## Supporting information

# Single Electron Transfer (SET) and Iodine-Atom Transfer Radical Addition (I-ATRA) Induced Cyclopropanation Reaction: Elucidating the Role of Iodine

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# Contents

## I. Computational methodology

All Density Functional Theory (DFT) calculations were conducted using Gaussian 16 (Revision C.01) quantum chemical programs.[1] Geometries were optimised using the hybrid functional B3LYP [2,3] with Grimme's D3 dispersion correction [4,5] using the 6-31+G** basis set[6] for all atoms, except for Br, for which the Stuttgart-Dresden double-ζ (SDD) basis set[7] and for iodine, LANL2DZ[8] along with effective core potential (ECP) was employed. Frequency calculations were also performed with optimisation to ensure the stationary points corresponded to either minima or a transition state. Intrinsic reaction coordinate calculations were conducted on the transition states to confirm their connections to the expected minima.[9] The effect of the solvent was evaluated using the SMD continuum solvation model[10] developed by Cramer and Truhlar in tetrahydrofuran (ε =7.42) solvent using the same functional but a different basis set, def2-TZVPP [11] for all the atoms except for Br and iodine. For those, an SDD and LANL2DZ basis set was employed along with effective core potential (ECP) respectively. Excited-state calculations were performed with the time-dependent DFT (TD-DFT) method. To elucidate the fine electronic features of significant transition states, we have carried out topological analysis of electron density using the atoms in molecule (AIM) formalism.[12]

Activation strain analysis was conducted to understand the contribution of distortion and interaction energies by the participating fragments in the transition states. [13,14] The activation strain energy can be written as the sum of interaction ($\mathbf{\Delta E_{int}}$) and distortion energies ($\mathbf{\Delta E_{dis}}$).

$$\mathbf{\Delta E_{act}^{\ddagger}} = \mathbf{\Delta E_{int}} + \mathbf{\Delta E_{dis}} \quad (1)$$

The component wise distribution to the interaction energy ($\mathbf{\Delta E_{int}}$) was further analysed using the second-generation energy decomposition analysis (EDA), which is based on absolutely localised molecular orbitals (ALMO-EDA)[15-17] using Q-Chem 6.2.[18] The interaction energy between two fragments is dissected according to the following equation.

$$\mathbf{\Delta E_{int}} = \mathbf{\Delta E_{pauli}} + \mathbf{\Delta E_{elstat}} + \mathbf{\Delta E_{pol}} + \mathbf{\Delta E_{ct}} + \mathbf{\Delta E_{disp}} \quad (2)$$

According to equation 2, the interaction energy ($\mathbf{\Delta E_{int}}$) is composed of Pauli repulsion ($\mathbf{\Delta E_{pauli}}$), electrostatic interaction ($\mathbf{\Delta E_{elstat}}$), polarisation ($\mathbf{\Delta E_{pol}}$), charge transfer ($\mathbf{\Delta E_{ct}}$) and dispersion ($\mathbf{\Delta E_{disp}}$ ). Therefore, the activation strain energy can be written as

$$\Delta E^{\ddagger}_{act} = \underbrace{\Delta E_{dis} + \Delta E_{pauli}}_{\text{Steric effects } (\Delta E_{steric})} + \Delta E_{elstat} + \underbrace{\Delta E_{pol} + \Delta E_{ct}}_{\text{Orbital Interactions } (\Delta E_{orbital})} + \Delta E_{disp} \quad (3)$$

The sum of distortion energy ($\mathbf{\Delta E_{dis}}$) and Pauli repulsion ($\mathbf{\Delta E_{pauli}}$) can be considered as the contribution to steric effects ($\mathbf{\Delta E_{steric}}$) while the polarization ($\mathbf{\Delta E_{pol}}$) and charge transfer ($\mathbf{\Delta E_{ct}}$) contributes to the orbital interactions ($\mathbf{\Delta E_{orbital}}$).The ALMO-EDA calculations were performed at the B3LYP-GD3BJ/def2-TZVPP-SDD(Br),SMD (THF) level of theory.

NBO (natural bonding orbital) analysis was carried out using NBO 7.0 software.[19] Spin density plots and NBO plots are generated using Chemcraft software.[20] The non-covalent interactions present in the selective transition states were plotted using interaction region indicator analysis [21] by Multiwfn version 3.8(dev).[22] IRI isosurfaces were rendered by visual molecular dynamics (VMD) software.[23] The discussion in the manuscript is presented on the basis of the Gibbs free energies obtained at 298.15 K.

## II. Estimation of activation barrier for the electron transfer process

Marcus-Hush theory was used to estimate the activation barrier for the single electron transfer (SET) process.[24-30] A detailed procedure is given below.

$$\Delta G^{\ddagger} = \frac{(\Delta G_r + \lambda)^2}{4\lambda} \quad (4)$$

$\Delta G^{\ddagger}$ = Activation energy barrier

$\Delta G_r$ = Free energy change for the SET process

$\lambda$ = Total reorganisation energy for the SET process

Total reorganization energy ($\lambda$) has two components, internal reorganization energy ($\lambda_{in}$) and solvent reorganisation energy ($\lambda_s$).

$$\lambda = \lambda_{in} + \lambda_s \quad (5)$$

Internal reorganization energy was estimated using the Nelsen four-point method.[31,32] A schematic diagram for the method is given below.

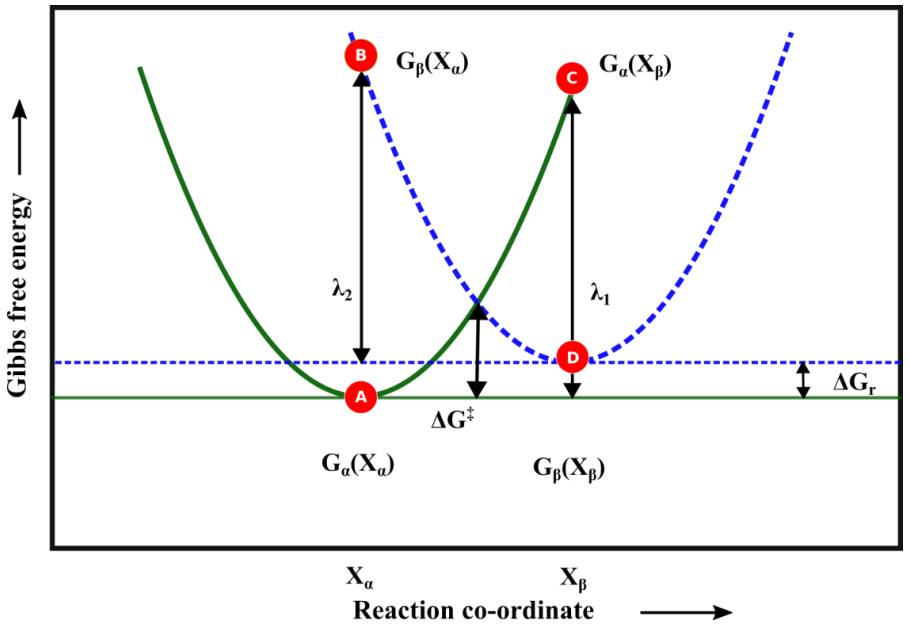



**Fig. S1.** Schematic representation of Nelsen four-point method.

$G_\alpha(X_\alpha)$ = Sum of Gibbs free energies of reactants in equilibrium geometries.

$G_\beta(X_\beta)$ = Sum of Gibbs free energies of products in equilibrium geometries.

$G_\alpha(X_\beta)$ = Sum of Gibbs free energies of reactants in products geometries.

$G_\beta(X_\alpha)$ = Sum of Gibbs free energies of products in reactants geometries.

$$\Delta G_r = G_\beta(X_\beta) - G_\alpha(X_\alpha) \quad (6)$$

$$\lambda_1 = G_\alpha(X_\beta) - G_\alpha(X_\alpha) \quad (7)$$

$$\lambda_2 = G_\beta(X_\alpha) - G_\beta(X_\beta) \quad (8)$$

For calculating $\lambda_{in}$ , arithmetic mean is widely applied [33]

$$\lambda_{in} = \frac{\lambda_1 + \lambda_2}{2} \quad (9)$$

The solvent contribution to the total reorganization energy is given by,

$$\lambda_s = (332 \text{ kcal mol}^{-1}) \left(\frac{1}{2r_D} + \frac{1}{2r_A} - \frac{1}{r_{DA}}\right)\left(\frac{1}{\varepsilon_{op}} - \frac{1}{\varepsilon_s}\right) \quad (10)$$

$\varepsilon_{op}$ and $\varepsilon_s$ are optical and static dielectric constants of solvent (THF) ($\varepsilon_{op}$= 1.97 and $\varepsilon_s$= 7.42). $r_D$, $r_A$, and $r_{DA}$ are hard-sphere radii of electron donor and acceptor species and distance between them ($r_{DA} = r_D + r_A$).

Finally, substituting the values of $\lambda$ and $\Delta G_r$ in equation (4) we can calculate the barrier for the single electron transfer process.[34]

**Table S1:** Calculated parameters for the calculations of SET barriers

| | $\lambda_{in}$ (kcal mol$^{-1}$) | $\lambda_s$ (kcalmol$^{-1}$) | $\Delta G_r$ (kcal mol$^{-1}$) | $r_A$ (Å) | $r_D$ (Å) | $\Delta G^{\ddagger}$(kcal mol$^{-1}$) |
|---|---|---|---|---|---|---|
| SET-1 | 7.3 | 10.1 | 18.1 | 6.0 | 6.4 | 18.1 |
| SET-2 | 15.7 | 15.7 | -56.7 | 3.3 | 6.0 | 5.2 |
| SET-1a | 14.8 | 14.3 | 13.2 | 6.0 | 3.7 | 15.4 |
| SET-3 | 10.9 | 10.1 | 42.3 | 6.4 | 6.0 | 47.8 |

**III. Formation of Hantzsch ester radical anion by SET**

A single electron transfer mechanism (**SET-3**) was evaluated, leading to the generation of the Hantzsch ester radical anion and the PLY(N,O) radical cation (Fig. S2). This pathway was found to be unfavourable due to its high energy barrier of 47.8 kcal mol$^{-1}$ (with respect to the intermediate **2**).

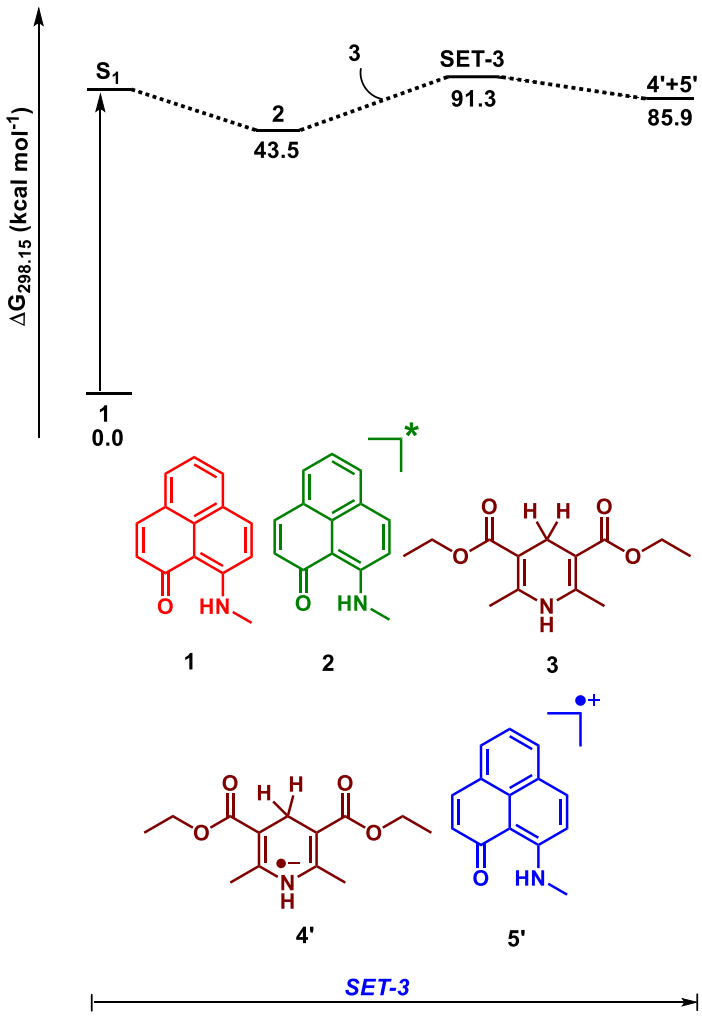



**Fig. S2.** Computed Gibbs free energy profile diagram for the **SET-3**

## IV. TD-DFT calculation on the diazo acetate molecule

It was observed that the dissociation of the nitrogen molecule in the diazoacetate molecule **6** takes place during the electronic transition from the orbitals 29 (HOMO-1) to 31 (LUMO) with a percentage contribution of 70.1% in the triplet excited state **3** (**T3**) (Table S2). The careful analysis of the Kohn-Sham molecular orbitals suggests that this level populates the nitrogen's antibonding orbital (π*) and thereby its release (Fig. 2a). Since the energy corresponds to this transition, **T3** (111.3 kcal $mol^{-1}$) is higher than the energy emitted by the PLY catalyst during its relaxation from the triplet state (43.5 kcal $mol^{-1}$) to the $S_0$, the energy transfer mechanism will not take place. Instead, a single electron transfer (**SET-1**), which is suggested in Fig. 1a, will occur.

**Table S2.** The four lowest triplet excited states of the diazoacetate molecule **6** obtained from TD-DFT calculation.

| Excited state | E (kcal $mol^{-1}$) | λ nm | Electronic transitions | Percentage contribution (%) |
|---|---|---|---|---|
| 1 | 61.9 | 461.80 | 30 → 31 | 70.4 |
| 2 | 74.7 | 382.94 | 30 → 32<br>30 → 34<br>30 ← 32 | 70.2<br>0.0<br>10.2 |
| 3 | 111.3 | 256.90 | 29 → 31 | 70.1 |
| 4 | 114.2 | 250.39 | 29 → 32<br>29 → 34 | 68.7<br>15.7 |

## V. PCET process involving deprotonation from the C4 position of Hantzsch ester

In **PCET-A**, a proton from the C4 position of Hantzsch ester radical cation **4** and an electron from the PLY radical anion **5** will be transferred to the diazoacetate **6** in a concerted manner. Instead of the PCET mechanism, we have looked into the energetics of the stepwise pathways that include either the proton transfer (PT) followed by the electron transfer (ET) or ET followed by the PT (Fig. S3). From the square scheme (Fig. S3), it is clearly evident that the PCET mechanism is more favorable compared to the stepwise mechanisms.

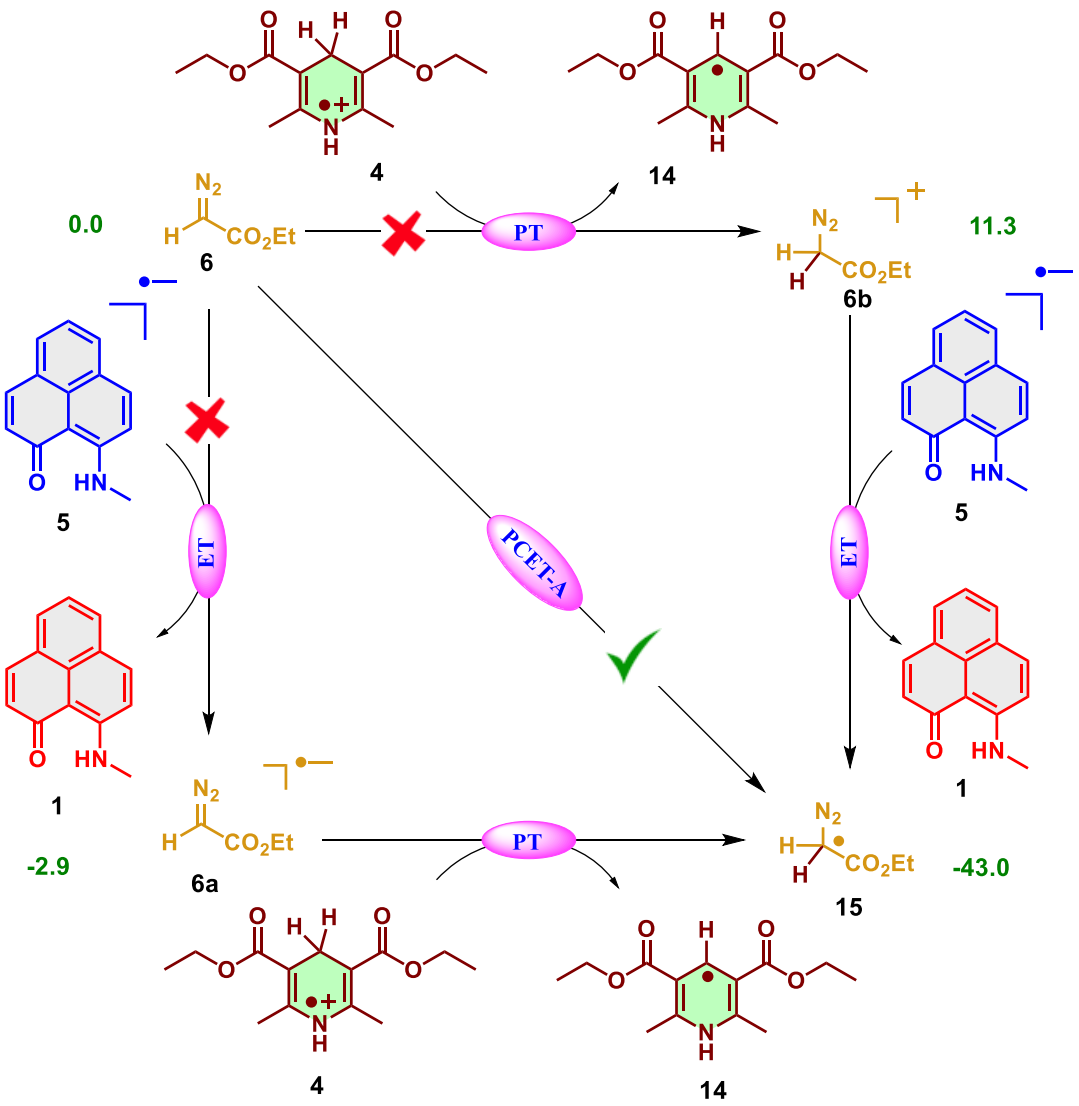



**Fig. S3.** Square scheme showing the energetics of stepwise reactions and **PCET-A**. The Gibbs free energies provided in kcal $mol^{-1}$ are with respect to the separated species involved in these steps.

## VI. PCET process involving deprotonation of the N-H proton of Hantzsch ester

The other possible mechanism for the transformation of the diazoacetate **6** to protonated diazoacetate radical **15** is depicted in Fig. S4 through **PCET-C**. Here the deprotonation occurs from the N-atom of the Hantzsch ester radical cation **4**. Even though the **PCET-C** is more favorable than **ET-1** followed by **PT-1** as well as **PT-1** followed by **ET-1** (Fig. S4), it clearly shows that the PCET process

given in Fig. S3 is more energetically feasible. This is reflected in the subsequent steps after the **PCET-C** as well (Fig. S5).

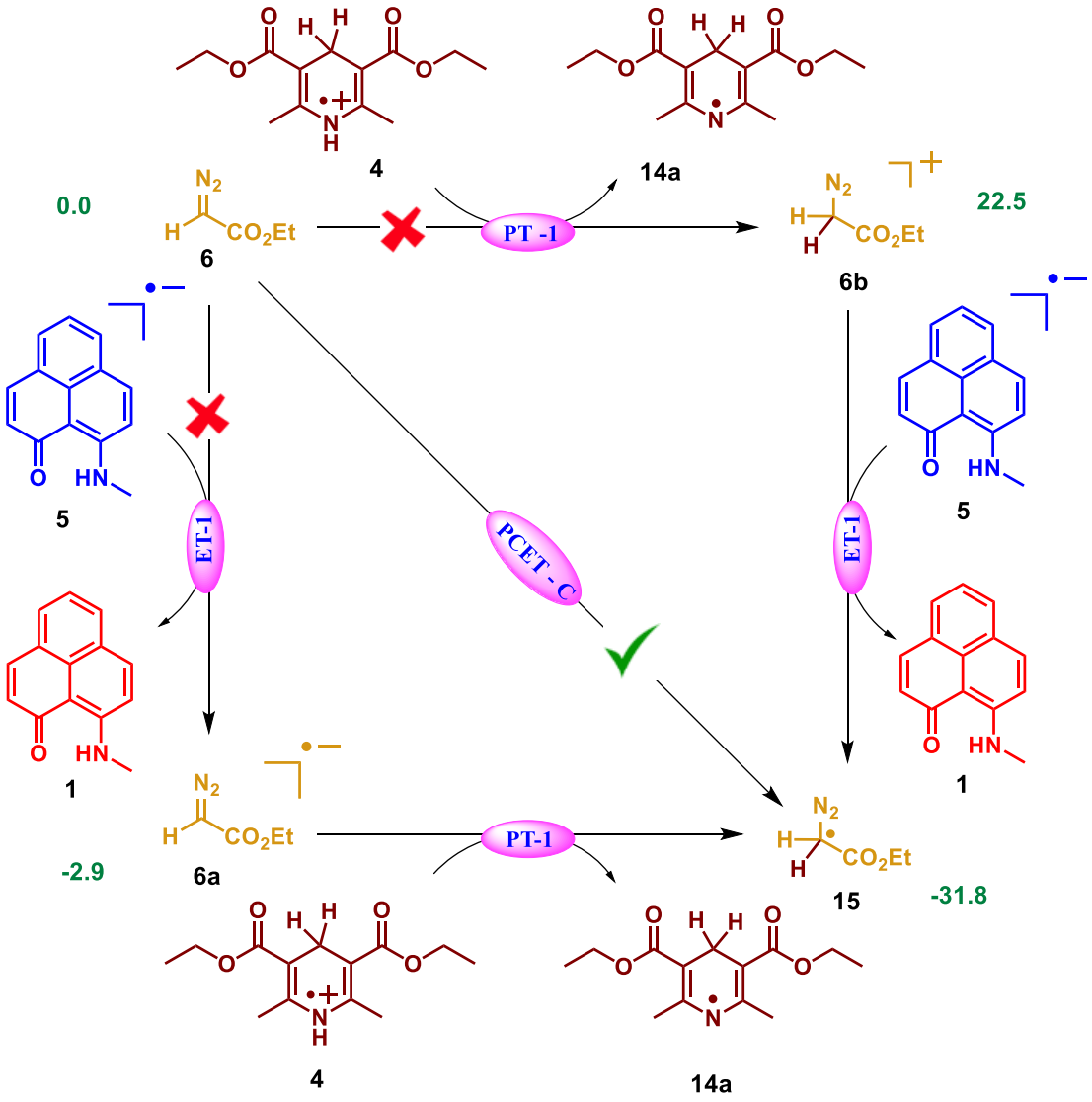



**Fig. S4.** Square scheme showing the energetics of stepwise reactions and **PCET-C**

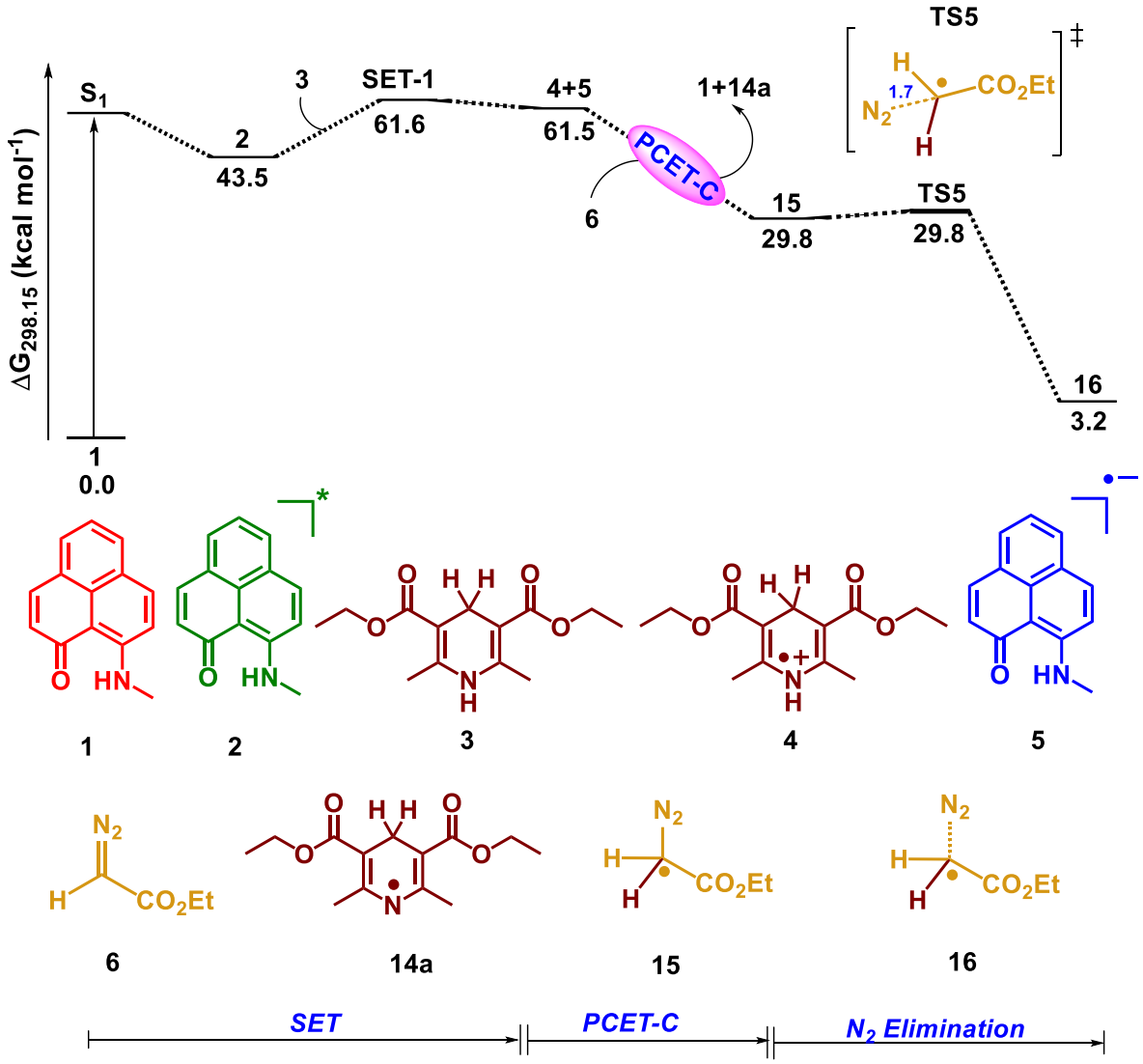



**Fig. S5.** Computed Gibbs free energy profile diagram involving **PCET-C** process and subsequent $N_2$ elimination step

## VII. Single Electron Transfer process (SET) from iodine radical anion to the triplet PLY (N,O) species

After the generation of $I_2$ radical anion in the first cycle, it will transfer an electron to the triplet PLY (N,O) species **2** via **SET-1a** with an energy barrier of 15.4 kcal $mol^{-1}$ and therefore initiates the next catalytic cycle (Fig. S6). This particular barrier is found to more favorable than the **SET-1** (Fig. 1a),

where the Hantzsch ester **3** acts as an electron donor to the triplet PLY (N,O) species **2**. Therefore, once the iodine radical anion is generated, it will be the preferred electron donor to the PLY system.

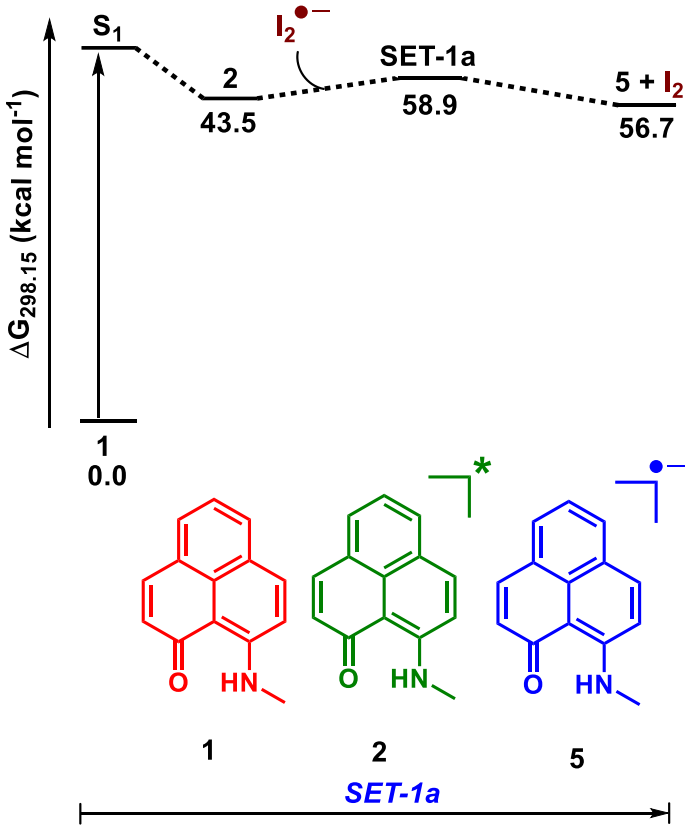



**Fig. S6.** Computed Gibbs free energy profile diagram for the **SET-1a**

## VIII. Formation of Hantzsch pyridine in the cyclopropanation reaction

After the completion of the reaction, Hantzsch ester radical cation **4** which was generated in the first cycle will get converted to Hantzsch pyridine with the assistance of iodine radical anion. This involves two steps. Initially a hydrogen atom transfer (HAT) will take place from the C4 position of species **4** to the iodine radical anion, leading to the formation of intermediate **16a** (Fig. S7). This step proceeds via the transition state **TS5a**, which has an energy barrier of 1.3 kcal $mol^{-1}$ (with respect to the stable intermediate **15a**. After the elimination of HI, the iodide ion abstracts a proton from the nitrogen atom, resulting in the formation of Hantzsch pyridine and another HI molecule (**17a**).

