*Electronic Supplementary Information*

*for*

# Role of Lewis Acid Additives in a Palladium Catalyzed Directed C–H Functionalization Reaction of Benzohydroxamic Acid to Isoxazolone

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**Monometallic Palladium Acetate**

In the following sections, additional details on various elementary steps are provided wherein monomeric palladium acetate is considered as the active catalyst.

## 1.1. N–H activation

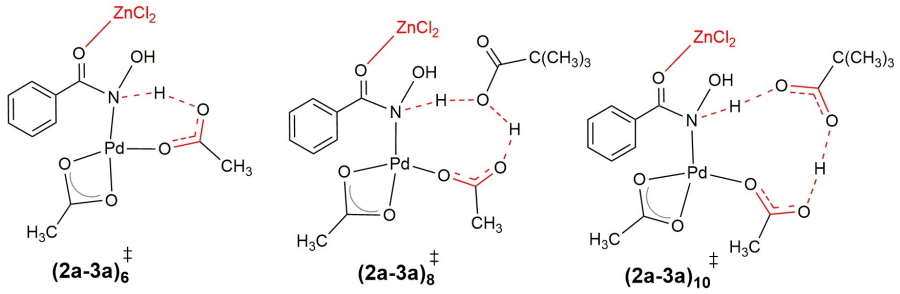



**Figure S1**. N−H bond activation transition states with and without pivalic acid assistance.

**Table S1**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for N–H Bond Activation via Monometallic Species (Acetate as Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1,S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(2a-3a)$_6$‡** | -20.9 | -8.6 | -14.2 | -3.3 | 7.9 | 8.2 | 13.9 | 10.8 | -18.9 | -5.4 | -8.7 | 2.2 |
| **(2a-3a)$_8$‡** | -22.3 | 5.7 | -13.7 | 12.8 | 15.9 | 30.6 | 21.4 | 32.4 | -18.0 | 11.8 | -7.4 | 21.1 |
| **(2a-3a)$_{10}$‡** | -28.9 | -1.1 | -19.8 | 6.7 | 1.9 | 17.7 | 9.6 | 21.7 | -27.6 | -0.2 | -15.7 | 10.6 |
| | **L3** | | | | **L3** | | | | **L3** | | | |
| | ΔE | | ΔG | | ΔE | | ΔG | | ΔE | | ΔG | |
| **(2a-3a)$_6$‡** | -13.1 | | -2.2 | | 12.3 | | 9.1 | | -6.7 | | 4.2 | |
| **(2a-3a)$_8$‡** | -12.6 | | 14.0 | | 19.3 | | 31.5 | | -5.9 | | 22.6 | |
| **(2a-3a)$_{10}$‡** | -16.7 | | 9.9 | | 20.3 | | 8.1 | | -11.9 | | 14.6 | |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S2**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the N–H Bond Activation via the Monometallic Species (Pivalate as the Ligand)

| | LA=0 | | LA=1 | | LA=1,S=1 | |
|---|---|---|---|---|---|---|
| | **L1** | **L2** | **L1** | **L2** | **L1** | **L2** |

| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **(2a-3a)$_6$**‡ | -21.1 | -5.5 | -15.2 | -0.8 | 7.3 | 9.5 | 13.2 | 12.0 | -19.4 | -2.9 | -10.4 | 4.8 |
| **(2a-3a)$_8$**‡ | -23.7 | 4.6 | -13.9 | 12.7 | 3.8 | 20.3 | 11.7 | 23.9 | -19.0 | 11.1 | -7.3 | 21.4 |
| **(2a-3a)$_{10}$**‡ | -27.4 | 2.4 | -18.1 | 11.9 | -1.0 | 17.5 | 6.6 | 22.3 | -29.2 | 2.5 | -14.2 | 17.0 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 1.2. C–H Activation

**Table S3**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the C–H Bond Activation via the Monometallic Species (Pivalate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1,S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(3a-4a)$_6$**‡ | -6.1 | 8.9 | 0.9 | 15.2 | 14.6 | 17.5 | 18.8 | 17.9 | -10.8 | 5.9 | -1.5 | 13.3 |
| **(3a-4a)$_8$**‡ | -20.8 | 8.3 | -10.4 | 17.9 | -1.8 | 15.5 | 6.2 | 19.9 | -24.9 | 5.5 | -11.8 | 17.5 |
| **(3a-4a)$_{10}$**‡ | -26.7 | 2.3 | -12.0 | 13.7 | -7.9 | 7.6 | 1.3 | 13.5 | -30.8 | -1.9 | -17.3 | 10.2 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

