Supporting Information

A Radical Mechanism of Isocyanide-Alkyne Cycloaddition by Multi-catalysis of Ag_2CO_3, Solvent, and Substrate

Pin Xiao, Haiyan Yuan, Jianquan Liu, Yiying Zheng, Xihe Bi,* and Jingping Zhang*

Faculty of Chemistry, Northeast Normal University, Changchun 130024, China

jpzhang@nenu.edu.cn; bixh507@nenu.edu.cn

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i. Experimental Evidence

We have ever contacted with authors about experimental details, and our co-workers Bi et. al. indeed observed a thin silver mirror on the wall of the reaction vessel during the reaction. Then we carried out experiments with BHT (3,5-di-tert-butyl-4-hydroxytoluene) and TEMPO ((2,2,6,6-tetramethyl-piperidin-1-yl)oxyl) as scavengers to test the possible radical mechanism.

Typical synthetic procedure (with Bi′s title reaction as an example): A mixture of **2** (0.16 ml, 1.5 mmol), Ag_2CO_3 (30 mg, 0.1 mmol) and TEMPO (312 mg, 2.0 mmol)/BHT (440 mg, 2.0 mmol) in 1,4-dioxane (4.0 ml) was heated to 80 ℃, then **1** (0.11 ml, 1.0 mmol was dissolved in 2.0 ml of 1,4-dioxane) was added drop by drop. About 30 min later, the reaction was indicated by TLC. We could not find product and substrate **2** was remained. The resulting mixture was filtered through a pad of calcite, the solvent was evaporated on a rotary evaporator. Then HNMR was carried out for the residue, no product was found either.

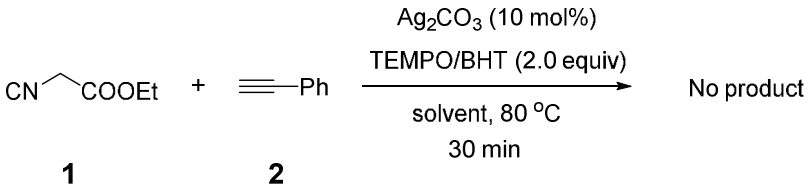


Table S1. Comparation of experiment yields for reations with BHT or TEMPO as scavengers and the standard.

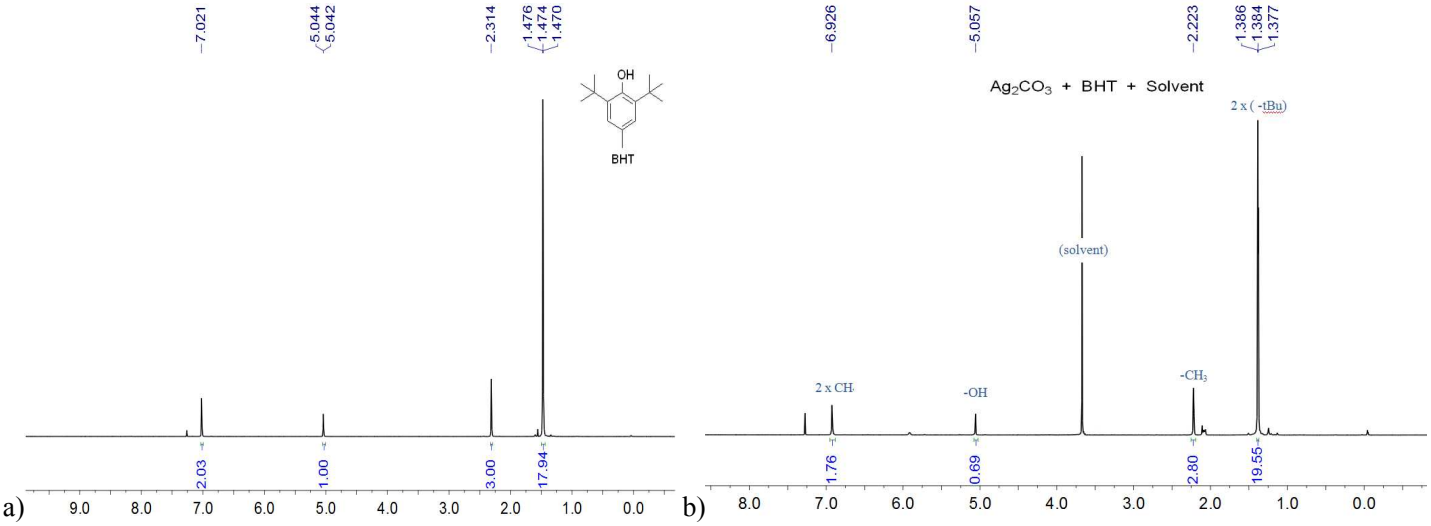
Entry	Standard[a]	BHT[b]	TEMPO[c]
Bi′s	90	0	0
Lei′s	89	0	0

[a]Reactions in optimized conditions reported by authors. [b]Adding BHT into the standard conditions. [c]Adding TEMPO into the standard conditions.

Although we could not isolate adducts of either scavenger with any radical intermediate, we found that the substrate 2 and solvent 1,4-dioxane survived while substate **1** disappeared by TLC. This shows that the reaction proceeds through a radical process in which **1** is the potential radical source to some extent. To exclude the possibility of scavenger reacting with Ag(I) salts, we conducted ^{1}H-NMR spectroscopy analyses for pure BHT before or after adding Ag_2CO_3.

NMR spectra (^{1}H NMR, 500 MHz)

a) the NMR spectrum of pure BHT； b) the NMR spectrum of BHT with Ag_2CO_3 in 1,4-dioxane.



No obvious shift was observed for the characteristic peaks of BHT after adding Ag_2CO_3, suggesting that BHT has no effect on the catalytic activity of Ag_2CO_3 in current reaction.

ii. Additional information on radical mechanism

The computed desublimation Gibbs energy of Ag (g):

$Ag_{(g)} \rightarrow Ag_{(s)}$; $\Delta_rG = \Delta_fG_s - \Delta_fG_g = -146.996138 - (-146.992853) = -0.003275$ a.u. (M06/SDD, 80 ℃, p = 1 atm)

The computed desublimation Gibbs energy of silver from gas to solid phase is negative (-2.1 kcal/mol), indicating this transformation of sliver from gas to solid phase is thermodynamically favorable.

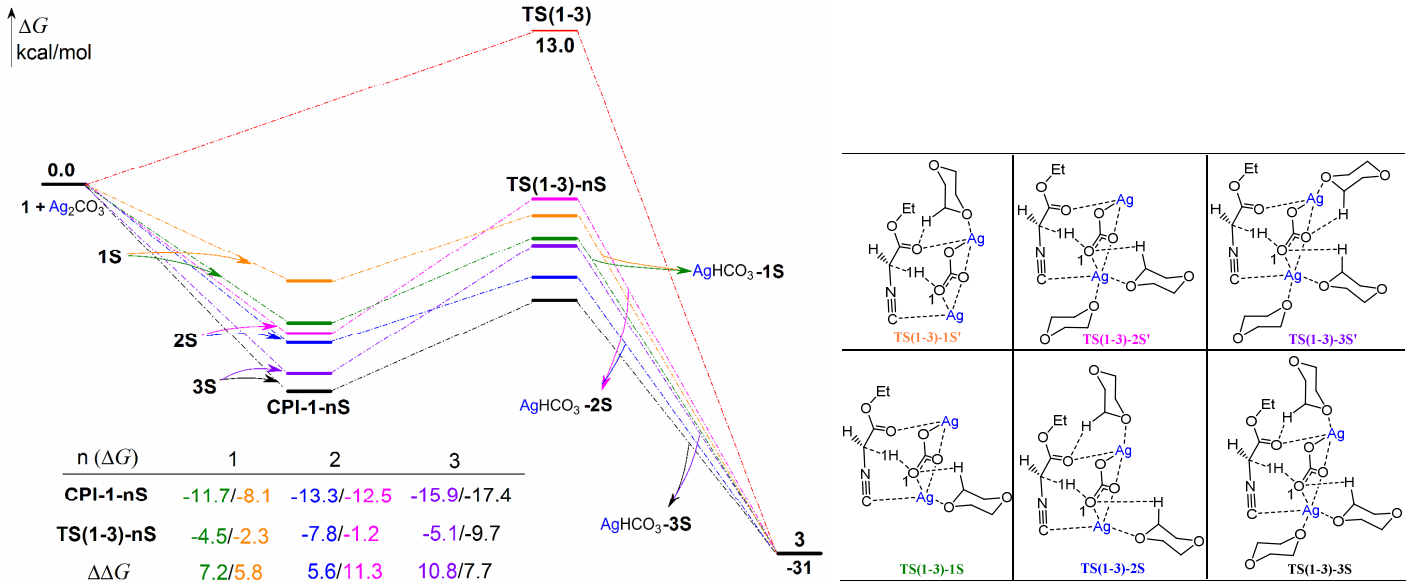


Figure S1. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile for the direct or 1-3 **S**-assisted deprotonation of isocyanide and the optimized structures of key transition states.

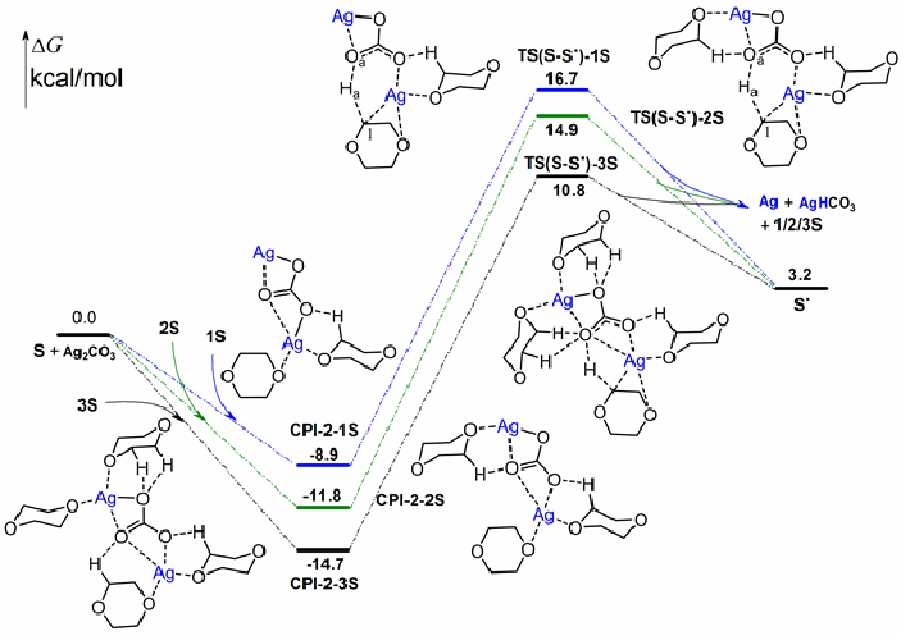


Figure S2. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile of 1-3 **S**-assisted deprotonation of dioxane to deliver radical **S**$^{\bullet}$.

The formation of silver-acetylide:

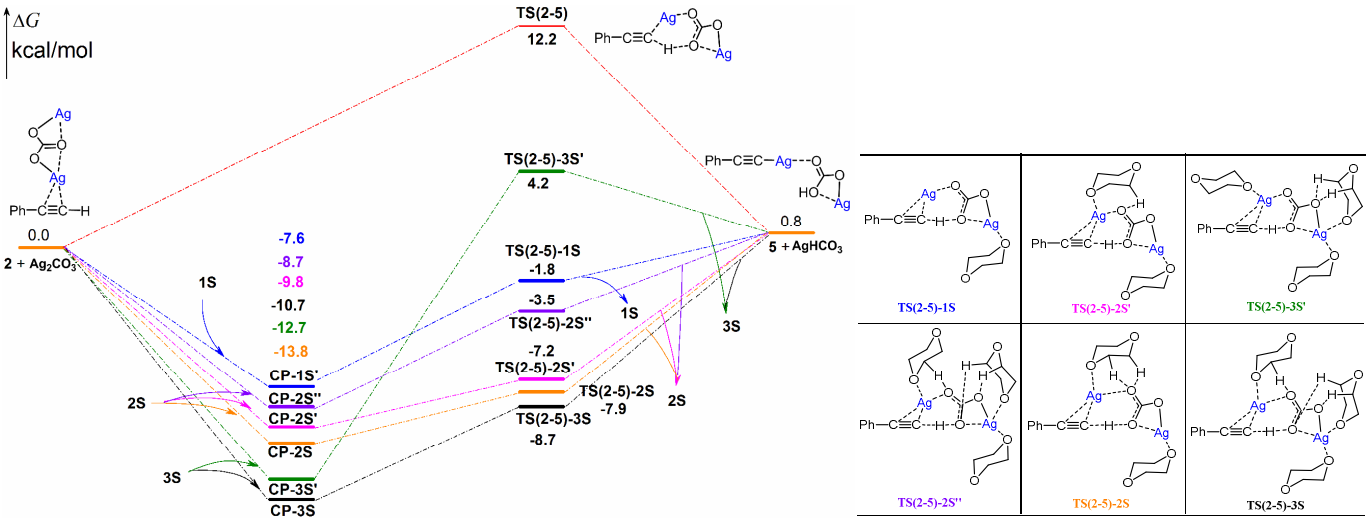


Figure S3. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile for the direct or 1-3 **S**-assisted formation of silver-acetylide and the optimized structures of key transition states.

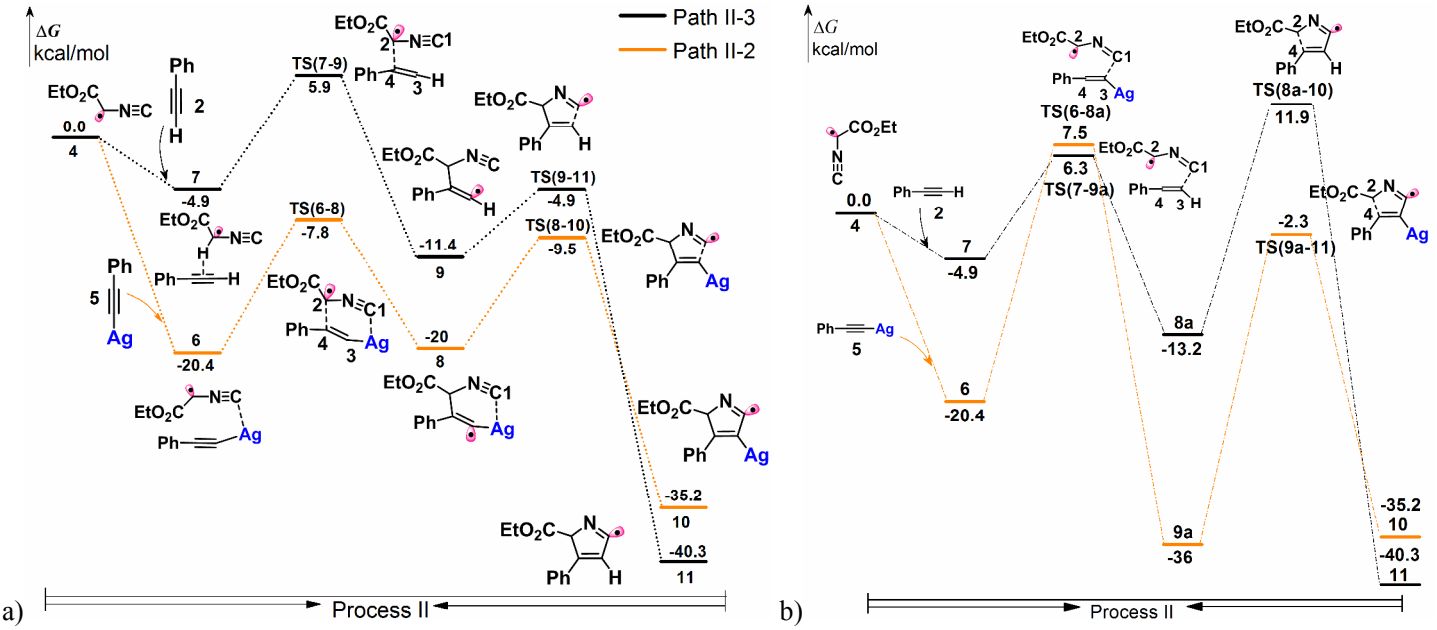


Figure S4. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile of unfavorable unassisted cycloaddition process II to give five membered intermediate **10** or **11**: a) C2-C4 bond forms before C1-C3 bond; b) C2-C4 bond forms after C1-C3 bond.

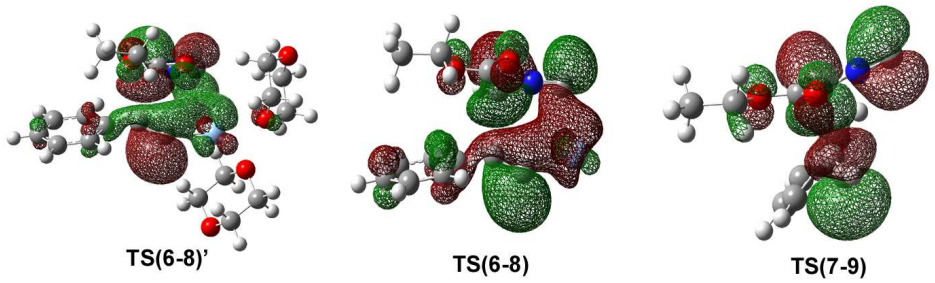
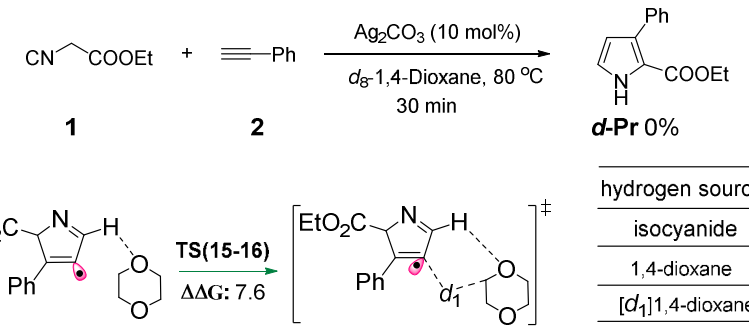


Figure S5. HOMOs of **TS(6-8)′**, **TS(6-8)** and **TS(7-9)**. No effective orbital interactions for C2-C4 bond formation. Thus, we choose HOMO-1s for discussion in paper.

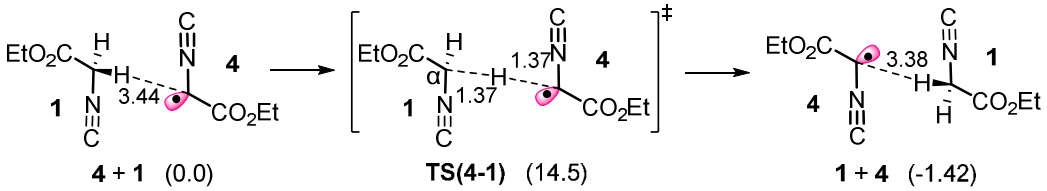
Table S2. Deuterium-labling experiment with [d_8]1,4-dioxane and the calculated activation barriers.



hydrogen source	ΔΔG
isocyanide	2.9
1,4-dioxane	5.9
[d_1]1,4-dioxane	7.6

The free energy barrier ($\Delta\Delta G_{sol}^{\ddagger}$, in kcal/mol) for the C-d_1 activation of [d_1]1,4-dioxane is less favorable by 1.7 and 4.7 kcal/mol than C-^{1}H of **S** and C$^{\alpha}$-H of isocyanide, respectively.

Typical synthetic procedure: A mixture of **2** (80 µl, 0.75 mmol) and Ag_2CO_3 (15 mg, 0.05 mmol) in [d_8]1,4-dioxane (2.0 ml) was heated to 80 ^{o}C then **1** (55 µl, 0.5 mmol was dissolved in 1.0 ml of [d_8]1,4-dioxane) was added drop by drop. About 30 min later, the reaction was indicated by TLC. The resulting mixture was concentrated and the residue was taken up in DCM. The organic layer was washed with 5% NaCl and water, dried over $MgSO_4$ and concentrated. Purification of the crude product by flash column chromatography (silica gel, petroleum ether: ethyl acetate = 10: 1) afforded **Pr** in 82% yield as a white solid. When we analyzed the HNMR of **Pr**, we found there was no deuterium-labling hydrogen in product.

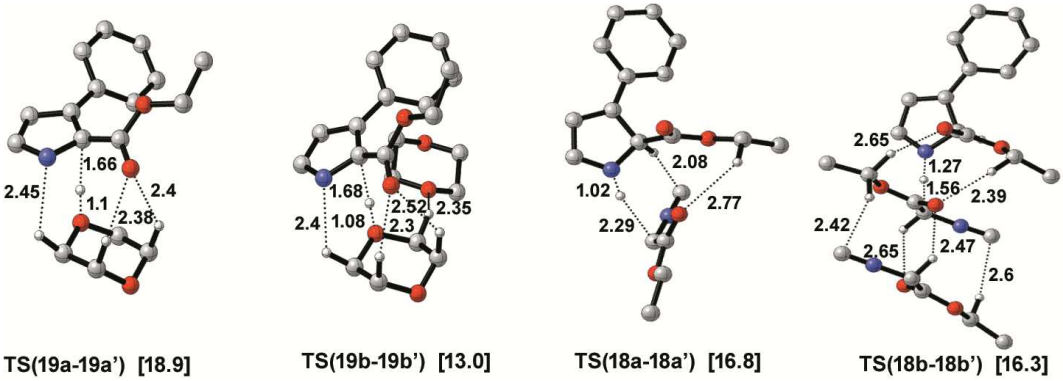


Scheme S1. Gibbs free energies (ΔG_{sol}) of self-initiation between **1** and **4**. Free energies in parentheses are in kcal/mol, and distances are in Å.

Table S3. Comparation of the activation barriers of the last (direct or 1-3 assistant (**S**/**1**/**W**)-assisted) H shift process IV ($\Delta\Delta G_{sol}^{\ddagger}$, in kcal/mol).

TS	assistant-assisted									Direct
	S			**1**			**W**			
number	3	2	1	3	2	1	3	2	1	
$\Delta\Delta G^{\ddagger}$	9.9	13.0	18.9	13.4	16.3	16.8	16.6/14.1	21.2	32.7	30.7

As shown in Table S3, each three molecules cluster catalyst is the most favorable in reducing the barrier of H shift process among combined clusters varing numbers of participants 1-3. Besides, **S**-assisted H-shift process is the most favorrable one.



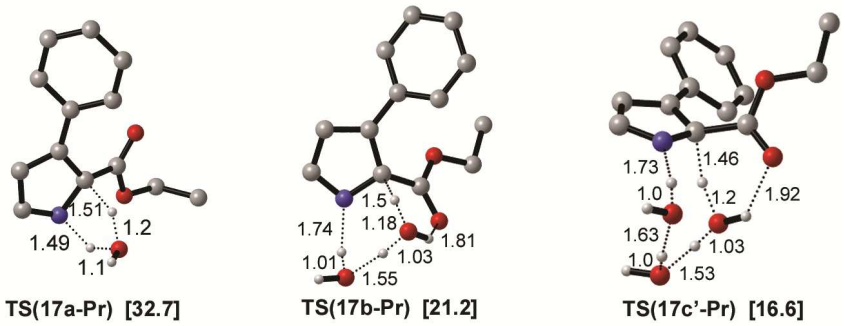


Figure S6. Optimized geometries of key transition states assisted by **S**/**1**/**W** for H shift process IV. Free energy barriers $\Delta\Delta G_{sol}^{\ddagger}$ in parentheses are in kcal/mol, and distances are in Å.

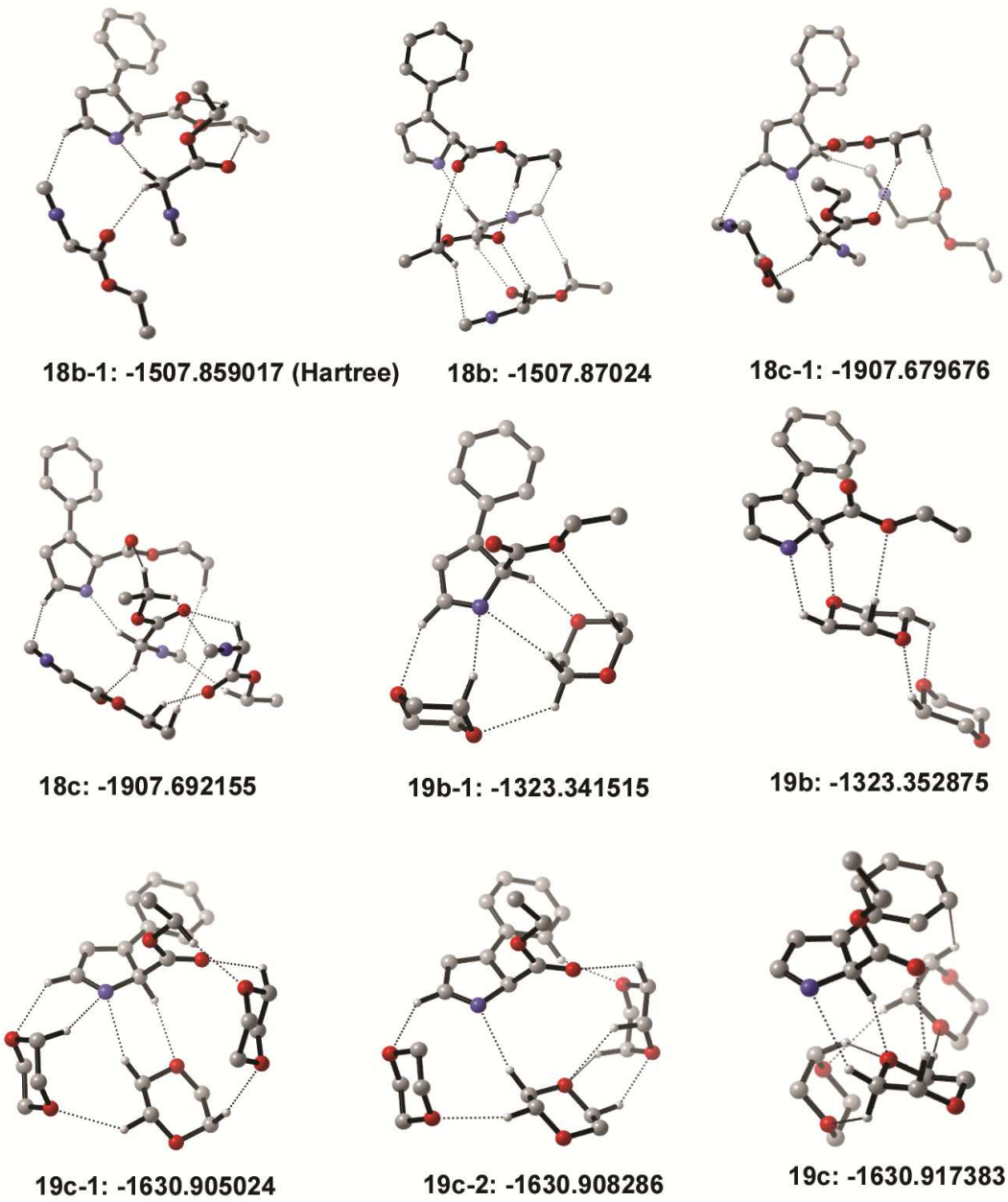
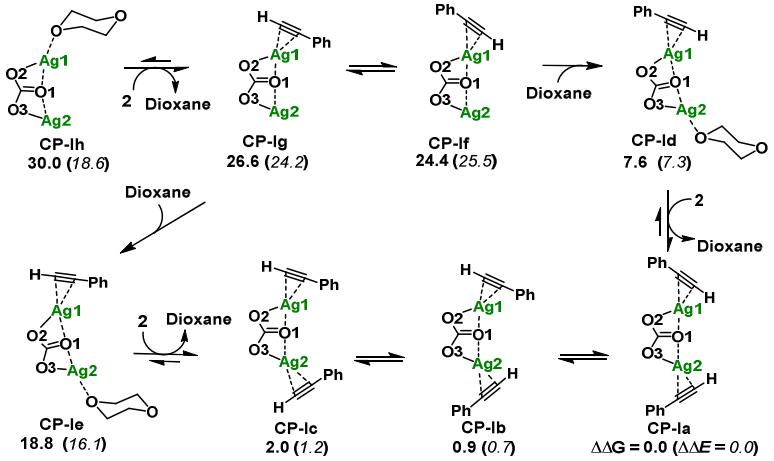


Figure S7. Optimized geometries and Gibbs free energies (G_{sol}, in Hartree) of nine models for 2-3 **S**/**1**-assisted reaction precursor. The intermediate **18b**/**18c**/**19b**/**19c** is the most stable one compared to the other geometries by 5.7~7.8 kcal/mol.

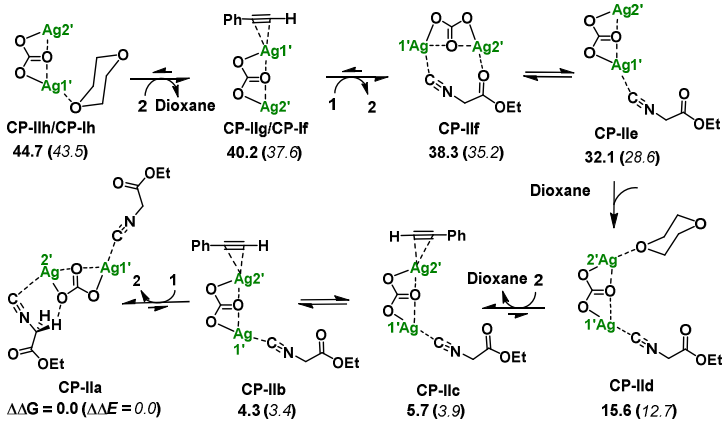
iii. The radical-free mechanisms proposed by Bi and Lei groups.

