	0.37994400	3.14990100	1.74261700

Me-TS1:

C	1.64861800	2.07554000	1.36753400
C	1.57842000	0.79083600	0.58672000
In	-0.41037700	0.47665100	-0.40753500
Cl	-0.57376900	-1.31886200	-1.85573600
C	2.39342700	-0.16698700	0.33464300
C	2.76793700	-1.39278400	-0.39111000
C	4.01654400	-1.19248500	-1.26651800
C	5.22894000	-0.81263500	-0.37387300
C	4.82037000	0.27586500	0.56836200
C	4.25452000	0.02508200	1.77818600
Cl	-1.37126500	2.54066900	-0.67611800
H	5.54893200	-1.69584100	0.19017000
H	6.06493600	-0.49435200	-1.00417200
H	3.82405700	-0.40509000	-2.00323100
H	4.23224200	-2.11346600	-1.81627800
H	2.90853000	-2.22477500	0.31040000
H	1.90707300	-1.65206400	-1.02504000
H	1.09120800	1.98227100	2.30708500
H	2.68404700	2.33754300	1.60075700
H	4.92445100	1.30806100	0.23568300
H	3.97661900	0.82305500	2.45819700
H	4.20077000	-0.98547300	2.17618700
Cl	-4.05259200	-0.06786400	-0.33491000
C	-4.10934100	-1.25525400	1.01527800
C	-2.78624000	-1.95522900	1.21707600
H	-4.85064000	-2.01683200	0.75363500
H	-4.43821300	-0.72915900	1.91261300

H	-2.83851800	-2.68663200	2.02556200
H	-2.39163500	-2.40669400	0.30673300
Cl	-1.46200000	-0.78027000	1.79127900
H	1.19905000	2.89943500	0.80638400

Me-10:

C	1.70394800	0.98674800	0.14436600
In	-0.25582500	0.29331800	-0.62425700
Cl	-1.56203300	2.07685200	-1.29493700
C	2.57962000	0.15181100	0.80466400
C	2.43001200	-1.35761600	0.95795500
C	3.40528900	-1.98716200	-0.05402000
C	4.68714300	-1.10179400	-0.06223100
C	4.26835800	0.31869900	0.21945100
C	3.86369600	0.72256800	1.53909000
Cl	-0.24116500	-1.76392700	-1.65889400
H	5.37394600	-1.42882500	0.72793800
H	5.21126000	-1.16908700	-1.01835300
H	2.94816000	-1.96343600	-1.04874000
H	3.64385600	-3.02774300	0.18087900
H	2.66895300	-1.65756700	1.98463000
H	1.40555400	-1.68473100	0.76054200
H	4.35754200	1.07467600	-0.55518100
H	3.82016400	1.78077100	1.77818900
H	4.14055700	0.08746000	2.37755200
C	1.95610800	2.43657400	-0.11689600
H	2.92289800	2.82457700	0.21750800
H	1.16175200	3.02653500	0.36375300
H	-3.95228900	-1.41291600	2.18682200
C	-4.05437700	-0.61253400	1.45241900
C	-3.15295700	0.55995300	1.75874200
H	-5.08591500	-0.24621000	1.46393100
Cl	-3.74120400	-1.30784400	-0.17596000
H	-3.17002200	1.33328400	0.99041100
H	-3.36027100	0.98108800	2.74400900
Cl	-1.36838900	0.03908000	1.88047700
H	1.84568600	2.65534600	-1.18821300

Me-TS2:

C	1.75502400	0.86928900	-0.56213200
In	-0.26106900	0.67324800	0.28999900
C	2.68275100	-0.26296300	-0.63073900

C	2.50779900	-1.66924300	-0.09310700
C	3.86048000	-2.02220200	0.57085700
C	4.89271000	-1.07534400	-0.08830100
C	4.06390700	0.07441600	-0.60462300
C	2.94220800	0.96267600	0.49523500
Cl	-1.48459300	2.60168000	0.06770700
Cl	-0.37971800	-0.71824400	2.15203600
H	5.69139100	-0.75124800	0.58551700
H	5.38236300	-1.53814400	-0.95642700
H	4.12120300	-3.07465600	0.44440700
H	3.80429800	-1.83218600	1.64736800
H	1.64738400	-1.78053700	0.57074600
H	2.31878400	-2.28878400	-0.98249800
H	4.50613000	0.86669800	-1.19859000
H	3.44083900	1.92478500	0.41982300
H	2.83331700	0.57143200	1.50252900
C	1.83471000	1.97973700	-1.61511700
H	2.85350800	2.17203200	-1.97193700
H	1.43080000	2.91575900	-1.21803100
H	-4.18460000	-1.58102900	-1.74560600
C	-3.87517700	-1.74341300	-0.71197300
C	-2.46373900	-2.27288100	-0.61824900
H	-4.53444600	-2.48888300	-0.25552300
Cl	-4.09027100	-0.20215000	0.18512000
H	-2.09299900	-2.33885300	0.40487900
H	-2.35870700	-3.22731600	-1.13706000
Cl	-1.25128900	-1.16867600	-1.50397600
H	1.22892100	1.70698200	-2.48574900

Me-11:

C	-3.05907400	-1.25740100	-0.00782500
C	-3.03912600	0.20527300	-0.46692000
C	-3.92844200	0.93952100	0.27346100
C	-4.65704000	0.10230400	1.26555200
C	-4.38517200	-1.34693300	0.79128600
C	-2.41682700	0.68471200	-1.82376200
C	-1.52248600	1.13366100	-0.78652900
H	-3.01313700	1.42033200	-2.36557000
H	-2.14992600	-0.18977800	-2.41678100
H	-4.08328400	2.00992700	0.17566300
H	-4.23653000	0.30312800	2.26620100
H	-5.71772200	0.37248600	1.33242000
H	-4.32439900	-2.05757300	1.61769300

H	-5.19507500	-1.67177000	0.13080800
H	-3.00950500	-1.96243400	-0.84124300
H	-2.21350000	-1.47803000	0.65796000
In	0.13696800	-0.15768900	-0.11097200
Cl	0.39216800	-1.96250800	-1.51753500
Cl	0.37693200	-0.15799200	2.19178400
C	-1.47808300	2.59725100	-0.42841300
H	-2.35916600	3.16114000	-0.75555900
H	-0.62089000	3.02292200	-0.97081500
H	2.88469500	1.17607400	1.57501000
C	3.44704800	1.40299000	0.66906100
C	4.47437800	0.35362300	0.31665500
H	3.88922300	2.39950500	0.71946300
Cl	2.16069600	1.57625600	-0.67092300
H	4.95305700	0.55310500	-0.64325600
H	5.23481400	0.36249200	1.10419500
Cl	3.77256300	-1.30032300	0.25544400
H	-1.30123400	2.77286000	0.63699100

Me-TS3:

C	-2.99116100	-1.10987000	0.35648000
C	-2.91105300	0.33463500	-0.09164800
C	-4.13338800	0.92817200	-0.08523100
C	-5.19396900	0.01397400	0.44945700
C	-4.51628500	-1.38298800	0.46722400
C	-1.92231700	1.01482000	-1.85575900
C	-1.64075000	1.11602800	-0.48262200
H	-2.02786900	1.88661000	-2.50846500
H	-2.05642500	0.04668500	-2.33357900
H	-4.32175500	1.96760200	-0.33689700
H	-5.50249900	0.34904600	1.45109500
H	-6.10157900	0.04369800	-0.16643700
H	-4.76406500	-1.95440200	1.36398200
H	-4.84924100	-1.96876900	-0.39424500
H	-2.49740000	-1.80522700	-0.33296500
H	-2.47885800	-1.20857800	1.32825200
In	0.16308800	-0.20892000	0.01866900
Cl	0.28778900	-2.01622200	-1.39832800
Cl	0.58470100	-0.06211000	2.28011900
C	-1.42551900	2.50658700	0.12305500
H	-2.26645100	3.17541700	-0.09220200
H	-0.52426600	2.97390700	-0.28603800
H	3.03137700	1.30236300	1.34425700

C	3.49817000	1.43999800	0.36883400
C	4.47717600	0.34862800	0.00745400
H	3.94822000	2.43071300	0.28471500
Cl	2.08042800	1.51523800	-0.84354500
H	4.86008200	0.45826600	-1.00819000
H	5.31168900	0.40980800	0.71342500
Cl	3.75985800	-1.29419400	0.15621800
H	-1.31489000	2.44393500	1.20917500

Me-TS$_a$:

C	-4.09103000	-0.15612000	-1.29168600
C	-3.17110900	0.36409200	-0.20127200
C	-3.09206200	-0.49328300	0.83932300
C	-3.91671100	-1.72978800	0.60302000
C	-4.26351300	-1.64947900	-0.90645500
C	-2.56572700	1.71204700	-0.19792200
C	-1.21445600	1.95014700	0.15992900
H	-3.25148700	2.56898900	-0.24576600
H	-1.85212400	1.85432700	-1.17458000
H	-2.59228300	-0.28947900	1.78425000
H	-3.38309800	-2.64696800	0.87703400
H	-4.81157400	-1.69266200	1.24146000
H	-3.55141200	-2.25362900	-1.47704500
H	-5.26551300	-2.02273400	-1.12868900
H	-5.04542000	0.38994200	-1.26770400
H	-3.67625600	-0.02652200	-2.29788100
In	0.06608100	0.11484000	0.24060200
Cl	0.03878600	-1.01367600	-1.77845000
Cl	0.37454400	-0.66066800	2.37795900
C	-0.75084300	3.33541500	0.44434400
H	-1.48638200	4.11213800	0.20666600
H	0.21171400	3.56614700	-0.02261300
Cl	2.39770200	1.48611100	-0.26700000
C	3.45788200	0.44493100	-1.39407600
C	4.36935200	-0.46925500	-0.61026100
H	4.02304100	1.18698800	-1.96064500
H	2.75388600	-0.08633200	-2.03453600
H	5.01657400	-0.98123700	-1.32968200
H	4.99012500	0.07894800	0.09995500
Cl	3.46477800	-1.72947100	0.29906500
H	-0.57721100	3.36366900	1.53383800

Me-TS$_b$:

C	-3.82338400	-0.73908300	-0.95766100

C	-3.03681400	0.36885100	-0.29043100
C	-2.85922800	0.11680400	1.03153400
C	-3.50800400	-1.18079700	1.44914400
C	-3.81514300	-1.87555100	0.09624100
C	-2.56529100	1.61069300	-1.02203400
C	-1.19996000	1.98551400	-0.47774800
H	-3.29792500	2.42601900	-0.93733300
H	-2.46524100	1.37344300	-2.08886800
H	-2.44209100	0.81711000	1.75401500
H	-2.87753300	-1.78093500	2.11371000
H	-4.42326000	-0.95161800	2.01412400
H	-3.01542000	-2.58353000	-0.14472500
H	-4.75316200	-2.43446300	0.11590400
H	-4.84090800	-0.37366100	-1.16392000
H	-3.39485200	-1.04211100	-1.91924800
In	-0.15940500	0.05272800	0.05207100
Cl	-0.17204900	-1.45169300	-1.68462700
Cl	0.51752300	-0.22931500	2.24394000
C	-0.91232500	3.27080900	-0.04526300
H	-1.63605000	4.08923600	-0.10874000
H	-0.47969100	2.63816400	-1.24242900
Cl	3.53032600	-1.78628300	-0.28218200
C	4.47747900	-0.27278200	-0.07461500
C	3.67275200	0.83472000	0.56522200
H	4.86931800	0.01686600	-1.05083100
H	5.31541300	-0.49683200	0.59333800
H	3.17429800	0.52967900	1.48517000
H	4.28098900	1.72677300	0.72460500
Cl	2.30904500	1.42192700	-0.55309700
H	0.07411800	3.51830000	0.34886600

M9

C	-3.15220800	2.90394200	0.81087600
C	-2.08396000	2.85861400	1.61014400
C	-2.95426900	0.36737400	-1.17249000
C	-2.69805700	1.54738200	-2.01494500
C	-3.63988900	2.73977700	-1.70694500
C	-3.20429600	3.61446600	-0.51517000
C	-3.37463400	-0.61969900	-0.58564700
In	-0.77994200	-0.97905200	0.06511900
Cl	0.51122900	1.02243000	-0.70051400
Cl	-0.79461300	-2.72404100	-1.45600600
Cl	-1.45982000	-0.95339600	2.27912800

H	-2.22363700	4.05907200	-0.73009600
H	-3.91623400	4.45093900	-0.44903000
H	-4.65986200	2.36651200	-1.55424900
H	-3.66920500	3.36873700	-2.60486900
H	-1.65665600	1.87313100	-1.93102400
H	-2.83636100	1.22993700	-3.05675600
C	-4.12295400	-1.73458600	0.02791800
H	-4.07339100	2.41145500	1.12678000
H	-2.10458100	2.34293000	2.56575700
H	-1.14735800	3.34223800	1.33932600
H	-4.56677200	-2.31864500	-0.78835600
H	-3.44871800	-2.41588700	0.55635600
C	-5.21155800	-1.23835500	0.99697000
H	-5.76423400	-2.09519300	1.39517300
H	-4.76442300	-0.69589300	1.83448500
H	-5.91986600	-0.57692700	0.48848100
Cl	1.81874600	-1.71395100	0.88893800
In	2.86694900	0.26560900	0.02649000
Cl	4.08415300	-0.04359500	-1.89795800
Cl	3.55435800	1.76448400	1.62846600

M10

C	-0.74978600	0.80679900	-0.57100300
In	1.18015700	-0.21599400	0.01404500
Cl	1.50600200	-2.08677300	-1.37809500
C	-1.92236000	0.08569700	-0.79524900
C	-2.07828500	-1.41664100	-0.54719600
C	-2.86211600	-1.53322500	0.77205500
C	-3.90313000	-0.38137400	0.75310200
C	-3.28012200	0.76704200	-0.01970400
C	-3.19146500	0.73434900	-1.46268200
Cl	2.84930600	1.41797800	-0.28238400
Cl	0.76461600	-0.79470800	2.27193500
H	-4.82082000	-0.70050900	0.24324900
H	-4.17521200	-0.06254500	1.76286600
H	-2.17053600	-1.38150200	1.60770500
H	-3.33833300	-2.51009300	0.89969800
H	-2.62713900	-1.87787100	-1.37725100
H	-1.11001900	-1.91887900	-0.50086800
H	-3.07384700	1.70194900	0.48961500
H	-3.02398100	1.65931500	-2.00530200
H	-3.77654900	-0.00514600	-2.00321700
C	-0.68261500	2.29627200	-0.66332300

C	-0.39390400	2.95383900	0.71295100
H	-1.57467800	2.75850100	-1.10499800
H	0.17044500	2.53572200	-1.31472000
H	-0.35781300	4.03963600	0.58410300
H	-1.17300700	2.71821900	1.44515600
H	0.56777200	2.62990400	1.11730500

M11

C	-2.43280100	-1.33301700	-0.41163700
C	-2.17853700	0.07365400	-0.93287800
C	-2.87609700	0.99239600	-0.21379500
C	-3.68504900	0.35654300	0.87728000
C	-3.65997000	-1.15185700	0.51959900
C	-1.22722300	0.37602600	-2.09601600
C	-0.38116700	0.95665600	-1.05504100
H	-1.63904900	1.05981500	-2.84474400
H	-0.86997600	-0.55768200	-2.53346500
H	-2.85784900	2.06354000	-0.38217800
H	-3.19408700	0.55401500	1.84207400
H	-4.69464100	0.77862300	0.94895100
H	-3.59910900	-1.78668000	1.40623500
H	-4.57691400	-1.41657900	-0.01744300
H	-2.61980900	-2.02733700	-1.23783700
H	-1.56944300	-1.72589900	0.13453000
In	1.07618900	-0.29533400	0.11973800
Cl	1.13388400	-2.32926500	-1.07395300
Cl	3.07287200	0.93929800	0.01035400
Cl	0.19098900	-0.52594500	2.29604400
C	-0.29506800	2.44682600	-0.97798200
C	-0.12591300	3.08126300	0.40752800
H	-1.09097500	2.94140500	-1.55401100
H	0.63449500	2.62265300	-1.55559100
H	0.00836000	4.16295400	0.30950900
H	-1.00469200	2.89928200	1.03525500
H	0.74971200	2.68282500	0.92765500

MTS1

C	-0.59123100	2.38168100	-0.50242700
C	-0.68319000	0.88489000	-0.40303000
In	1.27538800	-0.22376200	-0.01026800
Cl	0.94389900	-1.15419400	2.13673000
C	-1.66346000	0.04555000	-0.50828900

C	-2.06657400	-1.35407800	-0.18209500
C	-3.15759200	-1.35119000	0.89686800
C	-4.36039800	-0.48052900	0.42345900
C	-3.82635900	0.77723000	-0.18404100
C	-3.31371100	0.80356300	-1.45395400
Cl	1.42804000	-1.90063000	-1.65269300
Cl	2.92904100	1.43370700	-0.14434100
H	-4.93022000	-1.04073400	-0.32743300
H	-5.02617400	-0.26534700	1.26450900
H	-2.73943500	-0.94236200	1.82254900
H	-3.49981100	-2.37005800	1.10524000
H	-2.39672100	-1.88934000	-1.08098500
H	-1.18177000	-1.87676800	0.19737400
H	0.25895100	2.65030200	-1.13883700
H	-1.49425300	2.79148200	-0.97478800
H	-3.73762100	1.66488600	0.43941800
H	-2.96035000	1.72600500	-1.90069600
H	-3.49619000	-0.01705800	-2.14284400
C	-0.39811500	3.03709200	0.87969600
H	-1.22061700	2.78546100	1.55791200
H	0.53940800	2.71598800	1.34200900
H	-0.36209000	4.12559100	0.76775600

MTS2

C	3.30760800	1.02239200	0.35538600
C	1.97495700	0.32181300	0.14825400
C	2.20793900	-1.13759400	0.01399200
C	3.68607900	-1.40661200	0.26644000
C	4.38108500	-0.04306300	0.03241900
C	1.77230900	-0.51090100	-1.32289100
C	0.76438100	0.79373500	-0.38306500
C	0.69846300	2.22620900	-0.87871800
In	-1.20804500	-0.21624500	0.06699000
Cl	-2.87017400	1.43015600	-0.07278800
Cl	-0.92085700	-1.19615700	2.19356900
Cl	-1.41274700	-1.87702700	-1.62099500
H	0.89883800	-0.97709800	-1.77632400
H	2.51556400	-0.13916300	-2.02284900
H	1.47411400	-1.83914900	0.40444700
H	3.80012400	-1.73216800	1.30682900
H	4.08698500	-2.20142100	-0.36969800
H	5.27858500	0.07622700	0.64467300
H	4.69567700	0.05187200	-1.01271500

H	3.41850600	1.94953700	-0.21260400
H	3.32960400	1.29031300	1.42087200
H	-0.12297300	2.32410000	-1.59611200
H	1.62216200	2.50567300	-1.40452900
C	0.45509300	3.20630000	0.28758600
H	-0.48927800	2.99031300	0.79532900
H	1.26416200	3.16571700	1.02550700
H	0.39886300	4.22903800	-0.09812000

MTS$_{cis-a}$

C	-3.61900800	0.72783300	-0.82227800
C	-2.38287500	0.66568100	0.05774600
C	-2.39677400	-0.41123400	0.86312700
C	-3.62630800	-1.25128700	0.64921600
C	-4.55592300	-0.33149400	-0.18639000
C	-1.34121300	1.70368700	0.03684000
C	0.05415700	1.50494500	0.16806400
H	-1.71740600	2.73324100	0.06475200
H	-0.67563600	1.63657900	-1.01971000
H	-1.61953100	-0.67297300	1.57523600
H	-3.34141000	-2.16018300	0.09840400
H	-4.08087800	-1.58550300	1.58876200
H	-5.13242100	-0.88189100	-0.93460100
H	-5.27117800	0.16460800	0.47892700
H	-4.07150600	1.72756800	-0.85860600
H	-3.35121500	0.46436800	-1.85579300
In	1.08722400	-0.50874800	-0.05730200
Cl	-0.05015000	-1.55748000	-1.83525100
Cl	3.28470700	0.11505200	-0.61596200
Cl	0.94904200	-1.58429400	2.03231400
C	0.95920000	2.68836500	0.38287900
C	0.38997800	4.10893500	0.31405400
H	1.83610600	2.58016100	-0.26731700
H	1.36738400	2.49558800	1.39117900
H	1.18894900	4.82981800	0.51135700
H	-0.01584000	4.33811400	-0.67880200
H	-0.39799400	4.28084400	1.05575000

MTS$_{cis-b}$

C	2.51055700	-1.20646000	0.20554400
C	2.59036700	0.28702700	0.46818000
C	3.74140700	0.80350600	0.01707700

C	4.62881400	-0.23931900	-0.62011500
C	3.96691200	-1.57353800	-0.18141800
C	1.49297000	1.07878300	1.14713500
C	0.26268500	1.27767600	0.27718700
H	1.89771700	2.03112700	1.50813300
H	1.13747200	0.52511300	2.02822300
H	4.01827700	1.85419600	0.07906000
H	4.63429100	-0.12424800	-1.71482600
H	5.67429500	-0.16124300	-0.29722700
H	4.01286800	-2.34390200	-0.95614500
H	4.48943700	-1.96328200	0.69909200
H	2.14960400	-1.76515800	1.07788400
H	1.80956900	-1.42633100	-0.61176100
In	-1.29100000	-0.36430200	-0.01233000
Cl	-1.17532900	-1.58294400	1.98347500
Cl	-3.22582000	0.94993700	-0.33053200
Cl	-0.71962700	-1.51166300	-1.98396900
C	-0.05932300	2.53786500	-0.24337300
C	0.63188800	3.85424100	-0.04551600
H	-0.98459100	2.58665000	-0.82493900
H	0.55785900	1.55582400	-0.94013100
H	0.68223500	4.40864500	-0.98781300
H	0.00574800	4.44470700	0.63788400
H	1.62975200	3.76938700	0.38596100