After the N−H deprotonation, the carboxylic acid ligand attached to the palladium metal can form a different hydrogen bonding pair, say hydrogen bonding with the directing group or with the additive or with the carboxylate ligand. We have considered different hydrogen bonding patterns for the CMD step, with pivalate ligand at the SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** level of theory and the results are given in Table S4.

**Table S4.** Relative Free Energies (in kcal/mol) for the Effect of Hydrogen Bonding in C–H Bond Activation *via* CMD Mechanism when Pivalate Acts as Ligand at the SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** Level of Theory

| Transition State | H-bonding with the directing group | H-bonding with the additive | H-bonding with the ligand |
|---|---|---|---|
| LA=0 | | | |
| **(3a-4a)$_6$**‡ | 16.0 | -[a] | 15.7 |
| **(3a-4a)$_8$**‡ | 25.5 | 22.1 | -[a] |
| **(3a-4a)$_{10}$**‡ | 16.7 | 15.6 | 16.4 |
| LA=1 | | | |
| **(3a'-4a')$_6$**‡ | 15.8 | -[a] | 12.6 |

| | | | |
|---|---|---|---|
| **(3a'-4a')$_8$‡** | 21.6 | 21.6 | 21.0 |
| **(3a'-4a')$_{10}$‡** | 19.1 | 16.2 | 15.1 |
| LA=1, S=1 | | | |
| **(3a'-4a')$_{6\text{-}S}$‡** | 15.8 | - [a] | 14.5 |
| **(3a'-4a')$_{8\text{-}S}$‡** | 28.3 | 24.2 | 31.9 |
| **(3a'-4a')$_{10\text{-}S}$‡** | 20.2 | 18.5 | 18.1 |

[a] The transition states could not be located even after several attempts. Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.

The effect of breaking the hydrogen bonding patterns exhibits irregular trends. In acetic acid assisted ten-membered relay proton transfer transition states (**(3a-4a)$_{10}$‡**, **(3a'-4a')$_{10}$‡**, **(3a'-4a')$_{10\text{-}S}$‡**)), the pivalic acid when hydrogen bonded to the additive and ligand shows lower energy as compared to that when it is hydrogen bonded to the Directing Group (DG) (pivalate assisted pathway shows 1-2 kcal/mol higher in energy than with the acetate in all steps). In eight-membered acetic acid assisted (**(3a-4a)$_8$‡**) as well as in six-membered C–H activation transition states (**(3a'-4a')$_6$‡**) the trend is irregular. The lower energy CMD transition state among each set (**(3a-4a)$_6$‡**, **(3a-4a)$_8$‡** and **(3a-4a)$_{10}$‡**) is further considered for acetate assisted pathway.

### 1.3. Second N–H Activation or N–H Deprotonation

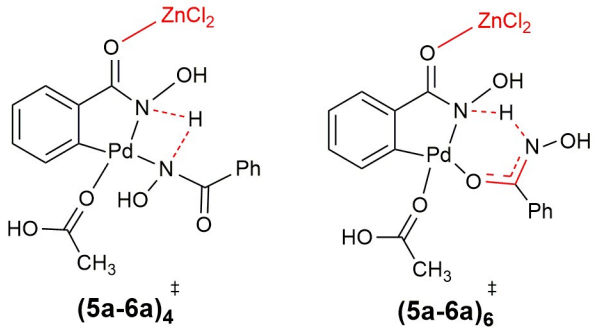



**Figure S2**. Different modes of deprotonation of second hydroxamic acid.

**Table S5**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the N–H Deprotonation of the Second Hydroxamic Acid via the Monometallic Species (Acetate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(5a-6a)$_4$‡** | 8.9 | 23.5 | 15.0 | 27.7 | 22.3 | 24.1 | 29.0 | 26.0 | -0.9 | 14.7 | 10.1 | 23.1 |
| **(5a-6a)$_6$‡** | -14.9 | -0.7 | -5.6 | 6.2 | 2.8 | 5.4 | 11.9 | 11.3 | -21.7 | -5.8 | -8.3 | 5.9 |
| | **L3** | | | | **L3** | | | | **L3** | | | |
| | ΔE | | ΔG | | ΔE | | ΔG | | ΔE | | ΔG | |