A number of Ag^I complexes may exist in equilibrium through ligand or substrate exchanges before reaction occurs in the reaction solution. Similar treatments were reported in many other previous metal-catalyzed reactions.[2] In Bi's work, to a mixture of phenylacetylene (**2**) and Ag_2CO_3 in 1,4-dioxane, ethyl isocyanoacetate (**1**) was slowly added, implying that initial Ag^I complex preferred coordinated with substrate **2** or 1,4-dioxane. We investigated two coordination modes for Ag^I complex with **2** and 1,4-dioxane: $\eta^{3,4}$-η^2 and η^4-$\eta^{3,4}$ for the two Ag atoms Ag1-Ag2. For the $\eta^{3,4}$-η^2 coordination (Scheme S2), we name the O atom of 1,4-dioxane-ligated with Ag_2CO_3 as η^3-η^2 complex **CP-Ih**. This complex can exchange O coordination with triple bond of **2** to form η^4-η^2 complexes **CP-Ig** and **CP-If**, respectively, considering the deprotonation mode of terminal H of **2** by different oxygen atoms O1 and O2 of catalyst Ag_2CO_3. For the η^4-η^3 coordination, another 1,4-dioxane molecule was added to **CP-Ig** and **CP-If** and coordinated with Ag2 atom, generating η^4-η^3 complexes **CP-Ie** and **CP-Id** respectively. A similar η^4-η^4 coordination for substrates **2** with Ag_2CO_3 is formed, including three kinds of complexes **CP-Ia/b/c**. Our calculations indicate that **CP-Ia** is the most stable specie among these Ag^I complexes. DFT calculations for Bi's work were carried out on the C-H activation pathways (terminal H of **2** in **CP-Ia** by O1) to form silver–acetylide. **1** in a drop by drop adding manner experimentally is likely to undergo 1,1-insertion process into C-Ag bond.

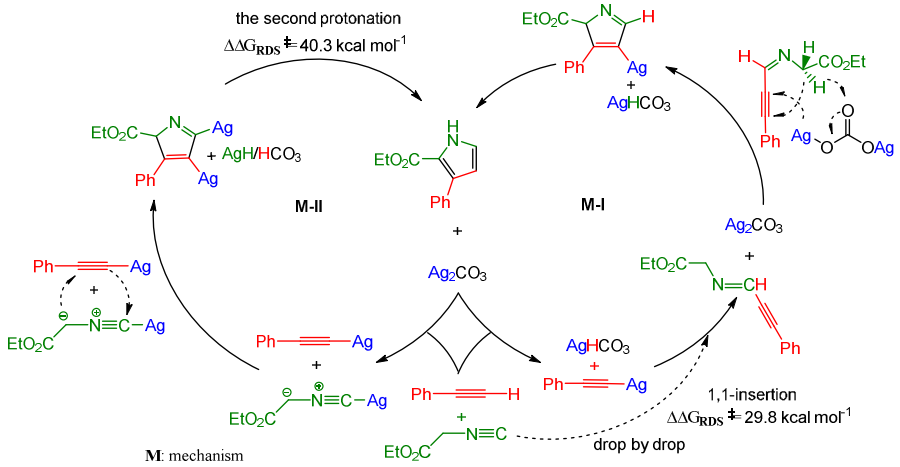


Scheme S2. Equilibrium between different Ag^I complexes of M-I. B3LYP/LANL2DZ + f (1.611)&6-31G**, gas phase, free energies and energies with respect to **CP-Ia** ($\Delta\Delta G$ and $\Delta\Delta E$) are in kcal/mol.

The similar treatment was employed in Lei's work to explore the most stable Ag^I complexes. In their work, a mixture of **1**, **2**, and Ag_2CO_3 was stirred in solvent, thus the initial Ag^I complex would also be coordinated with **1** besides **2** and solvent. As summarized in Scheme S3, **1** is more favorable than **2** and 1,4-dioxane coordinated with the catalyst Ag_2CO_3. The presence of **1** apparently changes the coordination modes of **2** and Ag_2CO_3 as compared with those in Bi's work due to its strong coordination ability. The calculated results suggest that the stable Ag^I complexes **CP-IIa** and **CP-IIb** are favorable to generate silver-isocyanide and silver-acetylide intermediates. Thereby, the more stable Ag^I complexes η^3-η^3 **CP-IIa** coordinated with two isocyanides and η^3-η^4 **CP-IIb** with one isocyanide as well as phenylacetylene molecule were employed in the mechanism discussion. Our finding is in good agreement with the experimental observation in Lei's work. After determining the most stable Ag^I complexes in these two systems, we focus on studying the mechanism in the following section using **CP-Ia** or **CP-IIa/CP-IIb** as the initial complexes.



Scheme S3. Equilibrium between different Ag^{I} complexes of M-II. B3LYP/LANL2DZ + f (1.611)&6-31G**, gas phase, free energies and energies with respect to **CP-IIa** (ΔΔG and Δ*ΔE*) are in kcal/mol.



Scheme S4. Two improved unfavorable radical-free mechanisms proposed by Bi and Lei groups at the level of M06/SDD/6-311++G**/SMD (1,4-dioxane, 353.15 K)//B3LYP/LANL2DZ/6-31G**.

iv. The detailed mechanism (M-I) proposed by Bi group.

The following calculations of the Gibbs free energies and electronic energies for discussion are carried out at the M06/SDD/6-311++G**/SMD (1,4-dioxane, 353.15 K)//B3LYP/LANL2DZ/6-31G** level. The calculated results indicate that the reaction mechanism of **2** and **1** catalyzed by Ag_2CO_3 is a concerted process for Bi's work. It includes mainly four processes: I) the C-H bond activation, II) isocyanide insertion, III) intermolecular cyclization, IV) hydrogen shift and protonation. The Gibbs free energy profiles are given in Figures S8a and S8b.

The reaction initiates from the most stable **CP-Ia** complex, and the free energy barrier for the C-H activation from **2** to afford the silver-acetylide intermediate (**Int1-I**) is calculated to be 14.1 kcal/mol (**TS1-I**), simultaneously releasing $AgHCO_3$. This process is promoted by the hydrogen bonding interaction between the terminal H1 of **2** and the O1 of Ag_2CO_3, namely, agnostic interaction (process I). To explore the reactive sites for the C-C bond formation between **Int1-I** and **1**, we performed NBO analysis (Figure S8a). It suggests that C1, C4 show electronegativity and C2, C3 electro-positivity. Subsequent isocyanide (**1**) insertion takes place from the **Int2-I** via two distinct pathways path I and path I1. Path I is a concerted process including C1-C3 bond formation and C3 protonation via **TS2-I** ($\Delta\Delta G^{‡}$ = 29.8 kcal/mol) to form the intermediate **Int3-I**. Path I1 is a stepwise process via transition states **TS2-I1** and **TS3-I1** with the $\Delta\Delta G^{‡}$ values of 35.1 and 17.4 kcal/mol respectively, which is less favorable than path I by 5.3 kcal/mol. Moreover, the NBO charge analysis on C1, C2, C3, and C4 (Figure S8a) indicates that

isocyanide insertion is a reasonable process. Although the intermediate **Int3-I1** in path I1 is more stable than **Int3-I** by 5.7 kcal/mol, **Int3-I1** is not beneficial to the following deprotonation of α-C4. Thus, path I1 can be excluded (process II). Subsequently, the abstraction of α-H2 by carbonyl O1 requires 11.5 kcal/mol of free energy barrier (**TS3-I**) to generate intermediate **Int4-I**. Then **Int4-I** furnishes the intramolecular cyclic **Int5-I** via **TS4-I** with a free energy barrier of 26.7 kcal/mol (Figure S8b, process III). Two pathways (path I and path I2**)** were considered in the hydrogen shift and protonation process (Figure S8b). In path I2, H3 shift from C4 to N via transition states **TS5-I2** ($\Delta\Delta G^{\ddagger}$ = 30.3 kcal/mol), then followed by H2 transfer from O1 to C1 via transition states **TS6-I2** ($\Delta\Delta G^{\ddagger}$ = 18.1 kcal/mol). The activation barrier of hydrogen shift step is quite high, changing completely the α-C4(sp^3) into C(sp^2) hybridization and leading to the aromatization of pyrrole ring. Therefore we computed a possible H_2O assisted hydrogen shift process, as shown in path I of Figure S8b. **Int5-I** can form a complex with water exothermically with energy loose of 12.3 kcal/mol. Path I is a water-accelerated mechanism regarding hydrogen shift. Here, the corresponding free energy barriers for H shift and protonation are 16.0 (**TS5-I**) and 18.3 kcal/mol (**TS6-I**), respectively. The computational result shows that the existing of a trace amount of water in the reaction system really plays a critical role in assisting the H shift process. The formation of product **Pr** + **2** + Ag_2CO_3 is exothermic by 28.3 kcal/mol with respect to **Int5-I**. The comparison of these two pathways shows that path I is the more favorable reaction channel (process IV).

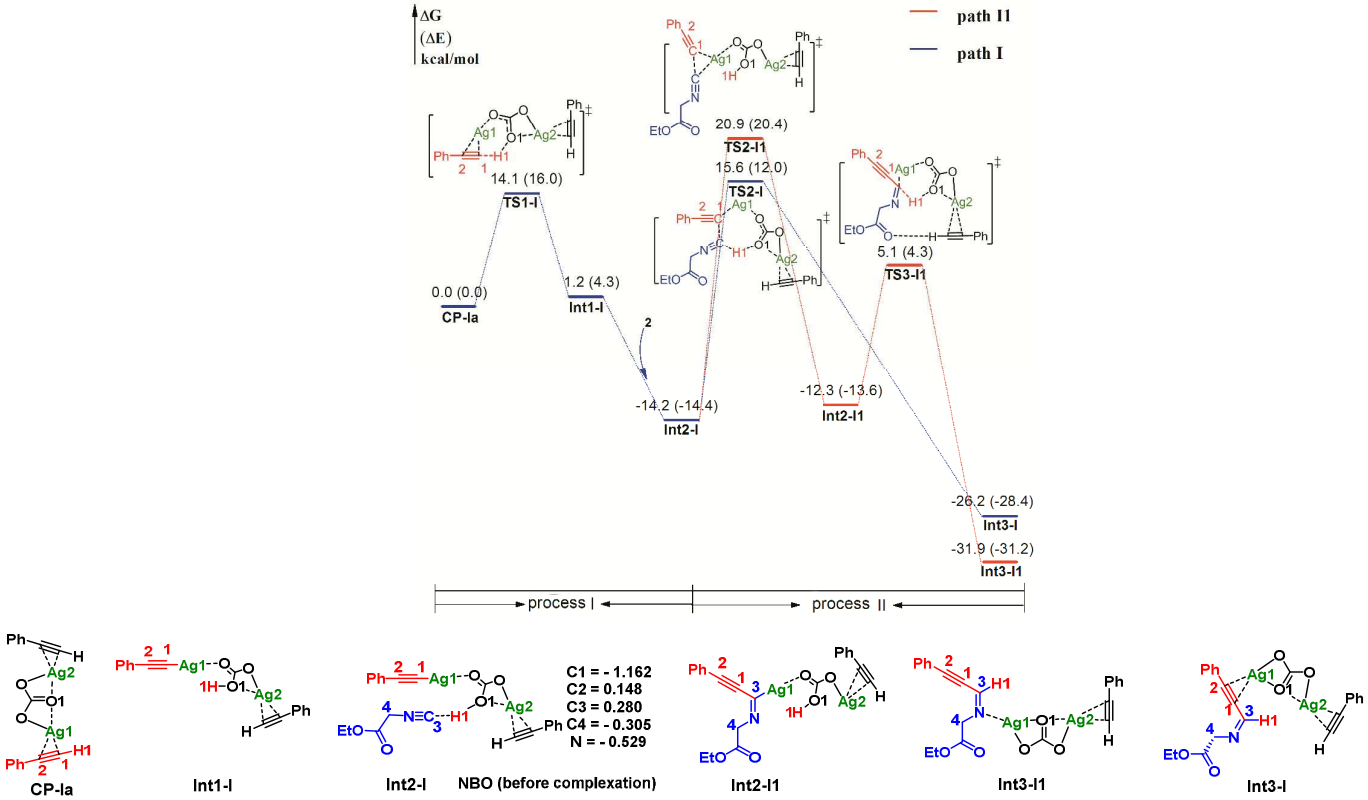


Figure S8a. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile for transformation from the most stable Ag^I complex to **Int3-I/Int3-I1** (energies are given in parentheses).

For isocyanide insertion process (process II, Figure S8a), the concerted transition state **TS2-I** is more favorable than **TS2-I1.** This is attributable to the fact that the reacting partners in **TS2-I1** must distort severely to achieve C1-C3 and C3-Ag1 bond formation, while the reacting partners in **TS2-I** with less ring strain have similar geometries and orientations as the intermediate **Int2-I**. For the hydrogen shift step, we discover that a trace amount of water could act as a catalyst for promoting H shift, which is in good agreement with the finding that a trace amount of water has an important catalytic role in some "anhydrous" reactions

involving [1,2] or [1,n] hydrogen shifts. Throughout the entire free energy profile, the rate-determining step in the catalytic cycle is the new C-C bond formation process with 29.8 kcal/mol of free energy barrier (**TS2-I**). The calculated results indicate that path I is a preferred reaction route for M-I.

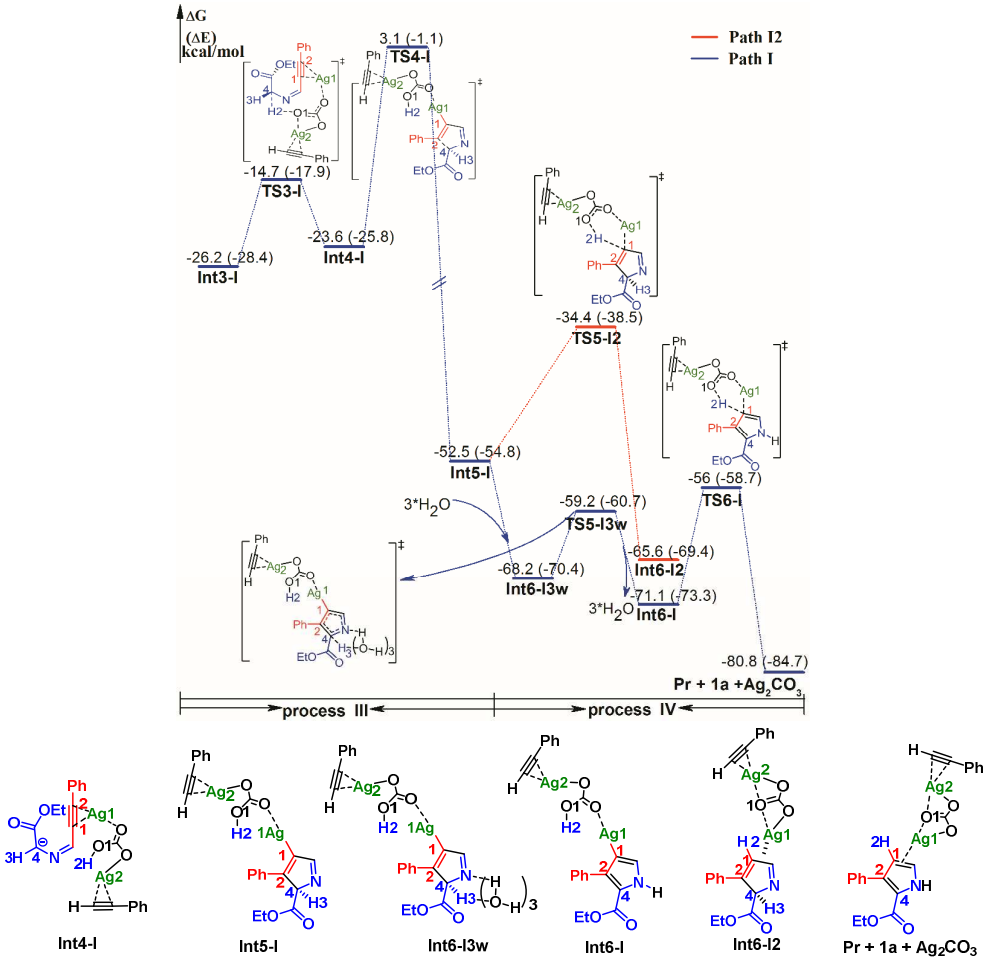


Figure S8b. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile for transformation from **Int3-I** to product (energies are given in parentheses).

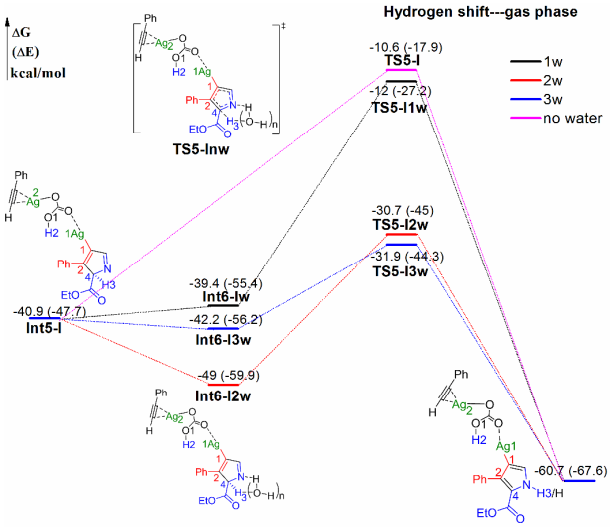


Figure S9. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile for [1, 5]-H shift using distinct equivalent water (w=water, energies are given in parentheses).

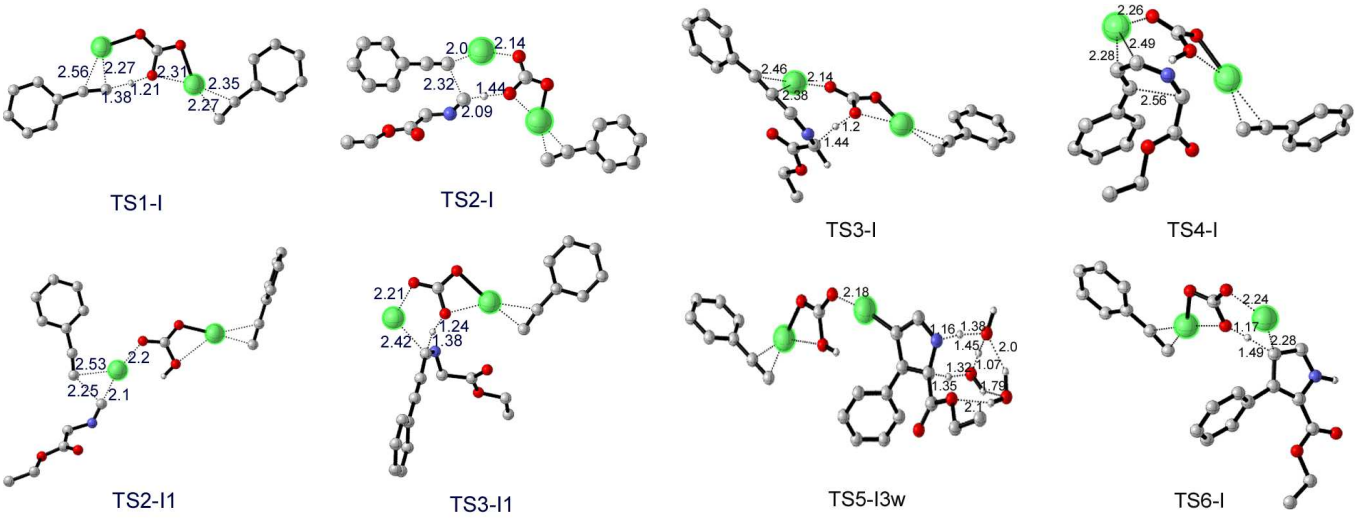
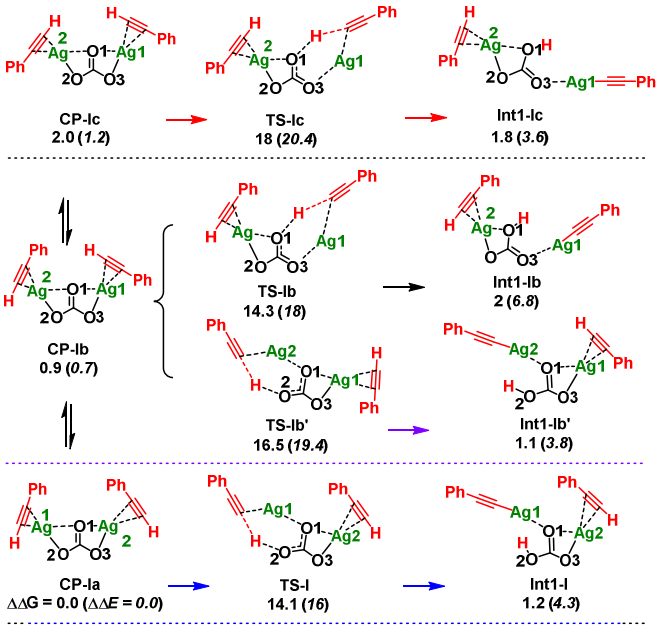


Figure S10. Optimized structures of the eight transition states in Figures S8a and 8b.

Additional information for M-I (the formation of silver-acetylide):



Scheme S5. Gibbs free energy (ΔG_{sol}, in kcal/mol) changes of process I form three stable Ag^{I} complexes in M-I.

v. The detailed mechanism (M-II) proposed by Lei group.

Note that the more stable complexes in M-II have been found to be **CP-IIa** and **CP-IIb** among all the possible Ag^{I} complexes (Scheme S4). The calculated results indicate the reaction mechanism of **1** and **2** catalyzed by Ag_2CO_3 herein is a stepwise process. The catalytic cycle begins with the formation of silver-acetylide complex **Int1-II** and silver-isocyanide complex **Int2-II** via (i), intermolecular cyclization via (ii), hydrogen shift via (iii), and protonation via (iv). The Gibbs free energy profiles are displayed in Figures S11a/b and Scheme S6.

In process i, the generation of **Int1-II** and **Int2-II** through C-H activation from **CP-IIb** and **CP-IIa** are very facile steps, requiring free energy barriers of 15.9 (**TS1-II)** and 12.6 kcal/mol (**TS2-II**), respectively (Figure S11a). The intermediate **Int1-II** is formed through H1' transfers from α-C to O2' of Ag_2CO_3 with simultaneously Ag1'–C3 bond formation. This is facilitated by

C4–H1'···O2' interaction of **CP-IIb** as well as the electron-withdrawing effect of -NC group, enhancing the acidity of α-C4-H1. Subsequently these two sliver-complexes combined together to form **Int3-II** exothermically.

The following intermolecular cyclization step from **Int3-II** to **Int5-II** via stepwise (path II) and concerted (path II1) transition states **TS3-II**/**TS4-II** and **TS3-II1**, requires the $\Delta\Delta G^{\ddagger}$ values of 5.8/16.6 and 24.6 kcal/mol. For path II, the consecutive C4-C2 (**TS3-II**) and C1-C3 bonds (**TS4-II**) formation leads to the cyclic intermediate **Int5-II**, featured by Ag-containing five-membered-ring structure. As depicted in Figure S11a, the frontier molecular orbital (FMO) analysis indicated that HOMO-5 of **TS4-II** has a larger electron delocalization over the N, C3, Ag1', and C1 as compared to **TS3-II1**. Therefore, the stepwise path II is more favorable. Five-membered cyclic **Int5-II** is generated with high exothermicity (-72 kcal/mol), verifying that the above processes can proceed smoothly.

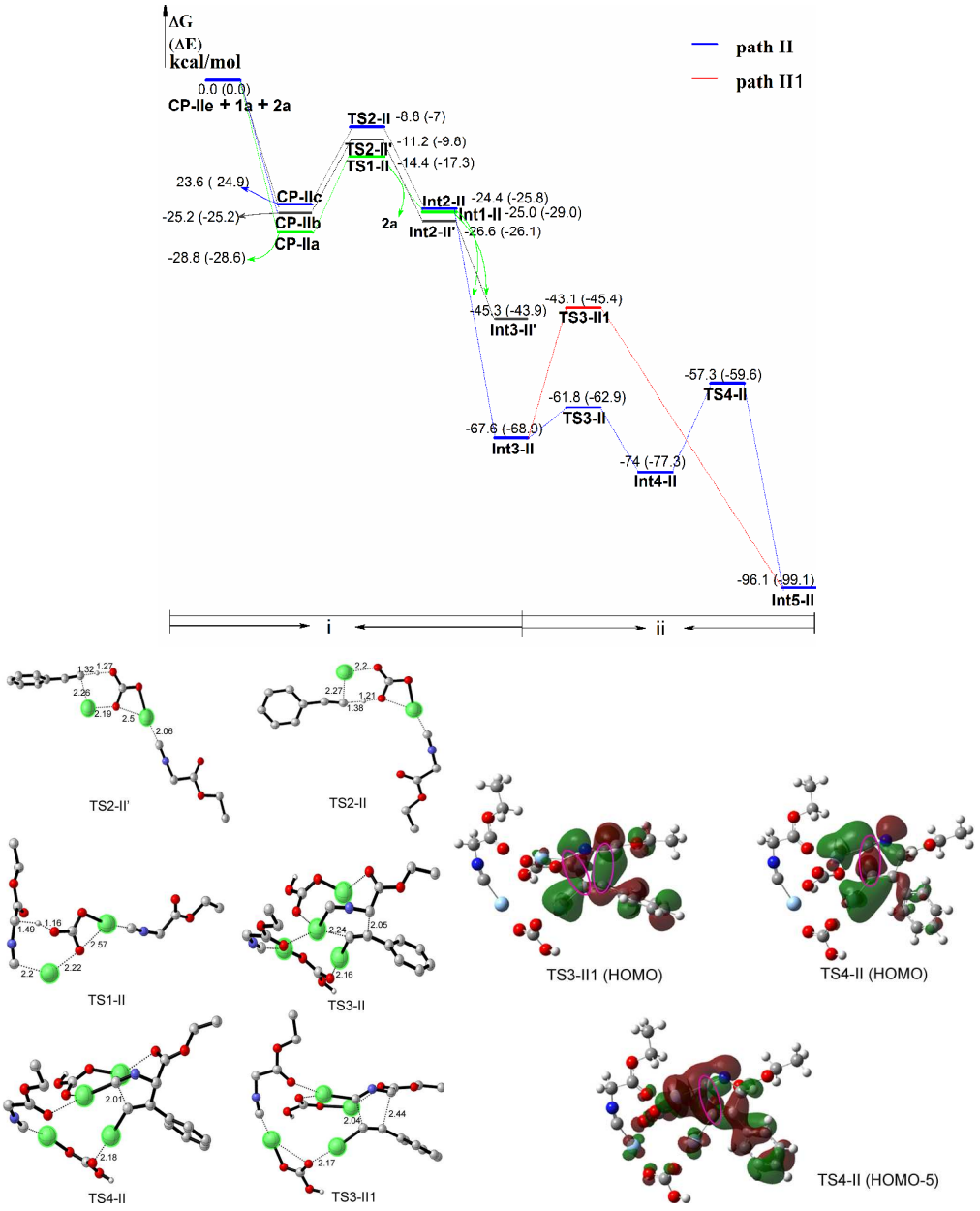


Figure S11a. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile from stable Ag^{I} complexes (**CP-IIa**/**CP-IIb**) to **Int5-II** (energies are given in parentheses) and the HOMOs/HOMO-5 of **TS3-II1** and **TS4-II** for C-C bonds formation (pink ellipse).