$MTS_{cis\text{-}c}$

C	-2.95883700	0.93017000	-0.90944100
C	-2.29055200	0.75895600	0.44255000
C	-2.81681100	-0.26476700	1.12602100
C	-3.91646700	-0.96066200	0.36419400
C	-3.78703000	-0.37205900	-1.06708100
C	-1.20859100	1.69173400	0.92603500
C	0.10599200	1.52593500	0.19225200
H	-0.95894900	1.44859200	1.96957900
H	-1.56607000	2.73186100	0.92116700
H	-2.51248300	-0.56009400	2.12674400
H	-3.80864500	-2.05157100	0.37688300
H	-4.89437300	-0.73887900	0.81808900
H	-3.22918400	-1.07315400	-1.69426200
H	-4.75655300	-0.19676900	-1.54261600
H	-3.59171900	1.83208300	-0.91298600
H	-2.23981900	1.05278200	-1.73247600
In	1.00068500	-0.55681700	-0.00561800

Cl	-0.11957800	-1.77287400	-1.67027300
Cl	3.17711900	0.04445600	-0.73041600
Cl	0.88049600	-1.38467800	2.18560800
C	0.87985700	2.62026000	-0.21403900
C	0.63262000	4.08504500	-0.00573500
H	0.07581700	1.91809300	-1.03511300
H	1.83619600	2.36657000	-0.68264000
H	0.89480900	4.65562300	-0.90188800
H	-0.38666200	4.32332900	0.30182300
H	1.31633200	4.41052100	0.79079700

MTS$_{trans-a}$

C	-3.69169900	0.71135100	-0.97765600
C	-2.41842800	0.81195000	-0.15586300
C	-2.44384800	-0.01092100	0.90741900
C	-3.72035700	-0.80475800	0.96803500
C	-4.64500500	-0.08666700	-0.05061200
C	-1.32899100	1.74158000	-0.49371900
C	0.06213100	1.52745400	-0.33278300
H	-1.65030900	2.76393700	-0.74170500
H	-0.72407700	1.35506400	-1.50380100
H	-1.64523100	-0.12054400	1.63527500
H	-3.50753300	-1.84284700	0.67199300
H	-4.14414400	-0.84996700	1.97776900
H	-5.28198300	-0.78120600	-0.60465700
H	-5.30341100	0.60822700	0.48221700
H	-4.09810900	1.69097700	-1.26163200
H	-3.48819600	0.17106800	-1.91349700
In	1.03008800	-0.50862600	-0.04547200
Cl	-0.18375200	-1.88329500	-1.52542500
Cl	3.24009300	-0.10505200	-0.73724700
Cl	0.88300400	-1.07299300	2.23443200
C	0.96563500	2.71868800	-0.47012000
C	1.44912200	3.10679100	0.95086800
H	0.45256000	3.57612400	-0.92840800
H	1.84264400	2.46304400	-1.07343800
H	2.10895200	3.97576200	0.87246300
H	0.60998300	3.36780900	1.60392900
H	2.01428200	2.29520800	1.41825700

MTS$_{trans-b}$

C	-3.64493900	-0.38394800	-1.05128000

C	-2.46135400	0.46357700	-0.62347000
C	-2.50808000	0.74449300	0.68702800
C	-3.72228700	0.14431400	1.35495500
C	-4.60997700	-0.28389800	0.15654900
C	-1.38346200	0.83131600	-1.61781900
C	-0.10484000	1.19357400	-0.89164100
H	-1.73501900	1.64696200	-2.27221700
H	-1.19799700	-0.03699900	-2.26243100
H	-1.74959400	1.28048600	1.25081300
H	-3.42274200	-0.71461700	1.97274500
H	-4.22995600	0.84702200	2.02716600
H	-5.14826300	-1.21771300	0.34186600
H	-5.35922400	0.49188700	-0.03782500
H	-4.10008600	-0.03495200	-1.98790500
H	-3.31140600	-1.41657100	-1.23015100
In	1.08300600	-0.46746600	0.09021700
Cl	0.11189600	-2.46169400	-0.65680200
Cl	3.22804900	-0.03692500	-0.81994400
Cl	0.99645100	-0.03624700	2.39992300
C	0.18853300	2.55052500	-0.72647200
C	1.32353900	3.12591300	0.06016400
H	-0.49306000	3.28013800	-1.18362400
H	0.73350700	1.70382900	-1.67735000
H	1.73132000	4.01927800	-0.42189300
H	0.91211000	3.43140300	1.03283300
H	2.12157700	2.40321400	0.24524400

$MTS_{trans\text{-}c}$

C	-2.70047100	-0.92985500	0.25313000
C	-2.69821800	0.28872500	-0.65406100
C	-3.86040600	0.95213000	-0.59030000
C	-4.84236400	0.30543000	0.35734100
C	-4.19397100	-1.07578300	0.64669000
C	-1.50463200	0.70383700	-1.48495700
C	-0.31120300	1.13314200	-0.62958800
H	-1.79436800	1.51413200	-2.16789100
H	-1.17113300	-0.14412700	-2.09762000
H	-4.08425500	1.86445600	-1.13929900
H	-4.95155400	0.90960200	1.27110700
H	-5.84791900	0.21552400	-0.07185800
H	-4.32515200	-1.39524400	1.68433300
H	-4.66185400	-1.83553400	0.01144100

H	-2.30379500	-1.82171500	-0.24524700
H	-2.06043300	-0.76787500	1.13415000
In	1.24650100	-0.38410700	0.03605500
Cl	0.64616600	-2.39861200	-0.99088500
Cl	3.28364500	0.50670800	-0.72524700
Cl	1.00505700	-0.27102800	2.38428900
C	-0.15739500	2.50073800	-0.38894000
C	0.95396900	3.16093400	0.36782500
H	-0.73003600	1.60632100	0.46797000
H	-0.90090600	3.18109400	-0.82528200
H	0.58523800	4.01237000	0.94761100
H	1.49712100	2.47249700	1.01870600
H	1.66587900	3.54380200	-0.37632700

syn-M9

C	3.15558200	0.31238700	1.07593400
C	2.46027900	-0.23740900	2.07432500
C	1.00942300	0.55944200	-1.31601600
C	1.99056500	-0.42303800	-1.80690500
C	3.45789000	-0.08561100	-1.44302000
C	3.86710300	-0.45735200	-0.00462800
C	0.25798900	1.49005500	-1.05336900
In	-1.02283800	-0.46401200	0.10166700
Cl	-0.09258900	-2.59673700	0.17419400
Cl	-2.83456200	-0.22909200	-1.34332100
Cl	-1.26525900	0.64098700	2.13739500
H	3.71512700	-1.53327600	0.15004100
H	4.94956100	-0.27898900	0.08125000
H	3.64680800	0.97851000	-1.63147200
H	4.09382400	-0.64409400	-2.14042900
H	1.73900500	-1.42402000	-1.43901700
H	1.88081000	-0.45715300	-2.89880300
C	-0.49275600	2.74506400	-0.85212900
H	3.24631000	1.39919500	1.02557300
H	1.97788500	0.36609200	2.83756100
H	2.34512000	-1.31556400	2.16417600
H	-0.51592100	3.25617600	-1.82367000
H	-1.53736700	2.52481400	-0.60587400
C	0.13006200	3.65472400	0.22224800
H	-0.44806200	4.58154300	0.29097500
H	0.11636700	3.16555300	1.19944700
H	1.16372200	3.91052600	-0.03060200

syn-MTS1

C	2.66369000	-1.35633600	0.41859800
C	2.12528600	-1.72234500	-0.76852700
C	1.78437200	0.73516500	-0.72684500
C	3.20680600	1.07610600	-0.87370200
C	4.05113900	0.70984800	0.35584300
C	4.06246600	-0.82973400	0.53767600
C	0.55404800	1.04888200	-0.60476900
In	-1.16769900	-0.27509600	0.04325600
Cl	-1.41856400	-1.97421300	-1.56782800
Cl	-3.02057500	1.16015500	0.10888900
Cl	-0.54480800	-1.11925300	2.15819400
H	4.69807100	-1.27382200	-0.23792100
H	4.49762200	-1.08156900	1.51041600
H	3.62663300	1.19383300	1.24224300
H	5.07377000	1.08136500	0.22954300
H	3.63357700	0.64238800	-1.78662800
H	3.20056300	2.17006200	-1.01016500
C	0.11160500	2.51582100	-0.84880100
H	2.04060500	-1.38551000	1.31097600
H	1.11251200	-2.10079300	-0.85979400
H	2.72730000	-1.75300800	-1.67483000
H	0.81858300	3.00681900	-1.52748300
H	-0.86411300	2.50242400	-1.34234100
C	0.01247600	3.29564600	0.46919300
H	-0.31012400	4.32149300	0.25959300
H	-0.72108700	2.84716900	1.14481200
H	0.97911100	3.33682200	0.98268500

D9

C	-2.10888700	0.53152500	2.31269900
C	-1.85628900	0.67201000	0.85870000
In	-1.46148400	-1.43521500	-0.34741200
Cl	-2.89703800	-1.66521800	-2.15033900
C	-1.69905300	1.17313900	-0.25481500
C	-1.51063500	1.77106100	-1.57972600
C	-2.17186900	3.16873800	-1.72033100
C	-1.50959600	4.28581300	-0.89175100
C	-1.77806400	4.21788500	0.58847900
C	-0.83955100	4.17079900	1.53792400
Cl	0.80283900	-1.33940500	-1.29744500
Cl	-1.61582300	-2.92104400	1.40595400
H	-0.42831400	4.29129000	-1.07632400
H	-1.89783100	5.24202400	-1.27276000
H	-3.23941200	3.09271300	-1.48030700

H	-2.10492100	3.42442100	-2.78386800
H	-0.43535900	1.84567700	-1.78481400
H	-1.94811000	1.10149800	-2.33100000
H	-1.44300500	-0.22594700	2.73516800
H	-1.80441500	1.49504800	2.74173700
H	-2.83011900	4.24686500	0.88040500
H	-1.09566200	4.16911100	2.59452800
H	0.22030100	4.14622500	1.29424000
C	-3.57611200	0.21791900	2.65060900
H	-4.24979400	0.97397100	2.23621500
H	-3.87185400	-0.76317800	2.26709700
H	-3.69900100	0.20359100	3.73785400
In	2.54171500	0.03041000	0.10702600
Cl	1.51095500	-0.12617900	2.19286200
Cl	2.29315200	2.12481300	-0.89132600
Cl	4.50571200	-1.11186200	-0.25911600