| | | | | | | |
|---|---|---|---|---|---|---|
| **(5a-6a)$_4$‡** | 14.5 | 27.1 | 25.7 | 22.7 | -5.9 | 6.7 |
| **(5a-6a)$_6$‡** | -5.6 | 6.2 | 9.5 | 10.1 | -6.0 | 8.3 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S6**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the N–H Deprotonation of the Second Hydroxamic Acid via the Monometallic Species (Pivalate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1,S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(5a-6a)$_4$‡** | 7.8 | 23.9 | 15.0 | 29.2 | 36.4 | 39.1 | 41.2 | 40.2 | -0.2 | 16.0 | 9.5 | 23.7 |
| **(5a-6a)$_6$‡** | -14.4 | 0.5 | 28.1 | 7.0 | 2.6 | 5.4 | 11.4 | 10.9 | -20.9 | -4.5 | -8.6 | 6.3 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

### 1.3.1. Role of Protic Additive in N–H deprotonation

Two modes of pivalic acid (protic additive employed in the present reaction) participation in the N–H deprotonation is shown below (Figure S4). These differ depending on the number of oxygen atoms of the carboxylic acid group that participate in the proton transfer.

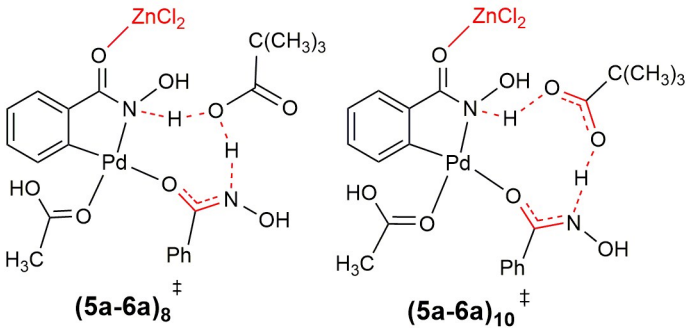



**Figure S3**. Role of protic additive in N–H deprotonation.

**Table S7**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants with an Explicit Protic Additive in the N–H Deprotonation of the Second Hydroxamic Acid in the Monometallic Species (Acetate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **(5a-6a)$_8$‡** | -31.6 | -3.4 | -20.7 | 6.7 | -[a] | -[a] | -[a] | -[a] | -[a] | -[a] | -[a] | -[a] |
| **(5a-6a)$_{10}$‡** | -43.6 | -14.9 | -30.5 | -2.0 | -14.2 | 3.0 | -2.1 | 11.4 | -40.1 | -9.9 | -21.9 | 5.9 |

| | **L3** | | **L3** | | **L3** | |
|---|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(5a-6a)$_8$‡** | -20.5 | 6.9 | -[a] | -[a] | -[a] | -[a] |
| **(5a-6a)$_{10}$‡** | -28.8 | -0.3 | -2.6 | 10.9 | -19.0 | 8.9 |

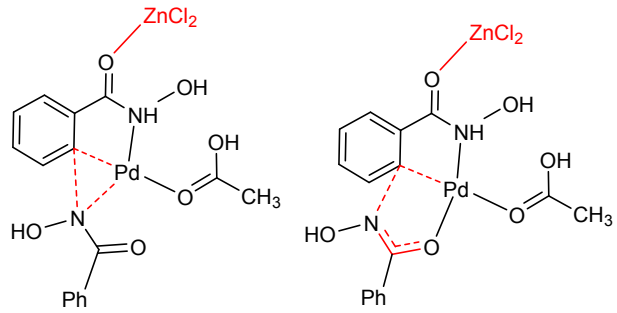
Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.[a] The transition states could not be located even after repeated attempts.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S8**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants with an Explicit Protic Additive in the N–H Deprotonation of the Second Hydroxamic Acid in the Monometallic Species (Pivalate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(5a-6a)$_8$‡** | -28.3 | -1.8 | -18.9 | 7.1 | -0.5 | 15.2 | 8.1 | 21.8 | -[a] | -[a] | -[a] | -[a] |
| **(5a-6a)$_{10}$‡** | -40.6 | -10.5 | -27.1 | 3.3 | -11.8 | 4.9 | -1.2 | 12.4 | -39.3 | -9.5 | -21.8 | 6.0 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.[a] The transition states could not be located even after repeated attempts
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 1.4. Reductive Elimination