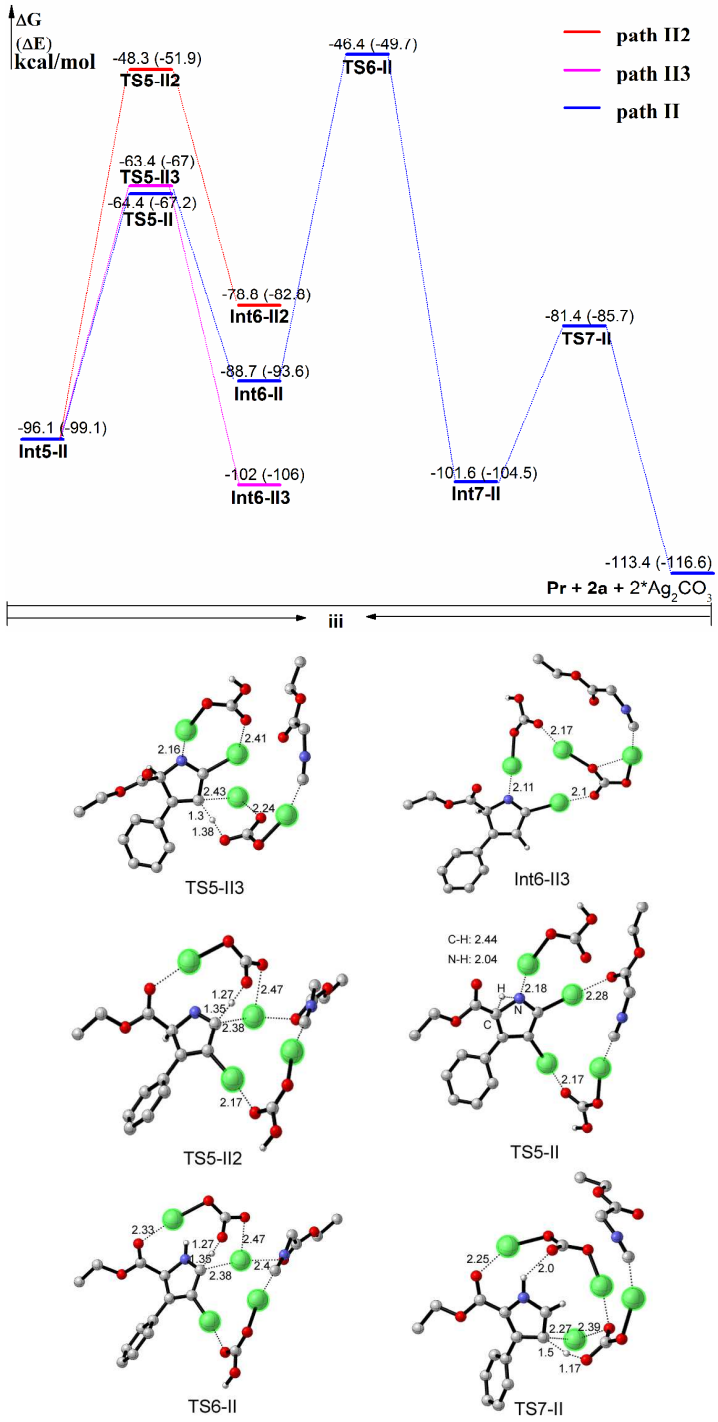
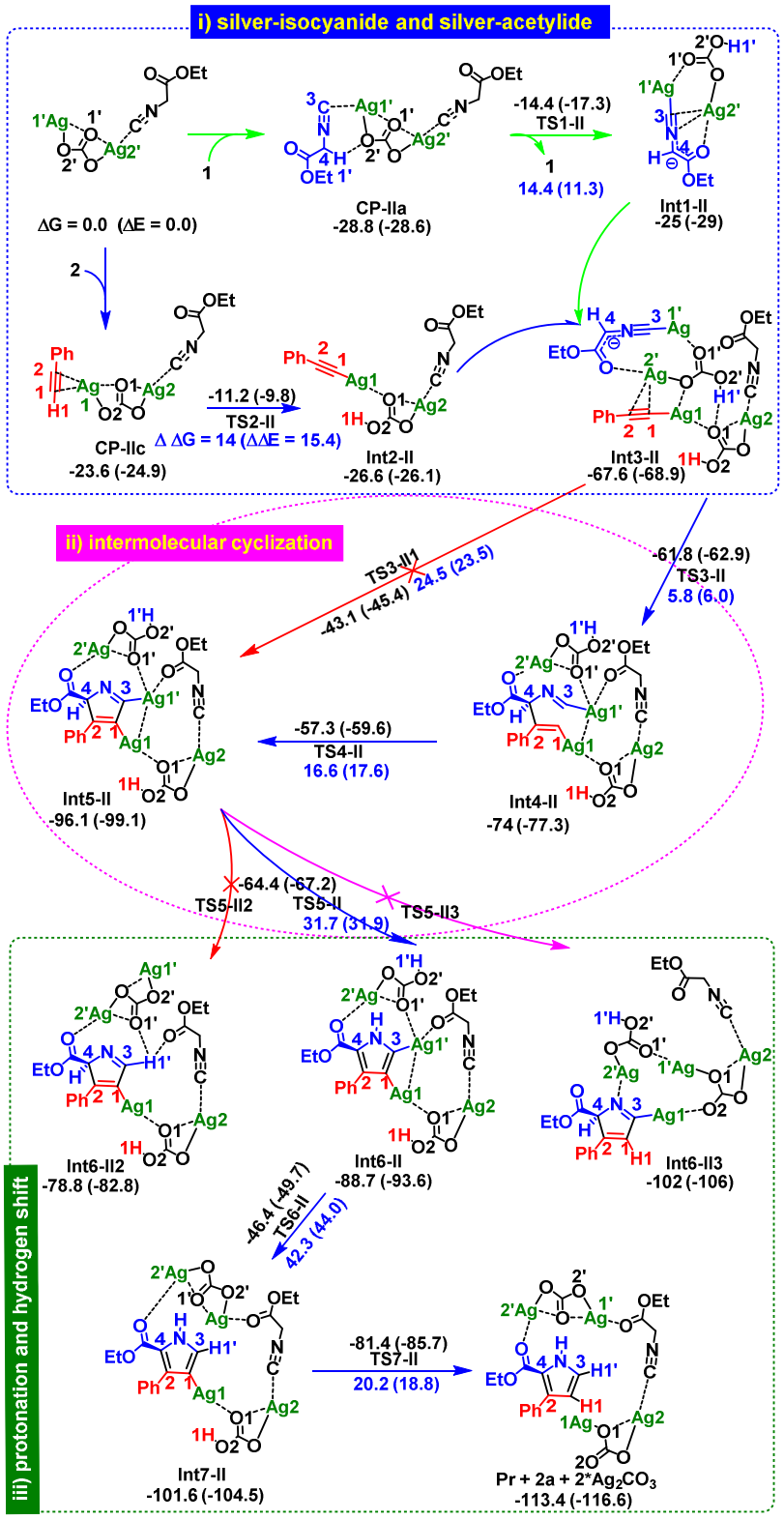


Figure S11b. Free energy (ΔG_{sol}, in kcal/mol) profile for transformation from **Int5-II** to product (energies are given in parentheses).

For process iii, we investigated three pathways path II, path II2 and path II3 differing in the sequence of the protonation of C1 as well as C3, and hydrogen shift. As illustrated in Figure S11b, path II2 requires a quite high activation barrier of C3 protonation being 47.8 kcal/mol (**TS5-II2**), eliminating it to be a possible pathway (Scheme S6). Although the energy barrier for protonation of C1 (**TS5-II3**, 32.7 kcal/mol) is reasonable, its direct product (**Int6-II3**) prevents the further protonation of C2, implying that the protonation of C1 should take place after C2. Therefore, a sole route can be accomplished wherein **TS5-II** is followed by **TS6-II** and **TS7-II** with free energy barriers of 42.3 and 20.2 kcal/mol, respectively. Then, the product is formed.



Scheme S6. Gibbs free energy (ΔG_{sol}, in kcal/mol) profile of mechanism M-II (energies are given in parentheses).

vi. References

(1) Cox, J. D.; Wagman, D. D.; Medvedev, V. A.; CODATA Key Values for Thermodynamics, Hemisphere Publishing Corp., New York, 1984, 1.

(2) (a) Yang, Y. F.; Cheng, G. J.; Liu, P.; Leow, D. S.; Sun, T. Y.; Chen, P.; Zhang, X. H.; Yu, J. Q.; Wu, Y. D.; Houk, K. N. *J. Am. Chem. Soc.* **2014**, *136*, 344-355. (b) Yu, H. Z.; Jiang, Y. Y.; Fu, Y.; Liu, L. *J. Am. Chem. Soc.* **2010**, *132*, 18078-18091. (c) Zhang, S. L.; Liu, L.; Fu, Y.; Guo, Q. X. *Organometallics* **2007**, 26, 4546-4554.

vii. Cartesian coordination and energies for the calculated key species of radical mechanism (in gas).

Gas Phase Optimization using B3LYP/LANL2DZ (f=1.611)-6-31G, $p^{\ominus}$ = 1 atm**

Single-point energies for discussion were calculated with M06/SDD/6-311++G/SMD (1,4-dioxane, 353.15 K), $c^{\ominus}$ = 1 M**

a) Process I

1

G-gas = -399.829471 Hartree

Symbol	X	Y	Z
C	0.2353060	0.1977450	0.0002280
O	0.4124780	1.3895830	-0.0002940
O	-0.9608890	-0.4171170	0.0008650
C	-2.1216630	0.4568450	0.0009030
H	-2.0721740	1.0990700	0.8850990
H	-2.0705860	1.1013550	-0.8815120
C	-3.3545300	-0.4241900	-0.0012440
H	-3.3811080	-1.0640480	0.8851340
H	-4.2526770	0.2006960	-0.0011040
H	-3.3797230	-1.0616620	-0.8893820
C	1.3320450	-0.8736820	0.0003100
H	1.1954810	-1.5114470	0.8806590
H	1.1953630	-1.5118810	-0.8796960
N	2.6287690	-0.3154500	0.0000910
C	3.7007290	0.1726720	-0.0009300

Ag_2CO_3

G-gas = -555.354719 Hartree

Symbol	X	Y	Z
C	-0.0003040	0.9869650	0.0001820
O	-0.0002170	-0.3526930	0.0002310
O	-1.1287300	1.5954310	-0.0003150
O	1.1280480	1.5952940	0.0002280
Ag	-2.3187530	-0.3045960	-0.0000010
Ag	2.3189450	-0.3044690	-0.0000460

1 + Ag_2CO_3

G-gas = -955.197170 Hartree

Symbol	X	Y	Z
C	1.7293140	-1.3209660	-0.4830520
O	1.5572420	-0.4247190	-1.2872420
O	2.8730220	-1.5888060	0.1415210
C	3.9644880	-0.6519070	-0.0591870
H	4.1506240	-0.5618360	-1.1335710
H	3.6430400	0.3225020	0.3226440
C	5.1676360	-1.1847960	0.6933330
H	5.4667030	-2.1663360	0.3121670
H	6.0102370	-0.4959010	0.5694920
H	4.9496870	-1.2753900	1.7616090
C	0.6710980	-2.3216920	-0.0158780
H	1.0726660	-3.3377140	-0.0662610
H	0.4239920	-2.0758470	1.0253570
N	-0.5356670	-2.2274180	-0.7611660
C	-1.6195390	-1.9601140	-1.1157860
C	-0.6959170	0.4408120	1.2786370
O	-1.2466970	1.2329270	0.3468090
O	0.5543520	0.5989750	1.5460320
O	-1.4114500	-0.4865710	1.7898140
Ag	0.8415890	1.8939390	-0.3473620
Ag	-2.8816210	-0.3509610	-0.0685350

TS(1-3)

G-gas = -955.172090 Hartree

Symbol	X	Y	Z
C	0.6553570	0.3743410	1.1095340
O	1.7560180	0.1129570	0.4363000
O	0.0598110	-0.6268060	1.7078990
O	0.2107530	1.5609420	1.1646150
Ag	1.4931620	-2.0289160	-0.2046090
Ag	1.7462570	2.3907180	-0.2544710
C	-2.5972390	-0.5443210	-0.3203920
O	-2.0429970	-0.1738350	-1.3431990
O	-3.7137030	0.0405130	0.1828390
C	-4.1747990	1.2133330	-0.5154210
H	-3.4016520	1.9878450	-0.4586590
H	-4.3197500	0.9694540	-1.5725910
C	-5.4662010	1.6564190	0.1475770

H	-5.3019560	1.8938900	1.2025890
H	-5.8560040	2.5497470	-0.3509570
H	-6.2243270	0.8699970	0.0869100
C	-2.1103250	-1.5928200	0.5938980
H	-1.0021450	-0.8885090	1.3540050
H	-2.8413780	-2.0268380	1.2705710
N	-1.2828570	-2.5251420	-0.0206490
C	-0.3875500	-3.1060300	-0.5149000

3 + **$AgHCO_3$**

G-gas = -955.249060 Hartree

Symbol	X	Y	Z
C	-3.0934680	-1.3616660	0.0003650
O	-3.4529620	-0.1530430	-0.0001470
O	-4.1087570	-2.2522450	0.0005630
O	-1.9208150	-1.8499090	0.0007470
Ag	-1.9552190	1.3329190	0.0000650
Ag	0.0529590	-0.9777220	-0.0004500
C	2.8520030	0.5319560	-0.0000520
O	2.1492700	-0.5258300	-0.0002940
O	4.2012890	0.4137940	-0.0000320
C	4.7488050	-0.9179680	-0.0004450
H	4.3921710	-1.4588040	0.8825600
H	4.3939300	-1.4574760	-0.8849980
C	6.2603760	-0.7790050	0.0011210
H	6.6014030	-0.2383070	0.8886030
H	6.7247670	-1.7701360	0.0007180
H	6.6031090	-0.2367940	-0.8847790
C	2.4206540	1.8641280	0.0001740
H	-3.7015130	-3.1310000	0.0009160
H	3.1110640	2.6932790	0.0003050
N	1.0958030	2.1152480	0.0001300
C	-0.0772900	2.1685720	0.0000320

3

G-gas = -544.990491 Hartree

Symbol	X	Y	Z
Ag	-1.8003120	-0.6013040	0.0098200
C	1.1149060	0.5397160	-0.0213120
O	0.4842900	-0.5455650	-0.0612140
O	2.4642160	0.5196110	0.0043990
C	3.0918940	-0.7613710	-0.0156450
H	2.7520200	-1.3518890	0.8443380
H	2.7958450	-1.3014260	-0.9237500
C	4.5755880	-0.5281160	0.0288260
H	4.8584740	0.0062770	0.9421050
H	5.1032380	-1.4878330	0.0117370
H	4.9026440	0.0625220	-0.8335370
C	0.5877160	1.8330020	0.0081420
H	1.1971030	2.7220700	0.0673090
N	-0.7652260	1.9236880	0.0002480
C	-1.9077890	1.6423310	-0.0195080

$AgHCO_3$

G-gas = -410.174676 Hartree

Symbol	X	Y	Z
H	3.1682500	-0.8474300	0.0006530
C	1.5276640	0.0428130	0.0000330
O	0.9680640	-1.1019580	0.0000960
O	0.9274780	1.1538680	0.0001650
O	2.8812080	0.0775130	-0.0002370
Ag	-1.0754940	-0.0094650	-0.0000220

4

G-gas = -399.195495 Hartree

Symbol	X	Y	Z
C	0.2597770	0.2112980	-0.0008850
O	0.4056860	1.4179500	-0.0000040
O	-0.9293050	-0.4310250	-0.0017080
C	-2.0991280	0.4235080	-0.0008890
H	-2.0583120	1.0708270	0.8807050
H	-2.0613100	1.0682570	-0.8845350
C	-3.3199520	-0.4745210	0.0023300
H	-3.3351040	-1.1121830	0.8905810
H	-4.2270010	0.1373530	0.0026360
H	-3.3376610	-1.1150550	-0.8838040

C	1.3512250	-0.7709720	-0.0010100
H	1.1493500	-1.8361280	-0.0018220
N	2.6234400	-0.3586660	-0.0009590
C	3.7572300	0.0110540	0.0032280

CPI-1-3S

G-gas = -1877.904497 Hartree

Symbol	X	Y	Z
C	0.3402880	-0.0131920	-1.4808810
O	0.1830980	0.8203520	-0.4644650
O	-0.6379700	-0.7326950	-1.8707960
O	1.5246420	-0.1025900	-2.0104850
Ag	-1.7865120	-0.0518260	0.2513530
Ag	2.6306080	0.9665090	-0.4332290
C	2.3908840	-2.5775260	-0.5664420
O	2.8851390	-1.8974830	0.3110620
O	3.0322760	-3.0350000	-1.6430220
C	4.3700860	-2.5256120	-1.8663980
H	4.3071330	-1.4363130	-1.9412360
H	4.9929450	-2.7791870	-1.0028390
C	4.8834650	-3.1515020	-3.1476130
H	4.2393590	-2.8879020	-3.9904590
H	5.8939510	-2.7862100	-3.3561460
H	4.9214510	-4.2413640	-3.0654840
C	0.9416610	-3.0531200	-0.6250680
H	0.4536670	-2.5533670	-1.4777870
H	0.9171320	-4.1371160	-0.7721510
N	0.2114680	-2.6951530	0.5381040
C	-0.4696300	-2.2332540	1.3732350
C	2.4552070	2.6027630	2.8681850
C	3.6871750	2.7933740	1.9912540
C	4.1993880	0.4780730	2.2511030
C	2.9653560	0.3265350	3.1304370
H	3.5283190	3.5494230	1.2176210
H	1.5784600	2.3892220	2.2347980
H	2.2556480	3.5097910	3.4483050
H	4.3770880	-0.4198280	1.6574140
H	5.0830360	0.7164290	2.8580410
H	2.1111020	0.0014040	2.5171230
H	3.1420870	-0.4253690	3.9057100
H	4.5514400	3.0775750	2.6063820
O	4.0054340	1.5612700	1.3054300
O	2.6702360	1.5507380	3.7998830
C	-4.0581810	2.7709930	-0.8164510
C	-3.0518390	3.9148660	-0.7810320
C	-1.7939320	2.8813160	-2.4573190
C	-2.7774790	1.7215530	-2.5158970
H	-3.5508760	4.8566500	-0.5296450
H	-4.8786460	3.0239040	-1.5066870
H	-4.4743560	2.5783760	0.1771660
H	-1.3698410	3.0716740	-3.4473060
H	-0.9814440	2.6319360	-1.7588790
H	-3.5433200	1.9049680	-3.2852090
H	-2.2507960	0.7843070	-2.7090660
H	-2.2847810	3.7058110	-0.0156820
O	-2.4507160	4.0868760	-2.0531660
O	-3.4322650	1.5581860	-1.2411320
C	-5.1644720	-2.2847400	0.0584830
C	-4.9909520	-0.8337230	0.4850460
C	-3.8558140	-1.5778990	2.4433340
C	-4.0589440	-3.0162210	1.9867150
H	-4.8422410	-0.1681760	-0.3678370
H	-4.3274100	-2.5838850	-0.5937540
H	-6.0996380	-2.4109160	-0.4959860
H	-2.9028330	-1.4618040	2.9624490
H	-4.6797220	-1.2644930	3.1005100
H	-3.1764220	-3.3452980	1.4168240
H	-4.1848630	-3.6762740	2.8506310
H	-5.8651240	-0.5073520	1.0670630
O	-3.8146580	-0.6941960	1.3079640
O	-5.2360780	-3.1375510	1.1954010

TS(1-3)-3S

G-gas = -1877.891050 Hartree

Symbol	X	Y	Z
C	0.9336640	-1.7903100	-0.3133990
O	0.1155680	-1.0370170	-0.9655650
O	0.5179050	-2.4243380	0.7646610
O	2.1739460	-1.8978700	-0.6477930
Ag	-1.5104290	-0.4296490	0.6053260
Ag	2.6082880	0.0589000	-1.4431850
C	2.8994690	-0.4300140	2.0564390
O	2.8731040	0.5498440	1.3141980
O	4.0337070	-1.0907280	2.3674510
C	5.2284750	-0.6921950	1.6676400
H	5.0710250	-0.8318590	0.5922680
H	5.4122780	0.3724790	1.8469210
C	6.3638490	-1.5586410	2.1812580
H	6.1584080	-2.6165480	1.9949190
H	7.2957080	-1.2922120	1.6721600
H	6.5063810	-1.4188610	3.2570680
C	1.7313520	-1.0996110	2.6554380
H	1.2385250	-1.9849670	1.6910280
H	1.9466070	-1.6255380	3.5837250
N	0.5929920	-0.2821670	2.7386020
C	-0.4200740	0.2724700	2.5207970
C	-4.6321460	1.1162990	1.1837660
C	-4.4362730	1.9990240	2.4100130
C	-3.0482080	3.4295790	1.1776170
C	-3.2348450	2.5685090	-0.0679970
H	-5.3416520	2.0034110	3.0253250
H	-5.5337420	1.4316280	0.6368370
H	-4.7268760	0.0624550	1.4593540
H	-2.9306230	4.4813690	0.8987370
H	-2.1508410	3.1118100	1.7330280
H	-4.0814250	2.9476810	-0.6601410
H	-2.3334580	2.5629950	-0.6890100
H	-3.6016600	1.6131430	3.0156320
O	-4.1953500	3.3459160	2.0185250
O	-3.5006820	1.2038230	0.3021080
C	1.7558990	2.7016560	-2.9729130
C	0.3161980	2.5915140	-2.4893370
C	0.9956650	2.9814130	-0.2773690
C	2.4468760	3.0943190	-0.7272170
H	-0.3640690	2.9698450	-3.2589470
H	1.9965620	3.7366100	-3.2521110
H	1.9496940	2.0444160	-3.8247750
H	0.8075870	3.6511480	0.5670130
H	0.7930520	1.9502230	0.0460920
H	2.7092120	4.1324650	-0.9702220
H	3.1210910	2.6977340	0.0334680
H	0.0787900	1.5340990	-2.2864870
O	0.0995480	3.3723480	-1.3223100
O	2.6557490	2.2922710	-1.9211200
C	-4.1174260	-1.8943080	-1.1127000
C	-3.4673860	-2.2371540	-2.4499390
C	-2.0996040	-3.8211040	-1.4139080
C	-2.7312930	-3.5211600	-0.0603060
H	-4.1896030	-2.1142090	-3.2652460
H	-5.0322480	-2.4924240	-0.9769810
H	-4.3610420	-0.8297630	-1.0524370
H	-1.8022500	-4.8731050	-1.4728320
H	-1.2141010	-3.1849370	-1.5532620
H	-3.5754570	-4.2014210	0.1306410
H	-1.9914660	-3.6078770	0.7385320
H	-2.6116000	-1.5650620	-2.6300380
O	-3.0417360	-3.5928110	-2.4654350
O	-3.2190430	-2.1622030	-0.0232720

CPI-2-3S

G-gas = -1785.642871 Hartree

Symbol	X	Y	Z
C	5.0415360	-1.1306830	-0.3456300
C	4.9055470	-2.3698940	0.5284820
C	3.5424150	-3.3938860	-1.0826030
C	3.6618670	-2.1696090	-1.9805200
H	5.8196210	-2.5380730	1.1054610

H	5.9223060	-1.2198450	-0.9970360	H	-3.0052210	-3.9649990	2.7790480
H	5.1021600	-0.2123720	0.2423000	H	-2.3039680	-2.4504860	2.1463590
H	3.4623850	-4.3059930	-1.6821070	H	-4.2838110	-4.2926190	0.6817810
H	2.6398680	-3.3038800	-0.4548500	H	-4.6272820	-2.6463250	1.2884340
H	4.5127710	-2.2823340	-2.6665530	H	-0.7459400	-2.6424160	0.2692320
H	2.7502180	-1.9974530	-2.5584860	O	-1.6487980	-4.2322480	1.2880880
H	4.0663740	-2.2382370	1.2313650	O	-3.4008950	-2.7194370	-0.3409580
O	4.7011750	-3.5314770	-0.2701950	C	3.4371640	3.8931860	-0.7615030
O	3.8703200	-0.9878730	-1.1827520	C	4.4560410	2.8156460	-0.4077850
C	-0.4038020	0.5183520	0.9942790	C	3.4382250	2.5773320	1.7191150
O	-0.3689900	-0.2478690	-0.0990080	C	2.4423460	3.6670440	1.3451140
O	-1.5362690	0.7963360	1.5197600	H	4.7414640	2.2303890	-1.2878650
O	0.7149140	0.9574580	1.4537030	H	2.5749750	3.4282750	-1.2697880
Ag	-2.7317270	-0.3634180	-0.1220960	H	3.8793020	4.6368450	-1.4334080
Ag	2.0128660	-0.0290600	-0.1112760	H	2.9564090	1.8216220	2.3435910
C	-3.3215090	3.3502810	0.0711150	H	4.3054980	3.0090780	2.2416290
C	-4.2228970	2.3606660	0.7937600	H	1.5365100	3.1961970	0.9410190
C	-5.2168670	1.7913940	-1.2874410	H	2.1708860	4.2544670	2.2270370
C	-4.2913290	2.7813630	-1.9871850	H	5.3561570	3.2856650	0.0186820
H	-3.6873030	1.9029480	1.6258830	O	3.9042250	1.8938050	0.5369410
H	-2.3669830	2.8574600	-0.1653350	O	3.0168260	4.5802880	0.4047870
H	-3.1167220	4.2171150	0.7064930	**TS(S-S$^{\bullet}$)-3S**			
H	-5.4393510	0.9280430	-1.9222450	G-gas = -1785.596977 Hartree			
H	-6.1594920	2.2884050	-1.0150480	Symbol	X	Y	Z
H	-3.3846110	2.2542200	-2.3315810	C	-3.5219250	-3.5127280	0.5494360
H	-4.7868540	3.2255760	-2.8570560	C	-2.1634580	-3.4649510	-0.1565410
H	-5.1424220	2.8520020	1.1426810	C	-1.3076680	-2.0655610	1.5364410
O	-4.5954010	1.2818830	-0.0981830	C	-2.6046640	-2.2382270	2.3009040
O	-3.9467320	3.8454830	-1.1147640	H	-1.9838960	-4.4029620	-0.6955710
C	-2.3325780	-3.4994740	-0.9149220	H	-3.5823040	-4.4095130	1.1834060
C	-1.1845850	-3.6342250	0.0776700	H	-4.3431130	-3.5327090	-0.1738720
C	-2.6837120	-3.4473920	1.8696170	H	-0.4869370	-2.0671870	2.2701220
C	-3.8484100	-3.3060400	0.8967040	H	-0.6201880	-0.9404430	0.7782940
H	-0.4119580	-4.2985560	-0.3240770	H	-2.6088590	-3.1563690	2.9134540
H	-2.7274120	-4.4896830	-1.1847130	H	-2.8228580	-1.3809060	2.9446260
H	-2.0207970	-2.9737500	-1.8213040	H	-2.1786810	-2.6370280	-0.8955410

O	-1.1074970	-3.2822500	0.7561990	C	-5.6516630	2.5564950	0.3571250
O	-3.7159550	-2.3506550	1.3684430	C	-5.7771980	1.3597580	-0.5787290
C	0.0013020	0.7856550	-0.3444940	C	-3.8900020	2.1376630	-1.7938590
O	0.2872470	-0.3357920	0.3330130	C	-3.7939030	3.3243940	-0.8474510
O	0.9973110	1.4314110	-0.8221750	H	-6.1478870	0.4747060	-0.0537230
O	-1.2006790	1.1700250	-0.4939940	H	-5.0378720	2.2771430	1.2309400
Ag	2.7369160	0.1391600	-0.2669110	H	-6.6378230	2.8724840	0.7126950
Ag	-2.8108040	-0.3205210	0.1054400	H	-2.8943360	1.8145080	-2.0999210
C	2.8326280	3.9314610	0.4607180	H	-4.5047550	2.3882040	-2.6704150
C	3.6017130	3.3046950	-0.6928640	H	-3.0884600	3.0837710	-0.0386000
C	5.1727920	2.4395350	0.8591130	H	-3.4274700	4.2081160	-1.3778380
C	4.3784800	3.0725040	1.9962560	H	-6.4615760	1.6014260	-1.4053550
H	2.9156830	2.9733920	-1.4735610	O	-4.4950960	1.0115550	-1.1198650
H	2.0369440	3.2424640	0.7781310	O	-5.0769510	3.6634080	-0.3188760
H	2.3749960	4.8744340	0.1479140	**S**			
H	5.6397960	1.4998500	1.1692290	G-gas = -307.573866 Hartree			
H	5.9554300	3.1339610	0.5191170	Symbol	X	Y	Z
H	3.6554740	2.3388170	2.3926040	C	0.0000000	0.7623610	1.1723880
H	5.0457580	3.3766480	2.8093960	C	0.0000000	-0.7623610	1.1723880
H	4.3336140	4.0155170	-1.1031320	C	0.0000000	-0.7623610	-1.1723880
O	4.3100180	2.1282240	-0.2435260	C	0.0000000	0.7623610	-1.1723880
O	3.7074660	4.2385300	1.5479110	H	0.5574930	-1.1568150	2.0276880
C	2.6480290	-2.9048240	0.6506400	H	1.0381820	1.1290000	1.2274690
C	1.8962760	-3.4359190	-0.5586440	H	-0.5574930	1.1568150	2.0276880
C	3.7904790	-3.1177780	-1.9065990	H	0.5574930	-1.1568150	-2.0276880
C	4.5698120	-2.5801420	-0.7124170	H	-1.0381820	-1.1290000	-1.2274690
H	1.1754790	-4.1959670	-0.2522800	H	1.0381820	1.1290000	-1.2274690
H	3.1408250	-3.7220530	1.1943150	H	-0.5574930	1.1568150	-2.0276880
H	1.9826450	-2.3587600	1.3197520	H	-1.0381820	-1.1290000	1.2274690
H	4.4589730	-3.6491980	-2.5916550	O	0.6366200	-1.2620120	0.0000000
H	3.3287950	-2.2766250	-2.4530280	O	-0.6366200	1.2620120	0.0000000
H	5.0999660	-3.3994420	-0.2074080	**S** + **Ag_2CO_3**			
H	5.2902960	-1.8121120	-1.0070470	G-gas = -862.933934 Hartree			
H	1.3415800	-2.6131450	-1.0333370	Symbol	X	Y	Z
O	2.8011150	-4.0404690	-1.4843670	C	-3.7615340	-0.0274920	1.0989280
O	3.6726880	-1.9651400	0.2326390	C	-3.5283410	1.4683290	1.2623460

C	-3.3665590	1.7255890	-1.0637800
C	-3.5967300	0.2337770	-1.2632010
H	-4.0790650	1.8503450	2.1272290
H	-4.8352370	-0.2440700	1.0211300
H	-3.3328740	-0.6058700	1.9207470
H	-3.8003160	2.2943910	-1.8917970
H	-2.2850870	1.9340280	-1.0191130
H	-4.6672390	0.0207620	-1.3833040
H	-3.0490760	-0.1577620	-2.1236360
H	-2.4539450	1.6647970	1.4119120
O	-4.0075450	2.1727960	0.1241190
O	-3.1226150	-0.4977240	-0.1097050
C	1.7779160	-1.0709410	0.0361390
O	1.2819570	0.1484150	-0.0205480
O	3.0486680	-1.2554300	0.0718270
O	0.9615930	-2.0762680	0.0551230
Ag	3.4587280	0.9517300	0.0063850
Ag	-0.9468590	-1.1361240	-0.0372850

TS(S-S(-Ag))

G-gas = -862.878911 Hartree

Symbol	X	Y	Z
C	-3.6638340	-1.7294640	-0.6625110
C	-2.2512590	-2.0716790	-1.1895060
C	-1.2572040	-1.8231020	0.9491490
C	-2.7166490	-1.4314540	1.4869750
H	-2.3399790	-2.7308450	-2.0276760
H	-4.1662620	-2.6273860	-0.3689100
H	-4.2256950	-1.2434950	-1.4326070
H	-0.7728530	-2.3306440	1.7570500
H	-0.1052370	-0.6651290	0.4163440
H	-3.1950330	-2.3226800	1.8359260
H	-2.6175850	-0.7330330	2.2915210
H	-1.7528620	-1.1743550	-1.4916820
O	-1.4894580	-2.7134680	-0.1556640
O	-3.5403850	-0.8642200	0.4602730
C	1.4047510	1.7134910	0.0775570
O	0.8971240	0.2537200	-0.3244390
O	2.7871290	1.9624900	0.4381660
O	0.6130440	2.7492610	0.0660490
Ag	3.6032050	-0.7616890	-0.0597310
Ag	-1.9874380	1.5016580	-0.1280350