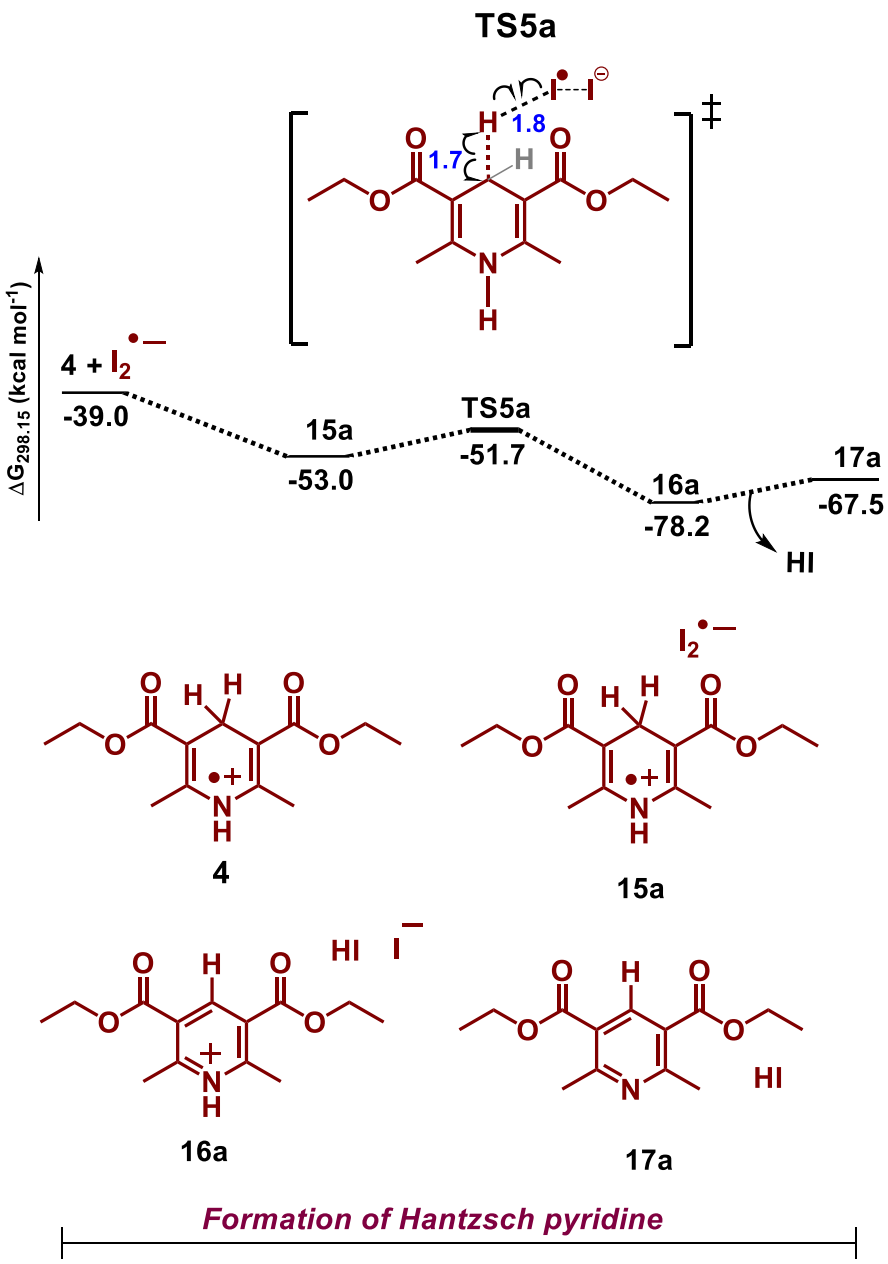



**Fig. S7.** Computed Gibbs free energy profile diagram for the formation of Hantzsch pyridine in the cyclopropanation reaction.

## IX. Regioselective Markovnikov radical addition in the cyclopropanation reaction

The possible Markovnikov radical addition transition state for the formation of the radical intermediate **11m** was considered (**TS3m**) (Fig. S8) instead of the anti-Markovnikov transition state **TS3** (Fig. 1a) for the cyclopropanation reaction. The estimated energy barriers for this transition state via Markovnikov

radical addition were found to be higher than the anti-Markovnikov transition state **TS3** by 7.8 kcal mol$^{-1}$. Hence this pathway was not considered for further mechanistic studies (Fig. S8).

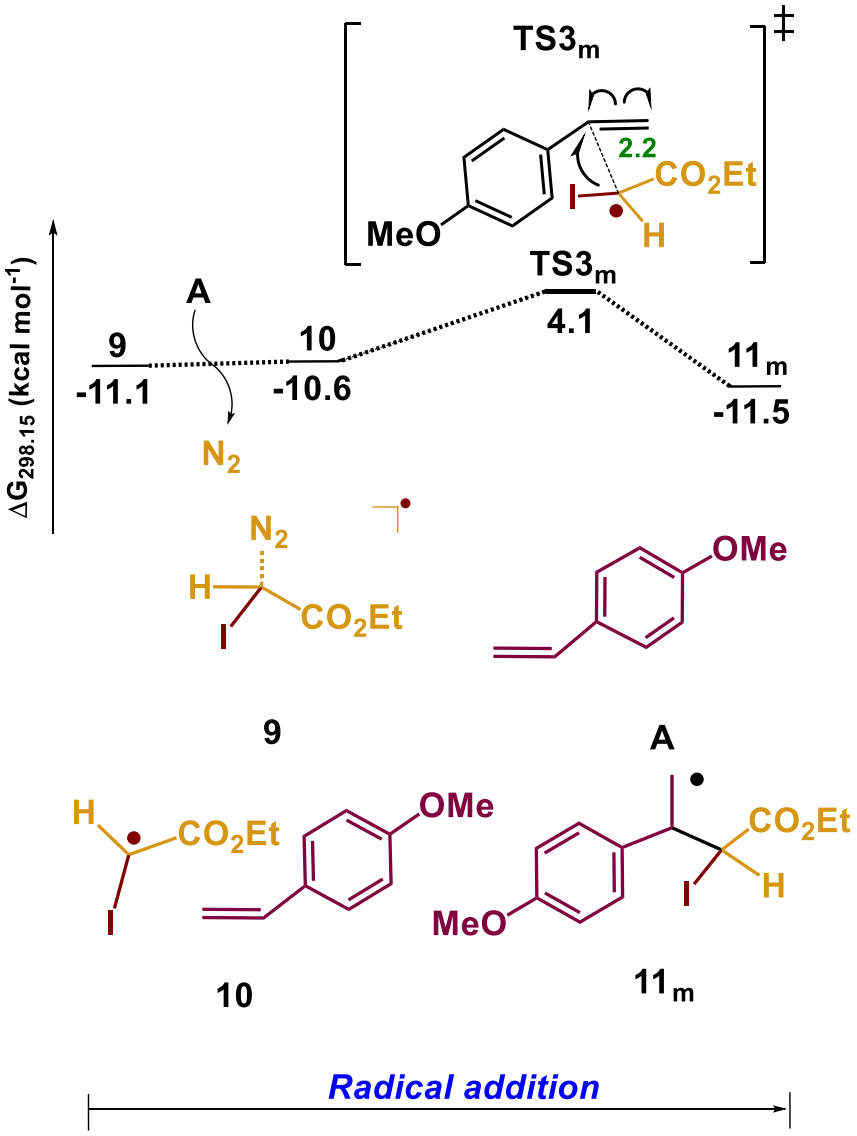



**Fig. S8.** Computed Gibbs free energy profile diagram for the possible Markovnikov radical addition in the cyclopropanation reaction.

### X. Hydroalkylation reaction involving propene and diazoacetate

The anti-Markovnikov radical addition and Markovnikov radical addition transition states **TS6b** and **TS6c** for the hydroalkylation reaction between propene (as the olefinic substrate) and diazoacetate were studied in order to analyse the effect of the substituent in the olefin (Fig. S9). The energy barrier for the

anti-Markovnikov radical addition transition state **TS6b** for the formation of **18a** was found to be 3.1 kcal $mol^{-1}$ more stable than the Markovnikov radical addition transition state **TS6c** for the formation of **18b**. This trend is the same as **TS6** and **TS6b,** where the styrene is the olefinic substrate (Fig. 3a).

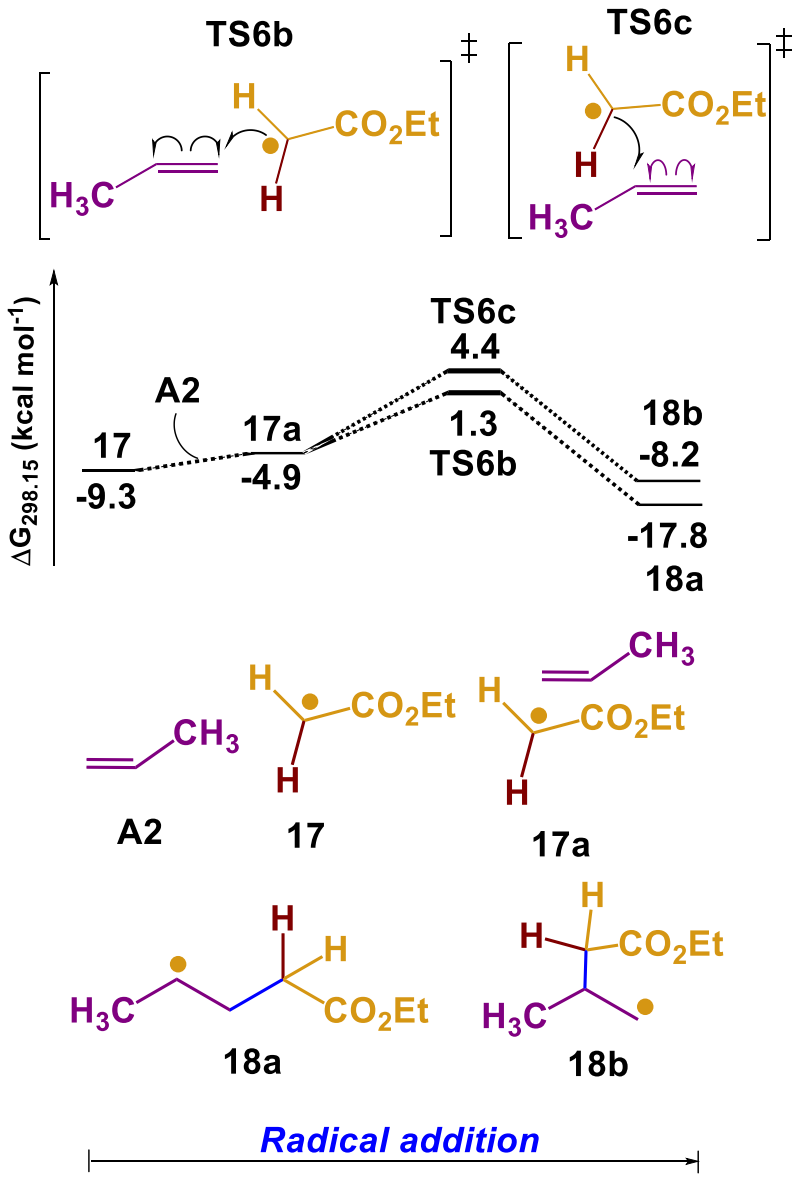



**Fig. S9:** Computed Gibbs free energy profile diagram for the AMRA and MRA transition states between propene and diazoacetate.

## XI. AIM analysis

A comprehensive study on the non-covalent interactions present in the transition states **TS6** and **TS6b** and their corresponding Markovnikov radical addition transition states **TS6a** and **TS6c** has been conducted using the AIM analysis. The topological maps obtained through AIM analysis were carefully analysed to identify the bond paths that correspond to weak non-covalent interactions in the radical addition transition states **TS6, TS6a, TS6b, TS6c** (Fig. 4a). The bond critical points correspond to the non-covalent interactions that were only found in the anti-Markovnikov transition states **TS6,** and **TS6b** and were absent in the Markovnikov transition states.[35] The quantification of these NCIs (non-covalent interactions) was carried out using the Espinosa formulation (Table S3), which is built on the topological parameters of the electron density approximation.[36]

**Table S3:** Estimated strengths of the important noncovalent interactions in the transition state **TS6** and **TS6b**

| **Transition states** | **ρ** | **$\nabla^2$ ρ** | **G** | **V=1/4$\nabla^2$ ρ-2G ($E_h$)** | **E=1/2(V) (kcal $mol^{-1}$)** |
|---|---|---|---|---|---|
| **TS6** | | | | | |
| 1. π(Phenyl)---H-C | 0.004 | -0.003 | 0.003 | -0.006 | -1.852 |
| 2. π(Phenyl)---H-C | 0.005 | -0.005 | 0.004 | -0.009 | -2.800 |
| 3. π(Phenyl)---O | 0.005 | -0.004 | 0.003 | -0.008 | -2.433 |
| **TS6b** | | | | | |
| 1. C-H--O | 0.005 | -0.005 | 0.004 | -0.009 | -2.882 |

## XII. Activation strain analysis

More insights into the additional stability of the transition state **TS6** are sought by employing activation strain analysis. The activation strain analysis was performed to calculate the extent of distortion ($E_{dis}$) and interaction energies ($E_{int}$) in the transition states **TS6, TS6a, TS6b,** and **TS6c**.

The activation strain energy ($E_{act}^{\ddagger}$) can be written as the sum of distortion ($\Delta E_{dis}$) and interaction energies ($\Delta E_{int}$).[37]

$$\Delta E^{\ddagger}_{act} = \Delta E_{int} + \Delta E_{dis} \quad (11)$$

For this analysis, at first, seven different points were selected from the reaction profile obtained from IRC calculations (Fig. S10a). The corresponding structures were made into two fragments: one acetate radical part and one alkene part. Single-point computations were carried out on those structures (Fig. S10b). The IRC points toward the product side (P1, P2, P3), and the reactant side (R1, R2, R3) along the reaction coordinate is shown in Fig. S10a. $\Delta E_{dis}$ and $\Delta E_{int}$ of the structures in each point are calculated.

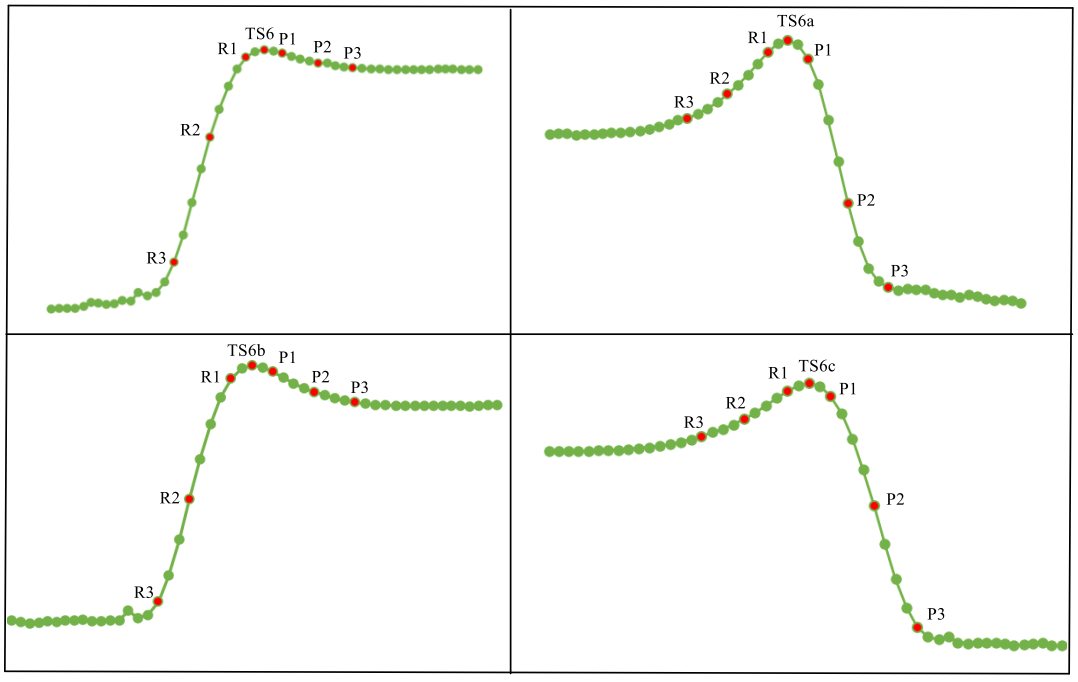
Equations used for calculating distortion energies and interaction energies are given below.[38]

$$\Delta E^{\ddagger}_{dis} = [\{ E_{f2(TS)} + E_{f1(TS)}\} - \{E_{f2} + E_{f1}\}] \quad (12)$$

$$\Delta E^{\ddagger}_{int} = \{ E_{(TS)} - (E_{f1(TS)} + E_{f2(TS)})\} \quad (13)$$

Where $E_{f1(TS)}$ is the single point energy of f1 fragment in the transition state, $E_{f2(TS)}$ is the single point energy of the f2 fragment in transition state, $E_{f1}$ is the single point energy of f1 fragment in the intermediates, and $E_{f2}$ is the single point energy of the f2 fragment in the intermediates.

**a)**



**b)**

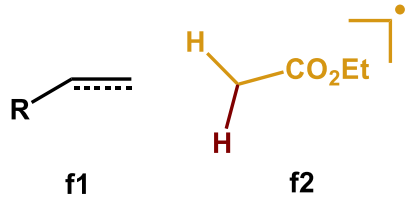



**Fig. S10.** a) The reaction profile along the intrinsic reaction coordinate (IRC) trajectory for **TS6, TS6a, TS6b,** and **TS6c**; b) Fragments f1 and f2 used for the calculation

From Table S4, it is noted that the total distortion energy, which has a destabilizing effect, is smaller for AMRA transition states **TS6** and **TS6b** compared to MRA transition states **TS6a** and **TS6c**. At the same time, the total interaction energy is stabilizing for both AMRA transition states **TS6** and **TS6b,** which in turn reduces the activation strain energy. In the case of MRA transition states **TS6a** and **TS6c**, the total interaction energy is lower compared to the AMRA transition states, and this increases their respective activation strain energy. This trend can be seen along the IRC path of these transitions. Since the activation strain energy is lower in the AMRA transition states compared to MRA transition states, the AMRA mechanism is more favorable.

**Table S4:** Relative distortion and interaction energies (in kcal $mol^{-1}$) for **TS6, TS6a, TS6b,** and **TS6c**

| Transition states | Distortion energy ($E_{dis}$) | | Total Distortion energy | Interaction Energy (Ei) | Activation Strain Energy |
|---|---|---|---|---|---|
| | **f1** | **f2** | **f1+f2** | | |
| **TS6** | 1.30 | 1.85 | 3.14 | -6.81 | -3.66 |
| P1 | 0.51 | 0.60 | 1.11 | -4.77 | -3.66 |
| P2 | 0.06 | 0.04 | 0.10 | -3.76 | -3.66 |
| P3 | 0.02 | 0.01 | 0.03 | -3.70 | -3.66 |
| R1 | 2.66 | 4.37 | 7.03 | -10.69 | -3.66 |
| R2 | 7.06 | 15.49 | 22.55 | -26.21 | -3.66 |

| | | | | | |
|---|---|---|---|---|---|
| R3 | 12.13 | 26.74 | 38.87 | -42.53 | -3.66 |
| **TS6a** | 2.22 | 4.64 | 6.86 | -3.31 | 3.55 |
| P1 | 4.31 | 10.19 | 14.50 | -10.95 | 3.55 |
| P2 | 9.75 | 26.13 | 35.88 | -32.33 | 3.55 |
| P3 | 12.51 | 32.05 | 44.56 | -41.01 | 3.55 |
| R1 | 0.85 | 11.65 | 12.50 | -8.95 | 3.55 |
| R2 | -0.01 | 0.37 | 0.35 | 3.19 | 3.55 |
| R3 | -0.03 | 0.16 | 0.13 | 3.42 | 3.55 |
| **TS6b** | 1.90 | 2.58 | 4.48 | -4.57 | -0.09 |
| P1 | 0.79 | 0.78 | 1.57 | -1.66 | -0.09 |
| P2 | 0.11 | 0.09 | 0.20 | -0.29 | -0.09 |
| P3 | 0.04 | 0.02 | 0.06 | -0.15 | -0.09 |
| R1 | 3.72 | 2.58 | 6.30 | -6.39 | -0.09 |
| R2 | 8.89 | 19.52 | 28.41 | -28.50 | -0.09 |
| R3 | 13.13 | 29.39 | 42.52 | -42.61 | -0.09 |
| **TS6c** | 2.15 | 4.51 | 6.67 | -3.15 | 3.52 |
| P1 | 3.92 | 8.81 | 12.74 | -9.21 | 3.52 |
| P2 | 8.67 | 22.74 | 31.42 | -27.89 | 3.52 |
| P3 | 13.06 | 34.91 | 47.97 | -44.45 | 3.52 |

| | | | | | |
|---|---|---|---|---|---|
| R1 | 0.99 | 2.02 | 3.01 | 0.51 | 3.52 |
| R2 | 0.18 | 0.54 | 0.72 | 2.80 | 3.52 |
| R3 | 0.11 | 0.16 | 0.28 | 3.25 | 3.52 |

**XIII. Substitutions for styrene – EDA analysis**

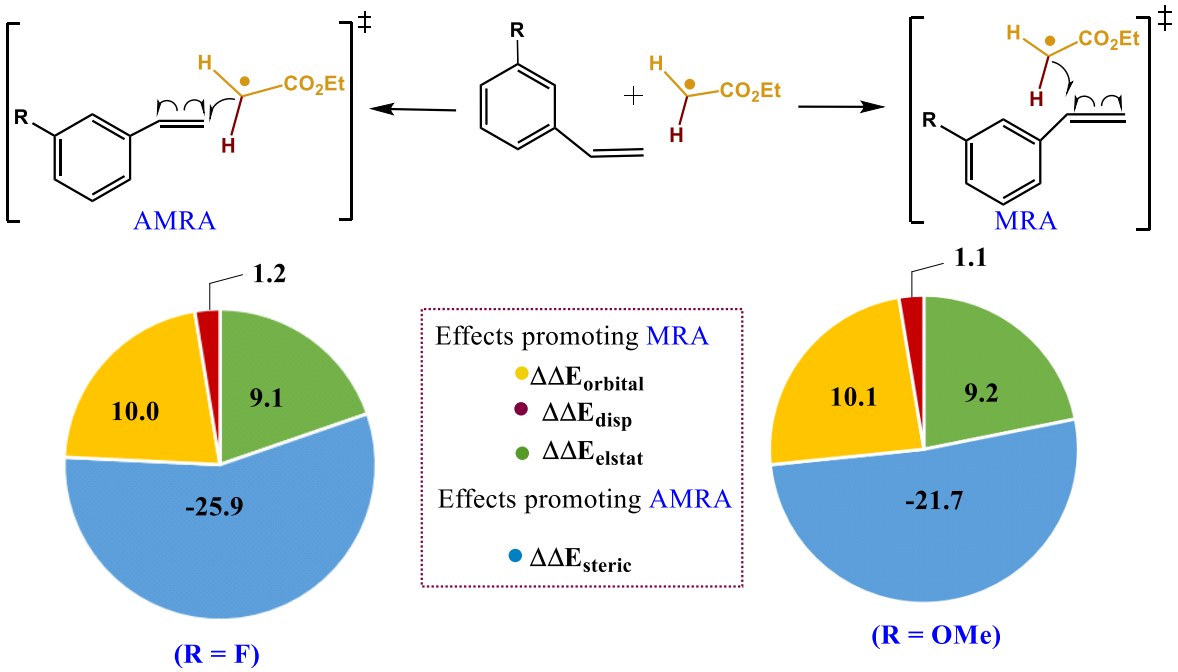
The substrate scope for the radical addition transition states **TS6** and **TS6a** was evaluated with substitutions on para, meta, and ortho positions of styrene. In all the substitutions, the Markovnikov radical addition transition states (MRA) are having a higher energy. The stability of the anti-Markovnikov radical addition (AMRA) is attributed to the formation of a stable secondary radical rather than a primary radical, which is generated after the Markovnikov addition. The details are given in the Table S5.

**Table S5**. Computed Gibbs free energy barriers with respect to the separated reactants, for anti-Markovnikov **(TS6)** and Markovnikov C-C (**TS6a)** radical addition transition states with different substitutions on styrene.

| Substitutions | Substitutions | Anti-Markovnikov Addition (**TS6**) | Markovnikov Addition (**TS6a**) |
|---|---|---|---|
| 1. Para position **TS6/6a** $_{\textbf{para}}$ | a). Fluorine | 10.3 | 16.9 |
| | b). Bromine | 10.1 | 16.9 |
| | c). Methoxy | 9.8 | 17.0 |
| | d). Methyl | 10.0 | 16.6 |
| 2. Meta position **TS6/6a** $_{\textbf{meta}}$ | a). Fluorine | 10.2 | 16.5 |
| | b). Methoxy | 10.2 | 16.4 |
| 3. Ortho position **TS6/6a** $_{\textbf{ortho}}$ | a). Chlorine | 9.5 | 19.0 |
| | b). Methyl | 10.4 | 18.8 |

In both meta- and ortho- substituted cases (Fig. S11), EDA analysis shows that the steric repulsions ($\Delta\Delta E_{steric}$) are the major effect that promotes the anti-Markovnikov radical addition, while orbital interactions ($\Delta\Delta E_{orbital}$), electrostatics ($\Delta\Delta E_{elstat}$), and dispersions ($\Delta\Delta E_{disp}$) promote Markovnikov addition. Since the sum of $\Delta\Delta E_{steric}$ is greater than $\Delta\Delta E_{orbital}$, $\Delta\Delta E_{elstat}$, and $\Delta\Delta E_{disp}$ the anti-Markovnikov addition is preferred. In the ortho methyl substituted case, $\Delta\Delta E_{disp}$ along with $\Delta\Delta E_{steric}$ are promoting the anti-Markovnikov transition state.

a)


AMRA
MRA
1.2
10.0
9.1
-25.9
(R = F)
Effects promoting MRA
ΔΔE orbital
ΔΔE disp
ΔΔE elstat
Effects promoting AMRA
ΔΔE steric
1.1
10.1
9.2
-21.7
(R = OMe)

b)

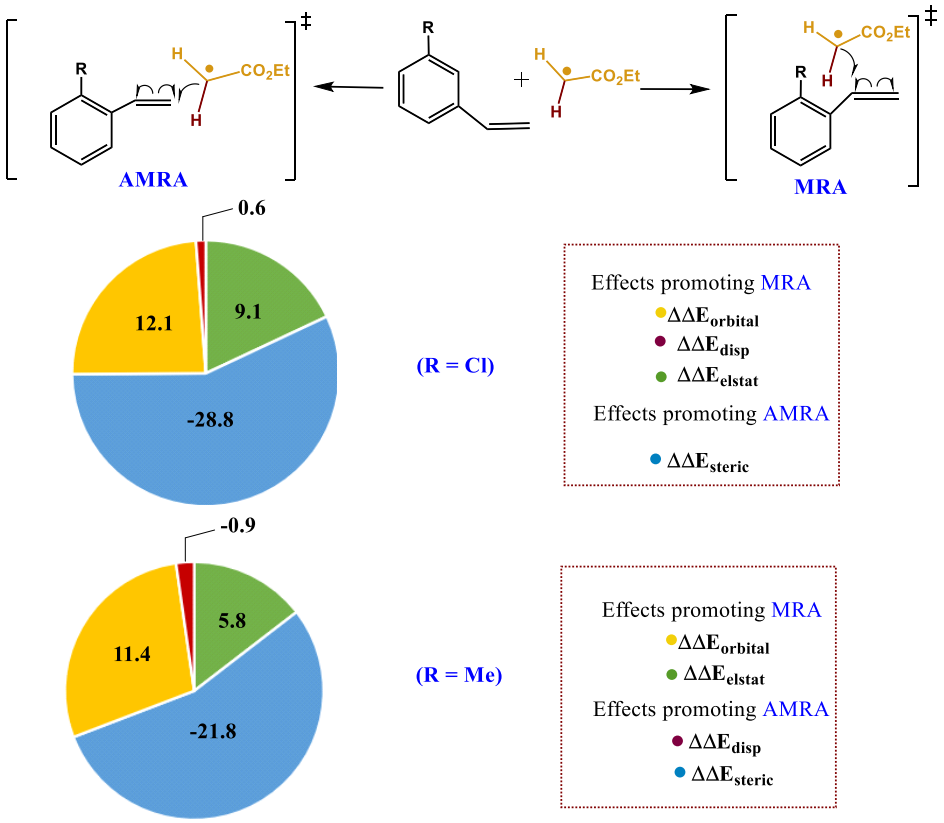

AMRA
MRA
0.6
12.1
9.1
-28.8
(R = Cl)
Effects promoting MRA
ΔΔE orbital
ΔΔE disp
ΔΔE elstat
Effects promoting AMRA
ΔΔE steric
-0.9
11.4
5.8
-21.8
(R = Me)
Effects promoting MRA
ΔΔE orbital
ΔΔE elstat
Effects promoting AMRA
ΔΔE disp
ΔΔE steric

**Fig. S11**. Contribution of different types of interactions obtained from the EDA for a) meta-substituted styrene and b) ortho-substituted styrene. Each component ($\Delta\Delta E_{orbital}$, $\Delta\Delta E_{disp}$, $\Delta\Delta E_{elstat,}$ and $\Delta\Delta E_{steric}$) is calculated from the energy difference between anti–Markovnikov (AMRA) and Markovnikov (MRA) transition states. Positive values indicate that the effect is promoting Markovnikov addition, while the negative values indicate the ones that are promoting anti–Markovnikov transition state.