**(6a$_1$-9)$_3$‡** **(6a-9)$_5$‡**

**Figure S4**.$C_{aryl}$–N bond formation via reductive elimination from five memebered and three memebered transition state.

**Table S9**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the $C_{aryl}$–N Bond Formation with Monometallic Species (Acetate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |

| | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **$(6a_1\text{-}9)_3$‡** | 2.9 | 16.1 | 9.5 | 22.8 | 7.4 | 23.1 | 25.8 | 25.1 | 0.9 | 15.3 | 9.0 | 23.4 |
| **$(6a\text{-}9)_5$‡** | 3.7 | 18.0 | 10.0 | 24.5 | 49.0 | 50.9 | 53.2 | 52.8 | -0.8 | 17.9 | 10.8 | 30.0 |
| | **L3** | | | | | | | | | | | |
| | ΔE | | ΔG | | ΔE | | ΔG | | ΔE | | ΔG | |
| **$(6a_1\text{-}9)_3$‡** | 11.7 | | 24.9 | | 26.0 | | 25.3 | | 13.0 | | 27.6 | |
| **$(6a\text{-}9)_5$‡** | 10.1 | | 24.6 | | 52.1 | | 51.7 | | 15.2 | | 34.4 | |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S10**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the $C_{aryl}$–N Bond Formation with Monometallic Species (with Pivalate as the Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **$(6a\text{-}7)_3$‡** | 3.3 | 16.5 | 9.8 | 22.8 | 22.5 | 24.3 | 26.0 | 25.9 | 1.5 | 16.4 | 9.4 | 24.3 |
| **$(6a\text{-}7)_5$‡** | 4.5 | 19.7 | 10.1 | 25.9 | 49.5 | 51.7 | 53.4 | 53.5 | 0.3 | 16.9 | 9.6 | 26.5 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 2. Potential Participation of a Pd-Zn Hetero-bimetallic Species

The formation of different palladium-zinc heterobimetallic species is studied in detail and shown in Figure S5. As can be noticed, we have examined different bridging combinations as well as binding of solvent molecules (S denotes solvent (DMA) coordination).