S(-Ag)

G-gas = -452.733244 Hartree

Symbol	X	Y	Z
C	-2.4867570	-0.0573680	-0.7313400
C	-1.6654280	-1.2765650	-0.3159550
C	-0.3519490	0.0861180	1.0786500
C	-1.1811430	1.2899500	0.6569900
H	-2.2898030	-2.1733800	-0.2610620
H	-3.3727570	0.0278820	-0.0808490
H	-2.8235010	-0.1536810	-1.7681310
H	0.0020170	0.1632570	2.1079020
H	-2.0210170	1.4076260	1.3699150
H	-0.5864450	2.2058270	0.6618500
H	-0.8527300	-1.4430820	-1.0448720
O	-1.0924120	-1.0975100	0.9743790
O	-1.7094680	1.1315110	-0.6547930
Ag	1.4568280	-0.0118990	-0.1632240

S$^{\bullet}$

G-gas = -306.925871 Hartree

Symbol	X	Y	Z
C	0.5997010	-1.1851680	0.2597590
C	1.3828300	0.0377140	-0.1957640
C	-0.6366830	1.2449210	-0.1468570
C	-1.4108510	-0.0119030	0.1086050
H	2.3640340	0.0891040	0.2841140
H	0.5372160	-1.2020980	1.3609110
H	1.0933040	-2.1025540	-0.0750470
H	-1.0978860	2.2123330	0.0324890
H	-1.6525630	-0.1150020	1.1884490
H	-2.3586210	0.0039240	-0.4383480
H	1.5132710	0.0082630	-1.2852200

O	0.6991000	1.2498250	0.1592210
O	-0.7001910	-1.1757450	-0.3119460

TS(S•-S)

G-gas = -706.72965 Hartree

Symbol	X	Y	Z
C	2.9609850	-0.9588240	0.9558270
C	1.4815030	-1.1843600	1.2239980
C	1.0864610	-0.9337560	-1.0972350
C	2.5439500	-0.5687850	-1.3074110
H	1.3226700	-1.9517370	1.9856180
H	3.4568290	-1.9178230	0.7331830
H	3.4429410	-0.5083730	1.8276720
H	0.5996560	-1.4011570	-1.9571090
H	3.0931770	-1.4695770	-1.6432720
H	2.6412670	0.1962370	-2.0830790
H	0.9986090	-0.2551190	1.5456900
O	0.8161160	-1.6706910	0.0362490
O	3.1337910	-0.0523890	-0.1279630
C	-1.3766910	0.8206600	0.2527550
O	-1.2918460	0.8946290	1.4611280
O	-2.3492720	0.1602990	-0.4114310
C	-3.3153440	-0.5318190	0.4168850
H	-2.7805730	-1.2353580	1.0622290
H	-3.8116640	0.1989590	1.0624510
C	-4.2905700	-1.2321120	-0.5085410
H	-3.7744600	-1.9550820	-1.1465030
H	-5.0400040	-1.7681430	0.0817590
H	-4.8082510	-0.5129850	-1.1495550
C	-0.3777410	1.3531740	-0.7254590
H	0.3835570	0.2689310	-0.9610360
H	-0.7959300	1.5752160	-1.7077840
N	0.4483630	2.3564970	-0.2394450
C	1.1980020	3.1667780	0.1828460

b) Process II

2 + **Ag_2CO_3**

G-gas = -863.686885 Hartree

Symbol	X	Y	Z
C	2.6543020	1.3139250	-0.0007380
C	1.7108490	2.1088220	-0.0013840
H	1.1931000	3.0464950	-0.0018370
C	3.8278610	0.4949320	0.0000730
C	4.4188220	0.1063390	1.2182410
C	4.4188370	0.1035840	-1.2172000
C	5.5828680	-0.6560610	1.2123230
H	3.9587510	0.4063060	2.1540450
C	5.5828760	-0.6588190	-1.2095490
H	3.9587820	0.4014170	-2.1536950
C	6.1665030	-1.0394720	0.0018220
H	6.0347660	-0.9534390	2.1535320
H	6.0347730	-0.9583260	-2.1500840
H	7.0735580	-1.6363380	0.0025070
C	-1.8587590	-1.0784120	-0.0001810
O	-1.9234790	0.2580310	0.0000860
O	-2.9511920	-1.7473480	0.0001630
O	-0.6931080	-1.6089720	-0.0008630
Ag	-4.2115470	0.1255080	0.0008960
Ag	0.4086440	0.3066450	-0.0013220

TS(2-5)

G-gas = -863.666029 Hartree

Symbol	X	Y	Z
C	2.0817550	0.5655890	0.0034720
C	0.8394370	0.6572750	0.0056920
H	-0.5506550	0.5462610	0.0050390
C	3.5044440	0.7602330	0.0013210
C	4.0265950	2.0698380	0.0015420
C	4.4027360	-0.3231520	-0.0009780
C	5.4029370	2.2803450	-0.0004870
H	3.3410730	2.9108630	0.0033290
C	5.7782170	-0.1049170	-0.0030210
H	4.0110140	-1.3366790	-0.0011380
C	6.2844800	1.1965090	-0.0027810
H	5.7888720	3.2957020	-0.0002700

H	6.4560720	-0.9536410	-0.0047910
H	7.3573110	1.3647130	-0.0043600
C	-2.2102200	-0.8961260	0.0003260
O	-1.7386230	0.3650290	0.0019000
O	-3.4857860	-1.0158990	-0.0016280
O	-1.4465150	-1.9095040	0.0007080
Ag	-4.0034890	1.1271410	-0.0008760
Ag	0.7333070	-1.6075200	0.0001070

5 + **$AgHCO_3$**

G-gas = -863.684121 Hartree

Symbol	X	Y	Z
C	3.5357640	-0.0874700	-0.0376930
C	2.3596340	-0.4282880	-0.1002690
H	-1.4028380	0.8126310	0.1535230
C	4.9090730	0.2955500	0.0365310
C	5.3851530	1.4303000	-0.6528340
C	5.8273500	-0.4539420	0.8015230
C	6.7264390	1.7980430	-0.5779630
H	4.6872760	2.0131700	-1.2458170
C	7.1672430	-0.0809590	0.8715560
H	5.4711310	-1.3297220	1.3347610
C	7.6246290	1.0458060	0.1833710
H	7.0734250	2.6755580	-1.1172770
H	7.8586320	-0.6728320	1.4655840
H	8.6705540	1.3341940	0.2391560
C	-2.6225730	-0.6753500	-0.1026410
O	-2.3648520	0.6653550	0.1273420
O	-3.8633430	-0.9481040	-0.1471760
O	-1.6877430	-1.4808460	-0.2427220
Ag	-4.9996280	0.8542630	0.1634320
Ag	0.4356510	-1.0199310	-0.1902180

2

G-gas = -308.324404 Hartree

Symbol	X	Y	Z
C	-2.0239090	-0.0000160	0.0000010
C	-3.2341800	0.0000050	-0.0000040
H	-4.2993540	0.0000180	-0.0000040
C	-0.5939700	-0.0000210	0.0000000
C	0.1200350	0.2130160	0.0000000
C	0.1200550	1.2130250	0.0000010
C	1.5123250	1.2083370	0.0000010
H	-0.4281630	2.1493560	0.0000060
C	1.5123610	-1.2083160	-0.0000010
H	-0.4281000	-2.1493910	-0.0000010
C	2.2125920	0.0000120	0.0000000
H	2.0526130	2.1503560	0.0000010
H	2.0526480	-2.1503350	0.0000020
H	3.2985050	0.0000370	0.0000010

5

G-sol = -453.493288 Hartree

Symbol	X	Y	Z
C	-0.4114670	-0.0001120	-0.0003050
C	0.8123600	0.0001380	-0.0003330
C	-1.8401650	-0.0000610	-0.0002930
C	-2.5603670	1.2116430	-0.0000600
C	-2.5604600	-1.2116960	-0.0000570
C	-3.9530380	1.2076290	0.0001210
H	-2.0123290	2.1484790	-0.0000730
C	-3.9531300	-1.2075660	0.0001170
H	-2.0125060	-2.1485830	-0.0000650
C	-4.6556820	0.0000540	0.0001550
H	-4.4926810	2.1506970	0.0002250
H	-4.4928360	-2.1505960	0.0002210
H	-5.7419290	0.0000950	0.0003180
Ag	2.8400850	-0.0000050	0.0000700

6′

G-gas = -1467.812180 Hartree

Symbol	X	Y	Z
C	2.7316350	-2.4433280	0.5769760
O	2.1334820	-2.8130080	1.5706630
O	4.0154530	-2.0300020	0.5498630
C	4.6871370	-1.9820760	1.8287170

H	4.1465740	-1.2865630	2.4789970
H	4.6378330	-2.9733770	2.2906990
C	6.1132880	-1.5324290	1.5760840
H	6.1297570	-0.5439580	1.1092560
H	6.6568090	-1.4793430	2.5248050
H	6.6344780	-2.2363520	0.9206360
C	2.1671580	-2.3876130	-0.7751520
H	2.7458040	-2.0303850	-1.6171270
N	0.8966520	-2.7525410	-0.9774000
C	-0.2635810	-2.9544110	-1.1380720
C	1.8708580	0.9677550	-0.5362500
C	0.7158240	0.5545750	-0.4425940
C	3.2141630	1.4404500	-0.6458440
C	3.9316200	1.8561350	0.4958670
C	3.8608460	1.5058010	-1.8981700
C	5.2423870	2.3156150	0.3859910
H	3.4421360	1.8171800	1.4640820
C	5.1716490	1.9645900	-2.0011360
H	3.3164310	1.1955610	-2.7848490
C	5.8704900	2.3706920	-0.8614470
H	5.7749800	2.6374180	1.2770840
H	5.6502690	2.0073640	-2.9757720
H	6.8918760	2.7304380	-0.9444850
Ag	-1.2174650	-0.1217220	-0.2845670
C	-4.0897290	-1.4948520	-1.1844190
C	-3.9998070	-3.0116100	-1.2980170
C	-3.6194820	-3.1994640	1.0004210
C	-3.7077450	-1.6883370	1.1617680
H	-4.6668100	-3.3687560	-2.0887920
H	-5.1338310	-1.1824740	-1.0394100
H	-3.6849120	-0.9959100	-2.0681930
H	-3.9988520	-3.6965450	1.8987430
H	-2.5729990	-3.5011380	0.8437310
H	-4.7402020	-1.3944990	1.3985860
H	-3.0376070	-1.3194150	1.9417090
H	-2.9682780	-3.3057980	-1.5311070
O	-4.4310540	-3.6247470	-0.0862280
O	-3.3166840	-1.0270290	-0.0605180
C	-4.0977180	3.5430870	1.2688710
C	-3.9796290	2.6446690	0.0414390
C	-1.7614550	3.3884840	-0.2752460
C	-1.8948130	4.2759970	0.9546410
H	-4.5556250	1.7233230	0.1674700
H	-3.8342330	2.9652520	2.1709420
H	-5.1200500	3.9191820	1.3804910
H	-0.7467820	2.9961640	-0.3836440
H	-2.0324630	3.9579810	-1.1778350
H	-1.5321750	3.7327300	1.8424940
H	-1.3083890	5.1926780	0.8410310
H	-4.3461120	3.1798070	-0.8489290
O	-2.6231810	2.2486720	-0.1540230
O	-3.2507590	4.6768340	1.1451490

TS(6-8)′

G-gas = -1467.796426 Hartree

Symbol	X	Y	Z
C	-2.0947330	-1.9458460	0.3948760
O	-1.1735730	-2.6005250	-0.0660010
O	-3.3836920	-2.0816430	0.0136680
C	-3.6328710	-3.0238440	-1.0507080
H	-3.0439610	-2.7311600	-1.9262710
H	-3.2884150	-4.0147590	-0.7371950
C	-5.1229520	-3.0016660	-1.3345020
H	-5.4465160	-1.9996350	-1.6299100
H	-5.3576520	-3.6965010	-2.1470040
H	-5.6934220	-3.3002810	-0.4502890
C	-1.9713220	-0.8656150	1.3928360
H	-2.8687030	-0.6010350	1.9400680
N	-0.8094360	-0.8667750	2.1204760
C	0.2718950	-0.8937310	2.5920850
C	-1.8761480	0.8100280	0.0932560
C	-0.7223350	0.8114650	-0.4272510
C	-3.1995620	1.4098430	0.1513210

C	-3.9295000	1.6048110	-1.0364620
C	-3.7669170	1.8356540	1.3662100
C	-5.1843410	2.2104500	-1.0065900
H	-3.4959610	1.2793070	-1.9765440
C	-5.0223820	2.4399380	1.3912940
H	-3.2084630	1.7060340	2.2887490
C	-5.7370780	2.6285750	0.2060360
H	-5.7327650	2.3552130	-1.9333080
H	-5.4420300	2.7681200	2.3381250
H	-6.7162160	3.0982750	0.2274600
Ag	1.1760450	0.0272530	-0.5450950
C	3.9486410	-1.4570220	0.2518550
C	3.5089730	-2.3466330	1.4086000
C	2.1399940	-3.5937960	-0.0264750
C	2.5693430	-2.7360670	-1.2091140
H	4.3342850	-2.4632500	2.1187370
H	4.8560560	-1.8593640	-0.2194820
H	4.1153670	-0.4266280	0.5677800
H	1.9550110	-4.6207940	-0.3571070
H	1.2116040	-3.1940200	0.4045990
H	3.4535830	-3.1665220	-1.6987350
H	1.7635670	-2.6235440	-1.9378700
H	2.6582770	-1.8846470	1.9333580
O	3.1790510	-3.6521900	0.9460530
O	2.9138050	-1.4007360	-0.7635590
C	3.0411720	3.3323380	-1.4873060
C	3.9871380	2.3382100	-0.8245850
C	2.9030340	2.6953120	1.2413270
C	1.9729260	3.6996320	0.5698490
H	4.2849570	1.5359130	-1.5095030
H	2.1686230	2.7991670	-1.8986270
H	3.5439410	3.8645170	-2.3011730
H	2.4016420	2.1507680	2.0455910
H	3.7819930	3.2169630	1.6492760
H	1.0497660	3.1967740	0.2455850
H	1.7118340	4.5044360	1.2639730
H	4.8865210	2.8673330	-0.4740820
O	3.3427480	1.7120530	0.2905420
O	2.6230610	4.3122470	-0.5443780

8′

G-gas = -1467.819843 Hartree

Symbol	X	Y	Z
C	-1.9177490	-1.9833400	0.7125250
O	-0.9814880	-2.7141840	0.4745130
O	-3.1996690	-2.2634760	0.4309320
C	-3.4412860	-3.5026910	-0.2799660
H	-2.8842020	-3.4772350	-1.2218070
H	-3.0492690	-4.3315030	0.3175100
C	-4.9369790	-3.6124090	-0.5034440
H	-5.3061020	-2.7669830	-1.0904430
H	-5.1629270	-4.5360100	-1.0454630
H	-5.4741860	-3.6320280	0.4489830
C	-1.8280920	-0.5800530	1.3256730
H	-2.6925910	-0.4467870	1.9794690
N	-0.6473220	-0.4767760	2.1112050
C	0.3748780	-0.3924300	2.6832690
C	-1.8761370	0.4650320	0.1618180
C	-0.8062490	0.6230480	-0.6134890
C	-3.1627190	1.1913960	-0.0387090
C	-3.5772580	1.5194410	-1.3428890
C	-3.9722650	1.6076700	1.0324020
C	-4.7500710	2.2366740	-1.5653910
H	-2.9637010	1.1958530	-2.1778680
C	-5.1497770	2.3223500	0.8093880
H	-3.6733520	1.3995740	2.0563490
C	-5.5462610	2.6397390	-0.4901170
H	-5.0493380	2.4740360	-2.5828330
H	-5.7541060	2.6371210	1.6559020
H	-6.4648990	3.1928600	-0.6634570
Ag	1.1348050	-0.0323130	-0.7888270
C	4.0293130	-1.2564730	0.0399900
C	3.6324480	-2.1870050	1.1782850

C	2.4486670	-3.5585420	-0.3043310	C	-7.0596970	0.4852320	0.3753180
C	2.8327560	-2.6587200	-1.4717670	H	-6.9566430	-0.5996070	0.4681320
H	4.4262790	-2.2202450	1.9310530	H	-7.7732260	0.8306130	1.1300050
H	4.9904490	-1.5685240	-0.3909730	H	-7.4690010	0.7107210	-0.6136550
H	4.0800250	-0.2139110	0.3584860	C	-2.6836280	0.4492190	-1.4442110
H	2.3748120	-4.5982530	-0.6386540	H	-3.3459420	-0.0130880	-2.1817590
H	1.4757440	-3.2494050	0.1056170	N	-1.8688890	1.4446590	-2.0972360
H	3.7679560	-3.0054390	-1.9320740	C	-0.6636800	1.5386170	-2.1042370
H	2.0472810	-2.6168440	-2.2302580	C	-1.7499460	-0.5873630	-0.7731600
H	2.7108800	-1.8233540	1.6588140	C	-0.4449920	-0.3434410	-0.8407210
O	3.4572630	-3.5168350	0.7005380	C	-2.3568670	-1.7546840	-0.0808430
O	3.0348280	-1.3017210	-1.0137070	C	-1.7901270	-2.2559090	1.1057230
C	2.5487420	3.9256410	-0.9235660	C	-3.4957820	-2.4036360	-0.5915420
C	3.5585340	2.8293390	-0.6024130	C	-2.3288960	-3.3699650	1.7456090
C	2.4852020	2.4733090	1.4758530	H	-0.9258510	-1.7488100	1.5225950
C	1.4888830	3.5736830	1.1334830	C	-4.0371910	-3.5167440	0.0518730
H	3.8687040	2.2943340	-1.5052960	H	-3.9596880	-2.0462860	-1.5052270
H	1.7038290	3.4964880	-1.4860440	C	-3.4564470	-4.0075590	1.2220490
H	3.0117850	4.7112450	-1.5295100	H	-1.8738710	-3.7354080	2.6624560
H	2.0179810	1.6796090	2.0644210	H	-4.9139140	-4.0036580	-0.3667530
H	3.3327320	2.8953460	2.0373010	H	-3.8799870	-4.8731840	1.7234030
H	0.5997920	3.1335030	0.6571560	Ag	1.5705180	-0.3422550	-0.5219080
H	1.1786300	4.1057490	2.0380320	C	1.6789000	3.9016710	-0.3387380
H	4.4466160	3.2711860	-0.1245940	C	2.7671000	3.0194960	0.2607990
O	2.9805490	1.8558330	0.2746280	C	1.2644680	2.3951950	1.9880550
O	2.0871530	4.5406060	0.2714690	C	0.2051230	3.3026850	1.3727180

TS(8-10)′

G-gas = -1467.805201 Hartree

Symbol	X	Y	Z

Symbol	X	Y	Z
C	-3.5552050	1.1280730	-0.3757670
O	-3.1560370	1.9276940	0.4397390
O	-4.8223430	0.6774940	-0.4419730
C	-5.7228400	1.1717200	0.5789460
H	-5.2916750	0.9545000	1.5608720
H	-5.7967450	2.2595170	0.4827440
H	3.3953560	2.5711460	-0.5148360
H	1.0970670	3.3315970	-1.0781220
H	2.1230700	4.7750080	-0.8278480
H	0.8130880	1.5041320	2.4332310
H	1.8231420	2.9437490	2.7623530
H	-0.4389290	2.7345940	0.6881990
H	-0.4228580	3.7353190	2.1577320
H	3.3983280	3.6151130	0.9389110
O	2.1889320	1.9266800	0.9916500
O	0.8291320	4.3909200	0.6940140

C	4.6531540	-1.6928280	1.4167740
C	4.5449940	-0.3214440	0.7663250
C	4.5107070	-1.3748310	-1.3707930
C	4.6228020	-2.7307650	-0.6864520
H	3.9668570	0.3866850	1.3626110
H	3.6470990	-2.0636540	1.6744720
H	5.2479830	-1.6362250	2.3332410
H	3.9149740	-1.4254090	-2.2851430
H	5.5088710	-0.9826240	-1.6068200
H	3.6163130	-3.1522320	-0.5285700
H	5.1974770	-3.4252930	-1.3064350
H	5.5459340	0.0855820	0.5698060
O	3.8500780	-0.4311690	-0.4990160
O	5.3113540	-2.6111020	0.5516320

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G-gas = -852.702209 Hartree

Symbol	X	Y	Z
C	3.2491630	0.6681680	0.0572820
O	2.0618590	0.9081530	0.1943920
O	4.2520780	1.5695660	0.0814190
C	3.8542830	2.9542610	0.2389590
H	2.9460710	3.1249580	-0.3442440
H	3.6224930	3.1233590	1.2958140
C	5.0099820	3.8186700	-0.2341500
H	5.2222580	3.6363610	-1.2912630
H	4.7541070	4.8748710	-0.1095730
H	5.9155920	3.6125800	0.3428300
C	3.8147900	-0.6922970	-0.1173370
H	4.8737200	-0.8928300	-0.2056890
N	2.9394820	-1.7040980	-0.1315730
C	1.9035760	-2.2784160	-0.0759380
C	-2.7928470	-0.6835240	0.0090930
C	-2.0222700	-1.6469240	0.0225360
C	-3.4729490	0.5605070	-0.0004050
C	-2.7046180	1.7554500	-0.0065150
C	-4.8778440	0.6520780	-0.0061870
C	-3.3497100	2.9893640	-0.0442000
H	-1.6249810	1.6739490	0.0453390
C	-5.5081830	1.8956540	-0.0220370
H	-5.4631030	-0.2616870	0.0054670
C	-4.7513100	3.0665890	-0.0461350
H	-2.7629070	3.9044700	-0.0478580
H	-6.5931870	1.9498110	-0.0182970
H	-5.2386320	4.0368030	-0.0677990
Ag	-0.1457800	-2.4475140	0.0097880

7

G-gas = -707.509363 Hartree

Symbol	X	Y	Z
C	2.4359360	0.7103760	0.0324120
O	3.4077930	1.2814280	0.4880770
O	1.2750000	1.3083510	-0.3176020
C	1.2193760	2.7386210	-0.1062400
H	1.3561140	2.9373770	0.9619050
H	2.0532230	3.2082320	-0.6365920
C	-0.1257010	3.2187000	-0.6138680
H	-0.9415780	2.7121040	-0.0920260
H	-0.2183990	4.2961810	-0.4501760
H	-0.2297870	3.0257490	-1.6850480
C	2.3410420	-0.7324240	-0.2199800
H	1.4262200	-1.1853930	-0.5950330
N	3.3921680	-1.5225120	0.0250690
C	4.3292840	-2.2238090	0.2513790
C	-1.0910140	-2.4443870	-0.2318860
C	-0.3460380	-3.3830610	-0.4148830
C	-1.9684060	-1.3364780	-0.0029170
C	-2.0453590	-0.7363250	1.2692830
C	-2.7648980	-0.8321100	-1.0494920
C	-2.8984730	0.3442870	1.4835670
H	-1.4353130	-1.1257070	2.0790230
C	-3.6145210	0.2488500	-0.8265300
H	-2.7072090	-1.2953050	-2.0297780
C	-3.6838890	0.8404510	0.4382330

H	-2.9529700	0.7987930	2.4691830
H	-4.2248310	0.6296710	-1.6413490
H	-4.3500310	1.6815530	0.6093440
H	0.2930220	-4.2200390	-0.5831990

8

G-gas = -852.677844 Hartree

Symbol	X	Y	Z
C	0.6825560	1.8457710	-0.0354140
O	0.1381510	2.4941200	-0.8966720
O	2.0025650	1.8147600	0.1982690
C	2.8310960	2.5622900	-0.7297420
H	2.6141990	2.2150810	-1.7442180
H	2.5518660	3.6187670	-0.6716710
C	4.2757000	2.3238640	-0.3367000
H	4.5186960	1.2587160	-0.3808900
H	4.9381710	2.8606650	-1.0227620
H	4.4697030	2.6814700	0.6785940
C	-0.0374990	0.8820200	0.9298890
H	0.5403720	0.8274380	1.8558810
N	-1.3267630	1.4060110	1.2204960
C	-2.4989650	1.5129560	1.1496430
C	-0.1104290	-0.5384140	0.2704000
C	-1.2248710	-1.0630790	-0.2244730
C	1.1882280	-1.2755830	0.1914260
C	1.5481910	-1.9217030	-1.0036970
C	2.0541870	-1.3807840	1.2927350
C	2.7338970	-2.6494050	-1.0937020
H	0.8869650	-1.8389660	-1.8602870
C	3.2419910	-2.1055990	1.2004860
H	1.7955740	-0.9103370	2.2370940
C	3.5883590	-2.7420410	0.0068070
H	2.9932790	-3.1396860	-2.0279670
H	3.8947260	-2.1783710	2.0660270
H	4.5144880	-3.3051930	-0.0639300
Ag	-3.2168310	-0.4064780	-0.2495330

9

G-gas = -707.505410 Hartree

Symbol	X	Y	Z
C	-2.0318250	0.5104020	0.1229070
O	-2.7296110	1.1510900	0.8728180
O	-2.3753230	-0.6492780	-0.4582190
C	-3.6871210	-1.1682050	-0.1105150
H	-3.7249750	-1.3149140	0.9731300
H	-4.4366700	-0.4154460	-0.3709080
C	-3.8805540	-2.4627580	-0.8737390
H	-3.1154090	-3.1956630	-0.6035270
H	-4.8615140	-2.8856500	-0.6370460
H	-3.8311660	-2.2923040	-1.9527110
C	-0.5937380	0.8784330	-0.2754450
H	-0.3718400	0.3762470	-1.2208710
N	-0.4807130	2.2822990	-0.4730340
C	-0.3830850	3.4479690	-0.6218510
C	0.4149910	0.3710320	0.7932360
C	0.0697240	0.3835270	2.0673360
C	1.7440860	-0.0926270	0.3135040
C	2.4800820	-1.0159310	1.0767260
C	2.3010210	0.3799430	-0.8857150
C	3.7329620	-1.4499980	0.6551650
H	2.0499770	-1.3972050	1.9977840
C	3.5569900	-0.0577970	-1.3065620
H	1.7731160	1.1170190	-1.4825260
C	4.2767180	-0.9743130	-0.5407900
H	4.2829680	-2.1682260	1.2561590
H	3.9738160	0.3251420	-2.2332960
H	5.2523320	-1.3168580	-0.8722650
H	-0.7876840	0.6792010	2.6549770

10

G-gas = -852.702022 Hartree

Symbol	X	Y	Z
C	2.1573710	-1.1760940	0.3592090
O	2.0075200	-1.3725440	1.5421510
O	3.3374770	-0.8665060	-0.2180650

C	4.4699670	-0.7834080	0.6810630
H	4.2555180	-0.0307280	1.4461470
H	4.5843000	-1.7461800	1.1884210
C	5.6866920	-0.4260690	-0.1507490
H	5.5490070	0.5359300	-0.6529660
H	6.5682700	-0.3541780	0.4938750
H	5.8778980	-1.1882380	-0.9115300
C	1.0431430	-1.2305280	-0.6874150
H	1.4736010	-1.0337020	-1.6745310
N	0.4505700	-2.5986820	-0.7098330
C	-0.7685280	-2.4128090	-0.4611600
C	-0.1164850	-0.2808550	-0.3629070
C	-1.2423150	-1.0401740	-0.2412130
C	0.0637750	1.1711170	-0.2252940
C	-0.7180850	1.9210900	0.6737060
C	1.0406920	1.8507600	-0.9778260
C	-0.5527730	3.2989800	0.7918080
H	-1.4330910	1.4039460	1.3060070
C	1.2057250	3.2298250	-0.8578850
H	1.6675730	1.2991900	-1.6714780
C	0.4071230	3.9615050	0.0227900
H	-1.1626490	3.8552960	1.4982630
H	1.9595650	3.7336890	-1.4561950
H	0.5383060	5.0355080	0.1171140
Ag	-3.2308530	-0.5086680	0.0703880

11

G-gas = -707.552892 Hartree

Symbol	X	Y	Z
C	-1.5683720	0.4036190	0.3728550
O	-1.5841140	0.5713180	1.5682750
O	-2.3011380	-0.5215610	-0.2807670
C	-3.1732370	-1.3304050	0.5504780
H	-2.5631210	-1.8438390	1.2996590
H	-3.8596070	-0.6647860	1.0819990
C	-3.9021730	-2.2976940	-0.3605620
H	-3.1978310	-2.9480110	-0.8872250
H	-4.5737260	-2.9272860	0.2311310
H	-4.4990280	-1.7615510	-1.1035360
C	-0.7200880	1.2139960	-0.6133550
H	-0.8647860	0.8181570	-1.6230510
N	-1.2098350	2.6269830	-0.5988820
C	-0.2098790	3.3085430	-0.2632220
C	0.7563330	1.2788520	-0.2262680
C	1.0400590	2.5916230	-0.0180240
C	1.6389760	0.1130990	-0.1332200
C	2.9336030	0.2247440	0.4099360
C	1.2168030	-1.1497980	-0.5890980
C	3.7744590	-0.8800550	0.4843700
H	3.2765060	1.1826100	0.7876350
C	2.0611090	-2.2558750	-0.5123550
H	0.2217660	-1.2718280	-1.0051400
C	3.3430180	-2.1263980	0.0217730
H	4.7678940	-0.7714230	0.9092660
H	1.7152900	-3.2204600	-0.8718470
H	4.0003500	-2.9885280	0.0817280
H	1.9834870	3.0445090	0.2516430

TS(6-8)