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## XV. Cartesian coordinates of the optimized geometries

**1**

SCF Energy (a.u.) = -670.454164

Thermal correction to Gibbs free energy (a.u.) = 0.177715

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.60331600 | -0.55093300 | 0.00000000 |
| C | 0.52976100 | 0.39258000 | -0.00000600 |
| C | 0.79560900 | 1.83070200 | -0.00000900 |
| C | 1.29970800 | -1.95283500 | 0.00001600 |
| C | -0.81285600 | -0.08188600 | -0.00000700 |
| C | -1.09462200 | -1.48195500 | -0.00000100 |
| C | 0.00406400 | -2.39017200 | 0.00001400 |
| C | -2.43074400 | -1.93175600 | -0.00000700 |
| H | -2.62354900 | -3.00125700 | -0.00000200 |
| C | -3.48664300 | -1.03016400 | -0.00001700 |
| C | -3.22117000 | 0.34517100 | -0.00001900 |
| C | -1.91116400 | 0.83380900 | -0.00001400 |
| C | -1.63066000 | 2.24592000 | -0.00000600 |
| C | -0.35909900 | 2.72023800 | 0.00000700 |
| H | -0.14296000 | 3.78341700 | 0.00002800 |
| H | -2.47265400 | 2.93424200 | -0.00000100 |
| H | 2.11076700 | -2.67081500 | 0.00002000 |
| H | -0.20330500 | -3.45707500 | 0.00002100 |

| | | | |
|---|---|---|---|
| H | -4.51144500 | -1.38644200 | -0.00002000 |
| O | 1.96042900 | 2.31060400 | 0.00007500 |
| C | 4.04507100 | -0.98105300 | -0.00001300 |
| H | 4.08039300 | -1.62187600 | 0.89018500 |
| H | 4.08036400 | -1.62193000 | -0.89017400 |
| H | 4.93417000 | -0.34889900 | -0.00004700 |
| H | -4.04443100 | 1.05472100 | -0.00002300 |
| N | 2.87988900 | -0.12242500 | -0.00002200 |
| H | 2.96656500 | 0.90206200 | -0.00006100 |

**2**

SCF Energy (a.u.) = -670.379843

Thermal correction to Gibbs free Energy (a.u.) = 0.172656

Charge = 0, Multiplicity = 3

| | | | |
|---|---|---|---|
| C | 1.62114500 | -0.56823900 | -0.00000600 |
| C | 0.51983300 | 0.39712700 | -0.00004100 |
| C | 0.75152700 | 1.85110700 | -0.00006800 |
| C | 1.33651900 | -1.94637400 | 0.00003800 |
| C | -0.80652500 | -0.08776700 | -0.00003700 |
| C | -1.07177600 | -1.50959600 | -0.00001500 |
| C | 0.03236300 | -2.40657500 | 0.00002700 |
| C | -2.40004200 | -1.96115400 | -0.00001500 |
| H | -2.59714600 | -3.02842700 | 0.00000400 |
| C | -3.47245100 | -1.04513400 | -0.00002900 |
| C | -3.25044500 | 0.31855300 | -0.00003100 |
| C | -1.92289200 | 0.83384600 | -0.00003800 |
| C | -1.67415500 | 2.23064000 | 0.00000800 |
| C | -0.38976800 | 2.71843500 | 0.00003000 |
| H | -0.18219900 | 3.78320900 | 0.00010200 |
| H | -2.52192700 | 2.90935600 | 0.00005300 |
| H | 2.15391500 | -2.65741600 | 0.00006000 |

| | | | |
|---|---|---|---|
| H | -0.16528900 | -3.47392600 | 0.00005300 |
| H | -4.49100300 | -1.42295700 | -0.00002200 |
| O | 1.92791200 | 2.35193200 | 0.00017000 |
| C | 4.06968600 | -0.93974200 | -0.00000400 |
| H | 4.10410900 | -1.58383700 | 0.88896900 |
| H | 4.10404800 | -1.58401200 | -0.88885100 |
| H | 4.95371000 | -0.30088300 | -0.00009700 |
| H | -4.08176900 | 1.01593600 | -0.00002000 |
| N | 2.89593800 | -0.10066300 | -0.00005100 |
| H | 2.97057300 | 0.92138300 | -0.00016900 |

**3**

SCF Energy (a.u.) = -862.936098

Thermal correction to Gibbs free Energy (a.u.) = 0.258556

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.22725400 | -2.09365200 | -0.00004500 |
| N | 0.00000000 | -2.73643000 | 0.00015500 |
| C | -1.22725400 | -2.09365200 | -0.00014700 |
| C | -1.26598400 | -0.73359200 | 0.00000600 |
| C | 1.26598400 | -0.73359100 | 0.00012000 |
| C | 0.00000000 | 0.10696500 | 0.00063100 |
| H | 0.00003800 | 0.78104700 | -0.86466100 |
| H | -0.00003800 | 0.77993200 | 0.86682000 |
| H | 0.00000100 | -3.74417100 | -0.00043700 |
| C | -2.55808700 | -0.04149800 | -0.00027900 |
| O | -2.38917600 | 1.30840300 | 0.00019000 |
| O | -3.67163400 | -0.55453700 | -0.00066800 |
| C | 2.55808700 | -0.04149800 | -0.00004200 |
| O | 2.38917500 | 1.30840300 | 0.00016500 |
| O | 3.67163400 | -0.55453600 | -0.00049500 |
| C | -3.59514500 | 2.10092700 | 0.00009100 |

| | | | |
|---|---|---|---|
| H | -4.18695600 | 1.84221200 | -0.88342400 |
| H | -4.18762200 | 1.84143400 | 0.88292800 |
| C | 3.59514400 | 2.10092700 | -0.00006900 |
| H | 4.18761000 | 1.84159900 | 0.88282500 |
| H | 4.18696800 | 1.84204900 | -0.88352800 |
| C | -2.41063000 | -3.02260200 | -0.00060500 |
| H | -3.04372400 | -2.84882300 | -0.87318400 |
| H | -2.08084100 | -4.06664800 | -0.00056800 |
| H | -3.04429600 | -2.84895900 | 0.87158400 |
| C | 2.41063000 | -3.02260100 | -0.00040200 |
| H | 2.08084100 | -4.06664800 | -0.00042900 |
| H | 3.04382100 | -2.84879900 | -0.87290600 |
| H | 3.04420100 | -2.84898200 | 0.87186200 |
| C | -3.17809500 | 3.55878500 | 0.00088200 |
| H | -2.58242700 | 3.79521900 | -0.88595700 |
| H | -4.06699000 | 4.19816600 | 0.00081400 |
| H | -2.58311600 | 3.79444900 | 0.88838800 |
| C | 3.17809400 | 3.55878600 | 0.00044700 |
| H | 2.58310300 | 3.79461500 | 0.88790100 |
| H | 4.06698800 | 4.19816700 | 0.00027100 |
| H | 2.58243700 | 3.79505400 | -0.88644500 |

**4**

SCF Energy (a.u.) = -862.740250

Thermal correction to Gibbs free Energy (a.u.) = 0.257002

Charge = 1, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.23552600 | -2.12544500 | -0.00033200 |
| N | -0.00000100 | -2.72627100 | -0.00040800 |
| C | -1.23552900 | -2.12544400 | -0.00030600 |
| C | -1.26259100 | -0.74471900 | -0.00008100 |
| C | 1.26259000 | -0.74472000 | -0.00010700 |

| | | | |
|---|---|---|---|
| C | 0.00000000 | 0.04175200 | 0.00005400 |
| H | -0.00000800 | 0.74887200 | -0.84839200 |
| H | 0.00000900 | 0.74853800 | 0.84878100 |
| H | -0.00000200 | -3.74212600 | -0.00056800 |
| C | -2.56494000 | -0.01376300 | 0.00003600 |
| O | -2.36950100 | 1.30644800 | 0.00025300 |
| O | -3.65098000 | -0.56324900 | -0.00013800 |
| C | 2.56494000 | -0.01376500 | -0.00001400 |
| O | 2.36950200 | 1.30644600 | 0.00019000 |
| O | 3.65097900 | -0.56325100 | -0.00020200 |
| C | -3.57222900 | 2.14755700 | 0.00033800 |
| H | -4.15612700 | 1.88839100 | -0.88618800 |
| H | -4.15625100 | 1.88804000 | 0.88667800 |
| C | 3.57223200 | 2.14755400 | 0.00024500 |
| H | 4.15626800 | 1.88804600 | 0.88657900 |
| H | 4.15611500 | 1.88837700 | -0.88628700 |
| C | -2.41097100 | -3.05426000 | -0.00045400 |
| H | -3.04273900 | -2.87507200 | -0.87335100 |
| H | -2.08438900 | -4.09760800 | -0.00056300 |
| H | -3.04280500 | -2.87527300 | 0.87243400 |
| C | 2.41096800 | -3.05426200 | -0.00050400 |
| H | 2.08438400 | -4.09761000 | -0.00063000 |
| H | 3.04273100 | -2.87506000 | -0.87340100 |
| H | 3.04280700 | -2.87529200 | 0.87238400 |
| C | -3.11559900 | 3.58898800 | 0.00065300 |
| H | -2.52207500 | 3.81654200 | -0.88924400 |
| H | -3.99317100 | 4.24215200 | 0.00071500 |
| H | -2.52220600 | 3.81619500 | 0.89072600 |
| C | 3.11560400 | 3.58898500 | 0.00055200 |
| H | 2.52222600 | 3.81620300 | 0.89063300 |
| H | 3.99317600 | 4.24214800 | 0.00059300 |

| | | | |
|---|---|---|---|
| H | 2.52206500 | 3.81653100 | -0.88933700 |

**5**

SCF Energy (a.u.) = -670.543265

Thermal correction to Gibbs free Energy (a.u.) = 0.170548

Charge = -1, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.59772200 | -0.58707700 | -0.01279000 |
| C | -0.53526400 | 0.38897900 | -0.00719100 |
| C | -0.82895400 | 1.82117400 | -0.00028600 |
| C | -1.28318800 | -1.95855100 | -0.00501200 |
| C | 0.81934800 | -0.07061900 | -0.00313300 |
| C | 1.11940900 | -1.48119800 | -0.00076500 |
| C | 0.04187500 | -2.39379500 | 0.00010200 |
| C | 2.47767900 | -1.90864800 | 0.00235600 |
| H | 2.68793600 | -2.97613700 | 0.00389200 |
| C | 3.51995300 | -0.98167300 | 0.00374300 |
| C | 3.24911500 | 0.38568200 | 0.00298800 |
| C | 1.91055200 | 0.86486600 | 0.00034500 |
| C | 1.60149600 | 2.24981900 | 0.00171900 |
| C | 0.29824600 | 2.70402000 | 0.00215900 |
| H | 0.07551600 | 3.76809700 | 0.00550200 |
| H | 2.42564400 | 2.96262700 | 0.00378800 |
| H | -2.08414400 | -2.69100200 | -0.00647500 |
| H | 0.25803100 | -3.46040200 | 0.00462500 |
| H | 4.55160500 | -1.32877600 | 0.00587900 |
| O | -2.02980100 | 2.29310200 | 0.00507100 |
| C | -4.03230700 | -1.01179700 | 0.02276600 |
| H | -4.08327700 | -1.69456200 | -0.84324100 |
| H | -4.04581500 | -1.64211200 | 0.93005300 |
| H | -4.94064900 | -0.40212500 | 0.02227700 |
| H | 4.06188800 | 1.10900900 | 0.00492900 |

| | | | |
|---|---|---|---|
| N | -2.89531800 | -0.14347100 | -0.02967700 |
| H | -2.96253900 | 0.88777200 | -0.00606100 |

**6**

SCF Energy (a.u.) = -416.143443

Thermal correction to Gibbs free Energy (a.u.) = 0.070829

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| N | 3.59711200 | 0.03157600 | -0.00052600 |
| N | 2.52760800 | -0.35194600 | 0.00071500 |
| C | 1.29575500 | -0.79338200 | -0.00015200 |
| C | 0.22193300 | 0.19163100 | 0.00005100 |
| O | 0.37049000 | 1.40283500 | 0.00043400 |
| C | -2.13955700 | 0.43232500 | -0.00056600 |
| H | -2.09473000 | 1.07536900 | 0.88347200 |
| H | -2.09543000 | 1.07418400 | -0.88551900 |
| O | -0.97796500 | -0.43365200 | -0.00051400 |
| C | -3.36643200 | -0.45793200 | 0.00045400 |
| H | -4.26926900 | 0.16148200 | 0.00069200 |
| H | -3.38734500 | -1.09733900 | -0.88717200 |
| H | -3.38634200 | -1.09655600 | 0.88866800 |
| H | 1.14967500 | -1.86386400 | 0.00045800 |

**$I_2$**

SCF Energy (a.u.) = -22.770239

Thermal correction to Gibbs free Energy (a.u.) = -0.025540

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 1.33000000 |
| I | 0.00000000 | 0.00000000 | -1.33000000 |

**$I_2$ radical anion**

SCF Energy (a.u.) = -22.955145

Thermal correction to Gibbs free Energy (a.u.) = -0.027223

Charge = -1, Multiplicity = 2

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 1.71884700 |
| I | 0.00000000 | 0.00000000 | -1.71884700 |

**Iodine anion**

SCF Energy (a.u.) = -11.560587

Thermal correction to Gibbs free Energy (a.u.) = -0.016848

Charge = -1, Multiplicity = 1

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 0.00000000 |

**Iodine radical**

SCF Energy (a.u.) = -11.364967

Thermal correction to Gibbs free Energy (a.u.) = -0.017503

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 0.00000000 |

**7**

SCF Energy (a.u.) = -427.523540

Thermal correction to Gibbs free Energy (a.u.) = 0.064633

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -0.42254800 | 2.83393700 | -0.83168600 |
| N | -0.34911300 | 2.08323200 | 0.01278900 |
| C | -0.23615600 | 1.15883600 | 0.95300300 |
| C | -1.28501300 | 0.12216900 | 1.06414800 |
| O | -1.39382500 | -0.59389900 | 2.03691900 |
| C | -3.07329800 | -0.95859800 | -0.06490900 |
| H | -2.56972600 | -1.92070100 | 0.06268900 |
| H | -3.74849100 | -0.80941400 | 0.78245700 |
| O | -2.06114100 | 0.08524700 | -0.03159300 |
| C | -3.78452000 | -0.85142400 | -1.39780000 |

| | | | |
|---|---|---|---|
| H | -4.55503500 | -1.62627700 | -1.46266600 |
| H | -4.26740100 | 0.12405100 | -1.50876200 |
| H | -3.08409500 | -0.99104400 | -2.22619600 |
| H | 0.37568400 | 1.41534700 | 1.80649400 |
| I | 1.90876100 | -0.44092100 | -0.20926400 |

**TS1**

SCF Energy (a.u.) = -427.516111

Thermal correction to Gibbs free Energy (a.u.) = 0.065135

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -0.05300400 | 2.83396500 | -0.49924400 |
| N | -0.19617600 | 2.05871000 | 0.33770200 |
| C | 0.06407300 | 0.84915500 | 0.94391800 |
| C | -1.13564100 | -0.06654800 | 1.02102100 |
| O | -1.28137900 | -0.86881900 | 1.91577800 |
| C | -3.09674700 | -0.78423200 | -0.10490000 |
| H | -2.71804400 | -1.80991900 | -0.11592100 |
| H | -3.70256900 | -0.65094900 | 0.79575300 |
| O | -1.95285900 | 0.11284900 | -0.01998600 |
| C | -3.85041000 | -0.43070100 | -1.36977800 |
| H | -4.71883200 | -1.08925300 | -1.47168400 |
| H | -4.20419900 | 0.60401400 | -1.34019400 |
| H | -3.21509900 | -0.55767500 | -2.25089400 |
| H | 0.55581700 | 0.98842100 | 1.90177300 |
| I | 1.76855500 | -0.43569100 | -0.27350800 |

**8**

SCF Energy (a.u.) = -427.518682

Thermal correction to Gibbs free Energy (a.u.) = 0.065241

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | 0.36579500 | 2.65704400 | -0.43941700 |

| | | | |
|---|---|---|---|
| N | -0.06423400 | 2.05908300 | 0.46926000 |
| C | 0.19412500 | 0.69550800 | 0.93568800 |
| C | -1.10050400 | -0.10492000 | 1.01183300 |
| O | -1.34417100 | -0.86364700 | 1.92432100 |
| C | -3.12182900 | -0.62698600 | -0.11397800 |
| H | -2.87132100 | -1.69137600 | -0.09364300 |
| H | -3.71014200 | -0.39609700 | 0.77848500 |
| O | -1.87865200 | 0.12736600 | -0.04481400 |
| C | -3.82248400 | -0.21983200 | -1.39316900 |
| H | -4.76481600 | -0.76959200 | -1.48309000 |
| H | -4.04583400 | 0.85091300 | -1.39376800 |
| H | -3.20457800 | -0.44746000 | -2.26641900 |
| H | 0.63433900 | 0.76370700 | 1.92843800 |
| I | 1.67430500 | -0.45085600 | -0.28975900 |

**TS2**

SCF Energy (a.u.) = -427.514973

Thermal correction to Gibbs free Energy (a.u.) = 0.062720

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | 0.62605300 | 2.24621900 | -1.55624900 |
| N | 0.07798200 | 2.22409300 | -0.54846500 |
| C | 0.26520700 | 0.96185600 | 0.60636200 |
| C | -1.14039600 | 0.51853300 | 0.92442300 |
| O | -1.65265400 | 0.71175900 | 2.00885900 |
| C | -3.10244100 | -0.50967300 | 0.07544100 |
| H | -3.10686600 | -1.22477400 | 0.90316200 |
| H | -3.70954300 | 0.35241600 | 0.36617000 |
| O | -1.73532300 | -0.05630500 | -0.12231900 |
| C | -3.56185500 | -1.12968500 | -1.22780800 |
| H | -4.59115100 | -1.48637400 | -1.11977600 |
| H | -3.53326100 | -0.39795000 | -2.04033100 |

| | | | |
|---|---|---|---|
| H | -2.92834600 | -1.97826800 | -1.50146100 |
| H | 0.70177500 | 1.49401700 | 1.44644600 |
| I | 1.59584700 | -0.61020900 | -0.01290600 |

**9**

SCF Energy (a.u.) = -427.559170

Thermal correction to Gibbs free Energy (a.u.) = 0.056248

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -1.85238200 | 2.48282400 | -0.28858400 |
| N | -0.89747300 | 2.80181600 | 0.16680300 |
| C | 0.49988100 | -0.28266300 | 1.29685200 |
| C | -0.92392900 | -0.52080800 | 1.18431300 |
| O | -1.64259400 | -0.59116500 | 2.17705900 |
| C | -2.79240100 | -0.86287700 | -0.23804900 |
| H | -3.05718200 | -1.79816100 | 0.26494900 |
| H | -3.32626500 | -0.04892600 | 0.26116100 |
| O | -1.37013600 | -0.64413000 | -0.08101000 |
| C | -3.07786100 | -0.90770300 | -1.72547200 |
| H | -4.14675800 | -1.07829900 | -1.88960300 |
| H | -2.80160100 | 0.03708800 | -2.20246600 |
| H | -2.52048600 | -1.71676400 | -2.20678100 |
| H | 0.92345300 | -0.16739000 | 2.28536600 |
| I | 1.81218000 | -0.13006300 | -0.29310200 |

**A**

SCF Energy (a.u.) = -424.384333

Thermal correction to Gibbs free Energy (a.u.) = 0.131295

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.86942700 | -1.03402100 | -0.00022700 |
| C | 0.50678500 | -1.27918500 | -0.00011200 |
| C | 1.44840600 | -0.24158000 | 0.00005000 |

| | | | |
|---|---|---|---|
| C | 0.95593200 | 1.08039100 | 0.00012300 |
| C | -0.40422400 | 1.34323000 | 0.00002600 |
| C | -1.33004100 | 0.28610100 | -0.00017000 |
| H | -1.55821200 | -1.86965100 | -0.00033400 |
| H | 0.85451800 | -2.30894000 | -0.00014900 |
| H | 1.64890200 | 1.91534100 | 0.00030300 |
| H | -0.78025400 | 2.36086800 | 0.00012400 |
| C | 2.88032300 | -0.56844200 | 0.00016800 |
| H | 3.09959600 | -1.63579500 | 0.00061600 |
| C | 3.91507200 | 0.28562700 | -0.00006800 |
| H | 4.93636800 | -0.07989300 | 0.00012600 |
| H | 3.78655000 | 1.36400500 | -0.00055700 |
| O | -2.64610900 | 0.64916400 | -0.00023500 |
| C | -3.62622900 | -0.38026800 | 0.00029100 |
| H | -3.54304100 | -1.00848500 | 0.89590400 |
| H | -4.59139700 | 0.12684100 | 0.00058500 |
| H | -3.54374800 | -1.00872600 | -0.89522100 |

**10**

SCF Energy (a.u.) = -742.379963

Thermal correction to Gibbs free Energy (a.u.) = 0.205785

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.27427300 | -1.04987200 | 0.22786200 |
| C | -2.78475800 | 0.28738700 | 0.02503800 |
| O | -3.81000100 | 0.68214400 | 0.57268200 |
| C | -2.50425700 | 2.39645600 | -1.02339200 |
| H | -3.51895600 | 2.35711600 | -1.43153300 |
| H | -2.55620300 | 2.91003900 | -0.05734800 |
| O | -2.03813900 | 1.04751500 | -0.80504800 |
| C | -1.52824200 | 3.06250900 | -1.97322800 |
| H | -1.84424300 | 4.09300200 | -2.16497500 |

| | | | |
|---|---|---|---|
| H | -0.52090600 | 3.08227800 | -1.54788900 |
| H | -1.48676600 | 2.52881500 | -2.92715600 |
| C | -0.12953400 | 0.20423000 | 2.81403500 |
| H | 0.04727300 | -0.63933100 | 3.48089100 |
| C | -1.27894600 | 0.88392100 | 2.94875600 |
| H | -2.01164900 | 0.60121300 | 3.69663700 |
| H | -1.53894200 | 1.73051600 | 2.32137700 |
| C | 0.93962800 | 0.44502900 | 1.83895100 |
| C | 2.05095700 | -0.40772400 | 1.81349200 |
| C | 0.89663900 | 1.48403700 | 0.88653200 |
| C | 3.08113400 | -0.25731400 | 0.88110500 |
| H | 2.10961400 | -1.22097000 | 2.53218100 |
| C | 1.90777900 | 1.64981900 | -0.04445100 |
| H | 0.05052800 | 2.16127000 | 0.86478400 |
| C | 3.00877000 | 0.77686300 | -0.05810000 |
| H | 3.91808000 | -0.94452700 | 0.89761100 |
| H | 1.86873900 | 2.44383400 | -0.78268200 |
| O | 3.94752000 | 1.01949600 | -1.01863400 |
| C | 5.08441700 | 0.16869200 | -1.07607300 |
| H | 4.79393500 | -0.87105700 | -1.27310700 |
| H | 5.69288400 | 0.53851600 | -1.90195100 |
| H | 5.66385400 | 0.21522500 | -0.14544200 |
| I | -0.59394300 | -1.83294900 | -0.67986900 |
| H | -2.79916400 | -1.69709800 | 0.91649400 |

**TS3**

SCF Energy (a.u.) = -742.373576

Thermal correction to Gibbs free Energy (a.u.) = 0.210323

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.97481900 | -1.18293700 | 0.14332700 |
| C | -3.09720000 | -0.52588400 | -0.50514900 |
| O | -3.94948400 | -1.15200300 | -1.12786000 |

| | | | |
|---|---|---|---|
| C | -4.14884400 | 1.51634300 | -1.10256900 |
| H | -4.13226400 | 1.24714600 | -2.16351700 |
| H | -5.10085300 | 1.17195300 | -0.68684300 |
| O | -3.07323800 | 0.82445100 | -0.43047400 |
| C | -3.93427400 | 3.00136600 | -0.88457200 |
| H | -4.73238200 | 3.56639600 | -1.37722000 |
| H | -3.94522000 | 3.24432300 | 0.18208800 |
| H | -2.97517200 | 3.32328200 | -1.30177700 |
| H | -2.06899600 | -2.24983000 | 0.28980900 |
| C | 0.52123100 | -1.87971600 | -1.48603600 |
| H | 0.63257600 | -2.96065900 | -1.41621000 |
| C | -0.70438800 | -1.38724200 | -1.83926100 |
| H | -0.85192300 | -0.33035700 | -2.03408400 |
| H | -1.47637500 | -2.05073300 | -2.21072100 |
| I | -0.79750000 | -0.24446000 | 1.60402600 |
| C | 1.69016700 | -1.11014600 | -1.10844700 |
| C | 2.85795000 | -1.78441300 | -0.68179300 |
| C | 1.73125000 | 0.29846000 | -1.13443600 |
| C | 3.99769500 | -1.09605700 | -0.30009300 |
| H | 2.85623900 | -2.87053700 | -0.64837200 |
| C | 2.86911600 | 1.00440200 | -0.75560400 |
| H | 0.85691800 | 0.85842200 | -1.44714400 |
| C | 4.01236300 | 0.30806800 | -0.33309300 |
| H | 4.88979600 | -1.61790400 | 0.02952700 |
| H | 2.85448700 | 2.08683400 | -0.78689200 |
| O | 5.17354800 | 0.90060700 | 0.06008200 |
| C | 5.24635000 | 2.32151400 | 0.05073200 |
| H | 4.50464700 | 2.76149300 | 0.72860700 |
| H | 6.24946300 | 2.56982400 | 0.39824600 |
| H | 5.10039500 | 2.71974900 | -0.96087000 |

**11**

SCF Energy (a.u.) = -742.417242

Thermal correction to Gibbs free Energy (a.u.) = 0.214957

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.09628000 | -0.18534700 | 0.30766300 |
| C | -1.77361500 | 1.14483000 | 0.56219300 |
| O | -2.13866500 | 1.53407800 | 1.65374500 |
| C | -2.62164300 | 3.10522100 | -0.47263100 |
| H | -3.61262500 | 2.91118600 | -0.05132700 |
| H | -2.07736300 | 3.74769100 | 0.22584400 |
| O | -1.91780600 | 1.84154900 | -0.57745100 |
| C | -2.69387900 | 3.69895200 | -1.86495800 |
| H | -3.22265900 | 4.65699300 | -1.82881700 |
| H | -1.69190600 | 3.87295900 | -2.26853400 |
| H | -3.23165100 | 3.03264400 | -2.54579200 |
| H | -0.47269000 | -0.12535600 | -0.58226500 |
| C | 0.81249600 | 0.21378700 | 1.79804400 |
| H | 0.64251100 | 1.02511500 | 2.49957100 |
| C | -0.33532300 | -0.70912700 | 1.52550100 |
| H | -0.00010800 | -1.73076800 | 1.32344300 |
| H | -1.01505000 | -0.74095200 | 2.38020500 |
| I | -2.69522500 | -1.62228200 | -0.31016700 |
| C | 2.05982700 | 0.15736000 | 1.13538100 |
| C | 3.07337200 | 1.12272200 | 1.42765500 |
| C | 2.38425700 | -0.83009800 | 0.16287800 |
| C | 4.30204800 | 1.09914600 | 0.80230100 |
| H | 2.86169000 | 1.89201900 | 2.16503700 |
| C | 3.62172200 | -0.85733300 | -0.47165300 |
| H | 1.65443900 | -1.58966800 | -0.09722300 |
| C | 4.59167400 | 0.10770200 | -0.15766500 |
| H | 5.06575200 | 1.83521800 | 1.03113000 |

| | | | |
|---|---|---|---|
| H | 3.82139400 | -1.62892900 | -1.20534900 |
| O | 5.83092900 | 0.17152000 | -0.71974600 |
| C | 6.18381800 | -0.80434700 | -1.69278600 |
| H | 5.51881500 | -0.75495700 | -2.56385200 |
| H | 7.20246600 | -0.56467600 | -1.99875700 |
| H | 6.15740500 | -1.81554000 | -1.26835800 |