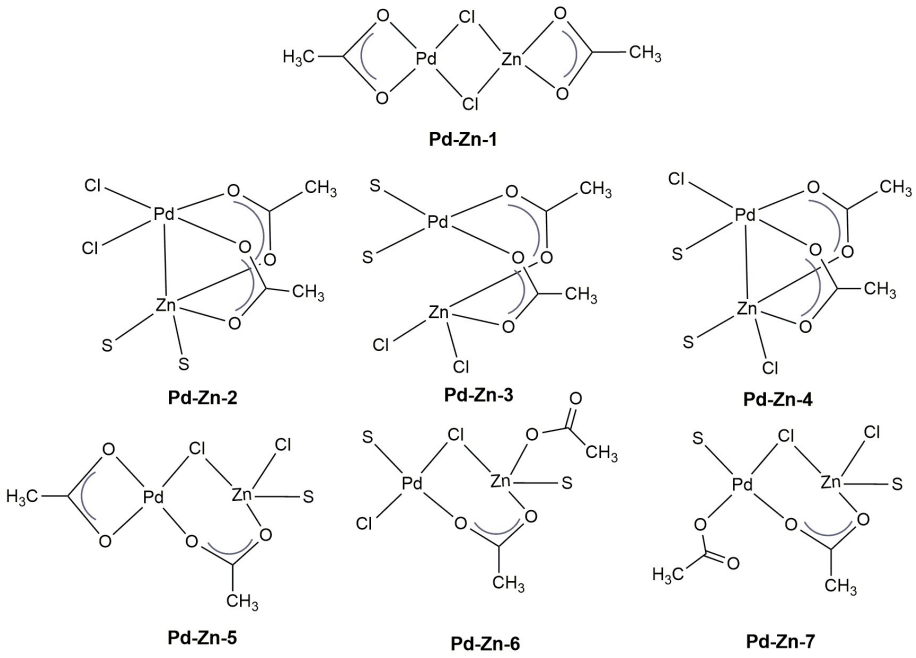



**Figure S5**. Various Pd-Zn heterobimetallic species.

**Table S11**. Energies (in kcal/mol) of the Formation of Various Pd-Zn Hetero-bimetallic Species Computed with Respect to the Infinitely Separated Reactants (with Acetate Ligand)

| Complex | **L1** | | **L2** | | **L3** | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | |
| **Pd-Zn-1** | 18.2 | 3.6 | 25.1 | 7.9 | 20.4 | 3.3 | 3.21 |
| **Pd-Zn-2** | -39.4 | -24.4 | -35.6 | -18.5 | -31.9 | -14.6 | 2.70 |
| **Pd-Zn-3** | -9.1 | 7.7 | -9.9 | 9.2 | -11.4 | 7.7 | 3.63 |
| **Pd-Zn-4** | -32.6 | -16.3 | -28.7 | -9.7 | -26.9 | -7.9 | 2.99 |
| **Pd-Zn-5** | -10.9 | -8.5 | -7.9 | -4.7 | -9.8 | -6.6 | 3.30 |
| **Pd-Zn-6** | -36.1 | -21.6 | -27.4 | -11.3 | -24.4 | -8.4 | 3.28 |
| **Pd-Zn-7** | -30.0 | -13.5 | -22.9 | -3.9 | -27.0 | -6.0 | 3.19 |

L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

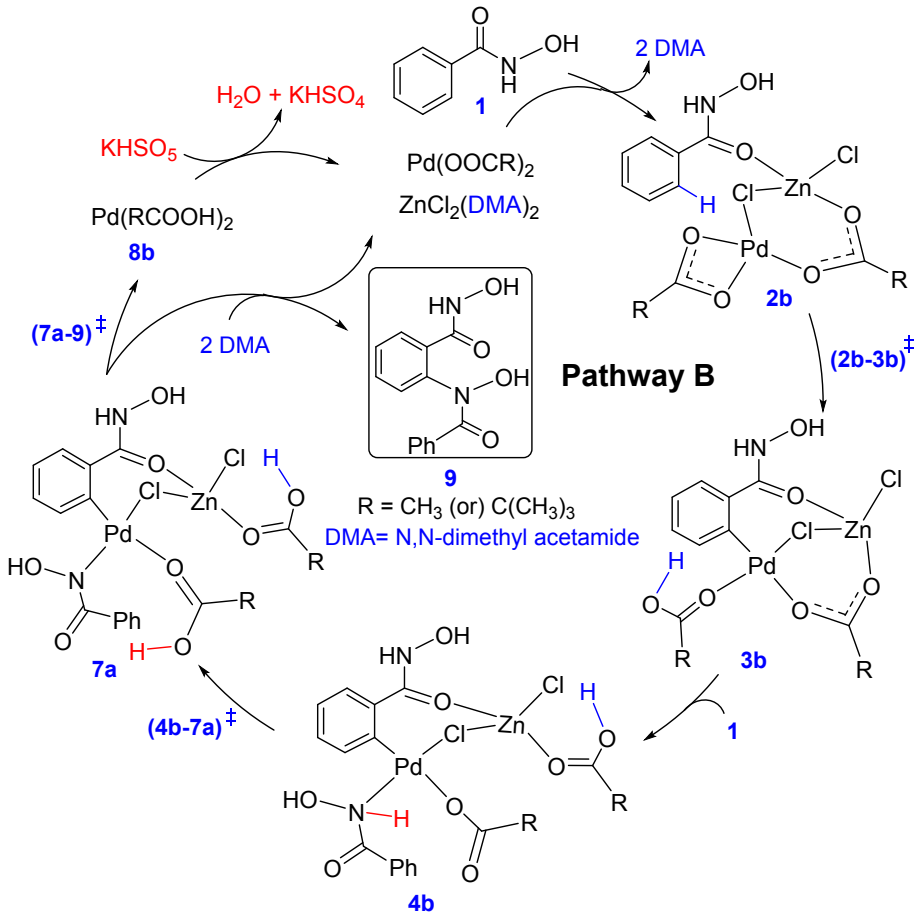
**Table S12**. Relative Energies (in kcal/mol) for the Formation of Various Pd-Zn Hetero-bimetallic Species Computed with Respect to the Infinitely Separated Reactants (with Pivalate Ligand)