D10

C	-2.48541900	0.75113400	-0.77618200
In	-1.07035700	-0.89321600	-0.21501600
Cl	-1.69947700	-2.88355100	-1.25832800
C	-3.85392200	0.55374500	-0.62303700
C	-4.49043100	-0.65643200	0.06340100
C	-4.90715000	-0.16136300	1.45963200
C	-5.43489600	1.28571900	1.25941400
C	-4.64696500	1.89474100	0.11627300
C	-4.91700100	1.53218200	-1.25475600
Cl	1.02119500	-0.18370300	-1.32130100
Cl	-0.90330000	-0.91775700	2.10985200
H	-6.49878100	1.27010900	0.99214200
H	-5.32442700	1.88639000	2.16582400
H	-4.02348800	-0.13597100	2.10657600
H	-5.65446700	-0.80427300	1.93373200
H	-5.35789300	-1.00064900	-0.51189100
H	-3.80371400	-1.50477900	0.11229200
H	-3.98772300	2.73408400	0.30943000
H	-4.55243200	2.17001900	-2.05362800
H	-5.84349100	1.01122800	-1.48250000
C	-1.88809800	2.02321200	-1.28148600
C	-1.08882900	2.76904500	-0.17867300
H	-2.62218700	2.70951900	-1.72111300
H	-1.17605500	1.75760400	-2.07574600
H	-0.65229000	3.67386100	-0.61065100

H	-1.73303600	3.06231300	0.65649000
H	-0.27044500	2.16861600	0.22482000
Cl	4.61218500	0.89838700	-1.54972700
In	3.16161400	0.26947000	0.14401100
Cl	2.36857800	2.01236500	1.47477900
Cl	3.50111900	-1.77200200	1.17566500

D11

C	-4.14092900	-0.03693600	-1.45597200
C	-3.32202400	1.14520400	-0.96496500
C	-3.93081300	1.75692600	0.08020400
C	-5.22503700	1.09360500	0.44759000
C	-5.50835100	0.15263300	-0.75242500
C	-1.95005100	1.48934100	-1.55423600
C	-1.31578900	1.12258400	-0.28483700
H	-1.84706000	2.53221300	-1.86118600
H	-1.72642200	0.81406000	-2.38204400
H	-3.54177700	2.61259000	0.62125400
H	-5.07802000	0.53162900	1.38243800
H	-6.02814300	1.81493000	0.63962700
H	-5.94687700	-0.79800900	-0.44064300
H	-6.21353600	0.63376200	-1.43781100
H	-4.21882100	-0.02190700	-2.55349100
H	-3.67537800	-0.99721000	-1.20605900
In	-1.05717400	-0.99230600	0.34283300
Cl	-1.26895600	-2.58084700	-1.33895500
Cl	1.25378500	-1.15569300	1.30719900
Cl	-2.43647100	-1.29196500	2.21366200
C	-0.82030700	2.16468500	0.66710600
C	-0.89179700	3.64889000	0.29163000
H	0.24387800	1.89836700	0.80069300
H	-1.24082500	1.96854300	1.66432500
H	-0.42280200	4.24030600	1.08339000
H	-0.34394000	3.84889400	-0.63445800
H	-1.91735100	4.01297500	0.16973200
In	2.88773200	0.18285400	-0.13113000
Cl	3.08581900	2.13224600	1.13124200
Cl	4.73406000	-1.13035800	-0.51770300
Cl	1.39001600	0.57664300	-1.91543200

DTS1

C	-1.95758600	0.33814700	2.33104500
C	-1.69367800	0.51986700	0.85801800

In	-1.51316200	-1.37388500	-0.32708800
Cl	-2.84427200	-1.32514700	-2.24328700
C	-1.47878700	1.52810400	0.08712500
C	-1.44419500	2.05983000	-1.29658000
C	-2.47729300	3.18290200	-1.48061200
C	-2.18644000	4.32845500	-0.47280200
C	-1.94357200	3.73346900	0.88020900
C	-0.72515300	3.25089200	1.25167200
Cl	0.81726800	-1.26676100	-1.27435800
Cl	-1.65056300	-3.22075200	1.06391700
H	-1.29484000	4.87363700	-0.80241800
H	-3.02529700	5.03122400	-0.45164300
H	-3.48368100	2.78160700	-1.31754500
H	-2.43418900	3.56617600	-2.50498600
H	-0.43390500	2.39900400	-1.55337900
H	-1.69705100	1.22719200	-1.96663300
H	-1.26266700	-0.40669300	2.73152900
H	-1.75119100	1.27844000	2.85438300
H	-2.79122300	3.61525300	1.55385200
H	-0.55118900	2.82788000	2.23480400
H	0.16183100	3.41040600	0.64297000
C	-3.40730400	-0.09948800	2.60892900
H	-4.12634100	0.62433400	2.21084100
H	-3.62393700	-1.07898200	2.17089400
H	-3.56256500	-0.17995900	3.68954800
In	2.55523200	0.06127700	0.05563000
Cl	1.68401000	-0.00734900	2.22572600
Cl	2.31533100	2.21361400	-0.86066300
Cl	4.54286700	-1.02329900	-0.36973500

DTS2

C	-2.20302300	0.95710400	0.07894300
In	-1.11397800	-0.96788500	0.08051100
Cl	-2.29411000	-2.38017700	-1.40429400
C	-3.67175300	0.95722000	0.23746400
C	-4.61936200	-0.22165900	0.36592300
C	-5.84762000	0.15508800	-0.49517700
C	-5.81071300	1.69998500	-0.59358400
C	-4.37356600	2.04981000	-0.31352800
C	-2.94182500	1.23897400	-1.25938100
Cl	0.89463900	-0.38282200	-1.26697600
Cl	-0.56736700	-1.88128200	2.14141200
H	-6.16591000	2.09559800	-1.55040400

H	-6.41910900	2.17836800	0.18828300
H	-6.78441200	-0.21431500	-0.07262700
H	-5.74415500	-0.28637200	-1.49176000
H	-4.16918100	-1.17529900	0.08333400
H	-4.86847000	-0.27737200	1.43554500
H	-4.02826200	3.07669800	-0.27389800
H	-2.64995300	2.17551300	-1.72621300
H	-3.20829300	0.43436400	-1.93961900
C	-1.41675700	2.16637400	0.61270100
C	-1.29830000	2.15119900	2.14126800
H	-1.88157400	3.11233600	0.29407200
H	-0.41575000	2.15831300	0.16840600
H	-0.70061300	3.00253500	2.47901600
H	-2.28454800	2.21212100	2.61804700
H	-0.80226500	1.24391100	2.50004100
In	3.12709600	0.30983400	-0.12270900
Cl	4.19029300	1.27801800	-1.94273700
Cl	2.29738800	1.83265100	1.44673300
Cl	3.98370100	-1.66735600	0.71455000

$DTS_{cis\text{-}a}$

C	3.39218300	-2.76504100	-0.79142500
C	3.13625500	-1.61062600	0.15903300
C	4.03292200	-0.62115300	-0.00133200
C	5.02247300	-0.92947900	-1.09276400
C	4.79529800	-2.44083100	-1.36980400
C	2.05686800	-1.60132800	1.16364600
C	1.22603200	-0.49881000	1.43158000
H	2.03379100	-2.45391400	1.85114900
H	0.93604500	-1.63090200	0.60732200
H	4.06209800	0.29709400	0.58183700
H	4.79150200	-0.30861400	-1.97050300
H	6.05398400	-0.69666900	-0.80509400
H	4.87304800	-2.68822200	-2.43149800
H	5.55428600	-3.02685500	-0.84047700
H	3.35323400	-3.74212900	-0.29316900
H	2.61906900	-2.78033800	-1.57236800
In	1.16290200	1.24846000	0.04023500
Cl	1.68793300	1.05010300	-2.21101200
Cl	-1.31946100	1.74042700	0.06128100
Cl	2.17342600	2.98210400	1.23024900
C	0.34647300	-0.46582000	2.64772600
C	0.29463400	-1.69175200	3.56336800

H	-0.66872900	-0.17022700	2.35442700
H	0.72837000	0.41118500	3.20065200
H	-0.37184400	-1.48355600	4.40498800
H	-0.10802600	-2.56655700	3.04062700
H	1.27846900	-1.94774400	3.97204700
In	-2.72229600	-0.35227200	-0.31954900
Cl	-3.52275100	-0.74277500	1.83087500
Cl	-4.18037600	0.09539100	-2.03902600
Cl	-0.98840800	-1.91211900	-0.79435000

$DTS_{cis\text{-}b}$

C	3.30373700	2.96215800	-0.05392800
C	2.35919400	2.04124900	0.69758300
C	1.08894900	2.46092400	0.60354200
C	0.95858900	3.71356400	-0.22721400
C	2.34622100	3.82713100	-0.91252400
C	2.86437700	0.87057500	1.50952000
C	2.03479400	-0.38354000	1.40403900
H	3.05987300	1.16794000	2.54902000
H	3.84103000	0.55447500	1.10695900
H	0.23677700	2.00866200	1.10468200
H	0.13098800	3.65964900	-0.94339800
H	0.74686500	4.57451200	0.42462200
H	3.88511900	3.57140900	0.65601200
H	4.03022100	2.41036200	-0.66288000
In	1.48788400	-1.11058600	-0.63603600
Cl	0.89914500	-3.34719100	-0.30182200
Cl	-0.58309700	-0.04479700	-1.55206900
Cl	3.19658600	-0.59292300	-2.11970700
C	1.73402000	-1.19193600	2.50148100
C	2.12186100	-1.01190000	3.94094600
H	1.20273400	-2.12152300	2.28024500
H	0.84841000	-0.33926200	2.02769600
H	2.89272700	-1.75982900	4.16943700
H	2.52249200	-0.02321600	4.16963200
H	1.26679200	-1.22146000	4.59117800
In	-2.58727000	0.18066500	0.02386400
Cl	-1.50432000	-0.14704500	2.12418900
Cl	-3.16578600	2.40066900	-0.27737100
Cl	-4.05658000	-1.49873500	-0.53942200
H	2.68627400	4.86192400	-1.01133400
H	2.28802400	3.40348300	-1.92068400