**TS4**

SCF Energy (a.u.) = -742.403561

Thermal correction to Gibbs free Energy (a.u.) = 0.214988

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -0.74939900 | 0.05351400 | 0.50932900 |
| C | -1.60082000 | 1.25695500 | 0.65650700 |
| O | -2.02386700 | 1.67386000 | 1.72291400 |
| C | -2.76176600 | 2.95013200 | -0.52861200 |
| H | -3.69888900 | 2.60394400 | -0.08267000 |
| H | -2.35987600 | 3.74776500 | 0.10403000 |
| O | -1.82716200 | 1.84458600 | -0.53162500 |
| C | -2.94125800 | 3.39148200 | -1.96741800 |
| H | -3.64835300 | 4.22639200 | -2.01085400 |
| H | -1.99080700 | 3.72142500 | -2.39800200 |
| H | -3.33328300 | 2.57246800 | -2.57719400 |
| H | -0.28649200 | -0.12760800 | -0.44967600 |
| C | 0.77999600 | 0.40943000 | 1.63535100 |
| H | 0.56179100 | 1.34544500 | 2.13905600 |
| C | -0.24548100 | -0.64095500 | 1.73418300 |
| H | 0.06890200 | -1.66779400 | 1.56621100 |
| H | -0.92715900 | -0.54689100 | 2.57658100 |
| I | -2.76022700 | -1.66076100 | -0.30613500 |
| C | 2.06343100 | 0.28522200 | 0.99652700 |
| C | 2.93221400 | 1.40576700 | 0.96052900 |

| | | | |
|---|---|---|---|
| C | 2.51334700 | -0.91032900 | 0.39474500 |
| C | 4.17873700 | 1.33290200 | 0.36858900 |
| H | 2.60722700 | 2.33869100 | 1.41222200 |
| C | 3.76130000 | -0.99299500 | -0.21257000 |
| H | 1.87746100 | -1.78937400 | 0.39357500 |
| C | 4.60481100 | 0.13114200 | -0.22804500 |
| H | 4.84525600 | 2.18822700 | 0.34545100 |
| H | 4.06859700 | -1.92687100 | -0.66628600 |
| O | 5.83811000 | 0.15624200 | -0.78981600 |
| C | 6.33020300 | -1.02554000 | -1.41796100 |
| H | 5.68669400 | -1.32495300 | -2.25339900 |
| H | 7.32064500 | -0.76912300 | -1.79337200 |
| H | 6.41177200 | -1.84930200 | -0.69923700 |

**12**

SCF Energy (a.u.) = -742.406772

Thermal correction to Gibbs free Energy (a.u.) = 0.215426

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -0.41346400 | 0.60053200 | 0.54391600 |
| C | -1.46977400 | 1.64228600 | 0.49890000 |
| O | -1.77919600 | 2.35846600 | 1.43513500 |
| C | -3.14113600 | 2.63788300 | -0.86976400 |
| H | -3.87487600 | 2.43969400 | -0.08328800 |
| H | -2.75573400 | 3.65197800 | -0.72534700 |
| O | -2.04478900 | 1.70262300 | -0.71765500 |
| C | -3.71670700 | 2.43086600 | -2.25659900 |
| H | -4.55501000 | 3.11743200 | -2.41406200 |
| H | -2.96338700 | 2.62338500 | -3.02649300 |
| H | -4.07987400 | 1.40584400 | -2.37465500 |
| H | -0.23854300 | 0.04913500 | -0.37239500 |
| C | 0.86856200 | 0.94794800 | 1.36525700 |

| | | | |
|---|---|---|---|
| H | 0.80556100 | 1.92842800 | 1.82911200 |
| C | -0.10167400 | -0.05739700 | 1.87257300 |
| H | 0.16267700 | -1.10889700 | 1.84404600 |
| H | -0.73698200 | 0.23948100 | 2.70029500 |
| I | -2.78508200 | -1.78293100 | -0.02535100 |
| C | 2.19469600 | 0.60597000 | 0.79826000 |
| C | 3.17687100 | 1.60876600 | 0.69021800 |
| C | 2.51921400 | -0.67776000 | 0.33856200 |
| C | 4.42951500 | 1.34086900 | 0.15642200 |
| H | 2.94988600 | 2.61325900 | 1.03656200 |
| C | 3.77115600 | -0.96390100 | -0.20838400 |
| H | 1.78929100 | -1.47948300 | 0.39901900 |
| C | 4.73603800 | 0.04928200 | -0.30010800 |
| H | 5.18709400 | 2.11358200 | 0.08014000 |
| H | 3.98059200 | -1.96900200 | -0.55298300 |
| O | 5.98739200 | -0.12075900 | -0.81147700 |
| C | 6.35268600 | -1.40869900 | -1.29280600 |
| H | 5.70412700 | -1.72196900 | -2.12020600 |
| H | 7.37799700 | -1.31243000 | -1.65068000 |
| H | 6.31336800 | -2.15759700 | -0.49219500 |

**TS3a**

SCF Energy (a.u.) = -742.373403

Thermal correction to Gibbs free Energy (a.u.) = 0.210221

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.92832100 | 0.75420000 | 0.55808200 |
| C | -2.64971200 | -0.06921000 | -0.40168600 |
| O | -2.29167700 | -0.36553800 | -1.53033300 |
| C | -4.56773000 | -1.45671800 | -0.64826300 |
| H | -4.85594600 | -0.93837100 | -1.56808400 |
| H | -3.93723300 | -2.30624700 | -0.93015800 |

| | | | |
|---|---|---|---|
| O | -3.79159100 | -0.55285300 | 0.16952600 |
| C | -5.77239600 | -1.88590300 | 0.16654600 |
| H | -6.39071700 | -2.57216000 | -0.42155100 |
| H | -5.46366500 | -2.39934000 | 1.08242000 |
| H | -6.38414800 | -1.02220300 | 0.44412000 |
| H | -2.45391900 | 1.13301300 | 1.42533300 |
| C | -0.18393500 | -1.69583200 | 0.84997500 |
| H | -0.68178300 | -2.45375700 | 0.24838500 |
| C | -0.94095900 | -1.00928100 | 1.76007200 |
| H | -1.93269400 | -1.36315000 | 2.01699900 |
| H | -0.49807400 | -0.28967300 | 2.44035100 |
| I | -0.38713800 | 1.98697000 | -0.12301300 |
| C | 1.19860200 | -1.43882200 | 0.50190900 |
| C | 1.75376400 | -2.06624200 | -0.63774200 |
| C | 2.03723100 | -0.58101700 | 1.24100400 |
| C | 3.06372100 | -1.84023100 | -1.02538900 |
| H | 1.12793600 | -2.72655900 | -1.23125100 |
| C | 3.35680300 | -0.34605700 | 0.86604600 |
| H | 1.65646800 | -0.08736800 | 2.12841900 |
| C | 3.87732300 | -0.97437100 | -0.27605800 |
| H | 3.48254600 | -2.31521900 | -1.90612100 |
| H | 3.96614500 | 0.32102400 | 1.46320600 |
| O | 5.15057200 | -0.81220400 | -0.73085500 |
| C | 6.01850200 | 0.06156000 | -0.01897300 |
| H | 6.17558000 | -0.28569500 | 1.00968100 |
| H | 6.96621600 | 0.04291400 | -0.55769300 |
| H | 5.62583000 | 1.08570100 | -0.00422700 |

**11a**

SCF Energy (a.u.) = -742.416425

Thermal correction to Gibbs free Energy (a.u.) = 0.215388

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.50901500 | -0.35937000 | 0.58969500 |
| C | 0.96304600 | 0.83448700 | -0.16389800 |
| O | 0.33868300 | 0.76615700 | -1.20384500 |
| C | 0.83005800 | 3.20297200 | -0.19338600 |
| H | 1.28349900 | 3.23367200 | -1.18870800 |
| H | -0.25597700 | 3.16108200 | -0.31710700 |
| O | 1.26199300 | 1.98396100 | 0.46432200 |
| C | 1.26742100 | 4.36502900 | 0.67522600 |
| H | 0.96097700 | 5.30734000 | 0.20948100 |
| H | 0.80943700 | 4.30591100 | 1.66711000 |
| H | 2.35482300 | 4.37629600 | 0.79454300 |
| H | 1.77532300 | -0.07752600 | 1.60645300 |
| C | -0.63455000 | -1.27115400 | 1.36455900 |
| H | -0.49696500 | -1.29070500 | 2.44405300 |
| C | 0.57912900 | -1.57208100 | 0.54049500 |
| H | 1.11311000 | -2.43656900 | 0.95016000 |
| H | 0.33515500 | -1.79564400 | -0.50001100 |
| I | 3.49883900 | -0.83835100 | -0.31943300 |
| C | -1.92299500 | -0.94190900 | 0.88831100 |
| C | -2.97900900 | -0.69556700 | 1.82213400 |
| C | -2.25742100 | -0.84444800 | -0.49207900 |
| C | -4.25810600 | -0.38706500 | 1.41004700 |
| H | -2.76048900 | -0.75892600 | 2.88472200 |
| C | -3.54544600 | -0.53307700 | -0.91055000 |
| H | -1.48700200 | -0.98099000 | -1.24031100 |
| C | -4.55783500 | -0.30365900 | 0.03499700 |
| H | -5.05331900 | -0.20446000 | 2.12540800 |
| H | -3.74875200 | -0.46199700 | -1.97215800 |
| O | -5.84837200 | 0.00733700 | -0.27219400 |
| C | -6.21212000 | 0.10470800 | -1.64415400 |

| | | | |
|---|---|---|---|
| H | -6.05526700 | -0.84793000 | -2.16478800 |
| H | -7.27344800 | 0.35442300 | -1.65350900 |
| H | -5.64511700 | 0.89579400 | -2.15001500 |

**TS4a**

SCF Energy (a.u.) = -742.403384

Thermal correction to Gibbs free Energy (a.u.) = 0.215610

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.03217400 | -0.58025300 | -0.66013700 |
| C | -0.59512000 | 0.59613800 | 0.11631000 |
| O | -0.05392400 | 0.54306600 | 1.20933400 |
| C | -0.59114400 | 2.96504700 | 0.18205800 |
| H | -1.16334000 | 2.93661900 | 1.11439600 |
| H | 0.47236100 | 3.00218900 | 0.43755500 |
| O | -0.85030800 | 1.74117200 | -0.54473700 |
| C | -1.00855600 | 4.11699600 | -0.71027500 |
| H | -0.83304800 | 5.06604700 | -0.19305600 |
| H | -0.43309200 | 4.11987700 | -1.64113500 |
| H | -2.07155400 | 4.04935300 | -0.95904100 |
| H | -1.47852200 | -0.40879200 | -1.62946600 |
| C | 0.54729300 | -1.58719700 | -1.12930000 |
| H | 0.40722200 | -1.75842900 | -2.19271900 |
| C | -0.58671900 | -1.94882400 | -0.25928200 |
| H | -1.23246700 | -2.74766200 | -0.61784200 |
| H | -0.38072100 | -2.03124600 | 0.80524500 |
| I | -3.67255900 | -0.53976100 | 0.28123700 |
| C | 1.84994600 | -1.12884400 | -0.73389400 |
| C | 2.76764800 | -0.72140000 | -1.73850500 |
| C | 2.28264000 | -1.07566500 | 0.60978400 |
| C | 4.04053300 | -0.29228700 | -1.42136200 |
| H | 2.45636700 | -0.74896900 | -2.77909300 |

| | | | |
|---|---|---|---|
| C | 3.56172700 | -0.64368700 | 0.94029300 |
| H | 1.60594200 | -1.35928400 | 1.40466800 |
| C | 4.44864800 | -0.24648200 | -0.07327000 |
| H | 4.74294700 | 0.01721200 | -2.18759200 |
| H | 3.85465500 | -0.61317200 | 1.98205900 |
| O | 5.71244100 | 0.19250200 | 0.14286900 |
| C | 6.18964900 | 0.27392000 | 1.48441000 |
| H | 6.19576400 | -0.71334200 | 1.96072600 |
| H | 7.20953000 | 0.65121500 | 1.41187100 |
| H | 5.58167900 | 0.96703000 | 2.07714100 |

**12a**

SCF Energy (a.u.) = -742.405389

Thermal correction to Gibbs free Energy (a.u.) = 0.214358

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.67994300 | -0.58623100 | 0.75941400 |
| C | 0.46455600 | 0.59301100 | -0.11833800 |
| O | -0.01820900 | 0.55559400 | -1.23591900 |
| C | 0.73822200 | 2.94430400 | -0.28153500 |
| H | 1.30026500 | 2.81104500 | -1.21065000 |
| H | -0.31396900 | 3.09584100 | -0.54110500 |
| O | 0.84987900 | 1.72780600 | 0.49620000 |
| C | 1.29053100 | 4.07363800 | 0.56520200 |
| H | 1.22706600 | 5.01531400 | 0.01002100 |
| H | 0.72159900 | 4.18159600 | 1.49370200 |
| H | 2.33888700 | 3.89165300 | 0.81923700 |
| H | 1.35312100 | -0.43568600 | 1.59527100 |
| C | -0.59161600 | -1.46599600 | 1.11194800 |
| H | -0.52456000 | -1.81897300 | 2.13801100 |
| C | 0.45982800 | -1.96835400 | 0.19169100 |
| H | 1.11902200 | -2.75443100 | 0.54338800 |

| | | | |
|---|---|---|---|
| H | 0.24865200 | -1.98930500 | -0.87220300 |
| I | 3.83124500 | -0.58110700 | -0.24625600 |
| C | -1.95482300 | -1.04145000 | 0.72112700 |
| C | -2.80919900 | -0.51907000 | 1.71433900 |
| C | -2.44653100 | -1.12471700 | -0.58849500 |
| C | -4.09661000 | -0.10291500 | 1.41554200 |
| H | -2.44900500 | -0.44185500 | 2.73683600 |
| C | -3.73923300 | -0.70929800 | -0.90781900 |
| H | -1.81335300 | -1.50630800 | -1.37965200 |
| C | -4.57102800 | -0.19310100 | 0.09527300 |
| H | -4.75530300 | 0.29492300 | 2.18009800 |
| H | -4.08033600 | -0.78817100 | -1.93243400 |
| O | -5.84473100 | 0.24131900 | -0.10749000 |
| C | -6.37842600 | 0.18504800 | -1.42598800 |
| H | -6.41539000 | -0.84728200 | -1.79454200 |
| H | -7.39099200 | 0.58248900 | -1.35338500 |
| H | -5.79087300 | 0.80085500 | -2.11752400 |

**13**

SCF Energy (a.u.) = -731.035483

Thermal correction to Gibbs free Energy (a.u.) = 0.222123

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.61499200 | -0.95584400 | -0.33012000 |
| C | -2.93373400 | -0.40260300 | 0.05786700 |
| O | -3.45267200 | -0.53942800 | 1.15293400 |
| C | -4.77656400 | 0.91356200 | -0.69435700 |
| H | -5.23454500 | 1.01019800 | -1.68108200 |
| H | -5.37474600 | 0.23947900 | -0.07666300 |
| O | -3.49568100 | 0.28819600 | -0.95952800 |
| C | -4.59825100 | 2.26718200 | -0.02448800 |
| H | -5.57438500 | 2.74895000 | 0.10000100 |

| | | | |
|---|---|---|---|
| H | -4.14432200 | 2.15222700 | 0.96310700 |
| H | -3.96657400 | 2.92117200 | -0.63356300 |
| H | -1.30795300 | -0.76629600 | -1.35237600 |
| C | -0.51177000 | -0.93958400 | 0.73850200 |
| H | -0.84353300 | -0.54210000 | 1.69353400 |
| C | -1.15315200 | -2.23275700 | 0.33925100 |
| H | -0.57949600 | -2.92713100 | -0.26664100 |
| H | -1.84530500 | -2.68278700 | 1.04345200 |
| C | 0.88380500 | -0.57835200 | 0.36699100 |
| C | 1.62053700 | 0.27348100 | 1.19479600 |
| C | 1.50824600 | -1.05443600 | -0.80012300 |
| C | 2.93435300 | 0.64671200 | 0.88946800 |
| H | 1.16421900 | 0.65754400 | 2.10329000 |
| C | 2.81004200 | -0.69250200 | -1.12178500 |
| H | 0.97336800 | -1.71827300 | -1.47353700 |
| C | 3.53437100 | 0.16206700 | -0.27701900 |
| H | 3.46696000 | 1.30729400 | 1.56263200 |
| H | 3.28879200 | -1.06079100 | -2.02313600 |
| O | 4.80750500 | 0.45883400 | -0.67734400 |
| C | 5.58234200 | 1.32182600 | 0.14277700 |
| H | 5.73134700 | 0.89460000 | 1.14268800 |
| H | 6.54689800 | 1.42217900 | -0.35613600 |
| H | 5.11467600 | 2.31039800 | 0.23537600 |

**HI**

SCF Energy (a.u.) = -11.993266

Thermal correction to Gibbs free Energy (a.u.) = -0.015071

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| I | 0.00000000 | 0.00000000 | 0.02990600 |
| H | 0.00000000 | 0.00000000 | -1.58499400 |

**TS3*m***

SCF Energy (a.u.) = -742.361565

Thermal correction to Gibbs free Energy (a.u.) = 0.210865

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.21932200 | -0.04789500 | 0.80269800 |
| C | -2.64483800 | -0.38653900 | 0.71234600 |
| O | -3.18819400 | -1.14151500 | 1.50672500 |
| C | -4.64671700 | -0.22840100 | -0.57031200 |
| H | -5.14757500 | -0.24574000 | 0.40066600 |
| H | -5.04899200 | 0.58670000 | -1.17553200 |
| O | -3.25922200 | 0.13180400 | -0.37255400 |
| C | -4.77176600 | -1.56747200 | -1.28090300 |
| H | -5.82576000 | -1.77596300 | -1.49495500 |
| H | -4.22463600 | -1.55570800 | -2.22880900 |
| H | -4.38526600 | -2.37484600 | -0.65371700 |
| H | -0.76192200 | -0.31428300 | 1.74734300 |
| C | -0.28971700 | -1.58260400 | -0.45357300 |
| H | -0.74233900 | -1.12385300 | -1.33049600 |
| C | -0.86463900 | -2.75686600 | 0.01036000 |
| H | -1.87715200 | -3.02761500 | -0.26383500 |
| H | -0.36344300 | -3.38990800 | 0.73470200 |
| I | -0.55311500 | 1.84710400 | 0.13076900 |
| C | 1.14100700 | -1.26825900 | -0.25387200 |
| C | 1.84800900 | -0.57515300 | -1.24166000 |
| C | 1.82983800 | -1.62588100 | 0.92062600 |
| C | 3.20173500 | -0.26012800 | -1.09235800 |
| H | 1.33501600 | -0.27332400 | -2.15003300 |
| C | 3.17061500 | -1.31517400 | 1.08962000 |
| H | 1.30397700 | -2.14039500 | 1.71965700 |
| C | 3.86827800 | -0.63062600 | 0.08025100 |
| H | 3.71224700 | 0.27385400 | -1.88412100 |

| | | | |
|---|---|---|---|
| H | 3.70105900 | -1.58333700 | 1.99719700 |
| O | 5.18241300 | -0.37053000 | 0.33929400 |
| C | 5.93302000 | 0.33550100 | -0.63988200 |
| H | 5.51083400 | 1.33165000 | -0.82241900 |
| H | 6.93830800 | 0.43616900 | -0.22968000 |
| H | 5.97775900 | -0.22101900 | -1.58450000 |

**$11_m$**

SCF Energy (a.u.) = -742.389223

Thermal correction to Gibbs free Energy (a.u.) = 0.213547

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.12839600 | -0.15925000 | 0.63075500 |
| C | -2.63167600 | -0.33495300 | 0.56802000 |
| O | -3.35477100 | -0.28513800 | 1.54249200 |
| C | -4.48724500 | -0.72580200 | -0.87666700 |
| H | -5.00885200 | -0.03776900 | -0.20759900 |
| H | -4.65407400 | -0.42690500 | -1.91335800 |
| O | -3.05833600 | -0.55746800 | -0.68836100 |
| C | -4.90432100 | -2.16685500 | -0.63077300 |
| H | -5.97320600 | -2.28166700 | -0.84084000 |
| H | -4.35238700 | -2.84870900 | -1.28541200 |
| H | -4.72814000 | -2.44914000 | 0.41033300 |
| H | -0.84065500 | -0.15998400 | 1.67963600 |
| C | -0.32424000 | -1.19730800 | -0.19057100 |
| H | -0.60883800 | -1.06210400 | -1.23883600 |
| C | -0.76063500 | -2.55915000 | 0.26206000 |
| H | -1.66790700 | -3.00311500 | -0.13187900 |
| H | -0.23228700 | -3.07120600 | 1.05819700 |
| I | -0.68127300 | 1.91858600 | -0.02154700 |
| C | 1.17294500 | -0.99951000 | -0.05556200 |
| C | 1.95804600 | -0.74644000 | -1.17958400 |

| | | | |
|---|---|---|---|
| C | 1.80939800 | -1.05849900 | 1.19501300 |
| C | 3.34009100 | -0.54974300 | -1.08087600 |
| H | 1.48739700 | -0.68740500 | -2.15703000 |
| C | 3.17914800 | -0.86481000 | 1.31534300 |
| H | 1.22922400 | -1.25414600 | 2.09316900 |
| C | 3.95467000 | -0.60700800 | 0.17428400 |
| H | 3.91272800 | -0.35044200 | -1.97822100 |
| H | 3.67156400 | -0.90493900 | 2.28119900 |
| O | 5.29111500 | -0.42837700 | 0.39152200 |
| C | 6.12139300 | -0.15320800 | -0.72840100 |
| H | 5.82140600 | 0.77690600 | -1.22741800 |
| H | 7.13114600 | -0.04316600 | -0.33159300 |
| H | 6.10121800 | -0.97817300 | -1.45182500 |

**A2**

SCF Energy (a.u.) = -117.970694

Thermal correction to Gibbs free Energy (a.u.) = 0.054553

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.23518900 | 0.16352000 | -0.00003800 |
| H | 1.80913900 | -0.14952300 | 0.88121000 |
| H | 1.81045000 | -0.15163600 | -0.87966100 |
| H | 1.17928800 | 1.25656300 | -0.00131400 |
| C | -0.13244400 | -0.45644000 | -0.00007900 |
| H | -0.16456800 | -1.54656500 | 0.00026700 |
| C | -1.28390700 | 0.22105800 | 0.00010400 |
| H | -2.24396600 | -0.28648900 | -0.00042800 |
| H | -1.30336900 | 1.30882400 | -0.00000200 |

**11b**

SCF Energy (a.u.) = -627.836368

Thermal correction to Gibbs free Energy (a.u.) = 0.186327

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.36565000 | -0.20964600 | -0.10775600 |
| C | 0.89569800 | 1.14440800 | -0.53279000 |
| O | 0.88485800 | 1.53883400 | -1.68102400 |
| C | 2.00339000 | 3.11922200 | 0.21127800 |
| H | 1.41851200 | 3.62457100 | -0.56078000 |
| H | 1.93424500 | 3.67540000 | 1.14824100 |
| O | 1.37271800 | 1.84614800 | 0.51161100 |
| C | 3.44672700 | 2.91749100 | -0.22048900 |
| H | 3.92339000 | 3.89167300 | -0.37451500 |
| H | 4.00765900 | 2.37407900 | 0.54549600 |
| H | 3.49610500 | 2.35907700 | -1.15860900 |
| H | -0.22093100 | -0.60570700 | -0.93379200 |
| C | -1.60430800 | 0.67140200 | 1.08780600 |
| H | -1.48711100 | 1.70622500 | 1.39798400 |
| C | -0.40983100 | -0.22327300 | 1.21515100 |
| H | 0.24424200 | 0.12092900 | 2.01908400 |
| H | -0.69754800 | -1.25470400 | 1.43964000 |
| I | 2.10477800 | -1.59700400 | -0.00655900 |
| C | -2.84006300 | 0.29167200 | 0.51066100 |
| C | -3.89260300 | 1.24726900 | 0.39518900 |
| C | -3.09699500 | -1.02488000 | 0.02674500 |
| C | -5.11539600 | 0.90806400 | -0.16376100 |
| H | -3.71963100 | 2.25789700 | 0.75494700 |
| C | -4.32462800 | -1.35341400 | -0.53229700 |
| H | -2.32492700 | -1.78416700 | 0.09498900 |
| C | -5.34324400 | -0.39476100 | -0.63342300 |
| H | -5.89917500 | 1.65600300 | -0.23982600 |
| H | -4.49488600 | -2.36282900 | -0.89522000 |
| H | -6.30016600 | -0.65842900 | -1.07262200 |

**TS4b**

SCF Energy (a.u.) = -627.818453

Thermal correction to Gibbs free Energy (a.u.) = 0.186340

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.00413400 | 0.05658000 | 0.00201400 |
| C | 0.71863600 | 1.27471200 | -0.45961700 |
| O | 0.83726200 | 1.58411800 | -1.62953700 |
| C | 2.03249500 | 3.13843100 | 0.23737700 |
| H | 1.59627400 | 3.64643700 | -0.62607700 |
| H | 1.96868200 | 3.78514400 | 1.11508400 |
| O | 1.19793700 | 2.00036900 | 0.57669100 |
| C | 3.46047600 | 2.69531200 | -0.03659000 |
| H | 4.08527400 | 3.57357500 | -0.23316600 |
| H | 3.87191900 | 2.15938800 | 0.82345700 |
| H | 3.50112100 | 2.03884100 | -0.90905800 |
| H | -0.45771300 | -0.51690000 | -0.78896700 |
| C | -1.53470900 | 0.71852200 | 0.95341000 |
| H | -1.39080500 | 1.78879500 | 1.05930400 |
| C | -0.43902800 | -0.14538700 | 1.41981400 |
| H | 0.23430500 | 0.29827400 | 2.14836100 |
| H | -0.68457300 | -1.17668800 | 1.66036600 |
| I | 2.16972500 | -1.61461600 | -0.09797100 |
| C | -2.81024500 | 0.27607900 | 0.43990000 |
| C | -3.74695200 | 1.24527400 | 0.01335500 |
| C | -3.16925700 | -1.08894200 | 0.35280900 |
| C | -4.99484600 | 0.86757600 | -0.47099700 |
| H | -3.47956500 | 2.29681400 | 0.06749600 |
| C | -4.41508300 | -1.46146300 | -0.13951200 |
| H | -2.46933200 | -1.85661200 | 0.66574200 |
| C | -5.33400600 | -0.48774600 | -0.55167800 |
| H | -5.70210100 | 1.62611100 | -0.79161400 |

| | | | |
|---|---|---|---|
| H | -4.67481000 | -2.51361100 | -0.20273300 |
| H | -6.30538200 | -0.78450000 | -0.93466100 |

**TS4c**

SCF Energy (a.u.) = -616.946761

Thermal correction to Gibbs free Energy (a.u.) = 0.193624

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.70664500 | -1.07389300 | -0.58386200 |
| C | 1.96187000 | -0.69787100 | 0.11071700 |
| O | 2.42921600 | -1.29064300 | 1.06776300 |
| C | 3.75739400 | 0.85329400 | 0.15264100 |
| H | 3.58645800 | 1.06858600 | 1.21167600 |
| H | 4.48442100 | 0.03826500 | 0.08866500 |
| O | 2.51211500 | 0.40499500 | -0.43530500 |
| C | 4.20405000 | 2.08056200 | -0.61605900 |
| H | 5.14697600 | 2.45166900 | -0.20150800 |
| H | 4.36054300 | 1.84376600 | -1.67253400 |
| H | 3.45868500 | 2.87846200 | -0.54670100 |
| H | 0.35448400 | -0.44017800 | -1.38651400 |
| C | -0.56304100 | -1.07185600 | 0.61095900 |
| H | -0.13845000 | -0.92011000 | 1.59754000 |
| C | -0.09193300 | -2.25858600 | -0.12188100 |
| H | 0.48383300 | -2.98340900 | 0.44685600 |
| H | -0.74246500 | -2.70293900 | -0.87005700 |
| C | -1.77185400 | -0.30392100 | 0.29633300 |
| C | -2.18291900 | 0.71037600 | 1.18154600 |
| C | -2.53954700 | -0.52667100 | -0.86228600 |
| C | -3.32147000 | 1.47103600 | 0.92325900 |
| H | -1.60060000 | 0.89545200 | 2.08004300 |
| C | -3.67442300 | 0.23928400 | -1.12329400 |
| H | -2.25120300 | -1.30093300 | -1.56634800 |

| | | | |
|---|---|---|---|
| C | -4.07278000 | 1.24079800 | -0.23278000 |
| H | -3.62193300 | 2.24482200 | 1.62328600 |
| H | -4.25231200 | 0.05135000 | -2.02323900 |
| H | 1.68762900 | -1.84864400 | -1.81516000 |
| H | -4.95867100 | 1.83372200 | -0.43743200 |