| Complex | **L1** | | **L2** | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | |
| **Pd-Zn-1** | 18.4 | 5.7 | 24.8 | 9.9 | 3.30 |
| **Pd-Zn-2** | -41.3 | -21.8 | -37.7 | -15.2 | 2.68 |
| **Pd-Zn-3** | -12.6 | 8.3 | -13.9 | 10.2 | 3.58 |
| **Pd-Zn-4** | -32.7 | -13.0 | -29.3 | -6.2 | 2.98 |
| **Pd-Zn-5** | -11.0 | -6.3 | -7.5 | -2.0 | 3.21 |
| **Pd-Zn-6** | -35.2 | -17.7 | -27.5 | -7.8 | 3.28 |
| **Pd-Zn-7** | -24.7 | -8.9 | -21.1 | -3.5 | 3.18 |

L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

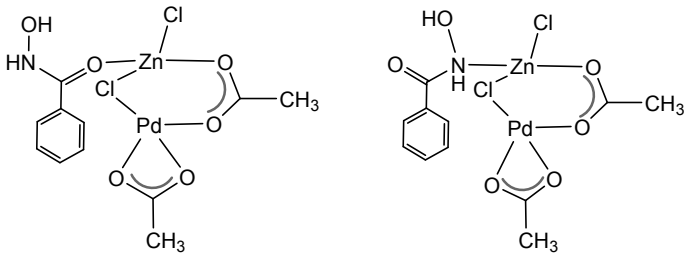
### 2.1. Pd-Zn Hetero-bimetallic Species in Various Catalytic Steps

The intermediate **2a** can rearrange to a Pd-Zn heterobimetallic species **2b** *via* ligand exchange process. The involvement of Pd-Zn hetero-bimetallic species in other catalytic steps from intermediate **2b** is also investigated and is shown in Scheme S1. The key events in the mechanism can be considered as beginning with the initial coordination of the substrate (**1**) to the Pd-Zn active species to give a catalyst-substrate complex **2b**. The *ortho* aryl C–H bond activation in this complex via **(2b-3b)**‡ results in a carbopalladated intermediate **3b**. Uptake of a second molecule of hydroxamic acid occurs next. This is accompanied by a concomitant proton transfer from the palladium-bound carboxylic acid to the bridging acetate, leading to the migration of the carboxylate-bridge from the palladium to the zinc. As the carboxylate-bridge breaks away during this process, only a chloro bridge prevails hereafter (Figure S8 and Figure S9). Now, a second molecule of benzohydroxamic acid gets coordinated to the palladium via the amido nitrogen (**4b**). The next step involves an intramolecular N–H deprotonation facilitated by the palladium-bound acetate via **(4b-7a)**‡. The carbopalladated intermediate **5b** thus produced provides an ideal arrangement for the $C_{aryl}$–N bond formation. The reductive elimination via transition state **(7a-9)**‡ results in a $C_{aryl}$–N bond formation to give the key species **9** for subsequent reaction.




**Scheme S1**. Mechanism for the Formation of **9** Involving from Pd-Zn Heterobimetallic Species.

## 2.2. Catalyst Substrate Coordination



**2b-O** **2b-N**

-1.4 2.1

**Figure S6**. N-coordination *versus* O-coordination of the substrate to the Pd-Zn heterobimetallic species.

## 2.3. C–H Activation

The following transition state models have been examined for the C–H activation step. The notations used indicate the identity of the intermetallic bridge (a = acetate, c = chloride) as well as other species involved in the C-H activation (e.g., w = water).