$DTS_{cis\text{-}c}$

C	-4.59795600	0.98545500	-1.67865000
C	-3.56606900	1.25370900	-0.59988400
C	-4.04652000	0.97315800	0.62295500
C	-5.47118900	0.47580400	0.57507900
C	-5.91237000	0.80322300	-0.87757900
C	-2.16705000	1.72097200	-0.94917500
C	-1.20944600	1.19150100	0.08691900
H	-2.13777700	2.81248600	-1.06172100
H	-1.89136400	1.29440600	-1.92270200
H	-3.49566500	1.05820100	1.55656500
H	-5.50081600	-0.60332100	0.78297500
H	-6.10903900	0.95315600	1.32857500
H	-6.55747900	0.03080200	-1.30488300
H	-6.47743400	1.74168900	-0.88352900
H	-4.65681300	1.80105300	-2.41108000
H	-4.32188500	0.07997800	-2.23750100
In	-1.17463100	-1.02807100	0.23228000
Cl	-1.98314600	-2.01606500	-1.70791500
Cl	1.30124500	-1.65285900	0.25133200
Cl	-1.88447800	-1.77735900	2.31438900
C	-0.50756900	2.01719600	0.96698900
C	-0.58848900	3.51060400	1.12930500
H	0.06141700	1.64054100	-0.14237900
H	0.13539700	1.52626900	1.70122400
H	0.41904900	3.93668700	1.16500100
H	-1.16785400	4.00833400	0.35076700
H	-1.05863000	3.71166400	2.10027400
In	3.00853200	0.16032500	-0.16301400
Cl	3.00828900	1.28747200	1.88588700
Cl	4.91774300	-0.83886200	-0.95472200
Cl	1.77550400	1.52342900	-1.67552400

$DTS_{trans\text{-}a}$

C	0.03396100	3.60644900	0.89001400
C	-1.08221700	2.61197000	0.62174000
C	-1.63908700	2.79867800	-0.58700000
C	-0.98491800	3.92937000	-1.33766400
C	-0.13399900	4.64260500	-0.25199000
C	-1.49616000	1.61107100	1.63228400
C	-1.98362600	0.30703400	1.38696900
H	-1.69558300	2.02629500	2.63083800

H	-0.58900400	0.84211400	1.83975000
H	-2.46025600	2.21843600	-0.99893800
H	-0.36242200	3.52122600	-2.14748700
H	-1.71550200	4.59326700	-1.81433100
H	0.82705800	4.99367500	-0.63583600
H	-0.67838800	5.51680400	0.12133700
H	-0.03642100	4.06043800	1.88715900
H	1.01084700	3.10567900	0.84317200
In	-1.71439400	-0.86140300	-0.50469600
Cl	0.50499400	-0.29614400	-1.50636100
Cl	-1.65331200	-3.10240700	0.11155400
Cl	-3.30021300	-0.27529400	-2.10764300
C	-2.64899500	-0.42789300	2.50324200
C	-4.17128800	-0.48759600	2.19146300
H	-2.49539700	0.07195900	3.46832900
H	-2.26723400	-1.45285900	2.56711900
H	-4.66802600	-1.02062100	3.00702200
H	-4.60618600	0.51362300	2.11613600
H	-4.38022800	-1.02772700	1.26273100
In	2.52208500	-0.36968600	0.07878500
Cl	3.69360000	-2.28101500	-0.43254800
Cl	3.46959700	1.71211200	-0.30602500
Cl	1.35461900	-0.41543500	2.14856900

$DTS_{trans\text{-}b}$

C	4.36320400	2.10322300	0.47394000
C	2.99257000	1.57579900	0.85701200
C	2.01461700	2.29105700	0.28466300
C	2.55513200	3.40525200	-0.57963500
C	4.05090600	3.47565900	-0.17302900
C	2.86080500	0.37300100	1.75619100
C	1.61432800	-0.47207800	1.58067000
H	3.00188800	0.65947100	2.81146000
H	3.68787800	-0.32047100	1.53101600
H	0.94913900	2.10949800	0.38907700
H	2.42982700	3.15209600	-1.64244100
H	2.02869800	4.35424800	-0.42242600
H	4.70856000	3.70073400	-1.01729700
H	4.18890600	4.26937600	0.56964600
H	5.04126000	2.18677400	1.33402200
H	4.83884400	1.41059600	-0.23577700
In	1.29762800	-1.29493700	-0.47942100
Cl	0.52428700	-3.48877000	-0.38025800

Cl	-0.55161300	0.04729400	-1.54698200
Cl	3.19931100	-0.98718600	-1.77505700
C	0.90080800	-0.84364200	2.71981500
C	-0.25436800	-1.78647400	2.81971800
H	0.54413400	0.19450300	1.93374300
H	1.24111100	-0.42445900	3.67451600
H	-0.62319600	-2.13968600	1.85584600
H	0.09804200	-2.65981700	3.38609500
H	-1.07241400	-1.33565400	3.38983300
In	-2.59003000	0.56643800	-0.10216600
Cl	-3.80617200	2.06641200	-1.35203300
Cl	-3.45234600	-1.50273100	0.48173800
Cl	-1.46187700	1.50077500	1.77873200

$DTS_{trans\text{-}c}$

C	-4.52104300	1.57644600	-1.52650800
C	-3.60162100	1.46682900	-0.32507900
C	-4.19125200	0.80773600	0.68630600
C	-5.59439900	0.36952300	0.34101900
C	-5.90205000	1.15843100	-0.96031500
C	-2.18866700	2.00584400	-0.36752500
C	-1.30763400	1.19776400	0.56196900
H	-2.17168000	3.07910800	-0.12156400
H	-1.80451600	1.91098400	-1.39123100
H	-3.73387700	0.57456500	1.64473700
H	-5.62143500	-0.71790700	0.18125200
H	-6.31121100	0.58153700	1.14343300
H	-6.48839600	0.57625900	-1.67638000
H	-6.48246500	2.05438800	-0.71432700
H	-4.52707300	2.58598300	-1.95765900
H	-4.17358200	0.89863000	-2.31949300
In	-1.22505200	-0.96516000	0.06843200
Cl	-1.82746700	-1.37096400	-2.13483400
Cl	1.26204300	-1.55049800	0.17035800
Cl	-2.06870000	-2.29601700	1.78064100
C	-0.78655600	1.79266000	1.70519800
C	0.00401800	1.13017400	2.78928500
H	-0.98795300	2.85979500	1.85574000
H	-0.10287400	1.68638900	0.51750900
H	0.96457800	1.63303400	2.94605800
H	-0.57126500	1.23173300	3.71905400
H	0.17799000	0.06749800	2.60949400
In	3.01910300	0.23186400	-0.21865300

Cl	3.77358900	0.66962800	1.93728900
Cl	4.45648800	-0.55435500	-1.83037700
Cl	1.60760300	2.03615100	-0.89377500

syn-D9

C	-3.15220800	2.90394200	0.81087600
C	-2.08396000	2.85861400	1.61014400
C	-2.95426900	0.36737400	-1.17249000
C	-2.69805700	1.54738200	-2.01494500
C	-3.63988900	2.73977700	-1.70694500
C	-3.20429600	3.61446600	-0.51517000
C	-3.37463400	-0.61969900	-0.58564700
In	-0.77994200	-0.97905200	0.06511900
Cl	0.51122900	1.02243000	-0.70051400
Cl	-0.79461300	-2.72404100	-1.45600600
Cl	-1.45982000	-0.95339600	2.27912800
H	-2.22363700	4.05907200	-0.73009600
H	-3.91623400	4.45093900	-0.44903000
H	-4.65986200	2.36651200	-1.55424900
H	-3.66920500	3.36873700	-2.60486900
H	-1.65665600	1.87313100	-1.93102400
H	-2.83636100	1.22993700	-3.05675600
C	-4.12295400	-1.73458600	0.02791800
H	-4.07339100	2.41145500	1.12678000
H	-2.10458100	2.34293000	2.56575700
H	-1.14735800	3.34223800	1.33932600
H	-4.56677200	-2.31864500	-0.78835600
H	-3.44871800	-2.41588700	0.55635600
C	-5.21155800	-1.23835500	0.99697000
H	-5.76423400	-2.09519300	1.39517300
H	-4.76442300	-0.69589300	1.83448500
H	-5.91986600	-0.57692700	0.48848100
Cl	1.81874600	-1.71395100	0.88893800
In	2.86694900	0.26560900	0.02649000
Cl	4.08415300	-0.04359500	-1.89795800
Cl	3.55435800	1.76448400	1.62846600

syn-DTS1

C	-2.44377000	2.67780800	0.90982700
C	-1.38591600	2.54439900	0.07899900
C	-3.20356100	0.95197900	-0.91127800
C	-4.09068200	2.04754100	-1.30604800
C	-4.70698600	2.81977600	-0.13106400
C	-3.59613300	3.59238600	0.62076800

C	-2.85311500	-0.27064600	-0.83911900
In	-1.10485100	-1.14099100	0.25100700
Cl	0.70114700	-0.32575200	-1.23046200
Cl	-1.21816600	-3.44443600	-0.00960800
Cl	-0.93137100	-0.28041700	2.40216200
H	-3.26212700	4.43028900	-0.00236400
H	-4.00506500	4.01054300	1.54680300
H	-5.20909400	2.11662300	0.54260600
H	-5.46273100	3.51732500	-0.50723700
H	-3.59394200	2.72664600	-2.01000700
H	-4.88542800	1.53024800	-1.87143100
C	-3.69160200	-1.35364500	-1.57749400
H	-2.47781700	2.07139300	1.81325800
H	-0.54324200	1.90995900	0.32581900
H	-1.27296800	3.16469900	-0.80764700
H	-4.24584400	-0.88821700	-2.39991500
H	-2.99978400	-2.07765500	-2.01781400
C	-4.65610100	-2.06461500	-0.62025400
H	-5.22406600	-2.81923900	-1.17523700
H	-4.12052500	-2.57811400	0.18340800
H	-5.36568500	-1.36073900	-0.17288800
Cl	3.23628500	-1.31010200	1.46391800
In	2.97899900	0.36209700	-0.11632100
Cl	4.35565800	0.35014400	-1.97624900
Cl	2.36246400	2.46598600	0.68006400

Toluene

C	-1.20168900	1.20559600	0.00219100
C	0.19421500	1.20272200	-0.00896100
C	0.91406700	0.00022200	-0.01134300
C	0.19447200	-1.20259100	-0.00895900
C	-1.20130300	-1.20580100	0.00219000
C	-1.90550900	-0.00014200	0.00845800
H	-1.73929700	2.15044700	0.00153400
H	0.73436100	2.14716200	-0.01785400
H	0.73487100	-2.14690300	-0.01786500
H	-1.73874000	-2.15075000	0.00153000
H	-2.99224900	-0.00032500	0.01388800
C	2.42598600	0.00009800	0.00934700
H	2.81042300	-0.01295100	1.03840400
H	2.83472600	-0.87975700	-0.49968200
H	2.83447200	0.89245100	-0.47749100