**14**

SCF Energy (a.u.) = -862.303821

Thermal correction to Gibbs free Energy (a.u.) = 0.240918

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.23761700 | -2.11087600 | 0.00069300 |
| N | 0.00000500 | -2.75335600 | 0.00035300 |
| C | 1.23761800 | -2.11087300 | 0.00067500 |
| C | 1.23748000 | -0.73343800 | -0.00017200 |
| C | -1.23747600 | -0.73344000 | -0.00015200 |
| C | -0.00000200 | -0.01021300 | -0.00063700 |
| H | -0.00000300 | 1.06622400 | -0.00127700 |
| H | 0.00000600 | -3.76163400 | 0.00352200 |
| C | 2.53244700 | -0.01503600 | -0.00091700 |
| O | 2.36312500 | 1.32718600 | 0.00077300 |
| O | 3.64073900 | -0.53362100 | -0.00290700 |
| C | -2.53244600 | -0.01503700 | -0.00087300 |
| O | -2.36312800 | 1.32718400 | 0.00076600 |
| O | -3.64073500 | -0.53362600 | -0.00286300 |
| C | 3.56916500 | 2.12217000 | -0.00017900 |
| H | 4.16145700 | 1.86266400 | 0.88264400 |
| H | 4.15943100 | 1.86363700 | -0.88463600 |
| C | -3.56917000 | 2.12216500 | -0.00020200 |
| H | -4.15944400 | 1.86359900 | -0.88464500 |
| H | -4.16145300 | 1.86268900 | 0.88263500 |
| C | 2.42482300 | -3.02801000 | 0.00121600 |

| | | | |
|---|---|---|---|
| H | 3.06269400 | -2.85212100 | 0.87107800 |
| H | 2.10021600 | -4.07391000 | 0.00744000 |
| H | 3.05660200 | -2.86096900 | -0.87497100 |
| C | -2.42481700 | -3.02801800 | 0.00125200 |
| H | -2.10020500 | -4.07391700 | 0.00744300 |
| H | -3.06266100 | -2.85215400 | 0.87113900 |
| H | -3.05662700 | -2.86096300 | -0.87491000 |
| C | 3.14873700 | 3.57874600 | 0.00113800 |
| H | 2.55421600 | 3.81269600 | 0.88932500 |
| H | 4.03651700 | 4.21958700 | 0.00058300 |
| H | 2.55234100 | 3.81376100 | -0.88551100 |
| C | -3.14874500 | 3.57874200 | 0.00105900 |
| H | -2.55235900 | 3.81372700 | -0.88560300 |
| H | -4.03652700 | 4.21958100 | 0.00049100 |
| H | -2.55421600 | 3.81272500 | 0.88923300 |

**15**

SCF Energy (a.u.) = -416.736530

Thermal correction to Gibbs free Energy (a.u.) = 0.078848

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -3.55836300 | -0.06348100 | 0.18325700 |
| N | -2.56998500 | -0.17182600 | -0.44552800 |
| C | -1.31326600 | -0.77909100 | 0.13359500 |
| C | -0.17857100 | 0.22570700 | 0.04241600 |
| O | -0.31674600 | 1.42736700 | 0.04088600 |
| C | 2.18932900 | 0.42598000 | -0.00201000 |
| H | 2.13992800 | 1.07821200 | -0.87818000 |
| H | 2.16684300 | 1.05632700 | 0.89147600 |
| H | -1.47693200 | -1.05759200 | 1.18038900 |
| O | 1.00242100 | -0.41603000 | 0.00440000 |
| C | 3.39497700 | -0.49003400 | -0.03179500 |

| | | | |
|---|---|---|---|
| H | 4.30985000 | 0.11093300 | -0.03815700 |
| H | 3.41616000 | -1.14001600 | 0.84778200 |
| H | 3.38894900 | -1.11715300 | -0.92800500 |
| H | -1.08657800 | -1.66962500 | -0.45493500 |

**TS5**

SCF Energy (a.u.) = -416.734196

Thermal correction to Gibbs free Energy (a.u.) = 0.076555

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -3.16940900 | -0.73918000 | -0.62677300 |
| N | -2.12922800 | -0.93836300 | -0.17509500 |
| C | -1.43037300 | 0.20923700 | 0.89702000 |
| C | -0.19607300 | 0.70126500 | 0.21675900 |
| O | -0.13708800 | 1.73108600 | -0.42825100 |
| C | 2.05714500 | 0.17134100 | -0.31856400 |
| H | 1.83641600 | 0.27494800 | -1.38482700 |
| H | 2.40572100 | 1.14067700 | 0.04955000 |
| H | -2.17926900 | 0.98575000 | 1.02239000 |
| O | 0.82398500 | -0.16268800 | 0.37138500 |
| C | 3.04771900 | -0.94044400 | -0.04080700 |
| H | 3.99318800 | -0.72355800 | -0.54810700 |
| H | 3.24502800 | -1.03110700 | 1.03137700 |
| H | 2.67147800 | -1.89986600 | -0.40737000 |
| H | -1.24778800 | -0.39961700 | 1.77853600 |

**16**

SCF Energy (a.u.) = -416.768785

Thermal correction to Gibbs free Energy (a.u.) = 0.068741

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | -0.30170300 | 2.46497300 | 0.36620600 |
| N | -1.29168600 | 2.39077500 | -0.11891000 |
| C | -1.87831600 | -1.12612400 | -0.92149300 |

| | | | |
|---|---|---|---|
| C | -0.81066100 | -1.03757900 | 0.05018400 |
| O | -0.93104900 | -1.30168600 | 1.24185300 |
| C | 1.47989000 | -0.49371600 | 0.39363700 |
| H | 1.19650800 | 0.16674300 | 1.21839200 |
| H | 1.69763200 | -1.48004900 | 0.81575200 |
| H | -2.85430700 | -1.44730100 | -0.58211700 |
| O | 0.35497800 | -0.61734000 | -0.50721700 |
| C | 2.64345500 | 0.05779200 | -0.40498600 |
| H | 3.51928300 | 0.16002500 | 0.24379400 |
| H | 2.90273500 | -0.60916200 | -1.23254600 |
| H | 2.40201700 | 1.04290100 | -0.81483700 |
| H | -1.70778200 | -0.87343000 | -1.96065000 |

**$N_2$**

SCF Energy (a.u.) = -109.568079

Thermal correction to Gibbs free Energy (a.u.) = -0.012858

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| N | 0.00000000 | 0.00000000 | 0.55256100 |
| N | 0.00000000 | 0.00000000 | -0.55256100 |

**17**

SCF Energy (a.u.) = -307.197100

Thermal correction to Gibbs free Energy (a.u.) = 0.072991

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.13413100 | -0.93243200 | -0.00004500 |
| H | -3.16517800 | -0.60390700 | -0.00024700 |
| C | -1.09518800 | 0.07446300 | 0.00000700 |
| O | -1.29880300 | 1.28373900 | -0.00009300 |
| O | 0.14838600 | -0.47367900 | 0.00015500 |
| C | 1.25151600 | 0.46131600 | 0.00016400 |
| H | 1.16641500 | 1.10187500 | -0.88333900 |

| | | | |
|---|---|---|---|
| H | 1.16667200 | 1.10153100 | 0.88394800 |
| C | 2.53392300 | -0.34626000 | -0.00016600 |
| H | 2.59565200 | -0.98264400 | -0.88795100 |
| H | 3.39479600 | 0.33011100 | -0.00016200 |
| H | 2.59590900 | -0.98298100 | 0.88735900 |
| H | -1.88765300 | -1.98698900 | 0.00013000 |

**A1**

SCF Energy (a.u.) = -309.804896

Thermal correction to Gibbs free Energy (a.u.) = 0.101978

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.78236900 | -1.04554300 | 0.00004900 |
| C | 0.40717000 | -1.28309100 | -0.00000500 |
| C | -0.51511800 | -0.22265100 | -0.00004600 |
| C | -0.01237800 | 1.09180800 | -0.00007200 |
| C | 1.35911100 | 1.33141300 | -0.00002100 |
| C | 2.26481300 | 0.26418600 | 0.00004500 |
| H | 2.47455800 | -1.88222800 | 0.00008300 |
| H | 0.03710400 | -2.30501900 | -0.00000500 |
| H | -0.69808100 | 1.93279700 | -0.00015900 |
| H | 1.72569900 | 2.35368600 | -0.00004000 |
| H | 3.33364300 | 0.45462000 | 0.00009000 |
| C | -1.95375100 | -0.53244100 | -0.00007200 |
| H | -2.18725900 | -1.59648400 | -0.00025200 |
| C | -2.97460400 | 0.33680500 | 0.00010700 |
| H | -4.00135100 | -0.01333600 | 0.00005800 |
| H | -2.82998700 | 1.41305000 | 0.00031300 |

**TS6**

SCF Energy (a.u.) = -617.007797

Thermal correction to Gibbs free Energy (a.u.) = 0.197237

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 2.95373600 | -0.54727500 | -0.26283700 |
| C | 2.05284300 | 0.28104700 | 0.51380000 |
| O | 1.77275600 | 0.10079100 | 1.69263000 |
| C | 0.51155200 | 2.09140200 | 0.43529600 |
| H | -0.29879900 | 1.45004600 | 0.79118200 |
| H | 0.98184600 | 2.55683000 | 1.30692100 |
| H | 3.28162700 | -0.21542300 | -1.24028300 |
| O | 1.49194300 | 1.26857300 | -0.23653600 |
| C | 0.02156800 | 3.11945100 | -0.56432500 |
| H | -0.72995500 | 3.76183100 | -0.09367000 |
| H | 0.84410600 | 3.74935900 | -0.91660200 |
| H | -0.43821600 | 2.63026200 | -1.42750900 |
| H | 3.55886700 | -1.25684600 | 0.28511400 |
| C | -2.67681400 | -0.49090700 | 1.15552500 |
| C | -1.54894800 | -1.30247300 | 1.05835800 |
| C | -0.78347700 | -1.34691500 | -0.12442900 |
| C | -1.20037500 | -0.55442700 | -1.21463000 |
| C | -2.32976200 | 0.25155600 | -1.11891000 |
| C | -3.07327900 | 0.29118600 | 0.06676400 |
| H | -3.24407900 | -0.46444000 | 2.08083200 |
| H | -1.23216500 | -1.89467900 | 1.91163600 |
| H | -0.63562000 | -0.57064300 | -2.14028100 |
| H | -2.63511300 | 0.85240800 | -1.97031900 |
| H | -3.95308800 | 0.92315000 | 0.13837800 |
| C | 0.40370000 | -2.18833400 | -0.16672800 |
| H | 0.54343900 | -2.84295500 | 0.69053400 |
| C | 1.39639500 | -2.13752800 | -1.10354500 |
| H | 2.18547300 | -2.88022700 | -1.09923400 |
| H | 1.29125000 | -1.55428900 | -2.01148600 |

**18**

SCF Energy (a.u.) = -617.051089

Thermal correction to Gibbs free Energy (a.u.) = 0.200561

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 2.08250400 | -1.81888200 | -0.29179500 |
| C | 2.01516100 | -0.58016600 | 0.57395900 |
| O | 1.96918500 | -0.57471600 | 1.78722900 |
| C | 1.78952000 | 1.78712400 | 0.53973400 |
| H | 0.84644500 | 1.71778100 | 1.08924900 |
| H | 2.59968100 | 1.90429500 | 1.26489800 |
| H | 2.98060900 | -1.77071000 | -0.91846400 |
| O | 1.98576800 | 0.54292100 | -0.17744400 |
| C | 1.77013900 | 2.90378200 | -0.48413000 |
| H | 1.62921200 | 3.86421400 | 0.02207100 |
| H | 2.71054400 | 2.94245400 | -1.04201500 |
| H | 0.94973000 | 2.76836900 | -1.19488700 |
| H | 2.16992200 | -2.67618200 | 0.37887300 |
| C | -3.37641700 | -0.02951100 | 0.80550700 |
| C | -2.47749900 | -1.06466200 | 0.60158100 |
| C | -1.34235700 | -0.90909000 | -0.25023600 |
| C | -1.17957100 | 0.35756600 | -0.88629100 |
| C | -2.08598500 | 1.38696000 | -0.67439400 |
| C | -3.19053900 | 1.20838600 | 0.17082500 |
| H | -4.22784300 | -0.17819900 | 1.46315900 |
| H | -2.62471300 | -2.01803400 | 1.10144600 |
| H | -0.32683600 | 0.52405900 | -1.53289600 |
| H | -1.93543600 | 2.34191900 | -1.17022400 |
| H | -3.89419900 | 2.01875500 | 0.33233600 |
| C | -0.44302100 | -1.98781300 | -0.42056700 |
| H | -0.65411600 | -2.89858800 | 0.13632900 |
| C | 0.83142600 | -1.96041400 | -1.20255600 |

| | | | |
|---|---|---|---|
| H | 0.94168300 | -2.89683100 | -1.76404300 |
| H | 0.83552800 | -1.14861000 | -1.93392700 |

**ArSH**

SCF Energy (a.u.) = -669.931025

Thermal correction to Gibbs free Energy (a.u.) = 0.091190

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.29470400 | 1.20661500 | -0.00280000 |
| C | -1.10154600 | 1.20106900 | -0.00758000 |
| C | -1.82884100 | 0.00556500 | -0.00809700 |
| C | -1.10563600 | -1.19587300 | -0.00741800 |
| C | 0.28739300 | -1.20689200 | -0.00238400 |
| C | 1.00159000 | -0.00052700 | 0.00072300 |
| H | 0.82566500 | 2.15395900 | -0.00463400 |
| H | -1.63159000 | 2.14995700 | -0.01238600 |
| H | -1.64045300 | -2.14231300 | -0.01222300 |
| H | 0.81935500 | -2.15371900 | -0.00340100 |
| S | 2.78576300 | -0.08295200 | 0.00388900 |
| C | -3.33810700 | 0.00257800 | 0.01113800 |
| H | -3.74072800 | 0.98783000 | -0.24061500 |
| H | -3.74497400 | -0.72094400 | -0.70317200 |
| H | -3.72119600 | -0.26833600 | 1.00265000 |
| H | 3.00438200 | 1.24558300 | 0.01007800 |

**ArS radical**

SCF Energy (a.u.) = -669.300681

Thermal correction to Gibbs free Energy (a.u.) = 0.083529

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.33854400 | 1.21658000 | -0.00451200 |
| C | -1.04797700 | 1.20910300 | -0.01174500 |
| C | -1.76887000 | 0.00000100 | -0.01263500 |

| | | | |
|---|---|---|---|
| C | -1.04797700 | -1.20910200 | -0.01174500 |
| C | 0.33854300 | -1.21657900 | -0.00451200 |
| C | 1.07259600 | 0.00000000 | 0.00011300 |
| H | 0.88704400 | 2.15245100 | -0.00532800 |
| H | -1.59021100 | 2.15082300 | -0.01846200 |
| H | -1.59021200 | -2.15082100 | -0.01846200 |
| H | 0.88704300 | -2.15245100 | -0.00532800 |
| S | 2.79661200 | -0.00000100 | 0.00743300 |
| C | -3.27379000 | 0.00000000 | 0.01607200 |
| H | -3.68351900 | 0.88764900 | -0.47438100 |
| H | -3.68351800 | -0.88758100 | -0.47450800 |
| H | -3.63882600 | -0.00007700 | 1.05133000 |

**TS7**

SCF Energy (a.u.) = -1286.984730

Thermal correction to Gibbs free Energy (a.u.) = 0.313317

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.42621000 | -1.97600400 | 1.88504100 |
| C | 0.21346300 | -1.77123100 | 0.51706000 |
| C | -0.25250700 | -0.54862400 | 0.05153300 |
| C | -0.52497900 | 0.51333600 | 0.94534600 |
| C | -0.28891200 | 0.29118400 | 2.32353000 |
| C | 0.17181400 | -0.93541900 | 2.78610100 |
| H | 0.79096300 | -2.93342000 | 2.24411000 |
| H | 0.42545500 | -2.56696600 | -0.19037400 |
| H | -0.39949900 | -0.40687700 | -1.01140400 |
| H | -0.48743900 | 1.09636300 | 3.02505000 |
| H | 0.33297200 | -1.08495800 | 3.84940100 |
| C | -0.96571000 | 1.82036100 | 0.49468200 |
| H | -1.25005900 | 2.49906000 | 1.30152200 |
| C | -1.73551100 | 2.02387500 | -0.78904600 |

| | | | |
|---|---|---|---|
| H | -1.35641700 | 1.37229500 | -1.58014800 |
| H | -1.59474000 | 3.05259500 | -1.13796600 |
| C | -3.25808000 | 1.79108800 | -0.61447300 |
| H | -3.75116100 | 1.93626500 | -1.58217400 |
| H | -3.67282100 | 2.50604200 | 0.09957500 |
| C | -3.58270900 | 0.40653100 | -0.09935300 |
| C | -3.41037700 | -1.91748500 | -0.56751000 |
| H | -4.46702500 | -2.09804100 | -0.34965700 |
| H | -2.84272200 | -2.04853900 | 0.35749100 |
| O | -4.05571400 | 0.16022700 | 0.99179200 |
| O | -3.25685500 | -0.54341500 | -1.00226900 |
| C | -2.89462600 | -2.80472500 | -1.68194000 |
| H | -3.45619400 | -2.64279500 | -2.60684200 |
| H | -1.83697600 | -2.60634900 | -1.87860700 |
| H | -2.99913000 | -3.85579600 | -1.39391500 |
| C | 2.89394800 | 0.75047400 | 0.72870800 |
| C | 3.41422100 | -0.53674800 | 0.65022000 |
| C | 3.47853900 | -1.22116000 | -0.57311400 |
| C | 3.01642400 | -0.56633000 | -1.72154500 |
| C | 2.48341300 | 0.72105500 | -1.65186300 |
| C | 2.40652800 | 1.39184500 | -0.42198300 |
| H | 2.84146600 | 1.26299700 | 1.68285700 |
| H | 3.76673100 | -1.02530700 | 1.55473900 |
| H | 3.06544500 | -1.07293000 | -2.68212900 |
| H | 2.11549300 | 1.21209400 | -2.54694000 |
| S | 1.68082100 | 3.01194100 | -0.31556600 |
| H | 0.34029700 | 2.48610700 | 0.15065300 |
| C | 4.00974100 | -2.63128600 | -0.63450500 |
| H | 4.14924600 | -2.96220900 | -1.66734600 |
| H | 4.97104900 | -2.71903700 | -0.11699500 |
| H | 3.31714500 | -3.33057000 | -0.14936200 |

**19**

SCF Energy (a.u.) = -1287.008240

Thermal correction to Gibbs free Energy (a.u.) = 0.317296

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.06046600 | -2.95424300 | 0.50348800 |
| C | -0.26044200 | -2.12729900 | -0.29192700 |
| C | -0.09843600 | -0.78257700 | 0.03641400 |
| C | -0.72760600 | -0.23185800 | 1.16215900 |
| C | -1.52938900 | -1.06780100 | 1.94784000 |
| C | -1.69647300 | -2.41783000 | 1.62470000 |
| H | -1.19084000 | -4.00172300 | 0.24787100 |
| H | 0.23770400 | -2.52969900 | -1.16958100 |
| H | 0.52371200 | -0.15203100 | -0.58898500 |
| H | -2.04389800 | -0.65447600 | 2.81028100 |
| H | -2.33042200 | -3.04462600 | 2.24468200 |
| C | -0.51793700 | 1.22594800 | 1.51725500 |
| H | -1.01317900 | 1.44206600 | 2.47133900 |
| C | -0.99610500 | 2.23498200 | 0.45495200 |
| H | -0.63382200 | 1.93539600 | -0.53323700 |
| H | -0.54210600 | 3.20806400 | 0.67159700 |
| C | -2.52237500 | 2.42714000 | 0.40823300 |
| H | -2.76429800 | 3.17726100 | -0.35416400 |
| H | -2.89515600 | 2.79117400 | 1.36917500 |
| C | -3.29988100 | 1.17016100 | 0.08314700 |
| C | -3.50303400 | -0.62764200 | -1.45781100 |
| H | -4.58997100 | -0.51678300 | -1.51381900 |
| H | -3.27075500 | -1.33850600 | -0.66099000 |
| O | -4.15916400 | 0.67829600 | 0.78886100 |
| O | -2.92339900 | 0.65158000 | -1.10319100 |
| C | -2.89912500 | -1.04417200 | -2.78336100 |

| | | | |
|---|---|---|---|
| H | -3.12617000 | -0.31442800 | -3.56657000 |
| H | -1.81348600 | -1.13983200 | -2.69673800 |
| H | -3.30794100 | -2.01402100 | -3.08559300 |
| C | 3.09268400 | 0.66887700 | 0.97299500 |
| C | 3.25278200 | -0.70362000 | 1.05274800 |
| C | 3.30412300 | -1.49888700 | -0.10845200 |
| C | 3.21263100 | -0.86296400 | -1.35960900 |
| C | 3.04476700 | 0.51110500 | -1.45471400 |
| C | 2.96477800 | 1.31563500 | -0.28660300 |
| H | 3.05035000 | 1.27372300 | 1.87240300 |
| H | 3.32433800 | -1.18100900 | 2.02599700 |
| H | 3.26196000 | -1.46192300 | -2.26481900 |
| H | 2.96119300 | 0.99347200 | -2.42278200 |
| S | 2.68932000 | 3.01311500 | -0.39038900 |
| H | 0.55328400 | 1.39193800 | 1.67608700 |
| C | 3.40395900 | -2.99464400 | -0.00055700 |
| H | 3.70558800 | -3.44886900 | -0.94803000 |
| H | 4.11982700 | -3.29287800 | 0.77190100 |
| H | 2.42875300 | -3.41299600 | 0.27945500 |

**20**

SCF Energy (a.u.) = -617.699973

Thermal correction to Gibbs free Energy (a.u.) = 0.215318

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -2.84650200 | 0.10178700 | 0.52184400 |
| C | -2.57178500 | -0.21035800 | -0.81364000 |
| C | -1.46849600 | -1.00082400 | -1.13377200 |
| C | -0.61820000 | -1.49422000 | -0.13295500 |
| C | -0.90749800 | -1.17999700 | 1.19982700 |
| C | -2.01016300 | -0.38581200 | 1.52731300 |
| H | -3.70570500 | 0.71600300 | 0.77411900 |

| | | | |
|---|---|---|---|
| H | -3.22042300 | 0.15826300 | -1.60315600 |
| H | -1.26009400 | -1.23805300 | -2.17423800 |
| H | -0.25621200 | -1.54420500 | 1.98874300 |
| H | -2.21064300 | -0.14828600 | 2.56770500 |
| C | 0.59041800 | -2.32597300 | -0.50321300 |
| H | 0.92332800 | -2.89854800 | 0.37096900 |
| C | 1.78092300 | -1.51552600 | -1.05803300 |
| H | 1.43929200 | -0.86905900 | -1.87281600 |
| H | 2.50281300 | -2.21947600 | -1.48858900 |
| C | 2.52458100 | -0.67065100 | -0.01153000 |
| H | 3.42796800 | -0.25020100 | -0.47210000 |
| H | 2.84912500 | -1.28660000 | 0.83171300 |
| C | 1.75531400 | 0.49759000 | 0.57109500 |
| C | 0.32436300 | 2.32626100 | 0.06451100 |
| H | 0.96331700 | 3.04511500 | 0.58634200 |
| H | -0.40689900 | 1.93637700 | 0.77645900 |
| O | 1.71688500 | 0.77897800 | 1.75341700 |
| O | 1.14583400 | 1.22124900 | -0.38758400 |
| C | -0.33837000 | 2.92633600 | -1.15851300 |
| H | 0.40688900 | 3.29364300 | -1.87073400 |
| H | -0.96613700 | 2.18306600 | -1.65691700 |
| H | -0.97180100 | 3.76738400 | -0.85779300 |
| H | 0.29591600 | -3.05891300 | -1.26397000 |

**21**

SCF Energy (a.u.) = -1531.675193

Thermal correction to Gibbs free Energy (a.u.) = 0.359694

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.62300100 | -1.20788600 | -1.73085400 |
| N | 0.49481300 | -1.94831000 | -1.57124900 |
| C | 1.65440500 | -1.62231200 | -0.75944600 |

| | | | |
|---|---|---|---|
| C | 1.73154800 | -0.13106000 | -0.59516900 |
| C | -0.59884100 | 0.12800200 | -1.34847200 |
| C | 0.63376300 | 0.64137700 | -0.83324600 |
| H | 0.69201700 | 1.70077000 | -0.62724000 |
| H | 0.43244500 | -2.92472300 | -1.82739700 |
| C | 2.96264000 | 0.46328100 | -0.04270800 |
| O | 2.83377800 | 1.79337300 | 0.20572300 |
| O | 4.00142600 | -0.13761800 | 0.18665300 |
| C | -1.78357600 | 0.97580400 | -1.46961300 |
| O | -1.52238500 | 2.26139000 | -1.10261500 |
| O | -2.89249300 | 0.61750900 | -1.84955700 |
| C | 4.00310100 | 2.45377000 | 0.73633800 |
| H | 4.29456100 | 1.95995500 | 1.66820600 |
| H | 4.82737600 | 2.33607100 | 0.02601400 |
| C | -2.62221500 | 3.19463400 | -1.16474500 |
| H | -2.14091900 | 4.16708600 | -1.29212300 |
| H | -3.22971700 | 2.96974600 | -2.04450600 |
| C | 2.87516300 | -2.31839700 | -1.36416900 |
| H | 3.73169300 | -2.24221300 | -0.69820900 |
| H | 2.64674600 | -3.37464300 | -1.54271700 |
| H | 3.12858300 | -1.84303800 | -2.31656400 |
| C | -1.78694600 | -1.90754800 | -2.36543000 |
| H | -1.51490300 | -2.92589800 | -2.65901900 |
| H | -2.62091000 | -1.94502700 | -1.66092400 |
| H | -2.14625700 | -1.35743900 | -3.23661700 |
| C | 3.63947200 | 3.90997300 | 0.95088100 |
| H | 2.81116400 | 4.00572300 | 1.65951000 |
| H | 4.50212400 | 4.45072400 | 1.35360700 |
| H | 3.34478800 | 4.38260900 | 0.00904900 |
| C | -3.45653100 | 3.14879900 | 0.10540300 |
| H | -2.83088200 | 3.32611700 | 0.98572900 |

| | | | |
|---|---|---|---|
| H | -4.23101100 | 3.92297200 | 0.07005600 |
| H | -3.94401100 | 2.17758600 | 0.20784800 |
| S | 1.44258200 | -2.46624600 | 0.97711700 |
| C | -0.14195800 | -1.78877700 | 1.42337500 |
| C | -1.32057900 | -2.48541600 | 1.11473300 |
| C | -0.23808700 | -0.52724700 | 2.02351700 |
| C | -2.56403400 | -1.91182300 | 1.36266600 |
| H | -1.25123600 | -3.47201300 | 0.66771800 |
| C | -1.48917900 | 0.04400400 | 2.25974400 |
| H | 0.66694100 | 0.01213800 | 2.27937600 |
| C | -2.66947400 | -0.62997900 | 1.92359800 |
| H | -3.46834300 | -2.45947800 | 1.10894800 |
| H | -1.54807600 | 1.03388000 | 2.70398500 |
| C | -4.02470500 | -0.01384700 | 2.16343200 |
| H | -4.61960100 | -0.62422400 | 2.85245100 |
| H | -3.93792900 | 0.98846500 | 2.59028200 |
| H | -4.58807000 | 0.06361300 | 1.22676500 |