G-gas = -852.657986 Hartree

Symbol	X	Y	Z
C	0.5497400	1.8369070	0.1113280
O	0.0373310	2.5311170	-0.7430490
O	1.8775530	1.7257410	0.3211810
C	2.7232040	2.4445050	-0.6065430
H	2.5029550	2.0983490	-1.6212780
H	2.4727160	3.5089520	-0.5587750
C	4.1617000	2.1731820	-0.2104820
H	4.3785860	1.1023800	-0.2532250
H	4.8385980	2.6943810	-0.8948010
H	4.3606430	2.5269930	0.8053230
C	-0.1870170	0.9588920	1.0580240
H	0.3445580	0.6144340	1.9379830
N	-1.4966000	1.2907390	1.2506490

C	-2.6754850	1.3437060	1.1566970
C	-0.1159250	-0.9520840	-0.0033470
C	-1.2883030	-1.2010060	-0.4117550
C	1.2769460	-1.3666590	0.0334930
C	2.0168880	-1.4428030	-1.1610270
C	1.9043410	-1.7202220	1.2411660
C	3.3459150	-1.8629010	-1.1440540
H	1.5343360	-1.1760360	-2.0958080
C	3.2330180	-2.1394250	1.2530240
H	1.3388530	-1.6791900	2.1674890
C	3.9600430	-2.2103220	0.0621120
H	3.9019460	-1.9230950	-2.0754990
H	3.7012910	-2.4153520	2.1935810
H	4.9951420	-2.5392140	0.0733660
Ag	-3.2477210	-0.4483670	-0.2836120

TS(8-10)

G-gas = -852.660055 Hartree

Symbol	X	Y	Z
C	-1.8702970	-1.7005590	-0.2379980
O	-1.7488860	-2.2793650	-1.2902680
O	-2.9812650	-1.0554720	0.1647020
C	-4.0694120	-1.0130420	-0.7915130
H	-3.6829910	-0.6363370	-1.7431130
H	-4.4260300	-2.0342730	-0.9590260
C	-5.1458520	-0.1154940	-0.2126920
H	-4.7574890	0.8922920	-0.0407320
H	-5.9871700	-0.0488920	-0.9095230
H	-5.5172780	-0.5101360	0.7374970
C	-0.7654750	-1.5403510	0.8190760
H	-1.2465420	-1.3560350	1.7849960
N	0.0266880	-2.7398480	0.8987700
C	1.1960370	-2.9347370	0.7058260
C	0.1708330	-0.3710690	0.4415740
C	1.4478000	-0.6858640	0.2490360
C	-0.3898980	0.9998280	0.3120160
C	-0.1557950	1.7582460	-0.8477720
C	-1.1584140	1.5695630	1.3420900
C	-0.6628230	3.0521900	-0.9680750
H	0.4122660	1.3136650	-1.6589090
C	-1.6657550	2.8621220	1.2193490
H	-1.3493050	1.0030530	2.2487310
C	-1.4189600	3.6091990	0.0647200
H	-0.4745850	3.6215480	-1.8740600
H	-2.2515750	3.2884990	2.0288610
H	-1.8162510	4.6157210	-0.0295320
Ag	3.3123280	0.0589010	-0.2009760

TS(7-9)

G-gas = -707.478794 Hartree

Symbol	X	Y	Z
C	-2.0486990	0.5344690	-0.0920260
O	-2.8507900	1.1197810	0.6058950
O	-2.1907610	-0.7332000	-0.5352750
C	-3.3923900	-1.4150910	-0.1034670
H	-3.4015560	-1.4492610	0.9907580
H	-4.2614600	-0.8313110	-0.4215230
C	-3.3765440	-2.8002020	-0.7191170
H	-2.4977630	-3.3638610	-0.3935040
H	-4.2715680	-3.3508300	-0.4138910
H	-3.3641900	-2.7423990	-1.8110780
C	-0.7374440	1.0762980	-0.5278220
H	-0.2091080	0.5219200	-1.2963100
N	-0.6283480	2.4371450	-0.6070810
C	-0.5151280	3.6165600	-0.6361830
C	0.5199250	0.5054620	1.1093100
C	-0.0944970	0.7534540	2.1680350
C	1.7320390	-0.0282520	0.5035570
C	2.1938400	-1.2977430	0.8914840
C	2.4633490	0.7079600	-0.4436980
C	3.3651420	-1.8157970	0.3430680
H	1.6280490	-1.8655800	1.6224850
C	3.6350590	0.1838820	-0.9852650
H	2.1193640	1.6939590	-0.7392380

C	4.0882990	-1.0783350	-0.5961800
H	3.7126590	-2.7977150	0.6501350
H	4.1965150	0.7648450	-1.7106290
H	5.0007130	-1.4844610	-1.0222390
H	-0.9185110	1.0960440	2.7594570

TS(9-11)

G-gas = -707.493225 Hartree

Symbol	X	Y	Z
C	1.6690200	0.6002520	0.2482790
O	2.2608110	0.6194040	1.2989970
O	1.0098020	1.6405310	-0.2912130
C	0.9721630	2.8508340	0.5099020
H	0.5931690	2.5975460	1.5040680
H	1.9955490	3.2196520	0.6276980
C	0.0812980	3.8426720	-0.2106250
H	-0.9293510	3.4419250	-0.3274720
H	0.0211720	4.7712420	0.3651090
H	0.4779610	4.0785800	-1.2021300
C	1.5161790	-0.6383170	-0.6553270
H	1.3188680	-0.2912440	-1.6741310
N	2.7202080	-1.4157160	-0.6376720
C	3.0033130	-2.5281180	-0.3020900
C	0.3670550	-1.5394520	-0.1492630
C	0.7007280	-2.7622140	0.2222960
C	-1.0221590	-1.0102770	-0.0934400
C	-1.8269450	-1.2626470	1.0300940
C	-1.5667860	-0.2742110	-1.1591970
C	-3.1413190	-0.8025090	1.0821200
H	-1.4059010	-1.8085420	1.8685620
C	-2.8808020	0.1869920	-1.1036860
H	-0.9675670	-0.0697440	-2.0406450
C	-3.6731700	-0.0762110	0.0154520
H	-3.7472920	-1.0048080	1.9603360
H	-3.2878100	0.7489130	-1.9392370
H	-4.6963200	0.2851890	0.0566530
H	0.2296990	-3.6589320	0.5955390

TS(6-8')

G-gas = -852.648284 Hartree

Symbol	X	Y	Z
C	2.8528070	-0.2760540	0.4384390
O	2.5241690	0.8967670	0.5322130
O	4.0680460	-0.6853640	-0.0155080
C	4.9717070	0.3689230	-0.4024910
H	4.4971820	0.9793810	-1.1782230
H	5.1500250	1.0203810	0.4596040
C	6.2502420	-0.2829400	-0.8951560
H	6.0541220	-0.9267160	-1.7575680
H	6.9682150	0.4864940	-1.1959560
H	6.7068660	-0.8911020	-0.1089000
C	2.0301460	-1.4320030	0.7689190
H	2.4033410	-2.4359550	0.6014050
N	0.8290450	-1.2739370	1.2873240
C	-0.2499780	-1.0902450	1.7992940
C	-1.6298450	0.6021440	0.0704310
C	-1.5619080	-0.6292830	0.2311510
C	-1.5898050	2.0160010	-0.0120050
C	-2.7690750	2.7817650	0.1305160
C	-0.3612300	2.6807880	-0.2343710
C	-2.7210570	4.1683910	0.0360110
H	-3.7107160	2.2723560	0.3091410
C	-0.3286880	4.0693090	-0.3176560
H	0.5527160	2.0991650	-0.2997190
C	-1.5031170	4.8172690	-0.1902690
H	-3.6344100	4.7469300	0.1419030
H	0.6209030	4.5720380	-0.4773130
H	-1.4693670	5.9007670	-0.2602300
Ag	-2.1919380	-2.4970590	-0.3811900

TS(7-9')

G-gas = -707.489018 Hartree

Symbol	X	Y	Z
C	-2.6429250	1.2016090	0.2909340
C	-2.6064590	2.4412770	0.3387750

H	-3.1000130	3.3578030	0.5848350
C	-2.3510140	-0.1749090	0.1666920
C	-2.9402330	-0.9500740	-0.8589590
C	-1.4693510	-0.7999150	1.0804940
C	-2.6557810	-2.3063570	-0.9619860
H	-3.6181350	-0.4725590	-1.5587870
C	-1.1949830	-2.1579160	0.9636490
H	-0.9899350	-0.2017680	1.8471750
C	-1.7864710	-2.9159170	-0.0514450
H	-3.1136410	-2.8932230	-1.7526670
H	-0.5125160	-2.6273670	1.6657980
H	-1.5697150	-3.9766990	-0.1348470
C	1.7757330	0.8412890	0.0793010
O	1.5618350	0.8531770	1.2798180
O	2.7531090	0.1095230	-0.5152230
C	3.5545580	-0.6947930	0.3757280
H	4.0125180	-0.0438740	1.1273580
H	2.9004770	-1.3950650	0.9059140
C	4.5921860	-1.4119750	-0.4661430
H	5.2333900	-0.6965020	-0.9886800
H	5.2232730	-2.0361700	0.1739750
H	4.1150200	-2.0546260	-1.2114580
C	1.0273500	1.5838530	-0.9306640
H	1.2562260	1.4792810	-1.9844890
N	0.0626340	2.4072130	-0.5639480
C	-0.7684320	3.1786060	-0.1669190

8'

G-gas = -852.724924 Hartree

Symbol	X	Y	Z
C	-3.0582120	-0.7354390	0.0312600
O	-2.8352020	0.2815130	-0.6389160
O	-4.2766510	-1.3255430	0.0481160
C	-5.3038940	-0.7059680	-0.7527810
H	-5.4702770	0.3152200	-0.3929300
H	-4.9557680	-0.6364910	-1.7884830
C	-6.5520680	-1.5597240	-0.6287890
H	-6.8832620	-1.6197260	0.4118870
H	-7.3609010	-1.1239980	-1.2236260
H	-6.3669370	-2.5752990	-0.9900320
C	-2.1299380	-1.4375560	0.9048330
H	-2.5442050	-2.2411730	1.5060700
N	-0.8514260	-1.1740900	1.0400490
C	-0.0580360	-0.1974570	0.7176950
C	2.5073650	-0.4141940	0.2644360
C	1.3028990	-0.3640770	0.4941860
C	3.8994450	-0.4851260	0.0056200
C	4.6553690	0.6917200	-0.1944570
C	4.5578970	-1.7336380	-0.0567840
C	6.0207630	0.6171190	-0.4501090
H	4.1546740	1.6534140	-0.1448960
C	5.9244440	-1.7969570	-0.3091230
H	3.9808320	-2.6397380	0.0962160
C	6.6603380	-0.6248150	-0.5075510
H	6.5901700	1.5293630	-0.6032470
H	6.4190200	-2.7630210	-0.3529650
H	7.7268790	-0.6787850	-0.7054890
Ag	-0.9147580	1.6984630	0.0962330

9'

G-gas = -707.516038 Hartree

Symbol	X	Y	Z
C	-2.6911210	1.4458790	0.2717760
C	-2.1093800	2.6396690	0.3027170
H	-2.6323680	3.5372650	0.6207010
C	-2.5327180	0.0539690	0.1342090
C	-3.3151750	-0.6658160	-0.8074590
C	-1.6329340	-0.6638920	0.9683450
C	-3.1879160	-2.0428360	-0.9173760
H	-4.0112250	-0.1229310	-1.4386430
C	-1.5263720	-2.0433240	0.8474750
H	-0.9995790	-0.1235200	1.6622290
C	-2.2996440	-2.7388140	-0.0881620
H	-3.7858200	-2.5813580	-1.6465470

H	-0.8235840	-2.5780990	1.4789480
H	-2.2093970	-3.8174520	-0.1740830
C	1.9256260	0.6132710	0.0687620
O	1.5166730	0.3229200	1.1842230
O	3.0508070	0.0798750	-0.4813640
C	3.7530590	-0.8711290	0.3419580
H	4.0392860	-0.3893070	1.2827400
H	3.0782680	-1.6965770	0.5926880
C	4.9619770	-1.3467710	-0.4415060
H	5.6241480	-0.5105350	-0.6835680
H	5.5275930	-2.0739580	0.1495240
H	4.6577910	-1.8251790	-1.3769430
C	1.3061370	1.5487950	-0.8558470
H	1.7231320	1.7457150	-1.8349580
N	0.2151390	2.1621240	-0.4859620
C	-0.6905490	2.7507840	0.0329040

TS(8'-10)

G-gas = -852.659101 Hartree

Symbol	X	Y	Z
C	-0.8039240	-1.9678100	0.1708990
O	-0.4219630	-2.3677330	1.2530570
O	-2.0560420	-2.1925190	-0.3178280
C	-2.9443180	-2.9067880	0.5677660
H	-2.5188620	-3.8945240	0.7733970
H	-3.0020520	-2.3712230	1.5207880
C	-4.2957380	-3.0019290	-0.1150710
H	-4.2155590	-3.5257640	-1.0721020
H	-4.9954490	-3.5530970	0.5210490
H	-4.7113760	-2.0068460	-0.2991450
C	-0.0155290	-1.1575800	-0.7786330
H	-0.3886970	-1.0905880	-1.7994390
N	1.3694140	-1.1404680	-0.6219620
C	1.8737260	-0.0144540	-0.2589260
C	-0.3547280	0.9616150	-0.1803810
C	0.9103980	1.0443070	-0.0607890
C	-1.6489660	1.5851670	-0.1033050
C	-1.7826870	2.8152900	0.5769100
C	-2.7893370	1.0103360	-0.6949830
C	-3.0197390	3.4463010	0.6567430
H	-0.9052240	3.2590200	1.0357590
C	-4.0235870	1.6519300	-0.6120450
H	-2.7021830	0.0576570	-1.2036170
C	-4.1452810	2.8687250	0.0617570
H	-3.1066580	4.3921530	1.1837910
H	-4.8945810	1.1991120	-1.0773640
H	-5.1097070	3.3643530	0.1240070
Ag	3.9367390	0.2260500	0.0379810

TS(9'-11)

G-gas = -707.47499 Hartree

Symbol	X	Y	Z
C	0.6354980	1.2239750	-0.5279400
C	0.0229420	2.0495560	-1.3711370
H	0.4599570	2.3181000	-2.3309050
C	1.7421860	0.3689400	-0.3386310
C	1.7131610	-0.9664430	-0.8195520
C	2.8832620	0.8039690	0.3846170
C	2.7887810	-1.8158420	-0.5988960
H	0.8391320	-1.3087570	-1.3637630
C	3.9529150	-0.0558910	0.5915130
H	2.9076600	1.8187320	0.7680420
C	3.9126100	-1.3675500	0.1042200
H	2.7556880	-2.8333700	-0.9767700
H	4.8239130	0.2929020	1.1382290
H	4.7502090	-2.0368220	0.2745810
C	-1.6753060	0.0211350	1.1719370
O	-1.3988270	-0.7078680	2.1072540
O	-2.3581110	-0.3728870	0.0741080
C	-2.7817700	-1.7540670	0.0704170
H	-1.8983380	-2.3969910	0.1421130
H	-3.3926700	-1.9401550	0.9594680
C	-3.5561820	-1.9886260	-1.2120200
H	-2.9309890	-1.7957340	-2.0885290

H	-3.8986570	-3.0272450	-1.2543290
H	-4.4307830	-1.3343740	-1.2648140
C	-1.2491290	1.4333070	1.1130590
H	-0.9173690	1.8554240	2.0571010
N	-1.6354160	2.2575450	0.1445130
C	-1.3163570	2.5861250	-0.9880730

c) Process III

12

G-gas = -1262.896250 Hartree

Symbol	X	Y	Z
C	4.4527370	-0.9741020	0.4587220
O	4.2318850	-1.0753000	1.6432550
O	5.6793080	-0.7545940	-0.0654910
C	6.7602730	-0.6695920	0.8920120
H	6.5564930	0.1567070	1.5806420
H	6.7797820	-1.5913470	1.4816210
C	8.0446700	-0.4620420	0.1122130
H	8.0025740	0.4607170	-0.4739060
H	8.8915390	-0.3928520	0.8022330
H	8.2250790	-1.2963020	-0.5717740
C	3.4033220	-1.0807860	-0.6462370
H	3.8832450	-0.8789960	-1.6094590
N	2.8831430	-2.4801400	-0.6837450
C	1.6429360	-2.3408680	-0.5166000
C	2.1773750	-0.1935130	-0.4087500
C	1.0713410	-0.9947150	-0.3468700
C	2.2816150	1.2679630	-0.2888210
C	1.3491970	2.0100120	0.4617640
C	3.3335600	1.9711430	-0.9078930
C	1.4463830	3.3953110	0.5632280
H	0.5641750	1.4790890	0.9912110
C	3.4312860	3.3581740	-0.8042220
H	4.0788870	1.4297780	-1.4824800
C	2.4859950	4.0790060	-0.0731060
H	0.7189620	3.9436360	1.1562140
H	4.2490910	3.8763670	-1.2974470
H	2.5643110	5.1592540	0.0099160
H	-2.5188210	-2.7345940	-0.0826580
C	-3.9581900	-1.5113240	0.0521660
O	-3.1436700	-0.5131830	-0.0370800
O	-5.1988680	-1.3622210	0.1758970
O	-3.4856090	-2.7610110	0.0122730
Ag	-5.0975170	0.9000690	0.1612480
Ag	-0.9530510	-0.6372600	-0.1790000

TS(12-13)

G-gas = -1262.873864 Hartree

Symbol	X	Y	Z
C	3.5640940	-1.6900820	0.4011200
O	3.3390930	-1.7840240	1.5839430
O	4.7271150	-2.0481360	-0.1846110
C	5.7412750	-2.5733050	0.7069700
H	5.9835440	-1.8074300	1.4503670
H	5.3245570	-3.4324480	1.2409910
C	6.9406000	-2.9513830	-0.1407520
H	7.3375860	-2.0802290	-0.6700240
H	7.7324810	-3.3560810	0.4971920
H	6.6721750	-3.7113490	-0.8800660
C	2.5816240	-1.1461590	-0.6401150
H	3.0396070	-1.2137490	-1.6316450
N	1.3665560	-2.0003760	-0.6427280
C	0.4191440	-1.2146930	-0.4027940
C	2.0718180	0.2711370	-0.3248250
C	0.7141230	0.2242460	-0.1841910
C	2.9668580	1.4308030	-0.2320800
C	2.5309120	2.6367870	0.3509070
C	4.2870870	1.3730280	-0.7199880
C	3.3745900	3.7396730	0.4311170
H	1.5229960	2.6879110	0.7483430
C	5.1319730	2.4792710	-0.6357200
H	4.6615850	0.4585980	-1.1692150
C	4.6806220	3.6687180	-0.0633690
H	3.0164350	4.6580120	0.8885570

H	6.1452580	2.4101880	-1.0216450
H	5.3390310	4.5302000	0.0016500
H	-0.8456720	-1.5951260	-0.3615640
C	-3.0733190	-1.3382010	-0.1999520
O	-3.0552840	-0.0547710	0.0212760
O	-4.1810900	-1.9592050	-0.2664730
O	-1.9993470	-2.0682020	-0.3654600
Ag	-5.4202800	-0.1125010	0.0698650
Ag	-1.1271200	1.1829230	0.1220240

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G-gas = -707.542743 Hartree

Symbol	X	Y	Z
C	-1.6186880	0.3854230	0.3507000
O	-1.7429990	0.6136250	1.5290700
O	-2.2114380	-0.6401010	-0.2970800
C	-3.0571120	-1.4906030	0.5203260
H	-2.4514840	-1.9103730	1.3290960
H	-3.8341010	-0.8701740	0.9761810
C	-3.6351470	-2.5618240	-0.3827150
H	-2.8432560	-3.1694600	-0.8299690
H	-4.2867940	-3.2216870	0.1981360
H	-4.2260320	-2.1172920	-1.1883270
C	-0.7627870	1.2137490	-0.6177110
H	-0.8866460	0.8168020	-1.6304580
N	-1.2758090	2.6031160	-0.6013140
C	-0.2921580	3.3488360	-0.2185000
C	0.7080630	1.2639850	-0.2060250
C	0.9130520	2.5757350	0.0229000
C	1.6315230	0.1362610	-0.1166630
C	2.9449630	0.3399320	0.3494920
C	1.2486910	-1.1624270	-0.4964240
C	3.8428730	-0.7177590	0.4302690
H	3.2480090	1.3387270	0.6495890
C	2.1521000	-2.2208830	-0.4130970
H	0.2415060	-1.3475160	-0.8560280
C	3.4505370	-2.0045300	0.0485870
H	4.8511840	-0.5414920	0.7931460
H	1.8396280	-3.2173070	-0.7114190
H	4.1525180	-2.8305280	0.1123660
H	-0.3938330	4.4249140	-0.1158680

14

G-gas = -1015.108192 Hartree

Symbol	X	Y	Z
C	0.5103870	1.2195390	0.0161200
O	-0.0956050	1.1620470	-1.0285310
O	1.2275680	2.2868800	0.4199320
C	1.2479510	3.4147670	-0.4946900
H	1.6674440	3.0816140	-1.4486220
H	0.2164820	3.7294590	-0.6770380
C	2.0761850	4.5087540	0.1486710
H	3.1032100	4.1752320	0.3225190
H	2.1068030	5.3823110	-0.5095970
H	1.6449810	4.8146050	1.1058520
C	0.5746290	0.0926680	1.0561570
H	1.0211530	0.4820210	1.9765980
N	-0.8141340	-0.3280270	1.3395270
C	-0.9014160	-1.5739560	1.0022730
C	1.3246700	-1.1355870	0.5335280
C	0.3703440	-2.0865760	0.5240640
C	2.7358940	-1.2190360	0.1654420
C	3.2441430	-2.4101210	-0.3893450
C	3.6175610	-0.1412070	0.3611620
C	4.5862720	-2.5186150	-0.7331730
H	2.5695600	-3.2461690	-0.5489040
C	4.9631780	-0.2541760	0.0142000
H	3.2507020	0.7888640	0.7824330
C	5.4534910	-1.4400860	-0.5324880
H	4.9592570	-3.4447110	-1.1605750
H	5.6303210	0.5878840	0.1737010
H	6.5020260	-1.5254440	-0.8015750
H	-1.8390330	-2.1158850	1.0573940
C	-5.4734890	-0.2896450	0.6284190

H	-4.9336160	-0.3088830	1.5896970
H	-6.5479510	-0.2286820	0.8310770
C	-5.1400450	-1.5489090	-0.1650200
H	-5.3392130	-2.4510330	0.4227160
H	-5.7563960	-1.5794670	-1.0784200
C	-3.3960800	-0.4021910	-1.2455660
H	-2.3210420	-0.4561080	-1.4314910
H	-3.9318590	-0.3930980	-2.2083250
C	-3.7354720	0.8512870	-0.4504330
H	-3.5407990	1.7506210	-1.0422300
H	-3.1165310	0.8810110	0.4583210
O	-5.1239630	0.8732840	-0.1107370
O	-3.7574720	-1.5758870	-0.5089320

15

G-gas = -1107.363026 Hartree

Symbol	X	Y	Z
C	0.9443540	-1.8741980	0.2021420
O	-0.1784760	-1.7291580	0.6307570
O	1.9934920	-2.2595810	0.9481540
C	1.7104330	-2.5318570	2.3485250
H	1.2934830	-1.6265760	2.7994540
H	0.9456880	-3.3118690	2.3983170
C	3.0101330	-2.9567650	3.0009250
H	3.7612590	-2.1644180	2.9361660
H	2.8348230	-3.1774180	4.0581450
H	3.4122790	-3.8549890	2.5245870
C	1.3619020	-1.6447470	-1.2551870
H	2.4222690	-1.8951340	-1.3632460
N	0.5831790	-2.5794260	-2.1013120
C	-0.0725470	-1.8494390	-2.9426440
C	1.0686580	-0.2280400	-1.7478490
C	0.1969400	-0.4340160	-2.7552530
C	1.6447560	1.0132490	-1.2384360
C	1.2339250	2.2495700	-1.7737240
C	2.6207960	1.0117390	-0.2259430
C	1.7827350	3.4410590	-1.3140660
H	0.4795200	2.2613650	-2.5548270
C	3.1672900	2.2090600	0.2343620
H	2.9572040	0.0729430	0.2026570
C	2.7528990	3.4264690	-0.3066680
H	1.4562920	4.3844340	-1.7416460
H	3.9224530	2.1891250	1.0145220
H	3.1824140	4.3574310	0.0507900
H	-0.7294920	-2.2839460	-3.6897390
C	-3.1501210	0.5733210	0.7395240
O	-4.1091460	0.5837160	1.4711250
O	-2.0568590	1.3464250	0.8803240
C	-2.0449040	2.2204890	2.0355500
H	-2.8886470	2.9135590	1.9595680
H	-2.1954900	1.6148410	2.9343010
C	-0.7109850	2.9403690	2.0447690
H	-0.5777590	3.5322050	1.1353250
H	-0.6597020	3.6129890	2.9066630
H	0.1167350	2.2289790	2.1094270
C	-2.9554560	-0.3273140	-0.4805330
H	-2.6313220	0.2876870	-1.3264960
H	-2.1357620	-1.0209430	-0.2582490
N	-4.1315730	-1.0374910	-0.8163080
C	-5.1140730	-1.6277950	-1.0847020

TS(14-16)

G-gas = -1015.097341 Hartree

Symbol	X	Y	Z
C	2.3760720	-1.3805050	0.3103020
O	1.9895640	-1.6042550	1.4319710
O	3.6762390	-1.3529530	-0.0559110
C	4.6290770	-1.6419920	0.9985910
H	4.4907700	-0.9146150	1.8043000
H	4.4058100	-2.6325740	1.4055170
C	6.0159900	-1.5711160	0.3911120
H	6.2179490	-0.5747480	-0.0125460
H	6.7665740	-1.7896130	1.1568970
H	6.1266410	-2.2994890	-0.4169670

C	1.4659750	-1.0936060	-0.8923280	O	3.0137860	-1.2784590	1.3183570
H	2.0920180	-0.9161140	-1.7730960	O	4.1818660	-0.5117890	-0.4633590
N	0.6537240	-2.3020310	-1.1312470	C	5.3862610	-0.4935030	0.3477170
C	-0.5768190	-1.9280190	-1.0049330	H	5.2191670	0.1665070	1.2042600
C	0.4971780	0.0618180	-0.6401390	H	5.5575810	-1.5021020	0.7344130
C	-0.7278690	-0.5085580	-0.7127320	C	6.5217380	-0.0161380	-0.5353120
C	0.8854500	1.4533070	-0.4060670	H	6.3287460	0.9914590	-0.9146460
C	-0.0876080	2.4457490	-0.1757330	H	7.4520360	0.0063550	0.0403710
C	2.2376080	1.8437570	-0.4161490	H	6.6610530	-0.6856890	-1.3884230
C	0.2761810	3.7701720	0.0393320	C	1.8771500	-0.9645440	-0.8131260
H	-1.1370580	2.1708140	-0.1704560	H	2.2015540	-0.5634080	-1.7787990
C	2.6001160	3.1721630	-0.2000320	N	1.4920960	-2.3788410	-1.0020150
H	3.0135240	1.1058960	-0.5925670	C	0.2676620	-2.4737770	-0.6049470
C	1.6237510	4.1413610	0.0289920	C	0.6566460	-0.2234550	-0.2713860
H	-0.4925130	4.5170730	0.2152340	C	-0.2765860	-1.1957000	-0.1622290
H	3.6501420	3.4494330	-0.2122530	C	0.6027690	1.2090740	0.0183690
H	1.9073590	5.1759500	0.1969320	C	-0.5737870	1.8056290	0.5125180
H	-1.4024160	-2.6237730	-1.1271170	C	1.7258660	2.0304540	-0.1944950
C	-5.5687960	-0.9000660	0.8841490	C	-0.6179170	3.1673830	0.7922450
H	-5.1493430	-1.7451100	1.4533790	H	-1.4617730	1.2029460	0.6657300
H	-6.6462600	-0.8501770	1.0693260	C	1.6764760	3.3948610	0.0843620
C	-5.2791030	-1.0905190	-0.6002550	H	2.6465600	1.6034650	-0.5785050
H	-5.6151890	-2.0699680	-0.9530860	C	0.5068400	3.9698270	0.5809450
H	-5.7868790	-0.3063930	-1.1824210	H	-1.5335900	3.6049710	1.1791570
C	-3.3102800	0.1643330	-0.3502700	H	2.5556160	4.0088570	-0.0868390
H	-2.0732800	0.0051960	-0.5086920	H	0.4697060	5.0325490	0.8005470
H	-3.5981370	1.0310160	-0.9658260	H	-0.2721800	-3.4158680	-0.6226140
C	-3.6013560	0.3585690	1.1244490	C	-3.8366740	-0.8806870	-0.0860590
H	-3.2475560	1.3305780	1.4789530	O	-4.5177390	-1.4869830	-0.8768430
H	-3.1090910	-0.4347600	1.7081460	O	-3.8325780	0.4586290	0.0720430
O	-5.0142860	0.3279360	1.3447390	C	-4.7099280	1.1998310	-0.8181930
O	-3.8668330	-1.0326660	-0.8363820	H	-4.4252080	0.9757370	-1.8503710

TS(15-16)

G-gas = -1107.354669 Hartree

Symbol	X	Y	Z
C	3.0670970	-0.9454640	0.1597140
H	-5.7330650	0.8429340	-0.6697890
C	-4.5609190	2.6711370	-0.4880620
H	-3.5302800	3.0040870	-0.6387060
H	-5.2116020	3.2609890	-1.1406900

H	-4.8448360	2.8705420	0.5492090
C	-2.8161500	-1.4927990	0.8523940
H	-1.7127940	-1.2319260	0.3835540
H	-2.8091820	-1.0078270	1.8315860
N	-2.9125500	-2.8818470	0.9534470
C	-2.9593790	-4.0606210	0.9953710