T9

C	1.83782000	1.83048100	1.28492400
C	1.54816900	0.58883200	0.48870600
In	-0.63480600	0.50316400	-0.41266400
Cl	-1.05753800	-1.18844100	-1.92115700
C	1.95584100	-0.47373500	-0.00811100
C	2.30165000	-1.72932400	-0.65900800
C	3.67831200	-1.71426200	-1.37843800
C	4.87314700	-1.71062200	-0.40742200
C	4.96804700	-0.46361000	0.42761900
C	4.88277300	-0.42658700	1.76270300
Cl	-1.03349900	2.73023700	-0.86855600
H	4.82132700	-2.59357300	0.24250900
H	5.78770800	-1.81546600	-1.00681200
H	3.72454600	-0.85354300	-2.05547500
H	3.71588400	-2.61322000	-2.00275000
H	2.26710600	-2.54260200	0.07791600
H	1.51623100	-1.93903600	-1.39959300
H	0.91993500	2.24662100	1.71107400
H	2.46704300	1.50470200	2.12182000
H	5.14677500	0.46393200	-0.11906700
H	5.00091100	0.50023000	2.31801900
H	4.74033400	-1.33025400	2.35203300
C	2.55891600	2.90414000	0.45226200
H	3.49647400	2.51576100	0.04534900
H	1.93386000	3.25597300	-0.37243300
H	2.78776900	3.75912500	1.09580800
H	-0.48038100	-1.18827200	2.56077300
C	-1.40211900	-1.08388100	1.99629700
C	-2.12986000	-2.20569500	1.60155700
C	-1.89821700	0.20530300	1.68197300
C	-3.34043000	-2.05333700	0.92032200
H	-1.76563700	-3.20084900	1.83658500
C	-3.13755500	0.33953100	1.00016900
H	-1.45531300	1.08662800	2.14753000
C	-3.86652900	-0.78733000	0.60073900
H	-3.89633000	-2.94053100	0.62855500
H	-3.52697300	1.33558000	0.80687600
C	-5.16837200	-0.65744200	-0.14728500
H	-5.93139000	-1.32112100	0.27241200
H	-5.55025000	0.36642200	-0.11763700
H	-5.03604200	-0.93682900	-1.19987300

T10

C	-1.75724100	0.38439000	-0.55901400
In	0.27922800	0.85590100	0.23696400
Cl	0.59121000	3.16411600	0.20342600
C	-2.21568600	-0.91195400	-0.69624700
C	-1.54513100	-2.16529600	-0.14042700
C	-2.38854300	-2.59444100	1.07475800
C	-3.87773400	-2.32852500	0.70986400
C	-3.91642500	-1.13826500	-0.21785200
C	-3.49373200	-1.25165800	-1.58461400
Cl	0.87163400	-0.39010000	2.10768300
H	-4.29947400	-3.19631600	0.18821900
H	-4.48141500	-2.14387800	1.60155500
H	-2.11194000	-1.97412100	1.93372500
H	-2.22709200	-3.63991400	1.35114000
H	-1.52242500	-2.95277500	-0.90333900
H	-0.51303200	-1.97093200	0.15844000
H	-4.37529500	-0.21110100	0.10946300
H	-3.77498600	-0.47927800	-2.29361700
H	-3.40204400	-2.24564300	-2.01653300
C	-2.56256800	1.59688800	-0.91853800
C	-3.02455600	2.38621500	0.33792700
H	-3.43917800	1.36373300	-1.53398400
H	-1.92634600	2.27240600	-1.50649900
H	-3.61718900	3.24559700	0.01254400
H	-3.64490400	1.77202000	0.99830100
H	-2.17667700	2.76748600	0.91229700
H	1.35216000	1.01446400	-2.31316600
C	1.87576200	0.32667700	-1.64897300
C	1.65328400	-1.06806200	-1.75320900
C	2.99585500	0.78833800	-0.91177400
C	2.48797700	-1.95976300	-1.08875900
H	0.84421800	-1.43853200	-2.37681800
C	3.81972900	-0.11955300	-0.25466800
H	3.20602300	1.85253300	-0.86644700
C	3.57873300	-1.50315600	-0.32523000
H	2.31077800	-3.02827400	-1.17371300
H	4.66943300	0.24546100	0.31472100
C	4.45935400	-2.47217200	0.41615800
H	5.48055100	-2.09267900	0.51411700
H	4.07023600	-2.62825800	1.43120500
H	4.49362700	-3.44740100	-0.07813000

T11

C	-3.02279800	-1.34009900	0.40414800
C	-3.01481800	-0.03844700	-0.40264800
C	-3.81070200	0.89613000	0.20310200
C	-4.46438000	0.36372600	1.43368700
C	-4.26469000	-1.16799700	1.31729900
C	-2.44699100	0.09048200	-1.84470600
C	-1.47430800	0.78933500	-1.03199700
H	-3.07281900	0.67134400	-2.52482000
H	-2.19350300	-0.89992600	-2.22268600
H	-3.96329900	1.90915200	-0.15580800
H	-3.95614600	0.78560900	2.31677200
H	-5.51070600	0.68205600	1.51253900
H	-4.13490900	-1.65061500	2.28796900
H	-5.14213700	-1.61358600	0.83834200
H	-3.07872100	-2.22387500	-0.23606300
H	-2.11851200	-1.44043100	1.01675700
In	0.24079100	-0.36833900	-0.20596100
Cl	0.11778300	-2.48191600	-1.19790800
Cl	0.52072500	-0.17092300	2.08939100
C	-1.44129800	2.29623400	-1.07704200
C	-1.11330700	3.02690500	0.22886500
H	-2.35449600	2.70273900	-1.53313700
H	-0.64986800	2.50421300	-1.81895200
H	-1.01168400	4.10104600	0.04800000
H	-1.90718600	2.88481000	0.97030400
H	-0.18199700	2.66942700	0.68010000
H	1.77256300	2.55202200	-1.49846500
C	2.30845900	1.78643800	-0.94534500
C	2.30461100	0.44713400	-1.40058000
C	3.05361900	2.12047700	0.18421200
C	3.08644600	-0.52655100	-0.72829700
H	1.88111100	0.20343600	-2.37562100
C	3.80319200	1.14309500	0.84425900
H	3.06896000	3.14491800	0.54309200
C	3.83540100	-0.19279600	0.40760400
H	3.11021300	-1.54164600	-1.11468200
H	4.38358300	1.42411900	1.71905700
C	4.64012200	-1.23057000	1.14722800
H	5.60876800	-0.83003500	1.46264500
H	4.10811000	-1.55240700	2.05131900
H	4.81792900	-2.11647300	0.53150600

TTS1

C	1.37014900	2.29123400	-0.29031700
C	1.43121400	0.81686300	0.05061700
In	-0.45732600	-0.28775200	-0.47799400
Cl	-0.13555700	-2.56172000	-0.87509300
C	2.34282100	0.05175700	0.54789100
C	2.82254600	-1.32633100	0.80005800
C	4.11609900	-1.63125100	0.02908900
C	5.23761900	-0.64400200	0.46404500
C	4.67501700	0.73926000	0.46668300
C	3.96749300	1.23770200	1.52021300
Cl	-1.71207900	0.98872500	-1.94040800
H	5.57925500	-0.91262900	1.46990000
H	6.08877100	-0.72616700	-0.21807500
H	3.92843700	-1.54215900	-1.04605600
H	4.43397300	-2.65943500	0.22594900
H	2.95968300	-1.49960800	1.87503000
H	2.02989000	-2.00544000	0.45616500
H	0.35636900	2.66990700	-0.12359700
H	2.02629300	2.84691600	0.38851500
H	4.75812800	1.33377900	-0.44180400
H	3.58928800	2.25362600	1.51770400
H	3.94705300	0.71964900	2.47580500
C	1.77377000	2.56640700	-1.75142400
H	2.79090000	2.21726900	-1.95585900
H	1.09241200	2.07786700	-2.45381000
H	1.73511300	3.64313800	-1.94248200
H	-0.72531000	1.32007200	2.52318200
C	-1.59628100	0.90842600	2.02181800
C	-1.65495700	-0.47424300	1.72615500
C	-2.68376900	1.71935900	1.69839800
C	-2.81956600	-1.02105200	1.13420800
H	-0.89671800	-1.14878200	2.12430900
C	-3.81965500	1.16409800	1.10400900
H	-2.65662200	2.78140700	1.92156700
C	-3.91085300	-0.20714800	0.80537800
H	-2.86433700	-2.09033900	0.94655700
H	-4.65953200	1.81066100	0.86393900
C	-5.13854800	-0.77438100	0.14020800
H	-6.05198800	-0.33409100	0.55240800
H	-5.12497300	-0.55516800	-0.93484100
H	-5.19586700	-1.85988900	0.25854500

TTS2

C	-1.77441100	0.75489500	0.15768700
In	0.37124500	0.68168900	-0.37544900
C	-2.55945400	-0.46371500	0.41102900
C	-2.11386400	-1.91430500	0.34629400
C	-3.26483400	-2.65902400	-0.37130800
C	-4.51115000	-1.76545200	-0.16268600
C	-3.94198600	-0.39775700	0.10820000
C	-2.71156600	0.35811000	-1.04560200
Cl	1.11422100	2.83860800	-0.83206300
Cl	0.68246500	-1.00666500	-1.96603500
H	-5.21212400	-1.77379700	-1.00286100
H	-5.08656000	-2.05870300	0.72729400
H	-3.40849400	-3.67095500	0.01236200
H	-3.03762300	-2.74739100	-1.43843100
H	-1.14048700	-2.05024200	-0.12968600
H	-2.02083600	-2.23324300	1.39478100
H	-4.57837500	0.44725300	0.34610200
H	-3.36554800	1.17647300	-1.33415300
H	-2.35720300	-0.26818900	-1.85947500
C	-2.20185800	2.07691600	0.81708500
C	-1.65512800	2.23044500	2.24086500
H	-3.29677900	2.16874400	0.84577700
H	-1.84060800	2.90316500	0.19424800
H	-2.00050100	3.17145100	2.67888700
H	-1.98739100	1.41455800	2.89336500
H	-0.55913100	2.25704500	2.25280400
H	0.42329800	-0.75825800	2.73201500
C	1.25856100	-0.86946300	2.04628600
C	1.71104000	-2.13398800	1.66761200
C	1.93973400	0.27589100	1.57284900
C	2.82993800	-2.25949100	0.84094900
H	1.20908500	-3.02499600	2.03267800
C	3.07697700	0.12868900	0.74386600

A6

C	0.16016600	3.19257600	0.41386900
C	-0.68060900	2.16267000	-0.29688500
C	0.03171900	1.58471500	-1.32430600
C	1.39642200	2.23601500	-1.47345100
C	1.59392800	2.94920400	-0.11390500
C	-2.11416000	1.88852300	0.06945500

C	-2.62348200	0.55444400	-0.42724700
H	-2.71831000	2.70820700	-0.35431300
H	-2.22685100	1.96368500	1.15713800
H	-0.43413900	1.01858900	-2.13278300
H	2.19753900	1.53326400	-1.71958600
H	1.34227200	2.95379600	-2.30396900
H	2.12676600	2.28939600	0.58052400
H	2.17336200	3.87077000	-0.19993000
H	-0.22113400	4.18241400	0.11575600
H	0.06644300	3.13877200	1.50368700
In	-0.01551400	-0.48867400	0.03914500
Cl	-0.33992000	-2.25719400	-1.40809000
Cl	-0.13565500	-0.31787300	2.34582300
C	-3.14467500	-0.39666600	0.37898600
C	-3.75542800	-1.68204200	-0.07975900
H	-2.66560300	0.40647600	-1.50690800
H	-3.15471200	-0.21410400	1.45456300
H	-3.66772000	-1.82403100	-1.15973100
H	-3.29845800	-2.53956300	0.42796600
H	-4.81969700	-1.69150300	0.19140500
C	3.33033000	-1.04376700	0.11705700
N	2.24743500	-0.65171900	0.00098100
C	4.69058500	-1.53426500	0.26438600
H	5.37796200	-0.69272200	0.39798100
H	4.74872700	-2.18872800	1.14052000
H	4.97767600	-2.09996700	-0.62794900