**TS8**

SCF Energy (a.u.) = -1531.667004

Thermal correction to Gibbs free Energy (a.u.) = 0.352822

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.47637100 | -0.15770800 | -1.53177000 |
| N | -1.43157900 | -1.50144800 | -1.31577400 |
| C | -0.31767900 | -2.17592700 | -0.94397100 |
| C | 0.87743400 | -1.46135400 | -0.78131800 |
| C | -0.31675000 | 0.59661000 | -1.30019700 |
| C | 0.84595600 | -0.07064900 | -0.91370700 |
| H | 1.74277700 | 0.49891200 | -0.71775600 |
| H | -2.40041600 | -1.90015400 | -0.83320400 |
| C | 2.14787200 | -2.15156600 | -0.42312500 |

| | | | |
|---|---|---|---|
| O | 3.07832100 | -1.28190200 | 0.01889000 |
| O | 2.34311400 | -3.34925600 | -0.51688800 |
| C | -0.30997900 | 2.08580500 | -1.41515900 |
| O | 0.79922100 | 2.61461700 | -0.86201700 |
| O | -1.17778500 | 2.75960500 | -1.93692500 |
| C | 4.36598300 | -1.84722400 | 0.37640900 |
| H | 4.20830900 | -2.59624000 | 1.15745000 |
| H | 4.77521700 | -2.35614300 | -0.50101600 |
| C | 0.89794800 | 4.06072700 | -0.88657500 |
| H | 0.81459900 | 4.39787600 | -1.92346300 |
| H | 0.04974300 | 4.46958200 | -0.32987300 |
| C | -0.50284100 | -3.64339600 | -0.72084200 |
| H | 0.12581100 | -4.00472700 | 0.09145700 |
| H | -1.55298400 | -3.84762100 | -0.50253200 |
| H | -0.20392900 | -4.19422500 | -1.61965300 |
| C | -2.79235500 | 0.34432800 | -2.02986800 |
| H | -3.59215200 | -0.27262300 | -1.60920200 |
| H | -2.94143200 | 1.39228000 | -1.78914000 |
| H | -2.81883300 | 0.24490300 | -3.12259900 |
| C | 5.24487500 | -0.70521900 | 0.84347600 |
| H | 4.80848400 | -0.20590100 | 1.71347500 |
| H | 6.22884000 | -1.09232500 | 1.12620500 |
| H | 5.38182600 | 0.03484400 | 0.04943300 |
| C | 2.22711600 | 4.43358200 | -0.26312300 |
| H | 3.05927700 | 4.00419300 | -0.82896400 |
| H | 2.33808800 | 5.52247300 | -0.26176600 |
| H | 2.28761500 | 4.07989800 | 0.76970700 |
| S | -3.52458700 | -1.97117200 | 0.62689200 |
| C | -2.50525000 | -0.70059500 | 1.33231800 |
| C | -2.84509900 | 0.66204000 | 1.22044500 |
| C | -1.26067100 | -1.00309500 | 1.92430900 |

| | | | |
|---|---|---|---|
| C | -1.96810000 | 1.66668300 | 1.63495000 |
| H | -3.80289600 | 0.92628400 | 0.78457400 |
| C | -0.38596600 | 0.00364200 | 2.32518100 |
| H | -0.98271700 | -2.04516200 | 2.04990100 |
| C | -0.71441800 | 1.36021800 | 2.17626700 |
| H | -2.25966400 | 2.70766900 | 1.51534200 |
| H | 0.57647500 | -0.26731800 | 2.75466400 |
| C | 0.24454500 | 2.44164600 | 2.61026800 |
| H | 0.31772800 | 2.49714400 | 3.70333400 |
| H | 1.25242700 | 2.25578200 | 2.22377100 |
| H | -0.07821400 | 3.42367800 | 2.25170700 |

**22**

SCF Energy (a.u.) = -1531.683874

Thermal correction to Gibbs free Energy (a.u.) = 0.350447

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.17223400 | -1.80390200 | -1.41529400 |
| N | 2.16499900 | -0.91709200 | -1.59500600 |
| C | 1.94566900 | 0.40643800 | -1.52810700 |
| C | 0.65003400 | 0.91421200 | -1.28134600 |
| C | -0.14970700 | -1.37061700 | -1.16868000 |
| C | -0.38899500 | 0.00144400 | -1.11523000 |
| H | -1.38536700 | 0.36073900 | -0.90676500 |
| H | 3.44154800 | -1.15436100 | 0.27343500 |
| C | 0.39156500 | 2.36673900 | -1.10393000 |
| O | -0.92126800 | 2.62546400 | -0.90036000 |
| O | 1.23806200 | 3.24255500 | -1.10977000 |
| C | -1.24979300 | -2.32268100 | -0.86897800 |
| O | -2.42101000 | -1.68452900 | -0.63727200 |
| O | -1.14044300 | -3.53433100 | -0.80327000 |
| C | -1.26686500 | 4.00692100 | -0.64917700 |

| | | | |
|---|---|---|---|
| H | -0.68967100 | 4.35880200 | 0.21130700 |
| H | -0.97128700 | 4.60535900 | -1.51589800 |
| C | -3.54449700 | -2.52098100 | -0.27665800 |
| H | -3.74610100 | -3.21115700 | -1.10121900 |
| H | -3.26810700 | -3.11765800 | 0.59781700 |
| C | 3.16510300 | 1.26514200 | -1.69631500 |
| H | 3.39836000 | 1.78296000 | -0.76065000 |
| H | 4.00380400 | 0.62747200 | -1.97760900 |
| H | 3.01017200 | 2.04537600 | -2.44486300 |
| C | 1.58774200 | -3.24601200 | -1.46405500 |
| H | 2.64233700 | -3.29493800 | -1.73737800 |
| H | 1.43580400 | -3.72471200 | -0.49153700 |
| H | 0.98428700 | -3.81494200 | -2.17548500 |
| C | -2.76044700 | 4.05952100 | -0.39770700 |
| H | -3.03198900 | 3.45390600 | 0.47179100 |
| H | -3.06605600 | 5.09316600 | -0.20697100 |
| H | -3.31623500 | 3.69043100 | -1.26476000 |
| C | -4.71718200 | -1.60253400 | 0.00313700 |
| H | -4.96792400 | -1.00774600 | -0.88020200 |
| H | -5.59397700 | -2.19714900 | 0.27850100 |
| H | -4.49084600 | -0.92019400 | 0.82778500 |
| S | 3.56122500 | -0.91644500 | 1.60205600 |
| C | 1.86490600 | -0.37073600 | 1.85733800 |
| C | 0.83191100 | -1.30154900 | 2.02116100 |
| C | 1.56663400 | 0.99495000 | 1.92788500 |
| C | -0.48076100 | -0.86898000 | 2.20480800 |
| H | 1.05749900 | -2.36236400 | 1.99127200 |
| C | 0.25079700 | 1.41772600 | 2.11905300 |
| H | 2.36194000 | 1.72373000 | 1.81345200 |
| C | -0.79632700 | 0.49562500 | 2.23861500 |
| H | -1.27377100 | -1.60466800 | 2.30988600 |

| | | | |
|---|---|---|---|
| H | 0.03472200 | 2.48212200 | 2.15535500 |
| C | -2.22794900 | 0.95485100 | 2.35212400 |
| H | -2.29504500 | 1.95341300 | 2.79378600 |
| H | -2.69406200 | 0.99885600 | 1.35996200 |
| H | -2.82179100 | 0.26957800 | 2.96465100 |

**B**

SCF Energy (a.u.) = -861.736940

Thermal correction to Gibbs free Energy (a.u.) = 0.235784

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.17139000 | 2.19581000 | -0.00023900 |
| N | 0.00000100 | 2.85091700 | -0.00037600 |
| C | 1.17139200 | 2.19580900 | -0.00027100 |
| C | 1.21347400 | 0.78047100 | -0.00005500 |
| C | -1.21347300 | 0.78047200 | -0.00002100 |
| C | 0.00000100 | 0.09164000 | 0.00003600 |
| H | 0.00000000 | -0.98914900 | 0.00017700 |
| C | 2.49826500 | 0.02935300 | 0.00013800 |
| O | 2.30239000 | -1.30937800 | -0.00017700 |
| O | 3.60901600 | 0.52959500 | 0.00058700 |
| C | -2.49826500 | 0.02935500 | 0.00021100 |
| O | -2.30239100 | -1.30937600 | -0.00017500 |
| O | -3.60901400 | 0.52959800 | 0.00065200 |
| C | 3.49580000 | -2.12907000 | 0.00012200 |
| H | 4.08988000 | -1.87912400 | -0.88380500 |
| H | 4.08954000 | -1.87900000 | 0.88423700 |
| C | -3.49580200 | -2.12906700 | 0.00009500 |
| H | -4.08953100 | -1.87904300 | 0.88423100 |
| H | -4.08989400 | -1.87907500 | -0.88381100 |
| C | 2.39319700 | 3.07057400 | -0.00041500 |
| H | 3.02246000 | 2.87024200 | -0.87221700 |

| | | | |
|---|---|---|---|
| H | 2.07160000 | 4.11248400 | -0.00112500 |
| H | 3.02178600 | 2.87132400 | 0.87214000 |
| C | -2.39319500 | 3.07057500 | -0.00035000 |
| H | -2.07159700 | 4.11248500 | -0.00107400 |
| H | -3.02248500 | 2.87023900 | -0.87213100 |
| H | -3.02175600 | 2.87132900 | 0.87222600 |
| C | 3.04856400 | -3.57704000 | 0.00012200 |
| H | 2.45041600 | -3.80215500 | -0.88788200 |
| H | 3.92526600 | -4.23263500 | 0.00029900 |
| H | 2.45012400 | -3.80206400 | 0.88795200 |
| C | -3.04856800 | -3.57703800 | 0.00001500 |
| H | -2.45011800 | -3.80210800 | 0.88782600 |
| H | -3.92527200 | -4.23263100 | 0.00016900 |
| H | -2.45043200 | -3.80210800 | -0.88800800 |

**TS6a**

SCF Energy (a.u.) = -616.996088

Thermal correction to Gibbs free Energy (a.u.) = 0.195031

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -0.56116600 | 0.55918600 | -0.90060700 |
| C | -1.90470800 | 0.89007300 | -0.45282000 |
| O | -2.24911300 | 1.97592000 | -0.00096600 |
| C | -4.07998500 | 0.02952600 | -0.01761200 |
| H | -4.01803400 | 0.35072800 | 1.02729000 |
| H | -4.54604600 | 0.84109000 | -0.58497000 |
| H | -0.40204600 | -0.37409900 | -1.42618200 |
| O | -2.74225600 | -0.18043500 | -0.51929600 |
| C | -4.83324800 | -1.27748400 | -0.16859100 |
| H | -5.85675600 | -1.15987100 | 0.20209000 |
| H | -4.87940400 | -1.58260900 | -1.21827100 |
| H | -4.34930500 | -2.07618600 | 0.40177300 |

| | | | |
|---|---|---|---|
| H | 0.08004400 | 1.39474300 | -1.15106200 |
| C | -0.24110700 | -0.95793400 | 1.53371200 |
| H | -1.18345700 | -0.78011800 | 2.03893700 |
| C | 0.46877200 | 0.09184200 | 0.98504700 |
| H | 0.06547800 | -1.99049000 | 1.40612300 |
| H | 0.21408600 | 1.09135300 | 1.33093500 |
| C | 1.84224200 | -0.04874500 | 0.44214300 |
| C | 2.71386400 | 1.04978600 | 0.49063500 |
| C | 2.30176000 | -1.24288500 | -0.13609400 |
| C | 4.01486000 | 0.95512700 | -0.00550700 |
| H | 2.36749500 | 1.98348700 | 0.92581800 |
| C | 3.60035600 | -1.33917200 | -0.63353700 |
| H | 1.63727100 | -2.09849800 | -0.20844800 |
| C | 4.46401500 | -0.24115300 | -0.56877800 |
| H | 4.67545900 | 1.81525500 | 0.04720400 |
| H | 3.93792200 | -2.27049100 | -1.07841600 |
| H | 5.47431100 | -0.31716400 | -0.95866600 |

**6a**

SCF Energy (a.u.) = -416.240476

Thermal correction to Gibbs free Energy (a.u.) = 0.067024

Charge = -1, Multiplicity = 2

| | | | |
|---|---|---|---|
| N | 3.68915600 | -0.53890900 | -0.00002000 |
| N | 2.61621000 | 0.01962100 | -0.00003200 |
| C | 1.35153500 | -0.51009400 | 0.00002500 |
| C | 0.22799700 | 0.34079700 | -0.00002200 |
| O | 0.13867500 | 1.57597900 | -0.00008400 |
| C | -2.16781800 | 0.31909400 | 0.00017600 |
| H | -2.20944100 | 0.97374200 | 0.88092800 |
| H | -2.20927300 | 0.97418100 | -0.88024600 |
| H | 1.22776200 | -1.59162500 | 0.00015500 |

| | | | |
|---|---|---|---|
| O | -0.96439400 | -0.43160300 | 0.00010100 |
| C | -3.32573800 | -0.66911400 | -0.00015900 |
| H | -4.28486900 | -0.13566900 | -0.00007900 |
| H | -3.28586000 | -1.31212300 | -0.88626400 |
| H | -3.28598000 | -1.31259600 | 0.88560900 |

**6b**

SCF Energy (a.u.) = -416.556179

Thermal correction to Gibbs free Energy (a.u.) = 0.081183

Charge = 1, Multiplicity = 1

| | | | |
|---|---|---|---|
| N | 3.48620100 | 0.23677200 | -0.00012700 |
| N | 2.54613000 | -0.34251400 | -0.00002500 |
| C | 1.24640200 | -0.97050700 | 0.00005700 |
| C | 0.17454700 | 0.18358700 | 0.00007100 |
| O | 0.48907100 | 1.34394700 | -0.00003300 |
| C | -2.19802500 | 0.49884400 | 0.00012400 |
| H | -2.11684200 | 1.12293300 | 0.89188000 |
| H | -2.11659100 | 1.12325600 | -0.89138100 |
| H | 1.19600600 | -1.59169600 | -0.90068900 |
| O | -0.99587900 | -0.39541200 | 0.00015100 |
| C | -3.41250200 | -0.39469200 | -0.00020200 |
| H | -4.30543300 | 0.23807500 | -0.00019600 |
| H | -3.44370100 | -1.02603200 | -0.89173700 |
| H | -3.44393000 | -1.02637100 | 0.89108600 |
| H | 1.19609600 | -1.59163900 | 0.90084800 |

**14a**

SCF Energy (a.u.) = -862.288759

Thermal correction to Gibbs free Energy (a.u.) = 0.243701

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.18742700 | -2.16397700 | -0.00035200 |

| | | | |
|---|---|---|---|
| N | 0.00000100 | -2.82381900 | -0.00043700 |
| C | -1.18742500 | -2.16397700 | -0.00032400 |
| C | -1.25482000 | -0.77370700 | -0.00010500 |
| C | 1.25482100 | -0.77370600 | -0.00013300 |
| C | 0.00000000 | 0.03360300 | 0.00002000 |
| H | -0.00000900 | 0.72947700 | -0.85480300 |
| H | 0.00000900 | 0.72917600 | 0.85509000 |
| C | -2.54193800 | -0.05413000 | 0.00001400 |
| O | -2.35247800 | 1.29080000 | 0.00024700 |
| O | -3.65459500 | -0.55852500 | -0.00009400 |
| C | 2.54193900 | -0.05412800 | -0.00004100 |
| O | 2.35247700 | 1.29080200 | 0.00018700 |
| O | 3.65459600 | -0.55852200 | -0.00017300 |
| C | -3.54976000 | 2.10271500 | 0.00036900 |
| H | -4.14311100 | 1.84942900 | -0.88331400 |
| H | -4.14314100 | 1.84911900 | 0.88394400 |
| C | 3.54975700 | 2.10271800 | 0.00028000 |
| H | 4.14315800 | 1.84912700 | 0.88384300 |
| H | 4.14309100 | 1.84942700 | -0.88341500 |
| C | -2.39307700 | -3.06628200 | -0.00045500 |
| H | -3.02564800 | -2.88212100 | -0.87301800 |
| H | -2.04803200 | -4.10071900 | -0.00058000 |
| H | -3.02568100 | -2.88233800 | 0.87212900 |
| C | 2.39308000 | -3.06628000 | -0.00051300 |
| H | 2.04803600 | -4.10071800 | -0.00064200 |
| H | 3.02563700 | -2.88211000 | -0.87308400 |
| H | 3.02569800 | -2.88234400 | 0.87206300 |
| C | -3.11255400 | 3.55395100 | 0.00063100 |
| H | -2.51541600 | 3.78327800 | -0.88702600 |
| H | -3.99343400 | 4.20392800 | 0.00072900 |
| H | -2.51544700 | 3.78296800 | 0.88838900 |

| | | | |
|---|---|---|---|
| C | 3.11255000 | 3.55395300 | 0.00054200 |
| H | 2.51546200 | 3.78297500 | 0.88831100 |
| H | 3.99342900 | 4.20393200 | 0.00061700 |
| H | 2.51539300 | 3.78327500 | -0.88710400 |

**4’**

SCF Energy (a.u.) = -862.994517

Thermal correction to Gibbs free Energy (a.u.) = 0.250426

Charge = -1, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.22891800 | -2.12720700 | -0.00026100 |
| N | -0.00000100 | -2.74710800 | -0.00033200 |
| C | -1.22892000 | -2.12720600 | -0.00030600 |
| C | -1.28254700 | -0.72802800 | -0.00002600 |
| C | 1.28254600 | -0.72802900 | 0.00002400 |
| C | 0.00000000 | 0.09373800 | 0.00039300 |
| H | 0.00001600 | 0.77141200 | -0.86437000 |
| H | -0.00001700 | 0.77059300 | 0.86581500 |
| H | -0.00000100 | -3.75543600 | -0.00062500 |
| C | -2.53436000 | -0.05257100 | -0.00003500 |
| O | -2.37564600 | 1.34505000 | 0.00032500 |
| O | -3.69102500 | -0.52419900 | -0.00037300 |
| C | 2.53436000 | -0.05257300 | 0.00006000 |
| O | 2.37564800 | 1.34504800 | 0.00026200 |
| O | 3.69102500 | -0.52420000 | -0.00032700 |
| C | -3.57908400 | 2.09809800 | 0.00023900 |
| H | -4.18353000 | 1.84558000 | -0.88081400 |
| H | -4.18396100 | 1.84509200 | 0.88085400 |
| C | 3.57908600 | 2.09809700 | 0.00008800 |
| H | 4.18396500 | 1.84519000 | 0.88072900 |
| H | 4.18353000 | 1.84548000 | -0.88093900 |
| C | -2.41220200 | -3.05295700 | -0.00055800 |

| | | | |
|---|---|---|---|
| H | -3.05561800 | -2.89383500 | -0.87307500 |
| H | -2.07769800 | -4.10039100 | -0.00072300 |
| H | -3.05573800 | -2.89415700 | 0.87193200 |
| C | 2.41220000 | -3.05295900 | -0.00046000 |
| H | 2.07769500 | -4.10039300 | -0.00068100 |
| H | 3.05567600 | -2.89380700 | -0.87292700 |
| H | 3.05567600 | -2.89418700 | 0.87208000 |
| C | -3.19376700 | 3.57005800 | 0.00073600 |
| H | -2.59655700 | 3.81370900 | -0.88431200 |
| H | -4.09210700 | 4.20002900 | 0.00068200 |
| H | -2.59700100 | 3.81322600 | 0.88621600 |
| C | 3.19376800 | 3.57005700 | 0.00042000 |
| H | 2.59700400 | 3.81332400 | 0.88587400 |
| H | 4.09210800 | 4.20002800 | 0.00029300 |
| H | 2.59655600 | 3.81360800 | -0.88465400 |

**5'**

SCF Energy (a.u.) = -670.249327

Thermal correction to Gibbs free Energy (a.u.) = 0.176242

Charge = 1, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.61685500 | -0.55157400 | 0.00000900 |
| C | -0.51101600 | 0.39570600 | -0.00005600 |
| C | -0.74295900 | 1.86241200 | -0.00011700 |
| C | -1.34166800 | -1.96189400 | 0.00010500 |
| C | 0.80358400 | -0.09260700 | -0.00006300 |
| C | 1.05851200 | -1.50872400 | -0.00001100 |
| C | -0.05715900 | -2.41124700 | 0.00009700 |
| C | 2.37332800 | -1.97359800 | -0.00003800 |
| H | 2.56285400 | -3.04231400 | -0.00000200 |
| C | 3.44976200 | -1.07320500 | -0.00010200 |
| C | 3.22217200 | 0.30550200 | -0.00012000 |

| | | | |
|---|---|---|---|
| C | 1.92112600 | 0.81912000 | -0.00009800 |
| C | 1.67930400 | 2.23899400 | -0.00000900 |
| C | 0.42007600 | 2.74109500 | 0.00008100 |
| H | 0.21590900 | 3.80584600 | 0.00026700 |
| H | 2.53749300 | 2.90427500 | 0.00005000 |
| H | -2.16630600 | -2.66280500 | 0.00013000 |
| H | 0.14202100 | -3.47843800 | 0.00015100 |
| H | 4.46622200 | -1.45175300 | -0.00011400 |
| O | -1.89453300 | 2.34010600 | 0.00044700 |
| C | -4.07565600 | -0.90964300 | -0.00006800 |
| H | -4.11767200 | -1.54158600 | -0.89254300 |
| H | -4.11787300 | -1.54116400 | 0.89269500 |
| H | -4.93281000 | -0.23818600 | -0.00032400 |
| H | 4.06270600 | 0.99199100 | -0.00013500 |
| N | -2.86492900 | -0.09719100 | -0.00013300 |
| H | -2.93708900 | 0.93160300 | -0.00046600 |

**18a**

SCF Energy (a.u.) = -425.173186

Thermal correction to Gibbs free Energy (a.u.) = 0.142986

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -0.59717500 | -1.84610400 | -0.93850400 |
| C | 0.27555100 | -1.25552400 | 0.04819100 |
| O | 0.22487700 | -1.47900400 | 1.25361600 |
| C | 2.10496400 | 0.22322100 | 0.40253400 |
| H | 1.53835600 | 0.74104300 | 1.18200700 |
| H | 2.69798800 | -0.55853800 | 0.88815200 |
| H | -0.52170200 | -1.57262200 | -1.98295200 |
| O | 1.17645000 | -0.40144200 | -0.51034800 |
| C | 2.96624000 | 1.17462000 | -0.40391600 |
| H | 3.69020900 | 1.66558500 | 0.25439400 |

| | | | |
|---|---|---|---|
| H | 3.51591500 | 0.64004100 | -1.18425500 |
| H | 2.35482400 | 1.94724800 | -0.88004900 |
| H | -1.33747700 | -2.56092500 | -0.60671900 |
| C | -2.38184900 | 1.13960600 | -0.33302800 |
| H | -2.73698000 | 1.57771600 | -1.26641900 |
| C | -2.94727900 | 0.00977200 | 0.10651300 |
| H | -3.75344200 | -0.47068700 | -0.44033000 |
| H | -2.62225500 | -0.46512300 | 1.02887100 |
| C | -1.27027600 | 1.87054200 | 0.36086700 |
| H | -0.96916200 | 1.35689700 | 1.27840300 |
| H | -0.39367400 | 1.95363600 | -0.29290300 |
| H | -1.57427800 | 2.89250400 | 0.61971200 |

**TS6b**

SCF Energy (a.u.) = -425.167869

Thermal correction to Gibbs free Energy (a.u.) = 0.147470

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.02068200 | -1.53226500 | -0.81864900 |
| C | 0.08698700 | -1.22455300 | 0.06516900 |
| O | 0.20688300 | -1.62187500 | 1.21882500 |
| C | 2.08780900 | 0.03962000 | 0.31165800 |
| H | 1.69554200 | 0.50015300 | 1.22398400 |
| H | 2.65712300 | -0.84669000 | 0.60879500 |
| H | -0.94821500 | -1.25934800 | -1.86383200 |
| O | 0.98022400 | -0.37296000 | -0.51555600 |
| C | 2.92583900 | 1.00797800 | -0.50008300 |
| H | 3.78269500 | 1.34435100 | 0.09271200 |
| H | 3.30125200 | 0.53190500 | -1.41080000 |
| H | 2.34047800 | 1.88680700 | -0.78828300 |
| H | -1.63566000 | -2.38084500 | -0.54641900 |
| C | -2.02326600 | 1.24237500 | -0.32659800 |

| | | | |
|---|---|---|---|
| H | -2.16925600 | 1.73222700 | -1.28851100 |
| C | -2.54990900 | -0.00527300 | -0.13797300 |
| H | -3.27197700 | -0.40369400 | -0.84365000 |
| H | -2.53974800 | -0.45618700 | 0.85046600 |
| C | -1.15999500 | 1.95073200 | 0.66813400 |
| H | -1.03244800 | 1.36153400 | 1.58085500 |
| H | -0.16696500 | 2.15344300 | 0.24733700 |
| H | -1.59038000 | 2.92333100 | 0.94123100 |

**19a**

SCF Energy (a.u.) = -425.200326

Thermal correction to Gibbs free Energy (a.u.) = 0.149568

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -1.02781600 | -1.24105700 | -0.72910300 |
| C | 0.10993400 | -0.88230800 | 0.19873200 |
| O | 0.10804500 | -1.07809200 | 1.39898000 |
| C | 2.26574300 | 0.10714100 | 0.35944200 |
| H | 1.90705200 | 0.79649200 | 1.12984100 |
| H | 2.66632400 | -0.77727200 | 0.86357100 |
| H | -0.76878300 | -0.97667100 | -1.75680100 |
| O | 1.13726500 | -0.29724900 | -0.45493200 |
| C | 3.28184100 | 0.75351300 | -0.56054500 |
| H | 4.15260400 | 1.07523600 | 0.01987900 |
| H | 3.61932300 | 0.04974900 | -1.32717800 |
| H | 2.85669300 | 1.62990100 | -1.05879100 |
| H | -1.16018200 | -2.32784500 | -0.67156700 |
| C | -2.33726000 | 0.93759000 | -0.45301500 |
| H | -2.61053900 | 1.35483300 | -1.42021800 |
| C | -2.35363100 | -0.54826000 | -0.29651500 |
| H | -3.15952900 | -0.98283300 | -0.89906500 |
| H | -2.53948200 | -0.81999500 | 0.75014800 |

| | | | |
|---|---|---|---|
| C | -1.68026700 | 1.83268700 | 0.54474300 |
| H | -1.76982100 | 1.43442100 | 1.56174100 |
| H | -0.59960700 | 1.94931100 | 0.34892500 |
| H | -2.10779300 | 2.84157300 | 0.52469900 |

**TS6c**

SCF Energy (a.u.) = -425.162157

Thermal correction to Gibbs free Energy (a.u.) = 0.146751

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.84231300 | 0.38704400 | -1.17501300 |
| C | -0.37607400 | 0.78575200 | -0.49193200 |
| O | -0.58022400 | 1.87822100 | 0.02020100 |
| C | -2.50301200 | 0.04153900 | 0.27928000 |
| H | -2.26320400 | 0.35760900 | 1.29957400 |
| H | -3.00640000 | 0.87817400 | -0.21545900 |
| H | 0.81506200 | -0.49409600 | -1.80504800 |
| O | -1.27328000 | -0.24099400 | -0.42214600 |
| C | -3.34216700 | -1.22105600 | 0.25655000 |
| H | -4.28817200 | -1.04617700 | 0.77937800 |
| H | -3.56669400 | -1.52281000 | -0.77092600 |
| H | -2.82188500 | -2.04610000 | 0.75271000 |
| H | 1.53224500 | 1.18029100 | -1.43151200 |
| C | 2.04573400 | -0.59543400 | 0.44913300 |
| H | 1.25678800 | -1.34039500 | 0.53598800 |
| C | 2.11461400 | 0.37490200 | 1.41572700 |
| H | 1.28670900 | 0.56365300 | 2.09011700 |
| H | 2.95513400 | 1.06234600 | 1.46113900 |
| C | 3.25332300 | -0.99911100 | -0.36439300 |
| H | 3.82246400 | -1.76849600 | 0.17171900 |
| H | 2.97781300 | -1.41648900 | -1.33665700 |
| H | 3.91979400 | -0.14714000 | -0.53157000 |

**19b**

SCF Energy (a.u.) = -425.186155

Thermal correction to Gibbs free Energy (a.u.) = 0.150688

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.74690400 | 0.14116200 | -0.86399100 |
| C | -0.30679500 | 1.08996800 | -0.32364200 |
| O | -0.10564000 | 2.27566000 | -0.17524800 |
| C | -1.88506100 | -0.78458200 | -0.18169200 |
| H | -1.93584800 | -0.95909300 | -1.26287900 |
| H | -1.13882600 | -1.46142000 | 0.24720900 |
| H | 0.30136800 | -0.64512600 | -1.47936300 |
| O | -1.50951200 | 0.58665800 | 0.06234600 |
| C | -3.24081400 | -0.99845300 | 0.46427300 |
| H | -3.57564600 | -2.02693500 | 0.29444600 |
| H | -3.18547200 | -0.82207800 | 1.54211300 |
| H | -3.98113100 | -0.31470900 | 0.04008500 |
| H | 1.40673200 | 0.73629000 | -1.49994400 |
| C | 1.59066000 | -0.50882700 | 0.26597800 |
| H | 0.89681000 | -1.05751300 | 0.92964300 |
| C | 2.31673400 | 0.50918200 | 1.08326800 |
| H | 2.00472600 | 1.54706400 | 1.10056000 |
| H | 3.10707800 | 0.18965900 | 1.75515400 |
| C | 2.55076900 | -1.55421200 | -0.33130900 |
| H | 3.14845900 | -2.02427700 | 0.45610200 |
| H | 1.99927500 | -2.34238500 | -0.85607200 |
| H | 3.23930900 | -1.08344400 | -1.04115500 |