16

G-gas = -708.223660 Hartree

Symbol	X	Y	Z
C	-1.5939380	0.4003020	0.3626510
O	-1.6960820	0.5683110	1.5543900
O	-2.2918230	-0.5521490	-0.3152310
C	-3.1703570	-1.3627590	0.4898190
H	-2.5858700	-1.8500280	1.2771110
H	-3.9020010	-0.7133380	0.9818330
C	-3.8339080	-2.3692290	-0.4327420
H	-3.0875780	-3.0077040	-0.9149240
H	-4.5166380	-3.0076470	0.1377420
H	-4.4071310	-1.8623710	-1.2146700
C	-0.7051960	1.2039120	-0.5873520
H	-0.8325010	0.7970780	-1.5971470
N	-1.1862080	2.5958420	-0.5811790
C	-0.1592700	3.2987110	-0.2231250
C	0.7661160	1.2393230	-0.1839870
C	1.0666570	2.5481100	0.0277130
C	1.6407370	0.0649430	-0.1062000
C	2.9982570	0.2035170	0.2530570
C	1.1532160	-1.2248390	-0.3980360
C	3.8222770	-0.9173960	0.3210060
H	3.4335880	1.1795820	0.4693830
C	1.9861170	-2.3407740	-0.3258350
H	0.1153980	-1.3612200	-0.6872410
C	3.3258880	-2.1930110	0.0363690
H	4.8643190	-0.7816210	0.5973180
H	1.5860680	-3.3257700	-0.5549990
H	3.9772240	-3.0619160	0.0924250
H	2.0162190	3.0076890	0.3071650
H	-0.2339710	4.3822120	-0.1390400

18

G-gas = -1160.281662 Hartree

Symbol	X	Y	Z
C	3.5559110	-1.3578100	0.3124750
O	3.3899330	-1.5850710	1.4881330
O	4.7656250	-1.1439390	-0.2529290
C	5.8950800	-1.2068940	0.6489860
H	5.7478110	-0.4750740	1.4494660
H	5.9196540	-2.1988740	1.1108020
C	7.1440340	-0.9236850	-0.1638430
H	7.0989000	0.0709990	-0.6169700
H	8.0261220	-0.9671430	0.4827740
H	7.2661490	-1.6608430	-0.9626800
C	2.4456680	-1.2608150	-0.7328630
H	2.8992620	-1.0801270	-1.7127980
N	1.7147720	-2.5580830	-0.7988950
C	0.5214480	-2.2444120	-0.5467200
C	1.3859080	-0.2086510	-0.3804910
C	0.1765910	-0.8383300	-0.2815640
C	1.7198640	1.2127150	-0.2046240
C	0.9611650	2.0448910	0.6411900
C	2.8242200	1.7834300	-0.8673160
C	1.2722060	3.3935910	0.7927200
H	0.1391360	1.6112850	1.2018150
C	3.1365530	3.1336330	-0.7131630
H	3.4411530	1.1684090	-1.5148600
C	2.3600210	3.9477190	0.1126350
H	0.6738140	4.0117990	1.4566690
H	3.9893490	3.5501970	-1.2421510
H	2.6051830	4.9989430	0.2339960
C	-4.6758690	0.9987810	-0.7049690
H	-5.3605070	1.7698530	-0.3280900
H	-3.9846580	1.4471260	-1.4222390
C	-5.4580510	-0.1590660	-1.3094710

H	-6.1333240	0.2024410	-2.0905280
H	-4.7611240	-0.8864890	-1.7568290
C	-5.4716250	-1.2680490	0.7573270
H	-6.1566680	-1.7161520	1.4829260
H	-4.7744280	-2.0458540	0.4055590
C	-4.6902790	-0.1283610	1.3962760
H	-4.0091590	-0.4822690	2.1734640
H	-5.3752220	0.6160900	1.8229050
O	-3.8727100	0.5288890	0.4013620
O	-6.2643730	-0.7860270	-0.3203740
Ag	-1.7451000	-0.1627800	0.0500000

TS(18-20)

G-gas = -1160.254518 Hartree

Symbol	X	Y	Z
C	-2.5857860	-1.6557360	-0.4337590
O	-2.4296230	-1.7128400	-1.6309450
O	-3.7296560	-2.0081310	0.1967360
C	-4.7982630	-2.4722470	-0.6617900
H	-5.0464110	-1.6790760	-1.3741130
H	-4.4375840	-3.3303880	-1.2370850
C	-5.9733090	-2.8325630	0.2271790
H	-6.3158540	-1.9631330	0.7959760
H	-6.8060930	-3.1920030	-0.3854510
H	-5.7006560	-3.6210880	0.9344200
C	-1.5351310	-1.1794330	0.5711560
H	-1.9476830	-1.2715900	1.5814160
N	-0.3528140	-2.0720070	0.4737710
C	0.6070110	-1.2894280	0.1776530
C	-1.0289770	0.2385640	0.2791420
C	0.3103380	0.1478710	0.0406410
C	-1.9071500	1.4163180	0.2953600
C	-1.5024740	2.6395430	-0.2739680
C	-3.1863760	1.3590680	0.8832250
C	-2.3287120	3.7582640	-0.2398820
H	-0.5324520	2.6949450	-0.7567250
C	-4.0144750	2.4806610	0.9154010
H	-3.5406560	0.4308670	1.3198690
C	-3.5902190	3.6873210	0.3585730
H	-1.9924050	4.6885840	-0.6899030
H	-4.9944470	2.4095960	1.3793460
H	-4.2356270	4.5606690	0.3837710
C	4.9146990	-0.1736120	0.6887170
H	5.8878730	-0.6230010	0.4433050
H	5.0802120	0.8121200	1.1325370
C	4.1374550	-1.0842350	1.6312580
H	4.7248980	-1.3054780	2.5272450
H	3.1992740	-0.5962350	1.9339270
C	3.1777200	-2.1820060	-0.2100120
H	3.0294060	-3.1731160	-0.6465840
H	1.9504970	-1.7596240	-0.0021710
C	3.8881800	-1.2310130	-1.1584620
H	3.2725600	-1.0136820	-2.0348610
H	4.8433870	-1.6659930	-1.4951280
O	4.1776690	0.0357000	-0.5267890
O	3.8553730	-2.3344290	1.0079610
Ag	1.9900890	1.3296860	-0.3839250

19

G-gas = -1252.556549 Hartree

Symbol	X	Y	Z
C	4.6735920	-1.0449040	0.1785850
O	4.6383150	-1.3021150	1.3593270
O	5.7847690	-0.6188870	-0.4669790
C	6.9673140	-0.4807330	0.3529820
H	6.7557540	0.2282640	1.1597400
H	7.1920780	-1.4469950	0.8155020
C	8.0922910	-0.0037780	-0.5458640
H	7.8458680	0.9581950	-1.0039780
H	9.0081650	0.1203150	0.0399040
H	8.2882700	-0.7251580	-1.3443000
C	3.4916250	-1.1385810	-0.7834130
H	3.8369860	-0.8779300	-1.7893740
N	2.9895390	-2.5403780	-0.8209320

C	1.7780180	-2.4317090	-0.4916740
C	2.2923030	-0.2875880	-0.3453810
C	1.2081020	-1.1070480	-0.1825210
C	2.3930120	1.1686210	-0.1643380
C	1.5699590	1.8511060	0.7525170
C	3.3313120	1.9274140	-0.8915260
C	1.6587960	3.2314280	0.9126400
H	0.8779180	1.2772000	1.3606790
C	3.4216760	3.3093110	-0.7287860
H	3.9916120	1.4341350	-1.5977490
C	2.5832790	3.9705420	0.1697670
H	1.0157130	3.7315030	1.6321090
H	4.1495310	3.8706110	-1.3084110
H	2.6556870	5.0468430	0.2978340
Ag	-0.7923810	-0.7695880	0.2555080
C	-6.1149020	0.0160670	-0.1386900
O	-5.6075640	0.0683220	-1.2302470
O	-7.4150140	0.1458390	0.1442610
C	-8.2971230	0.3735290	-0.9948000
H	-7.9718420	1.2866100	-1.5013230
H	-8.1763550	-0.4598290	-1.6926160
C	-9.7104850	0.4806160	-0.4601040
H	-9.8038400	1.3143070	0.2413230
H	-10.4018260	0.6517380	-1.2906240
H	-10.0085760	-0.4392900	0.0503990
C	-5.3541170	-0.2160310	1.1773500
H	-5.5214460	0.6321570	1.8487410
H	-5.7458450	-1.1106800	1.6716420
N	-3.9665950	-0.3718730	0.9468470
C	-2.8364150	-0.4984040	0.6948060

TS(19-20)

G-gas = -1252.521965 Hartree

Symbol	X	Y	Z
C	1.9867340	2.0804460	-0.7505570
O	1.9086690	1.9277650	-1.9464900
O	2.8693570	2.9033350	-0.1444370
C	3.7742120	3.6097590	-1.0282950
H	4.3144510	2.8765140	-1.6348010
H	3.1829440	4.2301790	-1.7088260
C	4.7050430	4.4363560	-0.1622770
H	5.2845550	3.7971750	0.5101100
H	5.4039880	4.9917770	-0.7953660
H	4.1436390	5.1544200	0.4423680
C	1.1197390	1.3591850	0.2851420
H	1.3194960	1.7851270	1.2735390
N	-0.3107340	1.5879650	-0.0360070
C	-0.7650680	0.4220840	-0.2105440
C	1.3145440	-0.1674190	0.2551680
C	0.1151540	-0.7458050	-0.0514080
C	2.6107270	-0.8046920	0.5251450
C	2.8944890	-2.1026570	0.0581690
C	3.6123510	-0.1339550	1.2539290
C	4.1156260	-2.7129100	0.3274130
H	2.1493950	-2.6181410	-0.5390520
C	4.8363550	-0.7460480	1.5216040
H	3.4348770	0.8722210	1.6190910
C	5.0936050	-2.0388620	1.0643010
H	4.3111280	-3.7134910	-0.0483720
H	5.5897480	-0.2102160	2.0922490
H	6.0475030	-2.5144940	1.2729860
Ag	-0.7676600	-2.6551260	-0.2828680
C	-4.2872300	0.4644880	0.2692850
O	-4.6680350	-0.1828870	1.2188880
O	-4.5198760	1.7723900	0.0701110
C	-5.2493290	2.4532740	1.1227110
H	-6.2386950	1.9940390	1.2132190
H	-4.7221150	2.2970270	2.0685590
C	-5.3285080	3.9189970	0.7437810
H	-5.8531930	4.0504780	-0.2068100
H	-5.8730810	4.4702770	1.5165600
H	-4.3286370	4.3514970	0.6500090
C	-3.4140270	-0.0577040	-0.8422840

H	-3.5991510	0.4158570	-1.8067750
H	-2.2090090	0.2563750	-0.5452390
N	-3.3808590	-1.4554220	-0.9238630
C	-2.9940190	-2.5659220	-0.8719760

20

G-gas = -853.411407 Hartree

Symbol	X	Y	Z
C	2.2189500	-1.2460570	0.3488690
O	2.1605740	-1.5039820	1.5293350
O	3.3936430	-0.9057000	-0.2659670
C	4.5412040	-0.8427020	0.5962650
H	4.3506720	-0.1224230	1.3992980
H	4.6917340	-1.8199650	1.0679930
C	5.7312240	-0.4379760	-0.2563380
H	5.5650500	0.5406180	-0.7168810
H	6.6351940	-0.3803000	0.3596400
H	5.9033070	-1.1659980	-1.0549980
C	1.0618010	-1.2385450	-0.6406090
H	1.4761750	-1.0428890	-1.6376140
N	0.4430280	-2.5700270	-0.6530920
C	-0.8040440	-2.3473990	-0.3704460
C	-0.0589550	-0.2495680	-0.2836050
C	-1.2238040	-0.9536360	-0.1348000
C	0.1650480	1.1972470	-0.1762450
C	-0.8135950	2.0451480	0.3868190
C	1.3590990	1.8010690	-0.6254570
C	-0.6123630	3.4181350	0.4821690
H	-1.7366550	1.6007260	0.7461830
C	1.5602810	3.1781640	-0.5244680
H	2.1416680	1.1873530	-1.0604200
C	0.5768490	3.9992330	0.0283070
H	-1.3896510	4.0406830	0.9195800
H	2.4921630	3.6101700	-0.8837440
H	0.7330970	5.0724390	0.1070050
Ag	-3.3853860	-0.4467980	0.0546120
H	-1.4947280	-3.1919470	-0.3308900

21

G-gas = -1339.985828 Hartree

Symbol	X	Y	Z
C	4.3843760	-1.1847840	0.3147850
O	4.2242400	-1.6101580	1.4349250
O	5.4762710	-0.4890480	-0.0779390
C	6.4569590	-0.2357910	0.9543230
H	5.9577560	0.2335370	1.8075140
H	6.8618390	-1.1936060	1.2968540
C	7.5289220	0.6561890	0.3575400
H	7.1018940	1.6058530	0.0223590
H	8.2957470	0.8693400	1.1090750
H	8.0105500	0.1730850	-0.4976370
C	3.3785370	-1.3086590	-0.8331310
H	3.8904510	-1.0468910	-1.7663020
N	2.8950400	-2.6839730	-0.9286370
C	1.6189350	-2.6078300	-0.7420310
C	2.1511670	-0.4296030	-0.5756070
C	1.0685870	-1.2574090	-0.5195480
C	2.2353020	1.0301370	-0.4140740
C	1.3764680	1.7221000	0.4620360
C	3.1911150	1.7840840	-1.1228810
C	1.4481940	3.1063410	0.6010300
H	0.6682270	1.1541230	1.0568410
C	3.2627200	3.1696180	-0.9841060
H	3.8766310	1.2824930	-1.7979810
C	2.3896910	3.8396860	-0.1253150
H	0.7778140	3.6126980	1.2905090
H	4.0033010	3.7273290	-1.5509900
H	2.4485060	4.9187870	-0.0152400
Ag	-0.9300270	-0.8136400	-0.2371020
H	-1.7983840	-0.5973160	2.1977790
C	-3.4610680	-0.0813490	1.4554500
O	-3.0232170	-0.3295100	0.2661020
O	-4.6264920	0.3298240	1.6770040
O	-2.6573350	-0.2640680	2.5088800

Ag	-5.2124890	0.3295580	-0.5144820
H	1.0115180	-3.5124390	-0.7704530

TS(21-16)

G-gas = -1339.960186 Hartree

Symbol	X	Y	Z
C	4.0359350	-1.0959420	0.7402990
O	3.8302180	--1.3204330	1.9083530
O	5.1834790	--0.5695300	0.2577190
C	6.1881970	--0.2545230	1.2527500
H	5.7518800	-0.4294060	1.9871320
H	6.4580720	--1.1750480	1.7793590
C	7.3718470	0.3585520	0.5296780
H	7.0811990	-1.2764950	0.0104700
H	8.1576160	-0.6060730	1.2502460
H	7.7862380	-0.3378250	-0.2050170
C	3.0288370	-1.3397220	-0.3922820
H	3.5542710	-1.2156000	-1.3462980
N	2.5107930	-2.7033590	-0.3041040
C	1.2361840	-2.5796500	-0.1415560
C	1.8196810	-0.4095880	-0.2773570
C	0.7023950	-1.1996070	-0.1067420
C	1.9159370	1.0558120	-0.2886620
C	0.9207040	1.8441320	0.3269030
C	3.0011100	1.7110930	-0.9022500
C	1.0019580	3.2333130	0.3063330
H	0.1034160	1.3548970	0.8466800
C	3.0749260	3.1033900	-0.9238890
H	3.7903420	1.1304880	-1.3680880
C	2.0751190	3.8706230	-0.3243800
H	0.2313460	3.8217970	0.7962880
H	3.9165520	3.5888100	-1.4099770
H	2.1353370	4.9550860	-0.3391260
Ag	-0.9940600	-0.6613910	-1.5076040
H	-0.4324960	-0.8620730	0.6918450
C	-2.4844770	-0.3142370	1.0908760
O	-2.7919480	-0.2840520	-0.1969460
O	-3.4021230	-0.0526830	1.9382580
O	-1.2938140	-0.5907260	1.5092500
Ag	-5.0114510	0.3094060	0.4608820
H	0.6130560	-3.4681960	-0.0402450

12′

G-gas = -2185.610461 Hartree

Symbol	X	Y	Z
C	5.6848900	-1.0580780	0.2470100
O	5.0875320	-1.2504180	1.2849170
O	7.0271100	-0.9598400	0.1644120
C	7.7495360	-1.1377420	1.4054610
H	7.4161270	-0.3771110	2.1186410
H	7.4929880	-2.1163490	1.8227730
C	9.2288660	-1.0202580	1.0917910
H	9.4639290	-0.0376180	0.6724870
H	9.8142700	-1.1527600	2.0071250
H	9.5365170	-1.7842540	0.3722430
C	5.0386400	-0.9122480	-1.1284370
H	5.7949720	-0.5770240	-1.8447290
N	4.5695240	-2.2666090	-1.5590570
C	3.3292870	-2.1044850	-1.7177460
C	3.7874040	-0.0293700	-1.1078070
C	2.7097780	-0.7915160	-1.4746530
C	3.8561770	1.3874580	-0.7154850
C	2.7168470	2.1018220	-0.2954650
C	5.0856670	2.0770980	-0.7280890
C	2.7951730	3.4411180	0.0778100
H	1.7620740	1.5877450	-0.2462240
C	5.1664890	3.4183250	-0.3556640
H	5.9909400	1.5631370	-1.0366190
C	4.0226240	4.1089880	0.0465150
H	1.8943580	3.9519390	0.4059280
H	6.1282340	3.9236140	-0.3810930
H	4.0870510	5.1532610	0.3392680
H	-1.0062040	-1.5732220	-3.4664870
C	-2.3643370	-0.9714400	-2.2967760

O	-1.5011220	-0.2760230	-1.6486790
O	-3.5812760	-1.0086750	-2.0026070
O	-1.9605530	-1.7044890	-3.3536080
Ag	-3.4756390	0.3720680	-0.1486130
Ag	0.6643440	-0.4885180	-1.5619080
C	-2.3948800	2.6113530	2.0810860
C	-0.8999670	2.6341240	1.7903170
C	-1.3111050	3.5542700	-0.3340220
C	-2.8085310	3.5573700	-0.0618060
H	-0.3408210	2.8317380	2.7095860
H	-2.7040220	3.5403710	2.5790330
H	-2.6751980	1.7580230	2.7036530
H	-1.0351580	4.4025230	-0.9672640
H	-1.0258740	2.6235560	-0.8483570
H	-3.1129920	4.5102450	0.3917970
H	-3.3900170	3.3871030	-0.9714480
H	-0.5679250	1.6652380	1.3896350
O	-0.5923100	3.6946000	0.8861540
O	-3.1502820	2.4897450	0.8525410
C	-7.3556090	-0.1617820	0.2443220
C	-6.4472880	-0.0240160	1.4606350
C	-5.4451860	-2.1059290	0.9116410
C	-6.3654060	-2.2155540	-0.2963830
H	-6.1890510	1.0205170	1.6573800
H	-6.8952560	0.3446070	-0.6215880
H	-8.3289550	0.2994190	0.4389360
H	-4.4677240	-2.5491640	0.7080660
H	-5.8951470	-2.5969340	1.7857040
H	-5.8608210	-1.8082130	-1.1842230
H	-6.6217230	-3.2619390	-0.4856660
H	-6.9380530	-0.4487900	2.3475910
O	-5.2061390	-0.7192450	1.2400310
O	-7.5920520	-1.5290960	-0.0489110
C	-0.6072920	-1.4831370	2.3177750
C	-0.1925740	-2.9461790	2.1922730
C	2.0585260	-2.3158350	2.1300760
C	1.6659890	-0.8503870	2.2486020
H	-0.8953980	-3.5951340	2.7264230
H	-0.7144340	-1.2255490	3.3849970
H	-1.5634050	-1.3011350	1.8116130
H	3.0168720	-2.4975820	2.6202920
H	2.1549750	-2.5903740	1.0699870
H	1.6734610	-0.5451590	3.3069820
H	2.3543170	-0.2205470	1.6837800
H	-0.1862660	-3.2335950	1.1272250
O	1.0856310	-3.1477650	2.7694750
O	0.3528660	-0.6281700	1.7040930

TS(12-13)′

G-gas = -2185.589483 Hartree

Symbol	X	Y	Z
C	-5.1857660	2.1594090	0.3838790
O	-4.9786150	1.9799110	1.5606240
O	-6.2939270	2.7622630	-0.1037480
C	-7.2442090	3.2173090	0.8895840
H	-7.5621430	2.3596740	1.4908970
H	-6.7389450	3.9200190	1.5591890
C	-8.4018640	3.8619560	0.1514300
H	-8.8902840	3.1452680	-0.5154270
H	-9.1440870	4.2238140	0.8699330
H	-8.0591250	4.7107860	-0.4469960
C	-4.2408550	1.7530940	-0.7544800
H	-4.7085090	1.9991060	-1.7122850
N	-3.0090000	2.5690260	-0.5942140
C	-2.1039990	1.7219790	-0.3552230
C	-3.7762540	0.2941840	-0.6514760
C	-2.4392380	0.2864660	-0.3570170
C	-4.6945570	-0.8377360	-0.8470400
C	-4.2200120	-2.1631880	-0.9211420
C	-6.0810850	-0.6348690	-0.9976960
C	-5.0895470	-3.2319950	-1.1126390
H	-3.1524210	-2.3384880	-0.8402410
C	-6.9520050	-1.7071760	-1.1900010

H	-6.4904490	0.3695280	-0.9671960
C	-6.4641540	-3.0125430	-1.2447940
H	-4.6933500	-4.2427100	-1.1700850
H	-8.0164600	-1.5182010	-1.2995930
H	-7.1423410	-3.8473930	-1.3968540
H	-0.8498490	2.1237990	-0.1812080
C	1.2939480	1.8029560	-0.0954700
O	1.1431930	0.5519100	0.1980270
O	2.4258420	2.3204720	-0.3166660
O	0.2598810	2.6233700	-0.1771390
Ag	3.4093070	0.1229020	0.0719160
Ag	-0.9477370	-1.0198500	0.2957740
C	3.8969310	-1.8209010	-2.9360740
C	2.5313220	-2.4720190	-3.1222420
C	1.5316480	-0.3652520	-3.3255890
C	2.8801900	0.3189490	-3.1504380
H	2.6319390	-3.4323530	-3.6382660
H	4.4031390	-1.7318530	-3.9085750
H	4.5284320	-2.4008200	-2.2549880
H	0.8902990	0.2148100	-3.9950240
H	1.0336110	-0.4520040	-2.3472470
H	3.3523390	0.4953620	-4.1274600
H	2.7782140	1.2611800	-2.6060300
H	2.0688470	-2.6513360	-2.1369660
O	1.6931070	-1.6536010	-3.9203410
O	3.7584210	-0.5147050	-2.3595230
C	6.3819580	2.2197360	-0.4944310
C	6.5462400	0.7191460	-0.2859300
C	5.8576350	0.9988160	1.9770010
C	5.6788950	2.4886530	1.7188360
H	6.2856160	0.1572750	-1.1837910
H	5.3762480	2.4372360	-0.8856040
H	7.1237990	2.5841440	-1.2117030
H	5.1309730	0.6149760	2.6977950
H	6.8732390	0.7941020	2.3416810
H	4.6454830	2.6985170	1.4004010
H	5.8950490	3.0609650	2.6260700
H	7.5757650	0.4835040	0.0151700
O	5.6550530	0.2513060	0.7542040
O	6.6014730	2.9195830	0.7238870
C	1.4066380	-2.3026420	2.1915060
C	1.1096470	-1.4276180	3.4012530
C	-0.9868800	-2.4523790	3.6544890
C	-0.7108500	-3.3447210	2.4497660
H	2.0294350	-1.2150720	3.9559400
H	1.9229780	-3.2229370	2.4982700
H	2.0101360	-1.7704900	1.4509880
H	-1.5951350	-2.9782060	4.3972940
H	-1.5284110	-1.5487860	3.3313080
H	-0.2320870	-4.2799290	2.7705040
H	-1.6152440	-3.5731690	1.8804420
H	0.6724820	-0.4748410	3.0644960
O	0.2330970	-2.0989970	4.2986580
O	0.1796440	-2.6689880	1.5291200

4 + **1**

G-gas = -799.014735 Hartree

Symbol	X	Y	Z
C	-0.2939020	1.7401830	-0.1133760
O	-0.8718060	1.6101260	-1.1773790
O	1.0386760	1.7520940	0.0616260
C	1.8433070	1.6186070	-1.1489190
H	1.6137180	0.6514070	-1.6018340
H	1.5402660	2.4072050	-1.8434860
C	3.2980430	1.7296690	-0.7424630
H	3.5796720	0.9204900	-0.0638920
H	3.9272170	1.6574900	-1.6349260
H	3.5006800	2.6883790	-0.2565180
C	-0.9697850	1.8996060	1.1835190
H	0.5206700	-1.0393750	1.9248240
H	-0.4117460	2.0873710	2.0945100
N	-2.3026390	1.8148230	1.2511580
C	-3.4894500	1.7071600	1.2822380

C	0.2665620	-1.7397930	-0.0944940
O	0.8620420	-1.6899410	-1.1441710
O	-1.0621360	-1.7183150	0.0615350
C	-1.8561520	-1.6266690	-1.1629240
H	-1.5894490	-0.6943780	-1.6656590
H	-1.5800710	-2.4651890	-1.8086470
C	-3.3153320	-1.6621750	-0.7578860
H	-3.5661260	-0.8145840	-0.1142980
H	-3.9404980	-1.6032210	-1.6542430
H	-3.5581240	-2.5889030	-0.2297140
C	0.9220840	-1.8389100	1.2911690
H	0.6312620	-2.7891260	1.7521810
N	2.3294100	-1.7360580	1.2219850
C	3.4964450	-1.5944500	1.1592730

TS(4-1)

G-gas = -798.983771 Hartree

Symbol	X	Y	Z
C	0.7033860	1.4367040	-0.0745060
O	0.0635340	1.7569890	-1.0516260
O	1.9685020	0.9983660	-0.0621910
C	2.5830060	0.7571890	-1.3616240
H	1.9253660	0.0870970	-1.9215980
H	2.6449190	1.7095600	-1.8960240
C	3.9436690	0.1436180	-1.1032840
H	3.8457380	-0.7892650	-0.5416940
H	4.4328890	-0.0751370	-2.0572610
H	4.5835610	0.8264230	-0.5372260
C	0.1505500	1.3544080	1.3256520
H	0.0000320	0.0004110	1.4273290
H	0.8651120	1.5467680	2.1264550
N	-1.0893740	1.9231020	1.5117200
C	-2.1882180	2.3500640	1.6181010
C	-0.7033050	-1.4365380	-0.0739060
O	-0.0634540	-1.7570740	-1.0509540
O	-1.9684770	-0.9983590	-0.0617130
C	-2.5830600	-0.7578160	-1.3612260
H	-1.9257910	-0.0874270	-1.9212850
H	-2.6443550	-1.7103210	-1.8954550
C	-3.9441110	-0.1450260	-1.1030840
H	-3.8467940	0.7880740	-0.5417470
H	-4.4334450	0.0731580	-2.0571330
H	-4.5835850	-0.8280850	-0.5368580
C	-0.1504130	-1.3536600	1.3261950
H	-0.8649550	-1.5457280	2.1270900
N	1.0895340	-1.9222200	1.5124760
C	2.1883870	-2.3491210	1.6190020

1 + **4**

G-gas = -799.015248 Hartree

Symbol	X	Y	Z
C	0.3001750	-1.7511330	-0.0952100
O	0.8855000	-1.6841170	-1.1492330
O	-1.0273930	-1.7544280	0.0721630
C	-1.8340430	-1.6684070	-1.1439880
H	-1.6021190	-0.7196310	-1.6328930
H	-1.5358760	-2.4860620	-1.8059280
C	-3.2874550	-1.7597340	-0.7282580
H	-3.5618690	-0.9301100	-0.0713570
H	-3.9219190	-1.7108310	-1.6182990
H	-3.4932000	-2.7013100	-0.2111600
C	0.9688180	-1.8419930	1.2832670
H	0.5714650	-1.0392550	1.9142880
H	0.6840900	-2.7906500	1.7530460
N	2.3752740	-1.7364900	1.2003150
C	3.5412970	-1.5934830	1.1267980
C	-0.3286030	1.7542680	-0.1183080
O	-0.8941520	1.6059710	-1.1865350
O	1.0021470	1.7878740	0.0686730
C	1.8217160	1.6641750	-1.1326950
H	1.6174800	0.6902510	-1.5840850
H	1.5101960	2.4427020	-1.8348710
C	3.2697080	1.8080070	-0.7116690
H	3.5641040	1.0037970	-0.0325670

H	3.9097880	1.7535680	-1.5975790
H	3.4442330	2.7700150	-0.2208090
C	-1.0180260	1.9172560	1.1710870
H	-0.4708040	2.1200510	2.0851240
N	-2.3505490	1.8193050	1.2287050
C	-3.5364980	1.7002710	1.2512100

d) Process IV

17c

G-gas = -937.474225 Hartree

Symbol	X	Y	Z
C	-1.2063240	-0.8631240	-0.7346540
C	-1.1775660	-1.8592890	-1.6591580
H	0.5731710	-2.9620560	-2.5627520
C	-2.3618460	-0.2198060	-0.1085990
C	-2.2916510	0.2308990	1.2225050
C	-3.5674030	-0.0608200	-0.8148220
C	-3.4002570	0.8205010	1.8258880
H	-1.3830390	0.0783730	1.7977030
C	-4.6702330	0.5338290	-0.2092650
H	-3.6233990	-0.3805160	-1.8508700
C	-4.5902860	0.9769700	1.1132580
H	-3.3351730	1.1534260	2.8573970
H	-5.5911250	0.6592200	-0.7711060
H	-5.4511500	1.4417010	1.5847530
C	0.6244490	0.9044890	-0.7229450
O	-0.0905770	1.7301620	-1.2377760
O	1.9073280	1.1447350	-0.3610300
C	2.4332240	2.4647220	-0.6824830
H	2.0967020	2.7341240	-1.6859830
H	2.0004560	3.1831620	0.0210260
C	3.9446760	2.3947640	-0.5739100
H	4.3556390	1.7077080	-1.3190500
H	4.3696950	3.3876050	-0.7501790
H	4.2572320	2.0533640	0.4166920
C	0.2315820	-0.5436550	-0.4065980
H	0.4601210	-0.7466390	0.6603420
N	1.0570330	-1.4601810	-1.2148200
C	0.2184930	-2.1773780	-1.8971930
O	3.3886980	0.0228290	1.9586140
H	3.5893690	-0.8040030	1.4744590
H	2.8710200	0.5113720	1.3004250
O	1.0532370	-1.4349680	2.4886010
H	1.8198910	-0.8351840	2.6028490
H	1.4766690	-2.1971700	2.0635300
O	3.0886550	-2.3385550	0.4994620
H	2.5240690	-2.0293280	-0.2510920
H	3.7132760	-2.9694030	0.1226840
H	-2.0225260	-2.3707360	-2.1021900