A7

C	2.75199900	-0.21793400	0.89267400
C	2.15212500	-1.17757000	1.63403800
C	0.87249300	1.27606500	-1.08023500
C	1.85733400	0.73588700	-2.04340100
C	3.29011600	0.63304300	-1.47413400
C	3.48256800	-0.45314000	-0.40107000
C	0.14674300	1.94792300	-0.35238900
In	-0.18761000	-0.53391900	0.34581600
Cl	0.18363400	-2.39507100	-0.98809900
Cl	-1.03536000	-0.12112000	2.45959800
H	3.23471500	-1.44384200	-0.79960100
H	4.55363800	-0.48143900	-0.14942600
H	3.59563400	1.61065400	-1.08281000
H	3.95463600	0.40905900	-2.31513100
H	1.52452700	-0.23723400	-2.42201700

H	1.84843000	1.42320800	-2.89925700
C	-0.68348900	2.87663600	0.43031100
H	2.78900800	0.79719000	1.29226100
H	1.77322800	-0.96390700	2.62953900
H	2.15801300	-2.21915700	1.31828000
H	-1.73912200	2.60589800	0.30884200
H	-0.45345800	2.76355400	1.49585100
C	-0.45160900	4.33631200	-0.02052900
H	-0.71042900	4.47238900	-1.07411600
H	-1.08564600	4.99431200	0.58029200
H	0.59004500	4.63446800	0.12603400
C	-4.68153000	-0.56595100	-1.51462400
H	-4.91448300	0.20135400	-2.25985600
H	-4.76796800	-1.55486000	-1.97689700
H	-5.39177200	-0.49245600	-0.68464800
C	-3.32732300	-0.38011000	-1.01814200
N	-2.24904600	-0.23555200	-0.62325500

A9

C	0.98390800	1.98223800	1.14323400
C	0.91209000	0.64476800	0.45856600
In	-1.15640000	0.14404100	-0.49034000
Cl	-1.20714900	-1.52393000	-2.07270800
C	1.49960200	-0.38618400	0.08765300
C	2.05217500	-1.63103400	-0.42580200
C	3.45488700	-1.48066500	-1.07567400
C	4.57109800	-1.20397100	-0.05206100
C	4.42883300	0.11860200	0.64937500
C	4.26084200	0.27247100	1.96848600
Cl	-2.22750400	2.16581300	-0.64548100
H	4.60482400	-2.01721400	0.68407100
H	5.52818300	-1.22745400	-0.59064800
H	3.41970500	-0.69164400	-1.83552100
H	3.66058100	-2.41971100	-1.60014300
H	2.08184200	-2.37615100	0.38005100
H	1.35046500	-2.00803000	-1.18488400
H	0.02186100	2.23389900	1.59843700
H	1.71059700	1.85295300	1.95400900
H	4.49820700	1.00490700	0.01625700
H	4.20849800	1.25631100	2.42743400
H	4.21967000	-0.58018500	2.64336700
C	1.42642300	3.10473300	0.18954000

H	2.39644100	2.87691400	-0.26140800
H	0.69531900	3.26542500	-0.60752600
H	1.51800500	4.03664200	0.75559400
C	-3.72264500	-1.96471300	2.97375200
H	-3.87533000	-1.30142000	3.83165800
H	-3.26782500	-2.90141700	3.31253600
H	-4.68962500	-2.17997800	2.50630200
C	-2.85305600	-1.31922700	2.00615400
N	-2.15909800	-0.80228200	1.23813200

ATS1

C	-1.36665600	1.90148000	-1.29856700
C	-1.07070700	0.54584900	-0.73525600
In	0.88309800	0.39611200	0.30425000
Cl	0.74393800	-0.42146900	2.47120000
C	-1.92374500	-0.53697600	-0.82597600
C	-1.75230200	-1.86341600	-0.08963100
C	-2.75791300	-1.83201100	1.07610400
C	-4.04384100	-1.13835200	0.54116400
C	-3.61998100	-0.12108000	-0.49091800
C	-3.17783400	-0.53019200	-1.79650000
Cl	2.29652600	2.13836900	-0.26696100
H	-4.69929800	-1.87565300	0.06168000
H	-4.60482200	-0.66065100	1.34784800
H	-2.33752800	-1.23144500	1.88938300
H	-2.97736200	-2.82723600	1.47209900
H	-1.95216300	-2.70188700	-0.76686300
H	-0.73176900	-1.98924600	0.28201700
H	-0.52223000	2.18088900	-1.94588800
H	-2.26826500	1.92627000	-1.92109400
H	-3.75268800	0.93798700	-0.29348500
H	-3.13509900	0.20335100	-2.59558900
H	-3.41297700	-1.53911000	-2.12768500
C	-1.47824400	2.98489500	-0.19402200
H	-2.27207500	2.75232100	0.52313500
H	-0.53919000	3.10619700	0.35487900
H	-1.70928200	3.94602700	-0.66133600
N	2.01018400	-1.27143000	-0.69093800
C	2.84890800	-1.98091700	-1.05468100
C	3.90342900	-2.87004700	-1.51205200
H	3.59014000	-3.37929200	-2.42914000
H	4.80815900	-2.28663000	-1.71356900

H	4.11876900	-3.61406100	-0.73810600

A10

C	-2.70737500	-1.18235200	-0.18889300
C	-2.41468300	0.16562300	-0.84742900
C	-3.15808600	1.15442000	-0.26538200
C	-4.03883900	0.62931600	0.81981300
C	-4.00997800	-0.90577100	0.60879700
C	-1.52587200	0.32589800	-2.09826000
C	-0.67208600	0.88534900	-1.06420100
H	-1.92349000	1.00521700	-2.85508900
H	-1.26784900	-0.65549200	-2.49738500
H	-3.12529700	2.20304100	-0.54329900
H	-3.61738600	0.92531800	1.79419900
H	-5.04189700	1.07075800	0.78244300
H	-4.04277600	-1.45832300	1.54972000
H	-4.87755800	-1.20912200	0.01513600
H	-2.82095700	-1.97717800	-0.93161200
H	-1.90389000	-1.49486500	0.48994800
In	0.66768900	-0.43626400	0.09687400
Cl	0.99266400	-2.42199200	-1.05220100
Cl	0.36767900	-0.40759100	2.39250200
C	-0.46972500	2.37534500	-1.02400200
C	-0.28651300	3.02540000	0.35125200
H	-1.23394400	2.90302600	-1.61096800
H	0.46163800	2.49764600	-1.60852000
H	-0.04460300	4.08619800	0.23937800
H	-1.19972400	2.94867100	0.95090900
H	0.51993600	2.55802900	0.92687400
C	3.81871500	0.72989500	-0.09302000
C	5.24351000	1.01397600	-0.07976100
H	5.57641000	1.17010200	0.95173700
H	5.78773700	0.16718200	-0.51134000
H	5.44923800	1.91417700	-0.66805300
N	2.68391900	0.50326600	-0.10279100

ATS2

C	0.82659000	2.14121000	0.89709100
C	0.88965900	0.68487100	0.47983900
In	-0.98678000	-0.02567500	-0.50053700
Cl	-0.92786000	-2.13152800	-1.46493100

C	1.80105500	-0.22460000	0.53869400
C	2.28490300	-1.55504600	0.10984200
C	3.57306100	-1.45801600	-0.72135800
C	4.70096500	-0.80141200	0.12596800
C	4.14839300	0.41839600	0.78765000
C	3.44841700	0.36428400	1.95552900
Cl	-2.10112000	1.73062600	-1.50237800
H	5.04141800	-1.51740000	0.88236300
H	5.55132000	-0.55458700	-0.51628800
H	3.38349800	-0.86610600	-1.62313000
H	3.88623300	-2.45658900	-1.04032200
H	2.42909700	-2.21103500	0.97758000
H	1.48451200	-2.00113200	-0.49752100
H	-0.19414700	2.39895600	1.19913900
H	1.45609300	2.28832200	1.78132600
H	4.23470100	1.37160600	0.26822300
H	3.07698000	1.26326500	2.43431500
H	3.42106600	-0.54442400	2.55163100
C	1.26933400	3.08921200	-0.23311700
H	2.29732100	2.88141000	-0.54688700
H	0.61677500	3.00143900	-1.10626600
H	1.22055400	4.12372600	0.12015500
N	-2.34313000	-0.40227900	1.23468100
C	-3.22932800	-0.63008400	1.94254500
C	-4.34306600	-0.91595400	2.83087700
H	-4.04131000	-0.75243200	3.87049200
H	-5.18199700	-0.25504500	2.58861800
H	-4.65521000	-1.95775700	2.70302900

A11

C	-2.70737500	-1.18235200	-0.18889300
C	-2.41468300	0.16562300	-0.84742900
C	-3.15808600	1.15442000	-0.26538200
C	-4.03883900	0.62931600	0.81981300
C	-4.00997800	-0.90577100	0.60879700
C	-1.52587200	0.32589800	-2.09826000
C	-0.67208600	0.88534900	-1.06420100
H	-1.92349000	1.00521700	-2.85508900
H	-1.26784900	-0.65549200	-2.49738500
H	-3.12529700	2.20304100	-0.54329900
H	-3.61738600	0.92531800	1.79419900
H	-5.04189700	1.07075800	0.78244300

H	-4.04277600	-1.45832300	1.54972000
H	-4.87755800	-1.20912200	0.01513600
H	-2.82095700	-1.97717800	-0.93161200
H	-1.90389000	-1.49486500	0.48994800
In	0.66768900	-0.43626400	0.09687400
Cl	0.99266400	-2.42199200	-1.05220100
Cl	0.36767900	-0.40759100	2.39250200
C	-0.46972500	2.37534500	-1.02400200
C	-0.28651300	3.02540000	0.35125200
H	-1.23394400	2.90302600	-1.61096800
H	0.46163800	2.49764600	-1.60852000
H	-0.04460300	4.08619800	0.23937800
H	-1.19972400	2.94867100	0.95090900
H	0.51993600	2.55802900	0.92687400
C	3.81871500	0.72989500	-0.09302000
C	5.24351000	1.01397600	-0.07976100
H	5.57641000	1.17010200	0.95173700
H	5.78773700	0.16718200	-0.51134000
H	5.44923800	1.91417700	-0.66805300
N	2.68391900	0.50326600	-0.10279100