**TS6$_{para}$ (R=F)**

SCF Energy (a.u.) = -716.289424

Thermal correction to Gibbs free Energy (a.u.) = 0.187821

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 3.30643200 | -0.14778400 | -0.21316900 |
| C | 2.27480300 | 0.53836000 | 0.53834400 |
| O | 1.98913100 | 0.31253700 | 1.70803600 |
| C | 0.50077800 | 2.11927000 | 0.42425900 |
| H | -0.21519400 | 1.37143600 | 0.77507800 |
| H | 0.88603200 | 2.65133500 | 1.29945300 |
| H | 3.60992500 | 0.23231800 | -1.18089400 |
| O | 1.59854500 | 1.43995500 | -0.22587200 |
| C | -0.11482700 | 3.06201600 | -0.58978300 |
| H | -0.95942100 | 3.59100000 | -0.13643600 |
| H | 0.61453900 | 3.80238500 | -0.93197600 |
| H | -0.48352400 | 2.50939600 | -1.45850100 |
| H | 3.99283400 | -0.76416300 | 0.35150200 |
| C | -2.27729300 | -0.90948000 | 1.12393000 |
| C | -1.04458400 | -1.55044500 | 1.03151500 |
| C | -0.26576900 | -1.48589900 | -0.14204600 |
| C | -0.77836500 | -0.75887000 | -1.23735600 |
| C | -2.00957100 | -0.11692400 | -1.16444800 |
| C | -2.73598400 | -0.20201800 | 0.01949800 |
| H | -2.87298000 | -0.94626600 | 2.02894800 |
| H | -0.65960700 | -2.09066700 | 1.89057300 |
| H | -0.20831400 | -0.69305800 | -2.15702500 |
| H | -2.41083600 | 0.44161100 | -2.00263800 |
| C | 1.02976500 | -2.14787900 | -0.16990000 |
| H | 1.24951100 | -2.78126800 | 0.68635200 |
| C | 2.01943200 | -1.94526800 | -1.08914100 |
| H | 2.90786100 | -2.56547200 | -1.07551600 |
| H | 1.84571400 | -1.37697000 | -1.99609400 |
| F | -3.93631500 | 0.42977500 | 0.09551700 |

**TS6a$_{para}$ (R=F)**

SCF Energy (a.u.) = -716.276745

Thermal correction to Gibbs free Energy (a.u.) = 0.185731

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.12600600 | 1.09383600 | -1.38298100 |
| C | 1.75865500 | -0.14906500 | -0.97040400 |
| O | 1.24970200 | -1.26084200 | -1.03664300 |
| C | 3.66204800 | -1.09827800 | 0.09685900 |
| H | 3.03044200 | -1.56360200 | 0.86074700 |
| H | 3.78634300 | -1.82246600 | -0.71417300 |
| H | 1.75826700 | 1.96588700 | -1.50250600 |
| O | 2.98507000 | 0.06761000 | -0.41896000 |
| C | 4.99238400 | -0.64036800 | 0.66161900 |
| H | 5.53924200 | -1.49925600 | 1.06410900 |
| H | 5.60615400 | -0.17373300 | -0.11463600 |
| H | 4.84643800 | 0.08443200 | 1.46835000 |
| H | 0.26172700 | 0.99701800 | -2.02780100 |
| C | 0.92556800 | 1.63027400 | 1.43704000 |
| H | 0.95342700 | 0.77493500 | 2.10345400 |
| C | 0.00794500 | 1.72236000 | 0.40538000 |
| H | -0.09355500 | 2.69533700 | -0.07093200 |
| C | -1.19675200 | 0.86577900 | 0.30590800 |
| C | -2.35476700 | 1.38144600 | -0.29673700 |
| C | -1.22184500 | -0.45422400 | 0.78379100 |
| C | -3.51744700 | 0.61866200 | -0.40654100 |
| H | -2.34958800 | 2.39798200 | -0.68061500 |
| C | -2.37271000 | -1.23233000 | 0.68236900 |
| H | -0.32875500 | -0.89450200 | 1.21088900 |
| C | -3.50069800 | -0.67754300 | 0.09057400 |
| H | -4.41778100 | 1.01226700 | -0.86463300 |
| H | -2.39743800 | -2.25632900 | 1.03727100 |

| | | | |
|---|---|---|---|
| H | 1.71422300 | 2.36628800 | 1.54263100 |
| F | -4.62640500 | -1.43352300 | -0.01206500 |

**$TS6_{para}$ (R=Br)**

SCF Energy (a.u.) = --629.789850

Thermal correction to Gibbs free Energy (a.u.) = 0.183977

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 4.16182900 | 0.27356000 | -0.19125800 |
| C | 3.02887200 | 0.80547700 | 0.54217000 |
| O | 2.77220100 | 0.55537000 | 1.71391500 |
| C | 1.03450200 | 2.09362400 | 0.39166800 |
| H | 0.43948200 | 1.25045800 | 0.75140700 |
| H | 1.32659200 | 2.69265100 | 1.25974900 |
| H | 4.40962800 | 0.67734000 | -1.16542200 |
| O | 2.23004600 | 1.58054600 | -0.23996700 |
| C | 0.28846200 | 2.91399000 | -0.64145100 |
| H | -0.63448700 | 3.30691900 | -0.20274300 |
| H | 0.89458100 | 3.75656500 | -0.98818200 |
| H | 0.02077200 | 2.29889300 | -1.50506500 |
| H | 4.93188800 | -0.21638200 | 0.38939200 |
| C | -1.23347200 | -1.19615300 | 1.10053800 |
| C | 0.06902900 | -1.68693000 | 1.03999400 |
| C | 0.84614600 | -1.57174500 | -0.12983700 |
| C | 0.25569900 | -0.96443500 | -1.25750200 |
| C | -1.04566600 | -0.47573000 | -1.21591000 |
| C | -1.77382800 | -0.58934300 | -0.03121300 |
| H | -1.81146500 | -1.27473300 | 2.01397900 |
| H | 0.50820400 | -2.13760300 | 1.92472400 |
| H | 0.81925000 | -0.86750500 | -2.17884600 |
| H | -1.48746400 | -0.00897600 | -2.08871000 |
| C | 2.22073400 | -2.04931400 | -0.11990400 |

| | | | |
|---|---|---|---|
| H | 2.51326700 | -2.62022900 | 0.75824800 |
| C | 3.18648400 | -1.72724800 | -1.03091600 |
| H | 4.15727100 | -2.20693400 | -0.98639600 |
| H | 2.94739200 | -1.21362800 | -1.95552000 |
| Br | -3.57959000 | 0.12918000 | 0.04124300 |

**TS6a$_{para}$ (R=Br)**

SCF Energy (a.u.) = -629.776866

Thermal correction to Gibbs free Energy (a.u.) = 0.181760

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.30715800 | 1.05303700 | 1.40489800 |
| C | -2.75824600 | -0.25709300 | 0.95973400 |
| O | -2.09028300 | -1.28333100 | 0.98307800 |
| C | -4.52159900 | -1.44245900 | -0.11103700 |
| H | -3.84156800 | -1.78921100 | -0.89622500 |
| H | -4.52665400 | -2.19986400 | 0.67907700 |
| H | -3.05787600 | 1.81973300 | 1.55766400 |
| O | -4.01208300 | -0.20605900 | 0.43232600 |
| C | -5.91354200 | -1.16600000 | -0.64572000 |
| H | -6.33738200 | -2.08330600 | -1.06749300 |
| H | -6.57560100 | -0.81514800 | 0.15169300 |
| H | -5.88689500 | -0.40518100 | -1.43195100 |
| H | -1.42676700 | 1.06605800 | 2.03507600 |
| C | -2.22391200 | 1.66841100 | -1.41211400 |
| H | -2.11741800 | 0.82988900 | -2.09208500 |
| C | -1.32808600 | 1.89094100 | -0.38143500 |
| H | -1.38126100 | 2.85950600 | 0.11146900 |
| C | -0.00129100 | 1.23598000 | -0.30037600 |
| C | 1.06382800 | 1.92071200 | 0.30412000 |
| C | 0.23139000 | -0.05559100 | -0.79717200 |
| C | 2.33430000 | 1.35106700 | 0.39747500 |

| | | | |
|---|---|---|---|
| H | 0.90157900 | 2.91869700 | 0.70310500 |
| C | 1.49287300 | -0.64192600 | -0.71008800 |
| H | -0.58146700 | -0.62914800 | -1.22706000 |
| C | 2.53057300 | 0.07252400 | -0.11616100 |
| H | 3.15100900 | 1.89299100 | 0.86012000 |
| H | 1.65876000 | -1.64477300 | -1.08586600 |
| H | -3.11926500 | 2.27219600 | -1.50648800 |
| Br | 4.29614100 | -0.74156900 | 0.00951400 |

**TS6$_{para}$ (R=OMe)**

SCF Energy (a.u.) = -731.588267

Thermal correction to Gibbs free Energy (a.u.) =0.226580

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 3.66003800 | 0.02166800 | -0.01602100 |
| C | 2.53897000 | 0.65794500 | 0.64209600 |
| O | 2.18537100 | 0.44645100 | 1.79657200 |
| C | 0.67453000 | 2.10769900 | 0.35530900 |
| H | -0.01767500 | 1.31890600 | 0.66137500 |
| H | 0.95310600 | 2.67625200 | 1.24808500 |
| H | 4.00465300 | 0.39531200 | -0.97233300 |
| O | 1.86131800 | 1.49451800 | -0.19382800 |
| C | 0.08095400 | 2.99374400 | -0.72140800 |
| H | -0.83015900 | 3.47120000 | -0.34593700 |
| H | 0.78527800 | 3.77650400 | -1.01925500 |
| H | -0.18154300 | 2.40515300 | -1.60465200 |
| H | 4.34378700 | -0.53359700 | 0.61164800 |
| C | -1.96620500 | -1.01332500 | 0.89365400 |
| C | -0.69891100 | -1.59408700 | 0.91798100 |
| C | 0.17356000 | -1.52565800 | -0.18255800 |
| C | -0.29008400 | -0.85574200 | -1.33851100 |
| C | -1.54748900 | -0.28054600 | -1.38111100 |

| | | | |
|---|---|---|---|
| C | -2.39556500 | -0.34776200 | -0.26172500 |
| H | -2.59696000 | -1.07775900 | 1.77134000 |
| H | -0.36336900 | -2.08846200 | 1.82464500 |
| H | 0.34757000 | -0.78442800 | -2.21270400 |
| H | -1.90217300 | 0.23235100 | -2.26869900 |
| C | 1.49877500 | -2.11010100 | -0.08156400 |
| H | 1.68294400 | -2.69947700 | 0.81397400 |
| C | 2.55023900 | -1.88005600 | -0.92398200 |
| H | 3.46734200 | -2.44676900 | -0.81505900 |
| H | 2.42025000 | -1.35444800 | -1.86339600 |
| O | -3.60653300 | 0.26221800 | -0.39861500 |
| C | -4.50826100 | 0.22623800 | 0.70166800 |
| H | -4.08084600 | 0.72257900 | 1.58137300 |
| H | -5.39724100 | 0.76595100 | 0.37495700 |
| H | -4.77951200 | -0.80485500 | 0.95864900 |

**TS6a$_{para}$ (R=OMe)**

SCF Energy (a.u.) = -731.574379

Thermal correction to Gibbs free Energy (a.u.) = 0.224215

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 1.63001200 | 1.21772500 | -1.30573500 |
| C | 2.08680700 | -0.12385600 | -0.98420100 |
| O | 1.44205000 | -1.15321900 | -1.14177000 |
| C | 3.82512000 | -1.39027100 | 0.03450000 |
| H | 3.11901600 | -1.82339200 | 0.75076800 |
| H | 3.87596000 | -2.06438000 | -0.82633600 |
| H | 2.37377400 | 2.00453600 | -1.35431400 |
| O | 3.32017900 | -0.11192400 | -0.40208500 |
| H | 0.77385400 | 1.28317200 | -1.96510200 |
| C | 1.45605100 | 1.59088300 | 1.53057800 |
| H | 1.38039600 | 0.69831400 | 2.14221800 |

| | | | |
|---|---|---|---|
| C | 0.56088100 | 1.85189900 | 0.50557600 |
| H | 0.57782500 | 2.85852700 | 0.09215800 |
| C | -0.73178700 | 1.15126900 | 0.34666200 |
| C | -1.81170400 | 1.82203500 | -0.25499900 |
| C | -0.93024400 | -0.17288000 | 0.75434600 |
| C | -3.04371500 | 1.20542300 | -0.42567500 |
| H | -1.68154400 | 2.84803000 | -0.59004200 |
| C | -2.16088300 | -0.80903400 | 0.58977600 |
| H | -0.10928400 | -0.73791700 | 1.18078900 |
| C | -3.22599400 | -0.11865400 | -0.00175000 |
| H | -3.87709800 | 1.72611400 | -0.88493600 |
| H | -2.26799600 | -1.83890600 | 0.90610300 |
| H | 2.32643500 | 2.21990700 | 1.67794300 |
| O | -4.46715900 | -0.64721900 | -0.21317400 |
| C | -4.69752600 | -1.99619300 | 0.17255100 |
| H | -5.73401600 | -2.20823600 | -0.09113000 |
| H | -4.03451800 | -2.68304600 | -0.36765200 |
| H | -4.56082400 | -2.13043700 | 1.25282600 |
| C | 5.18864400 | -1.15422500 | 0.65439900 |
| H | 5.11666700 | -0.47688300 | 1.51086500 |
| H | 5.60883200 | -2.10448300 | 0.99991700 |
| H | 5.87799200 | -0.71675400 | -0.07400500 |

**TS6$_{para}$ (R=Me)**

SCF Energy (a.u.) = -656.346378

Thermal correction to Gibbs free Energy (a.u.) = 0.221111

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 3.33684800 | -0.03857100 | -0.25919300 |
| C | 2.29965900 | 0.61716000 | 0.51090400 |
| O | 2.06275300 | 0.40721100 | 1.69449900 |
| C | 0.44138900 | 2.09893500 | 0.41636100 |

| | | | |
|---|---|---|---|
| H | -0.23333500 | 1.31976100 | 0.78026300 |
| H | 0.81553400 | 2.65327400 | 1.28256600 |
| H | 3.59033600 | 0.33205200 | -1.24476000 |
| O | 1.55842400 | 1.46958600 | -0.25010800 |
| C | -0.23508300 | 3.00665100 | -0.59119500 |
| H | -1.09445600 | 3.49931800 | -0.12425100 |
| H | 0.45267900 | 3.77822200 | -0.95055600 |
| H | -0.59377100 | 2.43121500 | -1.44900800 |
| H | 4.06962200 | -0.60874000 | 0.29563000 |
| C | -2.21437000 | -0.95111700 | 1.12326200 |
| C | -0.96424200 | -1.56143600 | 1.05765500 |
| C | -0.18607000 | -1.50677100 | -0.11440000 |
| C | -0.72679200 | -0.82535500 | -1.22563900 |
| C | -1.97628500 | -0.22466500 | -1.15607400 |
| C | -2.74570000 | -0.27101300 | 0.01950800 |
| H | -2.78398900 | -0.99696700 | 2.04746000 |
| H | -0.56359300 | -2.06414600 | 1.93294600 |
| H | -0.16031500 | -0.76241000 | -2.14839300 |
| H | -2.36758200 | 0.29503200 | -2.02709600 |
| C | 1.13175300 | -2.12125600 | -0.12459300 |
| H | 1.37824400 | -2.71436500 | 0.75322500 |
| C | 2.11041600 | -1.91661700 | -1.05590800 |
| H | 3.02133500 | -2.50265100 | -1.02416600 |
| H | 1.91071600 | -1.39004000 | -1.98239600 |
| C | -4.10680800 | 0.37528300 | 0.07460700 |
| H | -4.08546800 | 1.38496500 | -0.34960500 |
| H | -4.84059500 | -0.20216900 | -0.50120400 |
| H | -4.47307400 | 0.44591500 | 1.10246100 |

**TS6a$_{para}$ (R=Me)**

SCF Energy (a.u.) = -656.336335

Thermal correction to Gibbs free Energy (a.u.) = 0.221590

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.65519300 | -0.18825600 | -0.62220500 |
| C | -1.89793900 | -1.21466800 | 0.08009400 |
| O | -2.13267200 | -1.60595600 | 1.21809800 |
| C | 0.06256400 | -2.56350400 | 0.00707200 |
| H | 0.32592600 | -2.15085400 | 0.98420300 |
| H | -0.45675700 | -3.51390900 | 0.16933300 |
| H | -2.43079700 | -0.01245100 | -1.66712600 |
| O | -0.83944500 | -1.64850800 | -0.65074800 |
| H | -3.67596300 | -0.03957600 | -0.29369300 |
| C | -2.43252300 | 2.63331900 | -0.42784900 |
| H | -1.93735100 | 3.14750200 | -1.24465900 |
| C | -1.80868300 | 1.63229300 | 0.29375400 |
| H | -2.28092000 | 1.32008700 | 1.22258600 |
| C | -0.35332500 | 1.36691400 | 0.22999000 |
| C | 0.29515500 | 0.82806000 | 1.34935400 |
| C | 0.41038100 | 1.61002100 | -0.92228600 |
| C | 1.66311700 | 0.55514800 | 1.32346000 |
| H | -0.28013700 | 0.61257100 | 2.24478900 |
| C | 1.77403600 | 1.33530700 | -0.94445100 |
| H | -0.06685700 | 2.00008200 | -1.81609000 |
| C | 2.42728300 | 0.80011000 | 0.17703800 |
| H | 2.14158900 | 0.14215400 | 2.20768800 |
| H | 2.34289200 | 1.52959300 | -1.85025500 |
| H | -3.47222600 | 2.88094500 | -0.24332300 |
| C | 1.27674500 | -2.71846300 | -0.88710800 |
| H | 1.76402100 | -1.75111800 | -1.03528100 |
| H | 1.99349500 | -3.40415200 | -0.42297400 |
| H | 0.99661600 | -3.12188800 | -1.86494100 |
| C | 3.89843900 | 0.46841600 | 0.13078800 |

| | | | |
|---|---|---|---|
| H | 4.32338500 | 0.40164700 | 1.13635200 |
| H | 4.06878000 | -0.49646100 | -0.36364500 |
| H | 4.46090000 | 1.22334400 | -0.42766000 |

**$TS6_{meta}$ (R=F)**

SCF Energy (a.u.) = -716.289995

Thermal correction to Gibbs free Energy (a.u.) = 0.187894

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 3.14983200 | -0.11044900 | -0.58089000 |
| C | 2.25860500 | 0.49700300 | 0.38882400 |
| O | 2.17785900 | 0.17170300 | 1.56684400 |
| C | 0.49020400 | 2.05630800 | 0.70610300 |
| H | -0.14294100 | 1.26954900 | 1.12479700 |
| H | 1.02042500 | 2.53640200 | 1.53440000 |
| H | 3.28617500 | 0.35249800 | -1.55054000 |
| O | 1.46355000 | 1.44692300 | -0.17303100 |
| C | -0.30534400 | 3.05130900 | -0.11454900 |
| H | -1.05553900 | 3.53423500 | 0.52019600 |
| H | 0.34576600 | 3.82659200 | -0.52959800 |
| H | -0.82510800 | 2.55512400 | -0.93844100 |
| H | 3.91930300 | -0.76468300 | -0.19377500 |
| C | -2.17272700 | -1.09257300 | 1.54254000 |
| C | -0.96865500 | -1.70957200 | 1.21005700 |
| C | -0.36842200 | -1.50137800 | -0.04840500 |
| C | -1.02216500 | -0.65983800 | -0.97246700 |
| C | -2.21721000 | -0.06631600 | -0.61253000 |
| C | -2.81813100 | -0.25515800 | 0.62842900 |
| H | -2.61284800 | -1.25721500 | 2.52071500 |
| H | -0.46570200 | -2.34147900 | 1.93467300 |
| H | -0.61071600 | -0.46123900 | -1.95425500 |
| C | 0.90600900 | -2.14103200 | -0.34149800 |

| | | | |
|---|---|---|---|
| H | 1.25724600 | -2.84583000 | 0.40811900 |
| C | 1.73227800 | -1.84650200 | -1.38749100 |
| H | 2.61259200 | -2.45109200 | -1.57075300 |
| H | 1.41412800 | -1.20394300 | -2.20080600 |
| H | -3.75572100 | 0.23791700 | 0.85798700 |
| F | -2.83377600 | 0.74815000 | -1.51355200 |

**TS6a$_{meta}$ (R=F)**

SCF Energy (a.u.) = -716.279948

Thermal correction to Gibbs free Energy (a.u.) = 0.187842

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.24496600 | -0.85305600 | 0.93199700 |
| C | -2.15183400 | 0.40016000 | 0.19435400 |
| O | -2.75677900 | 0.64951300 | -0.84211800 |
| C | -0.99892900 | 2.47692100 | 0.03773300 |
| H | -0.74872400 | 2.22889200 | -0.99723000 |
| H | -1.91584600 | 3.07512800 | 0.02954900 |
| H | -1.75782900 | -0.91697800 | 1.89733500 |
| O | -1.25414100 | 1.24897000 | 0.75460800 |
| H | -3.15039100 | -1.42772500 | 0.78413800 |
| C | -0.89554700 | -3.31775200 | 0.44427700 |
| H | -0.07318100 | -3.56680100 | 1.10649300 |
| C | -0.92255500 | -2.14353400 | -0.28205100 |
| H | -1.65987000 | -2.06249800 | -1.07712000 |
| C | 0.26157600 | -1.26987900 | -0.45713200 |
| C | 0.38130200 | -0.50648200 | -1.62828100 |
| C | 1.25516400 | -1.16354100 | 0.52835500 |
| C | 1.47801900 | 0.33498100 | -1.82148600 |
| H | -0.39631400 | -0.56516200 | -2.38250800 |
| C | 2.32929300 | -0.31811200 | 0.30875600 |
| C | 2.47263900 | 0.44037500 | -0.84786300 |

| | | | |
|---|---|---|---|
| H | 1.55783300 | 0.91669900 | -2.73437100 |
| H | -1.74046900 | -3.99739400 | 0.42582400 |
| H | 3.33273500 | 1.08917100 | -0.96796700 |
| C | 0.14059600 | 3.18349300 | 0.74418000 |
| H | 1.04155400 | 2.56397800 | 0.73608500 |
| H | 0.36347900 | 4.12642500 | 0.23399100 |
| H | -0.11966800 | 3.40678800 | 1.78315800 |
| F | 3.28158900 | -0.21499000 | 1.27560900 |
| H | 1.19119600 | -1.70492300 | 1.46518600 |

**$TS6_{meta}$ (R=OMe)**

SCF Energy (a.u.) = -731.587539

Thermal correction to Gibbs free Energy (a.u.) = 0.226873

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 3.33748400 | 0.47798100 | -0.79959800 |
| C | 2.45305100 | 0.83791200 | 0.29121500 |
| O | 2.55514200 | 0.42976900 | 1.44165600 |
| C | 0.45679000 | 1.98487600 | 0.88641400 |
| H | 0.04220600 | 1.05827400 | 1.29171600 |
| H | 0.95635800 | 2.51588800 | 1.70289400 |
| H | 3.28520000 | 1.02070700 | -1.73542700 |
| O | 1.44085700 | 1.65070400 | -0.11778900 |
| C | -0.60409400 | 2.83649700 | 0.21752900 |
| H | -1.37036600 | 3.10880100 | 0.95156600 |
| H | -0.17182400 | 3.75778700 | -0.18490000 |
| H | -1.08612100 | 2.29032900 | -0.59754000 |
| H | 4.25261500 | -0.03497700 | -0.53628200 |
| C | -1.45414600 | -1.65442000 | 1.67569100 |
| C | -0.20209500 | -2.01712300 | 1.19631700 |
| C | 0.21632600 | -1.60448000 | -0.08762200 |
| C | -0.66455400 | -0.83796800 | -0.86662600 |

| | | | |
|---|---|---|---|
| C | -1.92130400 | -0.47698400 | -0.37888500 |
| C | -2.32715800 | -0.88096500 | 0.90072500 |
| H | -1.76367100 | -1.96562100 | 2.66866800 |
| H | 0.47505700 | -2.59593600 | 1.81575900 |
| H | -0.38912200 | -0.49641000 | -1.85717500 |
| C | 1.55159500 | -1.96544300 | -0.54443300 |
| H | 2.10009200 | -2.64230300 | 0.10638400 |
| C | 2.20291200 | -1.44203700 | -1.62469600 |
| H | 3.15728200 | -1.85190600 | -1.93382000 |
| H | 1.69043800 | -0.81936600 | -2.34929900 |
| H | -3.29743300 | -0.60801400 | 1.29581300 |
| O | -2.68390100 | 0.28503600 | -1.22221100 |
| C | -3.96146700 | 0.71435300 | -0.77109200 |
| H | -3.87692900 | 1.33973200 | 0.12644400 |
| H | -4.38189000 | 1.30437600 | -1.58588400 |
| H | -4.61871400 | -0.13861500 | -0.56179700 |

**TS6a$_{meta}$ (R=OMe)**

SCF Energy (a.u.) = -731.577645

Thermal correction to Gibbs free Energy (a.u.) = 0.226884

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 2.82712600 | -0.62784500 | 0.23985500 |
| C | 1.78158200 | -1.52743800 | -0.23010100 |
| O | 1.71609600 | -1.99085700 | -1.36317000 |
| C | -0.32878900 | -2.49108900 | 0.29348700 |
| H | -0.71771600 | -2.04527900 | -0.62574200 |
| H | -0.02220300 | -3.51755000 | 0.06741600 |
| H | 2.84296800 | -0.36101500 | 1.28952200 |
| O | 0.83226600 | -1.74214400 | 0.71518600 |
| H | 3.77331400 | -0.68530500 | -0.28280100 |
| C | 3.12810100 | 2.16043700 | -0.27072200 |

| | | | |
|---|---|---|---|
| H | 3.01349800 | 2.82691200 | 0.57725900 |
| C | 2.13853900 | 1.27244600 | -0.64645600 |
| H | 2.23968600 | 0.79683800 | -1.61933300 |
| C | 0.74886500 | 1.33706200 | -0.13322300 |
| C | -0.28260600 | 0.84175800 | -0.93281400 |
| C | 0.44185500 | 1.84663100 | 1.14166200 |
| C | -1.60792800 | 0.84964600 | -0.47927900 |
| C | -0.87549500 | 1.86274700 | 1.58159700 |
| H | 1.23122200 | 2.20920800 | 1.79107900 |
| C | -1.91457200 | 1.36770400 | 0.78275200 |
| H | -1.10982900 | 2.25455800 | 2.56688000 |
| H | 4.08676900 | 2.16361900 | -0.77795400 |
| H | -2.93157400 | 1.38518700 | 1.15374800 |
| C | -1.33789800 | -2.42985100 | 1.42292300 |
| H | -1.61536400 | -1.39260900 | 1.63026600 |
| H | -2.23945100 | -2.98506200 | 1.14264500 |
| H | -0.93190600 | -2.87117500 | 2.33821100 |
| H | -0.07198600 | 0.41946800 | -1.90984000 |
| O | -2.52598800 | 0.31129500 | -1.33715400 |
| C | -3.88623300 | 0.27329600 | -0.92667100 |
| H | -4.27870700 | 1.28296200 | -0.75330500 |
| H | -4.43202900 | -0.19229500 | -1.74767800 |
| H | -4.01096700 | -0.32784600 | -0.01732700 |

**$TS6_{ortho}$ (R=Cl)**

SCF Energy (a.u.) = -1076.636139

Thermal correction to Gibbs free Energy (a.u.) = 0.184851

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 2.95586300 | -1.20291000 | -0.60694600 |
| C | 2.67243600 | 0.14754200 | -0.15549600 |
| O | 3.16789100 | 0.68389300 | 0.82706600 |

| | | | |
|---|---|---|---|
| C | 1.24545300 | 2.02662600 | -0.48015500 |
| H | 0.85441100 | 1.91860100 | 0.53621800 |
| H | 2.08812700 | 2.72363600 | -0.44235000 |
| H | 2.59086900 | -1.52508300 | -1.57399800 |
| O | 1.72392900 | 0.73890200 | -0.92787200 |
| C | 0.17369700 | 2.47207300 | -1.45490100 |
| H | -0.23134100 | 3.43944900 | -1.14024600 |
| H | 0.58349600 | 2.58090400 | -2.46370000 |
| H | -0.64537700 | 1.74926500 | -1.48777400 |
| H | 3.79760700 | -1.71323000 | -0.15792000 |
| C | -2.80071500 | 0.35815400 | -0.10850000 |
| C | -1.70960200 | -0.04676700 | 0.65834600 |
| C | -0.78300300 | -1.01039700 | 0.20068700 |
| C | -1.01334700 | -1.53425700 | -1.09109500 |
| C | -2.09300000 | -1.13726400 | -1.86752900 |
| C | -2.99634300 | -0.18828900 | -1.37588300 |
| H | -3.48413300 | 1.09982700 | 0.28886300 |
| H | -0.31356800 | -2.25915700 | -1.49104800 |
| H | -2.23036000 | -1.56080900 | -2.85717900 |
| C | 0.35456900 | -1.42335700 | 1.00682400 |
| H | 0.50487100 | -0.88051100 | 1.93334400 |
| C | 1.28983600 | -2.35867900 | 0.66639900 |
| H | 2.04731800 | -2.63365700 | 1.39022500 |
| H | 1.15848700 | -3.03468500 | -0.17093300 |
| H | -3.84405800 | 0.12959800 | -1.97412200 |
| Cl | -1.51682200 | 0.70403800 | 2.23920900 |