TS(17c-Pr)

G-gas = -937.451871 Hartree

Symbol	X	Y	Z
C	1.1434010	0.8863470	-0.5519950
C	1.1071820	2.1401290	-1.1427040
H	-0.6462060	3.3773960	-1.7827840
C	2.3619750	0.1809270	-0.1245820
C	2.3861860	-0.6436580	1.0131650
C	3.5610770	0.3606160	-0.8374200
C	3.5650280	-1.2589670	1.4252170
H	1.4752330	-0.7986260	1.5801870
C	4.7401100	-0.2573060	-0.4266190
H	3.5573970	0.9727610	-1.7340710
C	4.7483210	-1.0688920	0.7087700
H	3.5596600	-1.8892320	2.3098710
H	5.6520030	-0.1095870	-0.9982910
H	5.6664590	-1.5520190	1.0301070
C	-0.6873100	-0.9244590	-0.4714410
O	0.0303720	-1.9019770	-0.4484670
O	-2.0639060	-1.0581180	-0.5457540
C	-2.5294830	-2.4121900	-0.7876890
H	-2.0593250	-2.7796920	-1.7038480
H	-2.1995370	-3.0576710	0.0317370
C	-4.0413920	-2.3629340	-0.9054750

H	-4.3490550	-1.7020550	-1.7205830
H	-4.4267720	-3.3663400	-1.1108440
H	-4.5029360	-2.0091520	0.0219380
C	-0.2528830	0.4876940	-0.3886820
H	-0.5720220	0.8844010	1.0454980
N	-1.0805110	1.4918110	-0.9724800
C	-0.2572370	2.4521200	-1.3664490
O	-3.2405010	-0.0655530	1.8333830
H	-3.6383070	0.7586710	1.4876180
H	-2.9673380	-0.5227470	1.0122200
O	-1.0541660	1.2803820	2.0259250
H	-1.8312620	0.6296370	2.1732370
H	-1.5696760	2.0593300	1.6885280
O	-3.0158620	2.3870160	0.6088790
H	-2.4642470	2.0360790	-0.1695660
H	-3.3913030	3.2325060	0.3357360
H	1.9534570	2.7831080	-1.3456190

TS(16-Pr)

G-gas = -708.176134 Hartree

Symbol	X	Y	Z
C	1.5098110	-0.4296520	-0.1157860
O	1.0931340	-1.5552990	-0.4029740
O	2.8778480	-0.2072600	0.0201760
C	3.6867920	-1.3575480	-0.1877110
H	3.4226750	-2.1465920	0.5292640
H	3.5069390	-1.7753480	-1.1864850
C	5.1364940	-0.9270340	-0.0233550
H	5.3102240	-0.5244600	0.9796160
H	5.8108100	-1.7775850	-0.1780730
H	5.3901960	-0.1455670	-0.7462370
C	0.7312050	0.7523630	0.2004430
H	1.2143950	1.2955360	1.2273360
N	1.4842190	2.0837610	0.2549210
C	0.4750160	2.9967500	0.1207510
C	-0.7036370	1.0277200	-0.0041820
C	-0.7752710	2.4534290	-0.0769090
C	-1.8405310	0.1492350	-0.0108610
C	-3.1329110	0.6310860	-0.3999510
C	-1.7948240	-1.2179350	0.4051430
C	-4.2647880	-0.1682850	-0.3525570
H	-3.2300900	1.6495990	-0.7655380
C	-2.9355740	-2.0047180	0.4475590
H	-0.8370180	-1.6482210	0.6666800
C	-4.1955890	-1.5020400	0.0791030
H	-5.2212630	0.2512120	-0.6645740
H	-2.8448410	-3.0398030	0.7758780
H	-5.0841640	-2.1272780	0.1161810
H	0.7162780	4.0534760	0.2059490
H	-1.6886950	3.0289370	-0.1721770

Pr

G-gas = -708.256351 Hartree

Symbol	X	Y	Z
C	-0.6624260	1.0484340	-0.1134760
C	-0.7529690	2.4675800	-0.1922920
H	0.8712000	4.0051330	-0.3156010
C	-1.8370490	0.1572470	-0.0367950
C	-1.8796010	-1.0984070	-0.6654950
C	-2.9848710	0.5964620	0.6481660
C	-3.0303270	-1.8822980	-0.6089020
H	-1.0047070	-1.4623790	-1.1878560
C	-4.1339440	-0.1892220	0.7038790
H	-2.9653980	1.5549970	1.1580530
C	-4.1625570	-1.4337130	0.0729550
H	-3.0411570	-2.8495480	-1.1032500
H	-5.0048190	0.1691480	1.2455510
H	-5.0566240	-2.0490780	0.1156530
C	1.4591920	-0.5008930	0.0173130
O	1.0064010	-1.6289230	0.0652510
O	2.8032840	-0.2452140	0.0807710
C	3.6535700	-1.4061790	0.1988160
H	3.3806910	-1.9544760	1.1057310
H	3.4688530	-2.0694160	-0.6519930

C	5.0894320	-0.9194750	0.2394050
H	5.2555120	-0.2579260	1.0946860
H	5.7680750	-1.7731120	0.3303990
H	5.3457170	-0.3750360	-0.6742970
C	0.7104670	0.7461070	-0.1140160
H	2.4054780	1.9896170	-0.1839360
H	-1.6675450	3.0398330	-0.2451290
N	1.3987390	1.9437130	-0.1885630
C	0.5270940	2.9842480	-0.2389300

19a

G-gas = -1015.788040 Hartree

Symbol	X	Y	Z
C	0.2183020	0.4775820	-1.6268300
O	0.8271720	0.6707180	-2.6515430
O	-0.6503590	1.3634060	-1.0860610
C	-0.8331170	2.5912160	-1.8377230
H	0.1383910	3.0837860	-1.9408330
H	-1.1809280	2.3344120	-2.8425120
C	-1.8339780	3.4469910	-1.0870440
H	-1.4675280	3.6942390	-0.0863610
H	-1.9995650	4.3824790	-1.6304100
H	-2.7945110	2.9337220	-0.9870000
C	0.3134630	-0.7949930	-0.7750130
H	-0.3035950	-0.6783740	0.1248790
N	-0.2491010	-1.9061530	-1.5585680
C	0.7014120	-2.7762910	-1.6571220
C	1.7464420	-1.1743390	-0.4404210
C	1.9436800	-2.3972930	-0.9954050
C	2.6690460	-0.3488060	0.3417200
C	4.0348150	-0.6786870	0.4407900
C	2.2143500	0.7976570	1.0199270
C	4.9062740	0.0998180	1.1945740
H	4.4164450	-1.5454880	-0.0891930
C	3.0895230	1.5774120	1.7735130
H	1.1686350	1.0815370	0.9590760
C	4.4377670	1.2319520	1.8668960
H	5.9558040	-0.1730190	1.2541740
H	2.7157140	2.4566130	2.2900990
H	5.1193430	1.8399410	2.4541740
H	2.8360620	-3.0089760	-0.9505780
C	-2.7592040	-0.5006690	2.4528130
H	-3.4885040	-1.0946160	3.0269460
H	-1.9848420	-0.1386670	3.1366780
C	-3.4723330	0.6564190	1.7634060
H	-4.0351510	1.2572710	2.4852450
H	-2.7263230	1.2993470	1.2695470
C	-3.7679550	-0.6664080	-0.1521620
H	-4.5519940	-1.0369660	-0.8196270
H	-3.0479500	-0.0799880	-0.7421790
C	-3.0420390	-1.8215540	0.5256150
H	-2.4608750	-2.3907440	-0.2041250
H	-3.7694230	-2.4835520	1.0217730
O	-2.1078330	-1.3276730	1.4915650
O	-4.4114160	0.1690710	0.8113290
H	0.5453160	-3.7141060	-2.1873260

TS(19a-19a')

G-gas = -1015.741038 Hartree

Symbol	X	Y	Z
C	-0.3480250	0.9354740	-1.0685050
O	-1.4306330	1.5105340	-1.1507260
O	0.8187010	1.6188350	-1.0181280
C	0.7210350	3.0571930	-1.0195490
H	0.1662170	3.3774340	-1.9066260
H	0.1468160	3.3810210	-0.1436870
C	2.1360290	3.6042250	-1.0005070
H	2.6884050	3.2815810	-1.8873290
H	2.1134940	4.6985640	-0.9859820
H	2.6769920	3.2538410	-0.1171890
C	-0.1643990	-0.5217800	-0.9933400
H	-1.4474300	-0.9009090	-0.0187390
N	-1.0693680	-1.3168860	-1.7239480
C	-0.5064660	-2.5292950	-1.7743630

C	1.0045880	-1.2891660	-0.6466550	H	-2.4882870	-1.2538910	3.4784680
C	0.7535410	-2.5709490	-1.1440530	H	-1.7163530	-2.7545690	2.9610860
C	2.1938390	-0.9032470	0.1323390	C	-0.3145520	-1.2324120	3.6421000
C	3.4429170	-1.4830940	-0.1559810	H	-0.2280510	-0.1420050	3.6591430
C	2.1315180	0.0036340	1.2058340	H	-0.2920430	-1.5925820	4.6753570
C	4.5754370	-1.1733580	0.5949860	H	0.5540620	-1.6397050	3.1169820
H	3.5222030	-2.1693160	-0.9934540	C	-2.5265570	-0.9722270	-0.5686720
C	3.2628570	0.3187610	1.9548730	H	-1.5957800	-0.3975100	-0.6575270
H	1.1814530	0.4668250	1.4539990	N	-2.4108780	-2.1404390	-1.4565490
C	4.4934510	-0.2698290	1.6554000	C	-3.3845790	-2.0316870	-2.2993810
H	5.5272240	-1.6340470	0.3448250	C	-3.7324000	-0.1782590	-1.0414940
H	3.1825780	1.0199950	2.7814230	C	-4.2266890	-0.8575500	-2.1077590
H	5.3756110	-0.0264320	2.2403180	C	-4.2009080	1.0699830	-0.4359980
H	1.3841820	-3.4421200	-1.0162520	C	-5.4336770	1.6408470	-0.8078530
C	-2.2095920	-0.3270170	1.9425320	C	-3.4294210	1.7357570	0.5348890
H	-2.6902220	-0.9490670	2.7013410	C	-5.8713270	2.8320100	-0.2392630
H	-1.1514590	-0.1994100	2.1771740	H	-6.0581550	1.1379520	-1.5392970
C	-2.9505100	0.9867580	1.7402010	C	-3.8704100	2.9285960	1.1046110
H	-3.0459010	1.4963230	2.7038920	H	-2.4767160	1.3191620	0.8459690
H	-2.4009030	1.6271790	1.0390260	C	-5.0909170	3.4835630	0.7197320
C	-4.2125650	0.1193560	-0.0266600	H	-6.8267220	3.2518570	-0.5400400
H	-5.2439590	0.0088850	-0.3732880	H	-3.2571840	3.4257120	1.8505210
H	-3.6459550	0.7394350	-0.7313180	H	-5.4343060	4.4128050	1.1643600
C	-3.5651030	-1.2490100	0.0723230	H	-5.0705530	-0.5895300	-2.7309990
H	-3.3441660	-1.6838790	-0.9016470	C	1.5852140	0.7170180	-0.9573530
H	-4.1266520	-1.9338400	0.7122470	H	2.4574820	0.8042360	-1.6217660
O	-2.2358730	-1.1256920	0.7105170	H	1.1743820	1.7172230	-0.7870060
O	-4.2660850	0.7349610	1.2620710	C	2.0115000	0.0735340	0.3551740
H	-1.0231370	-3.3548860	-2.2542040	H	2.8621390	0.6098960	0.7826120
19b				H	1.1686140	0.0837130	1.0633050
G-gas = -1323.352875 Hartree				C	1.4212370	-2.0401010	-0.4998580
Symbol	X	Y	Z	H	1.8397280	-3.0357840	-0.6768380
C	-2.6747150	-1.4869490	0.8690040	H	0.5517720	-2.1341830	0.1661490
O	-3.6296940	-2.0930180	1.2919080	C	0.9871330	-1.3927710	-1.8087870
O	-1.5836240	-1.1842250	1.6103100	H	0.1336310	-1.9277040	-2.2331250
C	-1.6066990	-1.6662860	2.9787790	H	1.8232730	-1.3987960	-2.5265300

O	0.5556630	-0.0486520	-1.5844690	C	-1.0921140	1.6300510	0.7219940
O	2.4440310	-1.2720170	0.1389170	C	-2.0903800	2.3931650	1.3565850
H	-3.5250590	-2.7705050	-3.0864220	C	-1.2126170	1.4263830	-0.6648830
C	6.0696040	2.0976760	-0.6051960	C	-3.1605040	2.9261990	0.6391480
C	7.0695610	1.8093100	0.5092470	H	-2.0074200	2.5840510	2.4221540
C	6.5634220	-0.4750450	0.3757470	C	-2.2766080	1.9653660	-1.3850150
C	5.5582640	-0.1958980	-0.7340340	H	-0.4662550	0.8318190	-1.1803700
H	7.9145130	2.5040500	0.4684290	C	-3.2601520	2.7173650	-0.7374080
H	6.5896500	2.0917810	-1.5767750	H	-3.9130670	3.5149740	1.1564220
H	5.5951060	3.0744230	-0.4667090	H	-2.3426410	1.7916100	-2.4559520
H	7.0419610	-1.4489940	0.2344190	H	-4.0906300	3.1356590	-1.2985250
H	6.0463450	-0.4758010	1.3491280	H	-1.0252010	0.5178920	3.4093880
H	6.0514180	-0.3018780	-1.7136900	C	1.3333060	-2.2557910	-0.8872240
H	4.7050420	-0.8763400	-0.6759280	H	1.0976060	-3.3205250	-0.8305790
H	6.5697020	1.9186680	1.4861300	H	0.4211030	-1.7002240	-1.1053420
O	7.6057180	0.4984410	0.3746460	C	2.4976330	-1.9938100	-1.8264220
O	5.0264090	1.1265620	-0.6032360	H	2.2546940	-2.3870180	-2.8183500

TS(19b-19b')

				H	2.6957070	0.9164640	-1.9021810

G-gas = -1323.306267 Hartree

C	4.0695840	-	2.1699190	-0.1032050			
H	4.9827640		-2.7032360	0.1765380			
H	4.2706490		-1.0944690	-0.1660680			
C	3.0049280		-2.4192400	0.9498590			
H	3.1945640		-1.8799020	1.8775950			
H	2.8196220		-3.4826040	1.1187810			
O	1.7053670		-1.8766380	0.4885570			
O	3.6555090		-2.6836420	-1.3702730			
H	1.4150770		-0.4155870	4.1304470			
C	-3.6084620		-1.4196350	0.8346490			
C	-2.2769360		-2.1475760	0.6964260			
C	-2.8441820		-2.7321890	-1.5167790			
C	-4.1657790		-1.9877400	-1.3646010			
H	-1.4929160		-1.6416410	1.2664300			
H	-3.4799460		-0.3579030	0.5804610			
H	-3.9839190		-1.4947850	1.8597290			
H	-2.4668970		-2.6629510	-2.5423290			
H	-2.9901730		-3.7948200	-1.2634800			

Symbol	X	Y	Z
C	2.1850210	1.3972530	0.0824920
O	3.2612700	0.9701580	-0.3254890
O	1.6174800	2.5088070	-0.4408860
C	2.3218880	3.1337330	-1.5327200
H	3.3429180	3.3643490	-1.2142690
H	2.3944260	2.4267630	-2.3673370
C	1.5459910	4.3805180	-1.9141490
H	1.4947460	5.0771390	-1.0728270
H	2.0379370	4.8853150	-2.7517260
H	0.5239000	4.1283980	-2.2098600
C	1.3727260	0.7839030	1.1460950
H	1.5884790	-0.8288810	0.7378370
N	2.0640510	0.2053410	2.2262650
C	1.1499520	0.0541700	3.1881320
C	0.0028210	1.0430540	1.5141480
C	-0.1187970	0.5492300	2.8167580

H	-4.0419940	-0.9472890	-1.7052430	C	1.2479800	-1.8174100	1.6779970
H	-4.9521910	-2.4643000	-1.9587160	H	2.0515980	-2.5513280	1.5145570
H	-2.3809340	-3.1827240	1.0596820	H	1.6580780	-0.8119530	1.5470670
O	-1.8468450	-2.1617200	-0.6703230	C	0.6520300	-1.9975570	3.0685210
O	-4.5943170	-2.0153360	-0.0090160	H	1.4302780	-1.9355140	3.8362890
19c				H	-0.0917790	-1.2055370	3.2567480
G-gas = -1630.908286 Hartree				C	-0.9563930	-3.4606390	2.1990380
Symbol	X	Y	Z	H	-1.3519400	-4.4722130	2.3354980
C	-3.5755840	-0.4472380	0.4915210	H	-1.7695060	-2.7322240	2.3436010
O	-3.4780220	-0.6872080	1.6769030	C	-0.3701950	-3.2924450	0.8025850
O	-4.7082000	-0.0472430	-0.1041740	H	-1.1553340	-3.3384610	0.0399880
C	-5.8727390	0.0621510	0.7513680	H	0.3818650	-4.0677460	0.6012240
H	-6.0466150	-0.9057330	1.2305830	O	0.2398290	-1.9974300	0.6777620
H	-5.6598220	0.7893540	1.5408550	O	0.0490130	-3.2783870	3.1951100
C	-7.0370800	0.4875780	-0.1208030	H	-2.7640060	-1.6478840	-3.5563370
H	-7.2267750	-0.2504700	-0.9048280	C	2.1758490	-1.2394410	-2.2287380
H	-7.9405190	0.5832120	0.4893000	C	1.9197970	-2.7405070	-2.2624700
H	-6.8383790	1.4524670	-0.5953910	C	4.0170630	-3.1186590	-1.2891770
C	-2.4235800	-0.5693400	-0.5110670	C	4.2744920	-1.6158160	-1.2491980
H	-1.5445400	-0.8939920	0.0604810	H	0.8552060	-2.9408480	-2.1167270
N	-2.7397960	-1.6221400	-1.4840400	H	1.7496650	-0.8284360	-1.3030490
C	-2.6036170	-1.0721950	-2.6462470	H	1.7099610	-0.7441840	-3.0867040
C	-2.1151140	0.6890060	-1.3060530	H	4.4900360	-3.6210030	-0.4394200
C	-2.2180950	0.3326450	-2.6132180	H	4.4298010	-3.5379260	-2.2216920
C	-1.7387900	1.9783270	-0.7203710	H	3.9575290	-1.2066440	-0.2779240
C	-1.6009250	3.1291540	-1.5220750	H	5.3379820	-1.3997790	-1.3958740
C	-1.5007440	2.1014580	0.6622400	H	2.2369830	-3.1540330	-3.2340470
C	-1.2331790	4.3495950	-0.9660280	O	2.6212950	-3.3925440	-1.2058150
H	-1.7951760	3.0668540	-2.5880870	O	3.5740400	-0.9577910	-2.3036800
C	-1.1352130	3.3272370	1.2174030	C	2.9403480	3.3811130	0.0908950
H	-1.6024920	1.2362920	1.3089600	C	2.8034170	1.8818320	-0.1408390
C	-0.9977040	4.4555370	0.4080500	C	4.5515440	1.4999670	1.3853890
H	-1.1358400	5.2233220	-1.6037520	C	4.6768190	3.0019690	1.6136130
H	-0.9590260	3.3982220	2.2864970	H	1.7597610	1.6121710	-0.3210760
H	-0.7156500	5.4100850	0.8420450	H	2.2411070	3.6961170	0.8815860
H	-2.0372090	0.9490540	-3.4851240	H	2.7085770	3.9387930	-0.8206540

H	4.7841620	0.9419830	2.2970930	H	2.4495450	5.1510470	0.5343480
H	5.2493740	1.1896080	0.5919350	H	0.7059640	0.0700440	3.6602270
H	4.0564650	3.2957490	2.4761390	C	-0.7486460 -	1.4088610	-1.4454900
H	5.7145350	3.2816670	1.8177300	H	-1.8279800	-1.5640430	-1.4396270
H	3.4050140	1.5680970	-1.0062860	H	-0.5307820	-0.3540930	-1.2729100
O	3.2159410	1.1586170	1.0230390	C	-0.0958090	-1.9901540	-2.6878070
O	4.2764630	3.7182240	0.4524900	H	-0.5317140	-1.5237370	-3.5766530

TS(19c-19c')

G-gas = -1630.868944 Hartree

Symbol	X	Y	Z
C	2.9725930	-1.4335520	-0.1895550
O	2.9622720	-2.3827280	-0.9667940
O	3.8647980	-0.4227040	-0.3113610
C	4.7657920	-0.4997720	-1.4343570
H	5.3236480	-1.4396370	-1.3807520
H	4.1838430	-0.5213910	-2.3629000
C	5.6775150	0.7109280	-1.3654330
H	6.2558900	0.7087550	-0.4373770
H	6.3761110	0.7009480	-2.2081670
H	5.0982290	1.6376400	-1.4029530
C	2.0424910	-1.2489260	0.9379130
H	0.6482750	-1.7936710	0.1797870
N	1.6750770	-2.3975820	1.6550770
C	1.1147470	-1.9444120	2.7814830
C	1.7381920	-0.0639220	1.7000320
C	1.1256150	-0.5354960	2.8659130
C	1.9423310	1.3538450	1.3582660
C	2.2038590	2.2941670	2.3732440
C	1.8610820	1.8317750	0.0369270
C	2.3779820	3.6459870	2.0820560
H	2.2945520	1.9481120	3.3982260
C	2.0468320	3.1816430	-0.2574810
H	1.6521160	1.1350920	-0.7681750
C	2.3044610	4.0994690	0.7638460
H	2.5848910	4.3455120	2.8873850
H	1.9854780	3.5186700	-1.2890230
H	0.9864250	-1.7988790	-2.6760310
C	0.2448580	-4.0679300	-1.6683080
H	0.0411070	-5.1341460	-1.8036450
H	1.3274590	-3.8973460	-1.6497940
C	-0.3604820	-3.6096200	-0.3540360
H	0.2038020	-3.9566290	0.5117990
H	-1.4279470	-3.8185590	-0.2670560
O	-0.2729140	-2.1312140	-0.2552230
O	-0.3556810	-3.3849830	-2.7710590
H	0.7139730	-2.6390890	3.5138860
C	-2.8621150	-0.4989600	2.0901110
C	-2.8712320	-2.0199320	2.0206660
C	-4.5436650	-1.9367350	0.3736960
C	-4.5264000	-0.4136330	0.4318630
H	-1.8708940	-2.4175230	2.2089840
H	-2.0772480	-0.1083810	1.4260290
H	-2.6566110	-0.1567620	3.1083770
H	-4.7745440	-2.2922280	-0.6355080
H	-5.3035280	-2.3273080	1.0687310
H	-3.8318640	-0.0228100	-0.3284870
H	-5.5241610	-0.0042780	0.2439570
H	-3.5697780	-2.4276960	2.7678190
O	-3.2589520	-2.4588980	0.7139180
O	-4.1343390	0.0369500	1.7247770
C	-1.7442990	3.9994770	-0.3455780
C	-1.9315970	2.5182820	-0.0448780
C	-2.8246190	2.2161570	-2.2094320
C	-2.6145150	3.6984860	-2.4946440
H	-1.1239550	2.1525450	0.5942110

H	-0.7257860	4.1709540	-0.7254510	H	-5.7772190	-3.8386690	-0.3146510
H	-1.8845430	4.5974410	0.5595720	H	-5.0911010	-0.2615570	1.9694060
H	-2.6867910	1.6172350	-3.1157610	H	-6.5375450	-2.2038420	1.4007340
H	-3.8478370	2.0583480	-1.8328250	H	-2.4833570	-1.6429720	-3.1973880
H	-1.6280650	3.8462910	-2.9649980	C	4.2438630	-1.4406050	0.6716680
H	-3.3859630	4.0771740	-3.1726830	H	4.4179720	-0.3653470	0.7704210
H	-2.8956190	2.3485150	0.4572060	H	3.8699730	-1.8544940	1.6098490
O	-1.8743110	1.7444100	-1.2535780	C	5.4687880	-2.1806270	0.1584180
O	-2.7085060	4.4525530	-1.2943560	H	6.3198260	-1.9976090	0.8207890

19c'

G-gas = -1630.898497 Hartree

Symbol	X	Y	Z
C	0.0455260	-1.3502350	0.7118620
O	1.2830330	-1.2335700	1.0137240
O	-0.8235630	-1.5055190	1.7163310
C	-0.3103850	-1.5718800	3.0625890
H	0.4679500	-2.3394000	3.1148640
H	0.1508850	-0.6118040	3.3172230
C	-1.4829100	-1.8916060	3.9704410
H	-1.9276150	-2.8544820	3.7057870
H	-1.1446910	-1.9370670	5.0104320
H	-2.2581510	-1.1255490	3.8889010
C	-0.4750120	-1.3242350	-0.6017030
H	2.1789700	-1.3873160	0.1572000
N	0.4189010	-1.1592940	-1.6503720
C	-0.3137480	-1.2755180	-2.7588780
C	-1.8084990	-1.5476950	-1.0909130
C	-1.6805680	-1.5256720	-2.4800300
C	-3.0818650	-1.7375570	-0.3649880
C	-3.9177770	-2.8208810	-0.6846060
C	-3.5281370	-0.8185860	0.6022190
C	-5.1509310	-2.9895390	-0.0543070
H	-3.5840050	-3.5392580	-1.4276980
C	-4.7611010	-0.9874270	1.2304590
H	-2.9099560	0.0419530	0.8361500
C	-5.5774980	-2.0747280	0.9088610
H	-5.5632400	-3.2628400	0.1404600
C	4.7737270	-1.8977440	-2.0650290
H	5.1287400	-1.5148910	-3.0257250
H	4.5370300	-2.9671840	-2.1770980
C	3.5379470	-1.1332160	-1.6313150
H	2.6511650	-1.3141870	-2.2368250
H	3.7365400	-0.0613820	-1.5421930
O	3.1723340	-1.6300930	-0.2987470
O	5.8392170	-1.7219100	-1.1328040
H	0.1405600	-1.1771160	-3.7408000
C	1.4777600	2.3331890	1.1845760
C	2.0331710	2.0168160	-0.1953440
C	4.1101710	2.9293880	0.4311200
C	3.5448680	3.2498020	1.8114580
H	1.5844880	1.1104110	-0.6094520
H	1.6091810	1.4549650	1.8360290
H	0.4136620	2.5753010	1.1213310
H	5.1764960	2.6871090	0.4851150
H	3.9773970	3.7978650	-0.2329920
H	3.7727520	2.4174380	2.4994930
H	3.9932590	4.1647350	2.2125710
H	1.8352160	2.8576320	-0.8778300
O	3.4511230	1.7909120	-0.1234380
O	2.1436690	3.4672710	1.7458820
C	-3.0047480	2.1131700	-2.0777220
C	-1.6596470	2.2533280	-1.3769760
C	-2.6607220	3.6441470	0.2375290

C	-4.0019370	3.4924150	-0.4722280	H	-2.7943280	-0.2503450	0.8014110
H	-1.0754320	1.3350460	-1.4671620	C	-5.4651410	-2.3191080	0.3846240
H	-3.5231440	1.2178850	-1.7047450	H	-5.5325780	-3.9737400	-0.9965370
H	-2.8699020	2.0157230	-3.1589070	H	-5.0891170	-0.6096970	1.6432050
H	-2.7934620	3.7411830	1.3196630	H	-6.4770070	-2.4712500	0.7496630
H	-2.1469380	4.5437460	-0.1382080	H	-1.8570730	-1.8200350	-3.2970590
H	-4.5600590	2.6520330	-0.0281800	C	4.1857250	-1.0857830	0.7587540
H	-4.6004140	4.4037940	-0.3714200	H	4.1141500	0.0043700	0.7503540
H	-1.0979010	3.0910160	-1.8215970	H	3.7456740	-1.4990620	1.6642940
O	-1.8453800	2.4926170	0.0238200	C	5.5936290	-1.5833370	0.4850100
O	-3.8077760	3.2749380	-1.8640070	H	6.2770240	-1.1764680	1.2355480

TS(19c'-Pr)