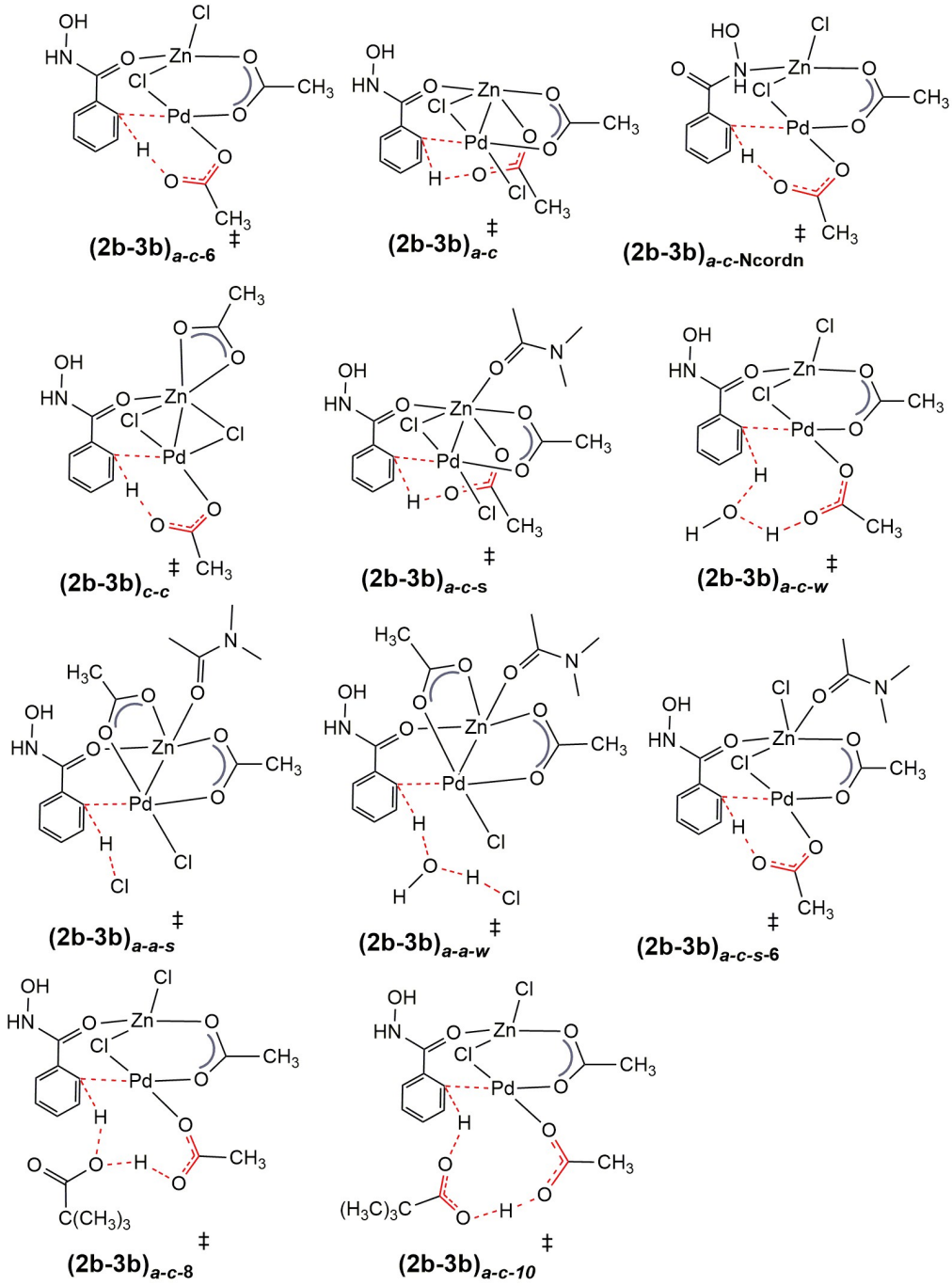



**Figure S7**. Transition states for C–H bond activation involving a Pd-Zn Heterobimetallic species.

**Table S13**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the C–H Bond Activation *via* Pd-Zn Hetero-bimetallic Species (with Acetate Ligands)