ATS2

C	-1.08309500	0.91406700	0.26282800
In	0.82705500	0.18048000	-0.53614400
C	-2.14200100	-0.01631700	0.67728800
C	-2.16015600	-1.53105700	0.59152700
C	-3.57879000	-1.89323000	0.08955100
C	-4.45626300	-0.66706000	0.44143600
C	-3.47214300	0.46674700	0.57458900
C	-2.28333700	0.83502800	-0.76512600
Cl	2.35538900	1.86471600	-0.95373100
Cl	0.44958400	-1.51215500	-2.09947500
H	-5.24413900	-0.46032300	-0.28918400
H	-4.95409000	-0.78068800	1.41487100
H	-3.95424100	-2.81560900	0.53679400
H	-3.55811500	-2.04623600	-0.99399800
H	-1.36054200	-1.94207400	-0.02939500
H	-1.99351400	-1.87819700	1.62201100
H	-3.78536500	1.45596100	0.88966100
H	-2.68433700	1.82178100	-0.97952700
H	-2.26359700	0.14474800	-1.60371000
C	-0.97957800	2.29085000	0.94039900

C	-0.18775400	2.23366300	2.25251100
H	-1.97534800	2.70999700	1.14076000
H	-0.48847900	2.98147100	0.24507200
H	-0.14400500	3.22638200	2.71003600
H	-0.65148800	1.55025000	2.97322000
H	0.84670700	1.90976400	2.08751400
N	1.96840100	-0.97195100	1.01396600
C	2.80272000	-1.52710700	1.59255400
C	3.85134300	-2.22411400	2.31808700
H	3.54617600	-2.37899100	3.35800600
H	4.04090300	-3.19407400	1.84660200
H	4.76875200	-1.62638700	2.29517700

$ATS_{trans\text{-}c}$

C	-3.44226700	-0.71718300	-1.11365600
C	-2.48376900	0.39409400	-0.73395900
C	-2.56767200	0.68997800	0.58046000
C	-3.59092900	-0.16127500	1.29020400
C	-3.91059900	-1.27346100	0.25558300
C	-1.59311600	1.08143900	-1.75090500
C	-0.31855600	1.47083200	-1.03072900
H	-2.09946800	1.93903200	-2.21783200
H	-1.35844700	0.36690400	-2.54927300
H	-2.04174100	1.49875100	1.08380800
H	-3.22296500	-0.55557700	2.24388100
H	-4.47280500	0.45130100	1.52837600
H	-3.33468300	-2.17298700	0.49522100
H	-4.96710700	-1.55173000	0.25349000
H	-4.27424100	-0.29517700	-1.69734300
H	-2.97143500	-1.48133000	-1.74224900
In	0.47180100	-0.23577800	0.16269900
Cl	0.04469400	-2.31189300	-0.76058900
Cl	0.70843800	0.22971100	2.41942700
C	0.01414900	2.82503100	-0.88740500
C	1.13209700	3.38326700	-0.06580900
H	-0.63299500	3.56176900	-1.37792100
H	0.52754500	2.00056200	-1.82908600
H	1.67084600	4.17102700	-0.60137400
H	0.67261000	3.85310400	0.81555800
H	1.82760800	2.61928700	0.28839300
N	2.69057700	-0.20384500	-0.35999400
C	3.79654000	-0.53705800	-0.44133400

C	5.18375800	-0.95924100	-0.54291000
H	5.65246600	-0.92053200	0.44595600
H	5.22474400	-1.98598100	-0.92173900
H	5.72673200	-0.29982800	-1.22765200

$(InCl_2+2)^+$

C	2.18688000	0.51766800	-0.57675600
C	3.23928100	0.99394500	0.40068400
C	2.74806900	1.13640200	1.63332500
C	1.28876200	0.80705400	1.76577000
C	0.85465400	0.42914900	0.26728600
C	5.31047200	0.05024800	-0.70569400
H	3.31986500	1.45607400	2.49904000
H	1.10196700	-0.03336600	2.44643600
H	0.69090000	1.64579600	2.14457000
H	2.06907800	1.20531400	-1.42129600
H	2.44409100	-0.45918600	-0.99697700
In	-2.67660700	-0.29511000	-0.11821800
Cl	-3.46940700	-0.83490500	-2.17903400
Cl	-3.72043300	-0.10016100	1.89540200
C	6.32957200	-0.63212400	-0.17663100
C	7.01546800	-1.80329000	-0.81712600
H	6.72076700	-0.31949900	0.79350300
H	4.92436000	-0.24530900	-1.68283600
H	8.07939900	-1.59034400	-0.98281200
H	6.97258300	-2.68922500	-0.16989700
H	6.56685000	-2.06015200	-1.78243000
C	4.65614500	1.24917800	-0.05187000
H	5.25010200	1.57642800	0.80806000
H	4.64599800	2.08898700	-0.76547400
C	0.30476100	-0.99024300	0.29555900
C	-0.14994300	1.48071000	-0.18449400
O	1.23264500	-1.87532900	0.50095900
O	0.40306500	2.63878700	-0.38373800
O	-1.38476100	1.33768200	-0.31996900
O	-0.89141900	-1.33999700	0.19248000
C	0.85852200	-3.28461200	0.62615400
H	1.80097500	-3.79984100	0.79581700
H	0.18094500	-3.40479100	1.47240400
H	0.38393700	-3.61606700	-0.29811900
C	-0.44083300	3.77657500	-0.75217300
H	0.25237400	4.60984800	-0.83956900
H	-0.93402300	3.56755300	-1.70218100

H	-1.17624800	3.95122100	0.03411300

TS3

C	1.87920800	-0.96009500	-0.95889900
C	1.89270800	0.07483300	0.14238100
C	3.16512000	0.37587100	0.52664400
C	4.18241700	-0.34342600	-0.30242000
C	3.35144900	-0.98478600	-1.45049200
C	0.90241000	0.05136400	2.06174600
C	0.68542400	0.72248600	0.83602900
H	1.04308900	0.58138900	3.00869900
H	0.94761000	-1.03452400	2.11257500
H	3.42630400	1.09203400	1.30104900
H	4.97941800	0.32025100	-0.65635200
H	4.67849600	-1.10444000	0.32041200
H	3.44701200	-0.37735900	-2.35482600
H	3.68736800	-1.99423100	-1.69424900
H	1.55361100	-1.94092300	-0.58590800
H	1.17022700	-0.67974900	-1.75693300
In	-1.21954800	-0.21863700	0.02177400
Cl	-1.32240300	-2.48284500	0.32586400
Cl	-2.87157200	1.11551000	-0.78767800
C	0.57473600	2.26036700	0.84564200
H	1.41057300	2.65793000	1.43758100
H	-0.33684100	2.54276800	1.38694000
C	0.58275500	2.90828600	-0.54256200
H	0.52947800	3.99591700	-0.44347200
H	1.49890800	2.66943900	-1.09238000
H	-0.27719900	2.60000200	-1.14766200

TS1′

C	-0.38454300	2.32355500	-0.01488300
C	-0.52485600	0.82385000	-0.16727500
In	1.41558500	-0.25214700	-0.05897300
Cl	1.41457300	-2.50728100	0.28308000
C	-1.45172100	-0.03470400	-0.33697400
C	-2.06511900	-1.36190800	-0.40208000
C	-3.22651800	-1.54345100	0.59668600
C	-4.39307500	-0.59645000	0.22704700
C	-3.88226900	0.80238000	0.06331600
C	-3.54454700	1.33374600	-1.13487900

Cl	3.21791100	1.09651800	-0.36584200
H	-4.85344500	-0.93997600	-0.70611500
H	-5.15688400	-0.64115900	1.01063600
H	-2.87063100	-1.34231500	1.61298500
H	-3.55993100	-2.58500200	0.56526100
H	-2.39010100	-1.57847000	-1.42768200
H	-1.26478200	-2.08053800	-0.16185400
H	0.35625600	2.69011500	-0.73384200
H	-1.34493800	2.77248000	-0.28370300
H	-3.75964500	1.40351300	0.96413600
H	-3.20198600	2.35890000	-1.23358500
H	-3.70352100	0.78823500	-2.06249000
C	0.01739100	2.73905600	1.41047800
H	-0.70339000	2.37958000	2.15101800
H	1.01203300	2.36593200	1.68177600
H	0.05663400	3.83043400	1.47148900

TS2′

C	-0.59745400	0.92413500	-0.25522000
In	1.21030400	-0.29793900	-0.02941400
C	-1.81687400	0.50998800	0.34975500
C	-2.07901900	-0.68404700	1.24182100
C	-3.42486500	-1.27615300	0.76262900
C	-4.15151800	-0.10630300	0.05720700
C	-3.03314900	0.80968000	-0.41671300
C	-1.85506900	0.20886100	-1.31078200
Cl	3.26021300	0.59616000	0.39135300
Cl	0.85772100	-2.53685300	-0.40467300
H	-4.79931500	-0.43161100	-0.76170100
H	-4.77566200	0.46064500	0.75762000
H	-4.00708600	-1.68899800	1.58857300
H	-3.23911100	-2.09666400	0.06241200
H	-1.26321200	-1.41235600	1.26934300
H	-2.16892900	-0.25325600	2.25104700
H	-3.27592600	1.81678300	-0.74193500
H	-1.68917200	0.85096600	-2.16954000
H	-1.80715500	-0.85803600	-1.50595100
C	-0.36641000	2.37437100	-0.68779400
C	0.24425400	3.19252300	0.46396800
H	-1.30449200	2.84803800	-1.00205200
H	0.30500600	2.39692100	-1.55454100
H	0.39932000	4.22333600	0.13218100

H	-0.42108500	3.21414700	1.33340900
H	1.21766400	2.80255000	0.77962800

10′

C	-0.63825600	0.94213100	-0.11977600
In	1.23235200	-0.20543500	-0.04967300
Cl	3.10445400	0.78022800	-0.90242200
C	-1.77027800	0.40401200	-0.68432800
C	-1.94577800	-1.04199500	-1.13198900
C	-2.80440600	-1.72609400	-0.05134800
C	-3.87533700	-0.68992300	0.40766700
C	-3.26660200	0.68246300	0.30549700
C	-3.04797100	1.30238400	-0.97247400
Cl	1.18421500	-2.30766100	0.85690700
H	-4.74790900	-0.73773400	-0.25516600
H	-4.20913300	-0.89185500	1.42795200
H	-2.16739500	-1.98132000	0.80206600
H	-3.27452700	-2.64613300	-0.40767400
H	-2.42982300	-1.07791300	-2.11444900
H	-0.98258500	-1.55193200	-1.23950600
H	-3.05046700	1.24927100	1.20690400
H	-2.84932500	2.36889600	-1.01637600
H	-3.59688200	0.91704300	-1.82906000
C	-0.51794300	2.32514300	0.44557400
C	0.22773500	2.37467400	1.79507700
H	-1.48419600	2.83320700	0.54195600
H	0.06194900	2.90502400	-0.29253400
H	0.26955200	3.40471200	2.15941400
H	-0.26957800	1.76587900	2.55713300
H	1.27074200	2.03875500	1.70363200