**TS6a$_{ortho}$ (R=Cl)**

SCF Energy (a.u.) = -1076.621568

Thermal correction to Gibbs free Energy (a.u.) = 0.185360

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.66280900 | 2.15762500 | -0.49848200 |
| C | 1.26049300 | 0.94289400 | -1.03539700 |
| O | 0.76904300 | 0.25497200 | -1.92122600 |
| C | 3.06555100 | -0.59197400 | -0.83893400 |
| H | 2.32620400 | -1.39663100 | -0.83331700 |
| H | 3.41121300 | -0.45957800 | -1.86969300 |
| H | 1.30655900 | 2.84864000 | 0.03265900 |
| O | 2.42446300 | 0.62855500 | -0.40853000 |
| H | -0.14379300 | 2.57415600 | -1.08976000 |
| C | 0.30010800 | 1.27414200 | 2.22733800 |
| H | 0.64873200 | 0.28782800 | 2.49182500 |
| C | -0.58288900 | 1.51811400 | 1.18929600 |
| H | -0.98812700 | 2.52722400 | 1.16465700 |
| C | -1.48952500 | 0.55111900 | 0.51989700 |
| C | -2.65563500 | 1.09315700 | -0.05761600 |
| C | -1.31197800 | -0.83605700 | 0.37135000 |
| C | -3.59105900 | 0.31757300 | -0.73185900 |
| H | -2.81843800 | 2.16360400 | 0.03326700 |
| C | -2.24048400 | -1.62953600 | -0.30380700 |
| C | -3.38213200 | -1.05689400 | -0.85740600 |
| H | -4.47363900 | 0.78270500 | -1.15871800 |
| H | -2.05329700 | -2.69313100 | -0.39622400 |
| H | 0.74111800 | 2.11792800 | 2.74784300 |
| H | -4.09609700 | -1.68118600 | -1.38471700 |
| C | 4.21196400 | -0.86296500 | 0.11503200 |
| H | 3.84233700 | -0.99485000 | 1.13651100 |
| H | 4.73421600 | -1.77771900 | -0.18402100 |
| H | 4.93097100 | -0.03809400 | 0.11138200 |
| Cl | 0.09415600 | -1.68190000 | 1.01411000 |

**TS6$_{ortho}$ (R=Me)**

SCF Energy (a.u.) = -656.344837

Thermal correction to Gibbs free Energy (a.u.) = 0.224558

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | -2.94700100 | -0.80545000 | 0.31079200 |
| C | -2.08976700 | -0.03328100 | -0.56460600 |
| O | -1.63308800 | -0.43141900 | -1.63116100 |
| C | -0.85124200 | 1.98568500 | -0.79719600 |
| H | 0.07226600 | 1.41688500 | -0.92811800 |
| H | -1.27568100 | 2.17662000 | -1.78785200 |
| H | -3.45549800 | -0.31757800 | 1.13314400 |
| O | -1.78600800 | 1.18337800 | -0.04006000 |
| C | -0.61993400 | 3.26552600 | -0.01971300 |
| H | 0.08810500 | 3.90162200 | -0.56096900 |
| H | -1.55344300 | 3.82094700 | 0.11300300 |
| H | -0.19902300 | 3.04631100 | 0.96541100 |
| H | -3.34747000 | -1.72868800 | -0.08566600 |
| C | 2.60431900 | -0.04838700 | -0.77793700 |
| C | 1.61772100 | -1.01893100 | -0.57375300 |
| C | 0.84906000 | -0.97048900 | 0.62053600 |
| C | 1.11391300 | 0.04888000 | 1.55866500 |
| C | 2.09834500 | 1.00432400 | 1.33577900 |
| C | 2.85026100 | 0.95790200 | 0.15838700 |
| H | 3.18434100 | -0.07799300 | -1.69617500 |
| H | 0.54450600 | 0.07957700 | 2.48141500 |
| H | 2.28450100 | 1.77569700 | 2.07671500 |
| C | -0.20149900 | -1.95254300 | 0.85927000 |
| H | -0.17577400 | -2.85030100 | 0.24986900 |
| C | -1.27628200 | -1.78746000 | 1.68724100 |
| H | -1.94444300 | -2.61829900 | 1.88278400 |
| H | -1.35037300 | -0.94141900 | 2.36134500 |
| H | 3.62392600 | 1.69644600 | -0.02864000 |

| | | | |
|---|---|---|---|
| C | 1.35284900 | -2.05252800 | -1.63929300 |
| H | 1.47585100 | -3.07357500 | -1.25921500 |
| H | 0.33121100 | -1.95479100 | -2.02092900 |
| H | 2.04530200 | -1.92663000 | -2.47539500 |

**TS6a$_{ortho}$ (R=Me)**

SCF Energy (a.u.) = -656.329837

Thermal correction to Gibbs free Energy (a.u.) = 0.223002

Charge = 0, Multiplicity = 2

| | | | |
|---|---|---|---|
| C | 0.70366800 | 1.73629200 | -0.98454500 |
| C | 1.35169100 | 0.44040800 | -1.11349600 |
| O | 0.92234800 | -0.50448100 | -1.76225600 |
| C | 3.22208400 | -0.87885100 | -0.45649600 |
| H | 2.54809400 | -1.69613800 | -0.18196400 |
| H | 3.53285200 | -1.04366400 | -1.49330600 |
| H | 1.31893700 | 2.57832400 | -0.69007900 |
| O | 2.50197200 | 0.36968200 | -0.38183600 |
| H | -0.09597200 | 1.92035700 | -1.69159100 |
| C | 0.28173200 | 1.67220900 | 1.86210000 |
| H | 0.55340200 | 0.79429700 | 2.42857400 |
| C | -0.58177300 | 1.65104100 | 0.77693000 |
| H | -0.92269900 | 2.63366700 | 0.45638300 |
| C | -1.53988500 | 0.57702700 | 0.40871900 |
| C | -2.69140200 | 0.99777500 | -0.28232100 |
| C | -1.37333900 | -0.80287400 | 0.67252900 |
| C | -3.67382400 | 0.10455900 | -0.69663700 |
| H | -2.81225100 | 2.05700400 | -0.49543700 |
| C | -2.37072700 | -1.68856900 | 0.24223500 |
| C | -3.51136000 | -1.25535300 | -0.43067300 |
| H | -4.55067100 | 0.46531300 | -1.22522700 |
| H | -2.23722000 | -2.74963100 | 0.43469100 |

| | | | |
|---|---|---|---|
| H | 0.78535600 | 2.59753700 | 2.12139000 |
| H | -4.25914900 | -1.97402900 | -0.75166400 |
| C | 4.40696700 | -0.77774900 | 0.48393600 |
| H | 4.07466200 | -0.61344100 | 1.51361300 |
| H | 4.98585300 | -1.70655500 | 0.45221000 |
| H | 5.06426100 | 0.04885400 | 0.19806200 |
| C | -0.18260400 | -1.37885400 | 1.40002000 |
| H | 0.75572000 | -0.91418900 | 1.09540500 |
| H | -0.27754800 | -1.25076600 | 2.48562300 |
| H | -0.10557100 | -2.45092500 | 1.20224200 |

**$A_{para\text{-}F}$**

SCF Energy (a.u.) = -409.086292

Thermal correction to Gibbs free Energy (a.u.) = 0.092402

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.27010400 | 1.19249400 | 0.00008500 |
| C | -0.11736200 | 1.34101800 | -0.00002700 |
| C | -0.97830300 | 0.22995500 | -0.00012600 |
| C | -0.39973600 | -1.05335500 | -0.00020100 |
| C | 0.98168800 | -1.22339400 | -0.00009700 |
| C | 1.79235300 | -0.09264200 | 0.00007900 |
| H | 1.93581400 | 2.04824300 | 0.00016600 |
| H | -0.54211000 | 2.34083400 | -0.00000800 |
| H | -1.03366800 | -1.93346600 | -0.00036000 |
| H | 1.43324200 | -2.20923700 | -0.00016600 |
| C | -2.43200400 | 0.45540200 | -0.00016700 |
| H | -2.72661300 | 1.50403000 | -0.00054600 |
| C | -3.40086900 | -0.47125400 | 0.00029200 |
| H | -4.44586500 | -0.18057700 | 0.00023500 |
| H | -3.19540600 | -1.53761400 | 0.00074900 |
| F | 3.14215400 | -0.25572800 | 0.00010100 |

**$A_{para\text{-}Br}$**

SCF Energy (a.u.) = -322.586355

Thermal correction to Gibbs free Energy (a.u.) = 0.088427

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.06637700 | 1.29707400 | -0.00005400 |
| C | -1.32735500 | 1.37702000 | -0.00001000 |
| C | -2.13223800 | 0.22541300 | 0.00009100 |
| C | -1.48980500 | -1.02648100 | 0.00019500 |
| C | -0.10092500 | -1.12689800 | 0.00016900 |
| C | 0.66242500 | 0.04058900 | 0.00002500 |
| H | 0.67154100 | 2.19630800 | -0.00010700 |
| H | -1.79915200 | 2.35590200 | -0.00003900 |
| H | -2.07664500 | -1.93904600 | 0.00037400 |
| H | 0.38077200 | -2.09799200 | 0.00029300 |
| C | -3.59541700 | 0.37867400 | 0.00010800 |
| H | -3.94252100 | 1.41110800 | 0.00082200 |
| C | -4.51469900 | -0.59755600 | -0.00030500 |
| H | -5.57366900 | -0.36204300 | -0.00007900 |
| H | -4.25366700 | -1.65180000 | -0.00103700 |
| Br | 2.60523300 | -0.09484200 | -0.00004400 |

**$A_{para\text{-}OMe}$**

SCF Energy (a.u.) = -424.384333

Thermal correction to Gibbs free Energy (a.u.) = 0.131201

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.86942700 | -1.03402100 | -0.00022700 |
| C | 0.50678500 | -1.27918500 | -0.00011200 |
| C | 1.44840600 | -0.24158000 | 0.00005000 |
| C | 0.95593200 | 1.08039100 | 0.00012300 |
| C | -0.40422400 | 1.34323000 | 0.00002600 |

| | | | |
|---|---|---|---|
| C | -1.33004100 | 0.28610100 | -0.00017000 |
| H | -1.55821200 | -1.86965100 | -0.00033400 |
| H | 0.85451800 | -2.30894000 | -0.00014900 |
| H | 1.64890200 | 1.91534100 | 0.00030300 |
| H | -0.78025400 | 2.36086800 | 0.00012400 |
| C | 2.88032300 | -0.56844200 | 0.00016800 |
| H | 3.09959600 | -1.63579500 | 0.00061600 |
| C | 3.91507200 | 0.28562700 | -0.00006800 |
| H | 4.93636800 | -0.07989300 | 0.00012600 |
| H | 3.78655000 | 1.36400500 | -0.00055700 |
| O | -2.64610900 | 0.64916400 | -0.00023500 |
| C | -3.62622900 | -0.38026800 | 0.00029100 |
| H | -3.54304100 | -1.00848500 | 0.89590400 |
| H | -4.59139700 | 0.12684100 | 0.00058500 |
| H | -3.54374800 | -1.00872600 | -0.89522100 |

**$A_{para\text{-}Me}$**

SCF Energy (a.u.) = -349.143048

Thermal correction to Gibbs free Energy (a.u.) = 0.125954

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.20721400 | 1.19475200 | -0.00002500 |
| C | 0.18082300 | 1.34280300 | -0.00000600 |
| C | 1.03363400 | 0.22852000 | -0.00000200 |
| C | 0.43792800 | -1.04727300 | -0.00001400 |
| C | -0.94424900 | -1.19123800 | -0.00002800 |
| C | -1.79642600 | -0.07339300 | -0.00003000 |
| H | -1.83955200 | 2.07866100 | -0.00004200 |
| H | 0.61247400 | 2.34040800 | -0.00000400 |
| H | 1.06146900 | -1.93553300 | -0.00001800 |
| H | -1.37592400 | -2.18923800 | -0.00005300 |
| C | 2.48884500 | 0.43931100 | 0.00001700 |

| | | | |
|---|---|---|---|
| H | 2.79399300 | 1.48521700 | 0.00001700 |
| C | 3.44920100 | -0.49687600 | 0.00001700 |
| H | 4.49726200 | -0.21693200 | 0.00002600 |
| H | 3.23193500 | -1.56089500 | 0.00002100 |
| C | -3.29502300 | -0.24782000 | 0.00004100 |
| H | -3.62945600 | -0.80663700 | -0.88174800 |
| H | -3.62945200 | -0.80568000 | 0.88244500 |
| H | -3.80786400 | 0.71791200 | -0.00046600 |

**$A_{Meta\text{-}F}$**

SCF Energy (a.u.) = -409.086611

Thermal correction to Gibbs free Energy (a.u.) = 0.092392

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -1.11666800 | 1.74550200 | 0.00004700 |
| C | 0.27121400 | 1.59693200 | 0.00001200 |
| C | 0.86494100 | 0.32275000 | -0.00004500 |
| C | 0.02668300 | -0.80729700 | -0.00003100 |
| C | -1.34539500 | -0.62817900 | 0.00003900 |
| C | -1.94907400 | 0.62549100 | 0.00005500 |
| H | -1.55464400 | 2.73859800 | 0.00007200 |
| H | 0.90718300 | 2.47708100 | 0.00000600 |
| H | 0.42512400 | -1.81491600 | -0.00011300 |
| C | 2.33280200 | 0.22001000 | -0.00011800 |
| H | 2.85283900 | 1.17664200 | -0.00041100 |
| C | 3.06704800 | -0.90127800 | 0.00012000 |
| H | 4.15075100 | -0.85464400 | 0.00000800 |
| H | 2.62533400 | -1.89331300 | 0.00046300 |
| H | -3.02989100 | 0.70752100 | 0.00006300 |
| F | -2.14288900 | -1.73117200 | -0.00006200 |

**$A_{Meta\text{-}OMe}$**

SCF Energy (a.u.) = -424.383659

Thermal correction to Gibbs free Energy (a.u.) = 0.130854

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.23725600 | 2.05353800 | 0.00001200 |
| C | -1.08041400 | 1.60653900 | 0.00011400 |
| C | -1.36461000 | 0.22714500 | 0.00000000 |
| C | -0.29607500 | -0.67763800 | -0.00009000 |
| C | 1.02602600 | -0.22491400 | -0.00019800 |
| C | 1.30369400 | 1.14941600 | -0.00015400 |
| H | 0.44685000 | 3.11902500 | 0.00007700 |
| H | -1.89821300 | 2.32093200 | 0.00024400 |
| H | -0.46333500 | -1.74874700 | -0.00014200 |
| C | -2.77203300 | -0.20565200 | 0.00002400 |
| H | -3.49471400 | 0.60923000 | -0.00016700 |
| C | -3.23726300 | -1.46280700 | 0.00011300 |
| H | -4.30411900 | -1.65962800 | 0.00004200 |
| H | -2.58393200 | -2.33019900 | 0.00041700 |
| H | 2.32154300 | 1.51830500 | -0.00022700 |
| O | 1.98370500 | -1.20156400 | -0.00042400 |
| C | 3.34841100 | -0.80596100 | 0.00039900 |
| H | 3.59441400 | -0.22195400 | 0.89612200 |
| H | 3.92642100 | -1.73055500 | 0.00070400 |
| H | 3.59549600 | -0.22190100 | -0.89499400 |

**A$_{\text{Ortho-Cl}}$**

SCF Energy (a.u.) = -769.433143

Thermal correction to Gibbs free Energy (a.u.) = 0.090801

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.68673200 | 0.76804800 | 0.06513000 |
| C | 0.29562800 | 0.70109800 | -0.01171700 |
| C | -0.39271400 | -0.52389200 | -0.09058400 |

| | | | |
|---|---|---|---|
| C | 0.39590400 | -1.69089500 | -0.10642700 |
| C | 1.78367200 | -1.64255300 | -0.02580700 |
| C | 2.43418900 | -0.40832100 | 0.06073300 |
| H | 2.17112000 | 1.73565700 | 0.13063900 |
| H | -0.10171900 | -2.64960500 | -0.20703400 |
| H | 2.35794100 | -2.56333500 | -0.04450800 |
| C | -1.86073000 | -0.58932200 | -0.17243900 |
| H | -2.35399800 | 0.29849800 | -0.55690700 |
| C | -2.61419500 | -1.63317100 | 0.20013600 |
| H | -3.69316000 | -1.60500000 | 0.09061000 |
| H | -2.19099200 | -2.53314100 | 0.63701400 |
| H | 3.51682900 | -0.35748100 | 0.11735100 |
| Cl | -0.59276100 | 2.22285000 | 0.01874600 |

**A$_{\text{Ortho-Me}}$**

SCF Energy (a.u.) = -349.141070

Thermal correction to Gibbs free Energy (a.u.) = 0.128320

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.76445100 | 0.72706000 | 0.07967400 |
| C | 0.38696700 | 0.96211100 | -0.00620800 |
| C | -0.49081000 | -0.14446100 | -0.09961500 |
| C | 0.04969200 | -1.44196900 | -0.12272600 |
| C | 1.42254100 | -1.65832500 | -0.03374500 |
| C | 2.28734200 | -0.56677800 | 0.06939600 |
| H | 2.43775200 | 1.57647400 | 0.15901000 |
| H | -0.61954100 | -2.28899000 | -0.23561900 |
| H | 1.81514000 | -2.67036000 | -0.05826100 |
| C | -1.94762400 | 0.06460900 | -0.18159700 |
| H | -2.27303400 | 1.01464500 | -0.59941300 |
| C | -2.89164000 | -0.79859500 | 0.22125100 |
| H | -3.94564000 | -0.56767100 | 0.10562900 |

| | | | |
|---|---|---|---|
| H | -2.64698300 | -1.74870200 | 0.68769700 |
| H | 3.36044100 | -0.71954900 | 0.13374900 |
| C | -0.13392300 | 2.37973600 | 0.02524400 |
| H | -0.65877100 | 2.64114300 | -0.90164100 |
| H | -0.83921200 | 2.53308100 | 0.84937400 |
| H | 0.68787000 | 3.08959500 | 0.14942600 |

**15a**

SCF Energy (a.u.) = -885.736976

Thermal correction to Gibbs free Energy (a.u.) = 0.248983

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 1.81707600 | -1.10968800 | -2.21205700 |
| N | 1.56537000 | 0.10481200 | -2.85543500 |
| C | 1.30917600 | 1.28281600 | -2.20273400 |
| C | 1.60959000 | 1.35982100 | -0.85499500 |
| C | 2.16525000 | -1.07837900 | -0.89940300 |
| C | 2.41259000 | 0.24827200 | -0.21246500 |
| H | 3.48617000 | 0.49970200 | -0.24701300 |
| H | 2.16342300 | 0.17403800 | 0.84354200 |
| H | 1.26022400 | 0.04678400 | -3.81675200 |
| C | 1.39875300 | 2.62451000 | -0.11808800 |
| O | 1.79441600 | 2.51182400 | 1.16809100 |
| O | 0.93828500 | 3.65693400 | -0.58269400 |
| C | 2.33146500 | -2.33222500 | -0.14217700 |
| O | 2.71739000 | -2.09055500 | 1.13199800 |
| O | 2.14985900 | -3.46298000 | -0.57113200 |
| C | 1.56882300 | 3.66850000 | 2.00844300 |
| H | 2.13692500 | 4.51093100 | 1.60224100 |
| H | 0.50654900 | 3.92565600 | 1.96283500 |
| C | 2.85920100 | -3.24879900 | 1.98698000 |
| H | 1.91124500 | -3.79483400 | 1.99113700 |
| H | 3.62278400 | -3.90630900 | 1.56008700 |

| | | | |
|---|---|---|---|
| C | 0.69432000 | 2.36417000 | -3.04098100 |
| H | 1.29413500 | 3.27534300 | -3.00248800 |
| H | 0.58945800 | 2.03509600 | -4.07911700 |
| H | -0.29096400 | 2.62921100 | -2.64951800 |
| C | 1.59495100 | -2.31944200 | -3.07262200 |
| H | 1.58807300 | -2.04088200 | -4.13186100 |
| H | 2.35866000 | -3.07640900 | -2.90001200 |
| H | 0.63313900 | -2.78289800 | -2.82813400 |
| C | 2.01067100 | 3.29876000 | 3.41044000 |
| H | 3.07198600 | 3.03284900 | 3.43003500 |
| H | 1.85577300 | 4.14994600 | 4.08139100 |
| H | 1.43287100 | 2.45075900 | 3.78976500 |
| C | 3.23906700 | -2.74701000 | 3.36618100 |
| H | 2.46441100 | -2.08721100 | 3.76823100 |
| H | 3.35681700 | -3.59598000 | 4.04745300 |
| H | 4.18365900 | -2.19533600 | 3.33623500 |
| I | -3.79447000 | -0.66795100 | 0.54690100 |
| I | -1.10077800 | 0.27222000 | -0.24575500 |

**TS5a**

SCF Energy (a.u.) = -885.728969

Thermal correction to Gibbs free Energy (a.u.) = 0.243102

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | -0.59714400 | 1.22133300 | 2.21331000 |
| N | -0.15320700 | 0.00133600 | 2.64676000 |
| C | -0.59592400 | -1.21943300 | 2.21423300 |
| C | -1.56001800 | -1.23216600 | 1.22112800 |
| C | -1.56125000 | 1.23236400 | 1.22018600 |
| C | -1.93978000 | -0.00032800 | 0.60626500 |
| H | -0.83482300 | -0.00046600 | -0.71464100 |
| H | -2.75833100 | -0.00100500 | -0.09978000 |

| | | | |
|---|---|---|---|
| H | 0.61183500 | 0.00197200 | 3.31013300 |
| C | -2.07390400 | -2.52261400 | 0.69294500 |
| O | -2.80972700 | -2.33774200 | -0.41569400 |
| O | -1.85872000 | -3.61487100 | 1.18981500 |
| C | -2.07651900 | 2.52187500 | 0.69105200 |
| O | -2.81346500 | 2.33524900 | -0.41656000 |
| O | -1.86151500 | 3.61486500 | 1.18638500 |
| C | -3.32323500 | -3.53511200 | -1.05776700 |
| H | -2.47860000 | -4.19511500 | -1.27314400 |
| H | -3.98352500 | -4.04699100 | -0.35156400 |
| C | -3.32849200 | 3.53155100 | -1.05940300 |
| H | -3.98842300 | 4.04371000 | -0.35306800 |
| H | -2.48456500 | 4.19194200 | -1.27636100 |
| C | 0.04015100 | -2.40970000 | 2.86055500 |
| H | 0.49388000 | -3.05073500 | 2.10077000 |
| H | 0.81240600 | -2.09920000 | 3.56960700 |
| H | -0.70577600 | -3.01834600 | 3.37615600 |
| C | 0.03789300 | 2.41271300 | 2.85860600 |
| H | 0.80858700 | 2.10344600 | 3.56988900 |
| H | 0.49346000 | 3.05199700 | 2.09840100 |
| H | -0.70889800 | 3.02268700 | 3.37131600 |
| C | -4.04646200 | -3.09493000 | -2.31394600 |
| H | -3.36552000 | -2.57459200 | -2.99363900 |
| H | -4.44668800 | -3.97242500 | -2.83163200 |
| H | -4.87974200 | -2.42732300 | -2.07465900 |
| C | -4.05272200 | 3.08949700 | -2.31434700 |
| H | -4.88547700 | 2.42181300 | -2.07345600 |
| H | -4.45383200 | 3.96617700 | -2.83273000 |
| H | -3.37219500 | 2.56863800 | -2.99405700 |
| I | 0.91510200 | -0.00002900 | -1.01615200 |
| I | 4.11151200 | 0.00105100 | -0.48202400 |

**16a**

SCF Energy (a.u.) = -885.768779

Thermal correction to Gibbs free Energy (a.u.) = 0.240695

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.00199900 | -1.20940200 | 1.11820800 |
| N | -0.59027100 | -0.00132900 | 1.26467900 |
| C | 0.00164200 | 1.20711600 | 1.11973000 |
| C | 1.36996000 | 1.21930500 | 0.80412400 |
| C | 1.37034400 | -1.22079200 | 0.80264900 |
| C | 2.02850500 | -0.00054200 | 0.63713800 |
| H | -0.26726000 | 0.00569600 | -3.31835900 |
| H | 3.07838400 | -0.00021800 | 0.37856000 |
| H | -1.66283100 | -0.00151800 | 1.31973300 |
| C | 2.11404200 | 2.50592300 | 0.64428700 |
| O | 3.36682400 | 2.29935100 | 0.19949800 |
| O | 1.65765100 | 3.60586500 | 0.88777900 |
| C | 2.11485500 | -2.50698500 | 0.64139200 |
| O | 3.36769400 | -2.29948100 | 0.19720300 |
| O | 1.65873500 | -3.60736600 | 0.88340600 |
| C | 4.18573300 | 3.48605300 | 0.01463000 |
| H | 3.68223400 | 4.13998300 | -0.70279700 |
| H | 4.24464800 | 4.01384400 | 0.97061700 |
| C | 4.18702400 | -3.48570500 | 0.01112700 |
| H | 4.24574600 | -4.01468900 | 0.96646700 |
| H | 3.68398000 | -4.13887400 | -0.70731100 |
| C | -0.87089600 | 2.40507800 | 1.30221900 |
| H | -0.77214300 | 3.07333500 | 0.44416100 |
| H | -1.91368500 | 2.10511400 | 1.41719800 |
| H | -0.54023800 | 2.97615900 | 2.17490300 |
| C | -0.87019100 | -2.40785800 | 1.29913000 |

| | | | |
|---|---|---|---|
| H | -1.91310300 | -2.10835700 | 1.41422000 |
| H | -0.77099100 | -3.07513600 | 0.44036600 |
| H | -0.53956500 | -2.97980100 | 2.17126600 |
| C | 5.54253100 | 3.02515600 | -0.47660900 |
| H | 5.45503600 | 2.48987900 | -1.42670900 |
| H | 6.18940300 | 3.89461100 | -0.63035300 |
| H | 6.02166600 | 2.36585600 | 0.25336500 |
| C | 5.54386400 | -3.02378300 | -0.47903000 |
| H | 6.02253500 | -2.36526900 | 0.25195700 |
| H | 6.19104900 | -3.89285100 | -0.63363900 |
| H | 5.45655800 | -2.48732700 | -1.42848200 |
| I | -1.44669200 | 0.00259000 | -2.19684600 |
| I | -3.88318000 | -0.00144800 | 0.79713000 |

**17a**

SCF Energy (a.u.) = -873.736231

Thermal correction to Gibbs free Energy (a.u.) = 0.233439

Charge = 0, Multiplicity = 1

| | | | |
|---|---|---|---|
| C | 0.59914400 | 1.17288800 | 1.21105600 |
| N | 1.20081500 | -0.00046800 | 1.46586300 |
| C | 0.59858900 | -1.17357100 | 1.21118800 |
| C | -0.70185100 | -1.21424000 | 0.65494300 |
| C | -0.70128800 | 1.21411300 | 0.65483500 |
| C | -1.33439400 | 0.00007300 | 0.38418100 |
| H | -2.32753100 | 0.00028200 | -0.04258400 |
| H | 4.44022300 | -0.00015600 | -2.15320500 |
| C | -1.39242300 | -2.49887200 | 0.35698800 |
| O | -2.62516900 | -2.30181900 | -0.16375700 |
| O | -0.93019600 | -3.60995800 | 0.54730800 |
| C | -1.39127500 | 2.49904100 | 0.35680600 |
| O | -2.62440000 | 2.30251300 | -0.16324800 |

| | | | |
|---|---|---|---|
| O | -0.92831700 | 3.60992400 | 0.54652000 |
| C | -3.37827700 | -3.49395200 | -0.49011000 |
| H | -2.80360400 | -4.08204000 | -1.21191600 |
| H | -3.49008800 | -4.09455700 | 0.41755200 |
| C | -3.37697000 | 3.49496300 | -0.48967500 |
| H | -3.48768300 | 4.09614900 | 0.41773400 |
| H | -2.80246200 | 4.08226800 | -1.21225400 |
| C | 1.40716000 | -2.39404100 | 1.54742600 |
| H | 1.58616400 | -3.00285800 | 0.65658000 |
| H | 2.35792600 | -2.07355900 | 1.97446200 |
| H | 0.87454100 | -3.03960500 | 2.25111600 |
| C | 1.40830000 | 2.39300400 | 1.54717800 |
| H | 2.35897100 | 2.07207700 | 1.97409500 |
| H | 1.58744200 | 3.00175800 | 0.65632700 |
| H | 0.87606300 | 3.03877900 | 2.25097300 |
| C | -4.71383300 | -3.04469400 | -1.04926400 |
| H | -4.57739100 | -2.43960600 | -1.95068700 |
| H | -5.31701400 | -3.92039400 | -1.31007400 |
| H | -5.26678100 | -2.45222300 | -0.31404100 |
| C | -4.71324900 | 3.04628200 | -1.04756400 |
| H | -5.26603900 | 2.45460900 | -0.31158000 |
| H | -5.31603600 | 3.92223700 | -1.30842800 |
| H | -4.57789600 | 2.44058000 | -1.94873900 |
| I | 3.50476100 | -0.00022100 | -0.83620500 |