G-gas = -1630.891049 Hartree

Symbol	X	Y	Z
C	0.1832820	-1.4798160	0.9195460
O	1.3834120	-1.3282510	1.2491150
O	-0.7664730	-1.6568960	1.8538050
C	-0.3354950	-1.6829230	3.2283920
H	0.4493860	-2.4371620	3.3451530
H	0.1003170	-0.7117540	3.4869550
C	-1.5532300	-1.9978350	4.0767200
H	-1.9777770	-2.9669500	3.8013230
H	-1.2725190	-2.0281880	5.1343540
H	-2.3277030	-1.2375040	3.9451580
C	-0.2352420	-1.4819230	-0.4491400
H	2.3070170	-1.4214070	-0.1521560
N	0.7924960	-1.3366810	-1.3606460
C	0.2250430	-1.4619930	-2.5715080
C	-1.4778960	-1.7112830	-1.1086970
C	-1.1587210	-1.7012730	-2.4778810
C	-2.8318480	-1.9225240	-0.5590720
C	-3.6354580	-2.9617510	-1.0610440
C	-3.3827740	-1.0788970	0.4229700
C	-4.9351180	-3.1591990	-0.5955930
H	-3.2216570	-3.6254520	-1.8145970
C	-4.6822800	-1.2776520	0.8881330
H	-2.7943280	-0.2503450	0.8014110
C	-5.4651410	-2.3191080	0.3846240
H	-5.5325780	-3.9737400	-0.9965370
H	-5.0891170	-0.6096970	1.6432050
H	-6.4770070	-2.4712500	0.7496630
H	-1.8570730	-1.8200350	-3.2970590
C	4.1857250	-1.0857830	0.7587540
H	4.1141500	0.0043700	0.7503540
H	3.7456740	-1.4990620	1.6642940
C	5.5936290	-1.5833370	0.4850100
H	6.2770240	-1.1764680	1.2355480
H	5.6202620	-2.6827120	0.5457380
C	5.2164840	-1.6190210	-1.8278350
H	5.6276300	-1.2395210	-2.7671460
H	5.2264880	-2.7197340	-1.8583760
C	3.7935770	-1.1176880	-1.6599910
H	3.0914890	-1.5534330	-2.3673310
H	3.7352920	-0.0266760	-1.6640540
O	3.3386090	-1.5833190	-0.3389750
O	6.0574980	-1.1427840	-0.7836960
H	0.8126190	-1.3717570	-3.4806840
C	1.2585420	2.3418060	0.9511900
C	1.7915750	1.9944410	-0.4291320
C	3.7995900	3.1270130	0.0628640
C	3.2523750	3.4787000	1.4432130
H	1.4189540	1.0247690	-0.7693690
H	1.4889980	1.5191650	1.6463030
H	0.1754920	2.4850570	0.9156580
H	4.8846970	2.9835520	0.0905010
H	3.5671310	3.9383250	-0.6445340
H	3.5802560	2.7154830	2.1703070
H	3.6280220	4.4534520	1.7719270
H	1.4953710	2.7708490	-1.1510260
O	3.2285630	1.9032590	-0.4019860
O	1.8365310	3.5637860	1.4209230
C	-3.6478120	2.1144010	-1.7769860

C	-2.1997740	2.1318040	-1.3041540
C	-2.7982320	3.6135090	0.4266830
C	-4.2441570	3.5847450	-0.0557250
H	-1.7222640	1.1623650	-1.4688940
H	-4.1770930	1.2704440	-1.3095390
H	-3.6999710	2.0040810	-2.8643240
H	-2.7452640	3.7232080	1.5143750
H	-2.2725670	4.4620420	-0.0402120
H	-4.7976470	2.8017400	0.4882990
H	-4.7337950	4.5478050	0.1221050
H	-1.6425140	2.9108150	-1.8494330
O	-2.1364270	2.3915960	0.1032490
O	-4.2983030	3.3445630	-1.4562950

18a

G-gas = -1108.045133 Hartree

Symbol	X	Y	Z
C	-0.4401880	1.7657860	0.5115410
O	-1.0953260	2.5881020	1.1046210
O	0.3779630	2.0476080	-0.5261230
C	0.4687020	3.4530440	-0.8852200
H	-0.5335560	3.8096180	-1.1402270
H	0.8069500	4.0132780	-0.0089540
C	1.4326430	3.5692900	-2.0487700
H	1.0884410	2.9822310	-2.9050220
H	1.5088770	4.6157380	-2.3592600
H	2.4327480	3.2251180	-1.7700430
C	-0.3981850	0.2673510	0.8425130
H	0.0560770	-0.2679640	0.0010840
N	0.4844090	0.0959770	2.0092320
C	-0.2403990	-0.4820020	2.9102430
C	-1.7465260	-0.3135810	1.2229690
C	-1.6081490	-0.7670270	2.4956760
C	-2.9095520	-0.3617330	0.3356420
C	-4.1634780	-0.8026660	0.8013100
C	-2.8036050	0.0287100	-1.0125080
C	-5.2628000	-0.8566710	-0.0483500
H	-4.2777350	-1.0950630	1.8401320
C	-3.9062120	-0.0249100	-1.8623710
H	-1.8517080	0.3759850	-1.4026800
C	-5.1396510	-0.4690480	-1.3854640
H	-6.2206090	-1.1975040	0.3332810
H	-3.8007440	0.2813390	-2.8988180
H	-5.9993250	-0.5101690	-2.0473700
H	-2.3498400	-1.2645650	3.1075950
H	0.1772420	-0.7329670	3.8832840
C	3.3160060	-1.3531570	-0.3001460
O	4.2815010	-2.0741560	-0.3368950
O	2.0751550	-1.7076560	-0.7031260
C	1.9377220	-3.0703080	-1.1824020
H	2.6258400	-3.2156690	-2.0202480
H	2.2407520	-3.7531540	-0.3831090
C	0.4913160	-3.2711070	-1.5884890
H	0.2067630	-2.5769760	-2.3844670
H	0.3506190	-4.2913000	-1.9583490
H	-0.1815770	-3.1199030	-0.7395480
C	3.2794510	0.0832040	0.2171330
H	2.7756880	0.7151490	-0.5215800
H	2.6518310	0.1128710	1.1192010
N	4.5739060	0.5830490	0.4899090
C	5.6546900	0.9897510	0.7189100

TS(18a-18a')

G-gas = -1107.995741 Hartree

Symbol	X	Y	Z
C	1.3834700	1.5805350	-0.1056580
O	2.2825910	1.8217290	-0.8722490
O	0.6012180	2.4624750	0.5142790
C	0.6921180	3.8499060	0.0584530
H	1.7355050	4.1664770	0.1355190
H	0.3827180	3.8621460	-0.9888900
C	-0.2397540	4.6665540	0.9268610
H	0.0436610	4.6084120	1.9818430
H	-0.1977680	5.7148780	0.6160660

H	-1.2678260	4.3152670	0.8121540
C	0.9234990	0.1551890	0.3009820
H	0.8698640	0.1132790	1.3962500
N	-0.4051600	-0.0678750	-0.2632400
C	-0.4074510	-1.1127750	-1.0640970
C	1.7285370	-0.9892000	-0.2756060
C	0.8835580	-1.7166920	-1.0779490
C	3.1296480	-1.2320450	0.0277480
C	3.8422850	-2.2537860	-0.6349530
C	3.8107050	-0.4660990	0.9949030
C	5.1767780	-2.4986770	-0.3383810
H	3.3495190	-2.8504010	-1.3952680
C	5.1463750	-0.7162290	1.2925090
H	3.2963020	0.3302430	1.5220540
C	5.8351470	-1.7323570	0.6281190
H	5.7080330	-3.2864830	-0.8632610
H	5.6510820	-0.1148700	2.0420180
H	6.8783410	-1.9249900	0.8585180
H	1.1217530	-2.6061880	-1.6426250
H	-1.3384630	-1.3830100	-1.5570910
C	-3.7648530	-0.4195670	-0.2602030
O	-3.2539080	-1.1094930	-1.1625840
O	-4.6732280	-0.9710650	0.6190300
C	-4.9631460	-2.3583910	0.4213870
H	-5.3373360	-2.5185790	-0.5959290
H	-4.0441650	-2.9497290	0.5188780
C	-5.9928750	-2.7601560	1.4631700
H	-6.9079000	-2.1711980	1.3511820
H	-6.2485040	-3.8192340	1.3539540
H	-5.6076220	-2.6004880	2.4748010
C	-3.5096980	0.9340550	0.0548180
H	-4.0367130	1.4297320	0.8582250
H	-1.2167030	0.5262200	-0.0912700
N	-2.7592010	1.7177750	-0.7789470
C	-2.0637810	2.3997440	-1.4587080

18b

G-gas = -1507.87024 Hartree

Symbol	X	Y	Z
C	-1.8900760	-0.3131500	-0.2351940
O	-1.6883630	0.5847610	-1.0208050
O	-1.5230270	-1.5910150	-0.4125400
C	-0.7901910	-1.8923380	-1.6375700
H	-1.4609550	-1.7194200	-2.4851250
H	0.0499310	-1.1990540	-1.7129000
C	-0.3336060	-3.3339080	-1.5407250
H	-1.1841330	-4.0135440	-1.4315480
H	0.2081170	-3.6061820	-2.4519810
H	0.3375590	-3.4671490	-0.6879340
C	-2.5862940	-0.1343470	1.1260330
H	-2.6265410	-1.1103140	1.6216970
N	-1.7616210	0.7683200	1.9411140
C	-2.5241500	1.7694480	2.2344590
C	-3.9619970	0.5045640	1.0191110
C	-3.8805800	1.6696820	1.7118890
C	-5.1040150	-0.0817990	0.3148180
C	-6.2967810	0.6459630	0.1353260
C	-5.0435120	-1.3920430	-0.1963320
C	-7.3858680	0.0830310	-0.5204350
H	-6.3650960	1.6644600	0.5037950
C	-6.1361340	-1.9536800	-0.8539920
H	-4.1371490	-1.9777150	-0.0819530
C	-7.3118270	-1.2212350	-1.0174210
H	-8.2945660	0.6636330	-0.6488110
H	-6.0672870	-2.9669510	-1.2383180
H	-8.1628830	-1.6594870	-1.5298570
H	-4.6644580	2.3972640	1.8795600
H	-2.1521060	2.5951620	2.8377030
C	1.5483460	0.8945160	0.0119110
O	1.8687570	0.2945850	-0.9947360
O	1.1636850	2.1668740	0.0715200
C	1.0281210	2.8792760	-1.1919090
H	1.8794590	2.6286030	-1.8268480

H	0.1112720	2.5172360	-1.6653220	H	-1.1167770	-4.0109330	-1.8352520
C	0.9802990	4.3592380	-0.8737380	H	0.2368240	-3.5423790	-2.8811790
H	1.9232700	4.6844960	-0.4267570	H	0.4174290	-3.4604990	-1.1157840
H	0.8245210	4.9259260	-1.7971230	C	-2.3617260	-0.2468340	0.9794430
H	0.1599430	4.5881430	-0.1875890	H	-2.3790250	-1.2401950	1.4388360
C	1.5261860	0.2998250	1.4204750	N	-1.4419910	0.6057150	1.7356610
H	2.3092070	0.7885380	2.0084920	C	-2.1001600	1.6551620	2.1192890
H	0.5463260	0.5073400	1.8697860	C	-3.7010240	0.4576200	1.0502220
N	1.7592850	-1.0979220	1.3942260	C	-3.4949240	1.6120730	1.7468260
C	1.9518300	-2.2550380	1.3365150	C	-4.9342180	-0.0619370	0.4638970
C	5.0666830	-0.0736100	0.0228880	C	-6.1115020	0.7121850	0.4549600
O	4.7016100	0.3845300	1.0804880	C	-4.9768010	-1.3514400	-0.1005730
O	5.5564640	-1.3030000	-0.1723850	C	-7.2875060	0.2120030	-0.0911680
C	5.5859100	-2.1824870	0.9892360	H	-6.1008860	1.7150190	0.8691330
H	6.0793710	-1.6533290	1.8089730	C	-6.1567810	-1.8491200	-0.6476690
H	4.5534590	-2.3904620	1.2825400	H	-4.0845610	-1.9690260	-0.1166460
C	6.3278410	-3.4395850	0.5836670	C	-7.3155440	-1.0718430	-0.6434420
H	7.3539260	-3.2128150	0.2800640	H	-8.1839170	0.8243910	-0.0909890
H	6.3637400	-4.1312010	1.4307710	H	-6.1702410	-2.8459190	-1.0772830
H	5.8219720	-3.9415190	-0.2456350	H	-8.2348370	-1.4609800	-1.0702520
C	5.0096380	0.6548120	-1.3228140	H	-4.2214860	2.3707460	2.0038830
H	5.9324020	0.4699270	-1.8800070	H	-1.6081790	2.4468740	2.6769500
H	4.1721520	0.2271770	-1.8844470	C	1.4140670	0.9346430	-0.1209340
N	4.8010990	2.0455520	-1.1640350	O	1.7007120	0.4015820	-1.1836420
C	4.5975440	3.1938160	-1.0083150	O	1.0867040	2.2397650	-0.0087950

TS(18b-18b')

G-gas = -1507.827906 Hartree

Symbol	X	Y	Z

Symbol	X	Y	Z
C	-1.8127610	-0.3733820	-0.4648750
O	-1.7122340	0.5642240	-1.2193840
O	-1.4530150	-1.6325880	-0.7086630
C	-0.7599900	-1.8772880	-1.9764870
H	-1.4659540	-1.6803220	-2.7890620
H	0.0663700	-1.1661870	-2.0423940
C	-0.2806910	-3.3133290	-1.9443380
C	1.0513240	3.0081650	-1.2347060
H	1.9228690	2.7550370	-1.8412330
H	0.1509620	2.7181580	-1.7866330
C	1.0456120	4.4754570	-0.8524250
H	1.9744820	4.7392080	-0.3403710
H	0.9626890	5.0921990	-1.7531650
H	0.2001190	4.7097860	-0.1981300
C	1.3145140	0.2753210	1.2109890
H	1.9885170	0.7524270	1.9254570
H	-0.1878090	0.4747860	1.6046060
N	1.5766760	-1.1085630	1.1354760

C	1.7319370	-2.2726220	1.0696700	C	6.8784450	1.0696770	0.2227860
C	4.9049180	-0.1206420	0.2167150	C	6.0353320	-1.1620630	-0.1491830
O	4.5305400	0.3490850	1.2646130	C	8.1013370	0.5413290	0.6211560
O	5.3666430	-1.3647820	0.0303690	H	6.7358940	2.1455050	0.2271160
C	5.3446180	-2.2470530	1.1878630	C	7.2612600	-1.6896270	0.2516050
H	5.8176770	-1.7284800	2.0264120	H	5.2401720	-1.8389680	-0.4454820
H	4.3004470	-2.4442480	1.4428520	C	8.2999630	-0.8420600	0.6365910
C	6.0834680	-3.5127320	0.8021580	H	8.9019910	1.2095110	0.9243960
H	7.1224630	-3.2994220	0.5340180	H	7.4041430	-2.7661100	0.2612330
H	6.0811960	-4.2091230	1.6463380	H	9.2551740	-1.2535250	0.9485490
H	5.5985370	-4.0034550	-0.0462200	H	4.8033570	2.9574510	-0.7338120
C	4.9051190	0.6066050	-1.1314560	H	2.2194750	2.9740800	-1.5178450
H	5.8330610	0.3834250	-1.6658490	C	-0.9096380	-0.2566840	0.2059040
H	4.0636560	0.2135070	-1.7118660	O	-0.9439020	-1.3088030	0.8136340
N	4.7542010	2.0058790	-0.9801460	O	-0.8205670	0.9524910	0.7654480
C	4.6046130	3.1633400	-0.8338050	C	-0.6044190	0.9937300	2.2057110

18c

G-gas = -1907.692155 Hartree

Symbol	X	Y	Z
C	2.7578860	-0.8409190	0.2670320
O	2.5302400	-0.3730130	1.3602280
O	2.5459040	-2.1193400	-0.0839260
C	1.9424220	-2.9854500	0.9194450
H	2.7139920	-3.2371380	1.6548010
H	1.1475320	-2.4312070	1.4200570
C	1.4121410	-4.2068710	0.1955330
H	2.2107810	-4.7326280	-0.3360880
H	0.9692700	-4.8979540	0.9198190
H	0.6406250	-3.9193650	-0.5235690
C	3.3008660	-0.0405830	-0.9273120
H	3.4823990	-0.7380090	-1.7525760
N	2.2559240	0.9068540	-1.3424650
C	2.7909770	2.0823130	-1.2660790
C	4.5358450	0.7837300	-0.6062340
C	4.1834240	2.0751610	-0.8313080
C	5.8203430	0.2288370	-0.1743770
H	1.3011740	0.3043690	2.6851440
H	0.4186600	0.6553150	2.3902470
C	-0.8358590	2.4216120	2.6555010
H	-1.8748730	2.7154220	2.4779580
H	-0.6388300	2.5050940	3.7285890
H	-0.1665460	3.1099850	2.1306060
C	-0.9151920	-0.1179930	-1.3122180
H	-1.6966340	0.5846230	-1.6172660
H	0.0591240	0.3059400	-1.5984980
N	-1.1001670	-1.3742290	-1.9414950
C	-1.2415420	-2.4326280	-2.4298480
C	-4.1298390	-2.1361610	0.3315730
O	-4.2463130	-1.1540920	-0.3656280
O	-4.2438100	-3.4030690	-0.0730480
C	-4.4661710	-3.6199040	-1.4993480
H	-5.2987540	-2.9860840	-1.8162090
H	-3.5644530	-3.3074310	-2.0320850
C	-4.7563360	-5.0945840	-1.6885660
H	-5.6501660	-5.3980640	-1.1357010
H	-4.9217030	-5.2989960	-2.7506580

H	-3.9134160	-5.7040610	-1.3517390	N	1.8373750	1.5794710	-0.3515250
C	-3.7958510	-2.1235950	1.8262150	C	2.4374610	2.6816120	-0.7152430
H	-4.3985440	-2.8735520	2.3455740	C	4.1266410	1.1787960	-0.4847050
H	-2.7386770	-2.3932650	1.9200350	C	3.8527590	2.4863530	-0.7977030
N	-4.0002720	-0.8459970	2.4024970	C	5.4174380	0.5006870	-0.4549230
C	-4.1472570	0.2281280	2.8573110	C	6.6155620	1.2433250	-0.4381740
C	-2.8643920	3.4066660	-0.7982310	C	5.4951230	-0.9061870	-0.4515740
O	-2.6081390	2.6769430	-1.7269400	C	7.8475850	0.6009060	-0.4251930
O	-3.9325840	3.3283590	-0.0025820	H	6.5773060	2.3275300	-0.4138070
C	-4.8887700	2.2623890	-0.2987670	C	6.7326300	-1.5441100	-0.4428340
H	-5.1987750	2.3686630	-1.3423240	H	4.5890230	-1.5021450	-0.4616680
H	-4.3854880	1.3002030	-0.1866510	C	7.9106030	-0.7956810	-0.4305460
C	-6.0428180	2.4137840	0.6696250	H	8.7607120	1.1876390	-0.4057500
H	-6.5166390	3.3951930	0.5732320	H	6.7758840	-2.6286700	-0.4478620
H	-6.7932580	1.6465750	0.4555510	H	8.8739720	-1.2963210	-0.4217890
H	-5.7022250	2.2779210	1.6991260	H	4.5565490	3.2552620	-1.0827900
C	-2.0194860	4.6126190	-0.3665130	H	1.8600520	3.5821690	-0.9114260
H	-2.5739620	5.5265210	-0.6084750	C	-1.0255520	0.0078320	0.6656280
H	-1.8920720	4.5864770	0.7192730	O	-0.6554470	-0.9160000	1.4026840
N	-0.7560480	4.6355500	-1.0002090	O	-1.8440640	1.0121680	1.1330370
C	0.2941480	4.6218880	-1.5276900	C	-2.2176210	0.9165680	2.5221040
TS(18c-18c')				H	-2.9643520	0.1242470	2.6421090
G-gas = -1907.652718 Hartree				H	-1.3409250	0.6376500	3.1124500
Symbol	X	Y	Z	C	-2.7791120	2.2600520	2.9517680
C	2.6673510	-0.0752320	1.2434140	H	-3.6541810	2.5279620	2.3519370
O	2.6051630	0.6129480	2.2327830	H	-3.0886080	2.2156220	4.0007530
O	2.5989340	-1.4019610	1.1885040	H	-2.0245990	3.0478630	2.8539240
C	2.2175210	-2.0848290	2.4209940	C	-0.6336320	0.2397950	-0.6927480
H	3.0627340	-2.0385990	3.1148380	H	-1.2543460	0.8580380	-1.3317280
H	1.3704740	-1.5425220	2.8434150	H	0.4344720	1.0508390	-0.4670010
C	1.8445710	-3.5004750	2.0359240	N	0.0521040	-0.7823540	-1.3260090
H	2.6886310	-4.0290450	1.5831580	C	0.7360390	-1.6022730	-1.8325230
H	1.5310710	-4.0517660	2.9279470	C	-3.3914290	-2.8079370	-0.4986470
H	1.0160550	-3.4800900	1.3244550	O	-4.2214440	-2.0531140	-0.9526710
C	2.8075660	0.5065880	-0.1892560	O	-2.5738810	-3.5886630	-1.2140090
H	2.5598180	-0.2892200	-0.9105850	C	-2.6641080	-3.4721860	-2.6611280

H	-3.6096960	-3.9253710	-2.9773130	H	2.5283450	-3.6540180	2.1947590
H	-2.6954610	-2.4119580	-2.9230950	H	1.8934670	-3.5511170	3.8481040
C	-1.4577540	-4.1748840	-3.2494180	H	0.8782790	-3.0312940	2.4841970
H	-1.4299380	-5.2260120	-2.9468460	C	2.2895780	0.6694090	0.1011860
H	-1.5096760	-4.1341150	-4.3422420	H	1.3130790	0.1375990	0.2949260
H	-0.5369140	-3.6828100	-2.9246520	N	1.8461480	2.0322720	0.0071070
C	-3.0819210	-3.0005930	0.9868980	C	2.5940920	2.7284330	-0.8283820
H	-2.9777570	-4.0688530	1.1986210	C	3.4662740	0.6257410	-0.7985210
H	-2.1191120	-2.5117520	1.1973490	C	3.6415250	1.9133510	-1.3011670
N	-4.0854220	-2.4356880	1.8119860	C	4.3818500	-0.4914050	-0.9985050
C	-4.9122670	-1.9328020	2.4801320	C	5.7350620	-0.2541760	-1.3292560
C	-3.3192450	2.9539280	-1.0477690	C	3.9203680	-1.8185010	-0.9213090
O	-2.7977920	2.4912060	-2.0352640	C	6.5935350	-1.3192410	-1.5859850
O	-4.4166830	2.4991960	-0.4434740	H	6.1129270	0.7619600	-1.3580470
C	-5.0020510	1.2828180	-1.0099210	C	4.7896790	-2.8798960	-1.1885290
H	-5.3512180	1.5194080	-2.0196070	H	2.8836040	-2.0152770	-0.6833290
H	-4.2189920	0.5263580	-1.0839340	C	6.1229880	-2.6306640	-1.5213490
C	-6.1257320	0.8387950	-0.0993340	H	7.6314860	-1.1245560	-1.8331140
H	-6.8936880	1.6123050	-0.0032670	H	4.4148810	-3.8967690	-1.1430030
H	-6.5838850	-0.0605080	-0.5197580	H	6.7924000	-3.4653050	-1.7276930
H	-5.7517140	0.5810340	0.8946040	H	4.4165980	2.2384390	-1.9856110
C	-2.8228750	4.2139970	-0.3235280	H	2.3516410	3.7576200	-1.0749730
H	-3.4267740	5.0670330	-0.6539200	C	-0.6761420	-0.4532140	1.0359670
H	-2.9608530	4.0998440	0.7532280	O	-0.9400190	-1.3113290	1.8822890
N	-1.4573440	4.4625670	-0.6076480	O	-0.5182820	0.8886580	1.3827930
C	-0.3171110	4.5925950	-0.8500350	C	-0.7617250	1.2514760	2.7560960

18c'

G-gas = -1907.635899 Hartree

Symbol	X	Y	Z	H	-1.0993550	0.3594160	3.2917870
				H	0.1989560	1.5744240	3.1773530
C	2.5974680	0.2784370	1.6107580	C	-1.7902840	2.3690370	2.8161350
O	2.8167770	1.0390340	2.5205320	H	-2.7572210	2.0315430	2.4272740
O	2.4198000	-1.0415930	1.6933590	H	-1.9358050	2.6877100	3.8566220
C	2.4326830	-1.6522830	3.0196770	H	-1.4594870	3.2385870	2.2463510
H	3.4602060	-1.6202060	3.4009740	C	-0.3895050	-0.6482630	-0.3431960
H	1.8037220	-1.0447190	3.6735920	H	-0.4424040	0.1824770	-1.0401980
C	1.9024800	-3.0641930	2.8706800	H	0.9171620	2.3027800	0.3324260
				N	-0.5113220	-1.9069410	-0.8762930

C	-0.5901210	-2.9900550	-1.3462810	O	2.3596910	-1.1001970	1.6825960
C	-4.0717360	-2.4722400	-0.3699330	C	2.4026230	-1.6940370	3.0117210
O	-4.3683990	-1.6901240	-1.2424430	H	3.4352820	-1.6501030	3.3718990
O	-3.8081500	-3.7723540	-0.5442900	H	1.7803820	-1.0874070	3.6731890
C	-3.7731270	-4.2498250	-1.9238960	C	1.8792100	-3.1090420	2.8779540
H	-4.7966880	-4.2849050	-2.2952590	H	2.5043730	-3.6978090	2.2004630
H	-3.2128980	-3.5229640	-2.5157790	H	1.8838180	-3.5949730	3.8587690
C	-3.0970810	-5.6017060	-1.9113700	H	0.8560310	-3.0879860	2.4952270
H	-3.6259490	-6.3018690	-1.2467710	C	2.3221800	0.6606690	0.1283450
H	-3.1036480	-6.0220890	-2.9221730	H	1.1800910	-0.1067590	-0.2779250
H	-2.0657140	-5.5034280	-1.5788840	N	1.8428440	2.0138550	0.0342880
C	-3.8957180	-2.1399050	1.1164510	C	2.5953220	2.7290920	-0.7841600
H	-4.4323280	-2.8792310	1.7180830	C	3.5538320	0.6761040	-0.7158080
H	-2.8255370	-2.2085010	1.3644870	C	3.6820170	1.9537530	-1.2410090
N	-4.3575480	-0.8355970	1.4253110	C	4.4243240	-0.4671030	-0.9665930
C	-4.7113700	0.2582500	1.6671000	C	5.7732880	-0.2628540	-1.3225730
C	-1.7122710	3.7410940	-1.0734640	C	3.9340340	-1.7869160	-0.9030840
O	-0.7564390	2.9960350	-1.1125530	C	6.6047010	-1.3416710	-1.6004660
O	-2.9873090	3.4008610	-1.1903240	H	6.1727720	0.7460760	-1.3512460
C	-3.2780340	1.9664870	-1.3384570	C	4.7704230	-2.8620530	-1.1914250
H	-2.7618820	1.6230580	-2.2398020	H	2.8959860	-1.9691500	-0.6507520
H	-2.8494100	1.4519800	-0.4768030	C	6.1054340	-2.6457120	-1.5376570
C	-4.7779170	1.8027090	-1.4257340	H	7.6439500	-1.1673860	-1.8619540
H	-5.1829330	2.3342430	-2.2892880	H	4.3739640	-3.8718160	-1.1519130
H	-5.0007440	0.7365600	-1.5248600	H	6.7544450	-3.4877440	-1.7585240
H	-5.2575050	2.1677600	-0.5203050	H	4.4362710	2.2970480	-1.9338380
C	-1.6032090	5.2610280	-0.8694320	H	2.3278450	3.7486230	-1.0378680
H	-2.1337770	5.7729940	-1.6783990	C	-0.6558030	-0.4553870	1.0094000
H	-2.1082120	5.5294440	0.0679120	O	-0.9248650	-1.3108730	1.8566530
N	-0.2483170	5.6678920	-0.8307380	O	-0.5054460	0.8899940	1.3633940
C	0.9086890	5.8769090	-0.8254760	C	-0.7506410	1.2408670	2.7438680

TS(18c'-Pr)

G-gas = -1907.64458 Hartree

Symbol	X	Y	Z
C	2.5130540	0.2195390	1.5953040
O	2.7508710	0.9746790	2.5094240
H	-1.0928750	0.3473920	3.2683560
H	0.2102970	1.5521160	3.1689330
C	-1.7750870	2.3620150	2.8131570
H	-2.7424100	2.0360800	2.4204000
H	-1.9158690	2.6700610	3.8549170

H	-1.4396960	3.2390780	2.2485470
C	-0.3844620	-0.6445350	-0.3759840
H	-0.4621160	0.1840140	-1.0688750
H	0.9082620	2.2567410	0.3529740
N	-0.5275350	-1.9059270	-0.9039430
C	-0.6152680	-2.9922380	-1.3619040
C	-4.0794160	-2.4543290	-0.3731160
O	-4.3770190	-1.6666770	-1.2423110
O	-3.8262670	-3.7545380	-0.5534790
C	-3.7899090	-4.2251360	-1.9295100
H	-4.8186450	-4.2603390	-2.3033610
H	-3.2255760	-3.5033200	-2.5223240
C	-3.1249250	-5.5855290	-1.9223220
H	-3.6520630	-6.2811330	-1.2624860
H	-3.1307810	-6.0007520	-2.9352600
H	-2.0880570	-5.4869610	-1.5929090
C	-3.8996320	-2.1243070	1.1094310
H	-4.4345150	-2.8646240	1.7119840
H	-2.8302900	-2.1923310	1.3536360
N	-4.3572130	-0.8198330	1.4238670
C	-4.7074330	0.2741120	1.6704090
C	-1.6947950	3.7534690	-1.0633360
O	-0.7417110	3.0049860	-1.1099470
O	-2.9708450	3.4186870	-1.1789070
C	-3.2666720	1.9862000	-1.3349810
H	-2.7556690	1.6394820	-2.2368890
H	-2.8419700	1.4657020	-0.4749850
C	-4.7669620	1.8285760	-1.4205820
H	-5.1738870	2.3660180	-2.2823390
H	-4.9936060	0.7637990	-1.5197260
H	-5.2472260	2.1908530	-0.5084970
C	-1.5804330	5.2719230	-0.8513390
H	-2.1072080	5.7900000	-1.6588930
H	-2.0806510	5.5375030	0.0862120
N	-0.2240990	5.6734260	-0.8134140
C	0.9336770	5.8780090	-0.8103730