| | L1 | | L2 | | L3 | | Pd-Zn distance |
|---|---|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | (Å) |
| **(2b-3b)**$_{a\text{-}c\text{-}6}^{\ddagger}$ | 5.9 | 8.7 | 17.6 | 16.2 | 17.5 | 16.1 | 3.48 |
| **(2b-3b)**$_{a\text{-}c\text{-}8}^{\ddagger}$ | 8.7 | 23.3 | 24.0 | 34.9 | 23.6 | 34.5 | 3.51 |
| **(2b-3b)**$_{a\text{-}c\text{-}10}^{\ddagger}$ | 2.8 | 18.8 | 18.7 | 31.0 | 18.6 | 31.0 | 3.43 |
| **(2b-3b)**$_{c\text{-}c}^{\ddagger}$ | 12.1 | 13.8 | 21.2 | 18.4 | 24.3 | 21.5 | 2.80 |
| **(2b-3b)**$_{a\text{-}c}^{\ddagger}$ | 19.5 | 22.0 | 26.5 | 24.4 | 27.9 | 25.8 | 2.53 |
| **(2b-3b)**$_{a\text{-}c\text{-}\mathrm{Ncordn}}^{\ddagger}$ | 15.3 | 17.5 | 23.6 | 21.2 | 19.9 | 17.5 | 3.11 |
| **(2b-3b)**$_{a\text{-}a\text{-}w}^{\ddagger}$ | -25.0 | 2.4 | -13.0 | 15.2 | -2.1 | 26.1 | 2.99 |
| **(2b-3b)**$_{a\text{-}a\text{-}s}^{\ddagger}$ | -3.6 | 11.5 | 6.6 | 18.4 | 11.3 | 23.1 | 2.64 |
| **(2b-3b)**$_{a\text{-}c\text{-}s}^{\ddagger}$ | -9.7 | 6.6 | 0.4 | 14.0 | 5.3 | 18.9 | 2.65 |
| **(2b-3b)**$_{a\text{-}c\text{-}s\text{-}6}^{\ddagger}$ | -11.9 | 4.5 | 1.5 | 15.8 | 6.2 | 20.5 | 3.65 |
| **(2b-3b)**$_{a\text{-}c\text{-}w}^{\ddagger}$ | -12.3 | 14.2 | 3.9 | 29.8 | 11.6 | 37.4 | 3.74 |

L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S14**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for the C–H Bond Activation *via* Pd-Zn Hetero-bimetallic Species (with Pivalate Ligands)

| | L1 | | L2 | | Pd-Zn distance |
|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | (Å) |
| **(2b-3b)**$_{p\text{-}c\text{-}6}^{\ddagger}$ | 4.1 | 9.6 | 15.4 | 17.3 | 3.40 |
| **(2b-3b)**$_{p\text{-}c\text{-}8}^{\ddagger}$ | 6.7 | 25.5 | 21.2 | 37.9 | 3.45 |
| **(2b-3b)**$_{p\text{-}c\text{-}10}^{\ddagger}$ | 2.0 | 19.9 | 19.3 | 33.5 | 3.49 |
| **(2b-3b)**$_{c\text{-}c}^{\ddagger}$ | 11.4 | 15.9 | 19.7 | 20.3 | 2.81 |
| **(2b-3b)**$_{p\text{-}c}^{\ddagger}$ | 19.6 | 24.0 | 26.4 | 26.6 | 2.52 |
| **(2b-3b)**$_{p\text{-}c\text{-}\mathrm{Ncordn}}^{\ddagger}$ | 15.2 | 19.7 | 21.9 | 22.4 | 3.23 |
| **(2b-3b)**$_{p\text{-}a\text{-}w}^{\ddagger}$ | -26.9 | 3.6 | -15.4 | 16.4 | 2.94 |
| **(2b-3b)**$_{p\text{-}p\text{-}s}^{\ddagger}$ | -4.2 | 16.5 | 4.4 | 23.5 | 2.64 |
| **(2b-3b)**$_{p\text{-}c\text{-}s}^{\ddagger}$ | -11.3 | 8.5 | -1.5 | 16.6 | 2.66 |
| **(2b-3b)**$_{p\text{-}c\text{-}s\text{-}6}^{\ddagger}$ | -14.6 | 5.4 | -2.0 | 16.5 | 3.69 |
| **(2b-3b)**$_{p\text{-}c\text{-}w}^{\ddagger}$ | -16.4 | 13.7 | -0.1 | 29.9 | 3.74 |

L1-M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 2.4. Ligand Exchange

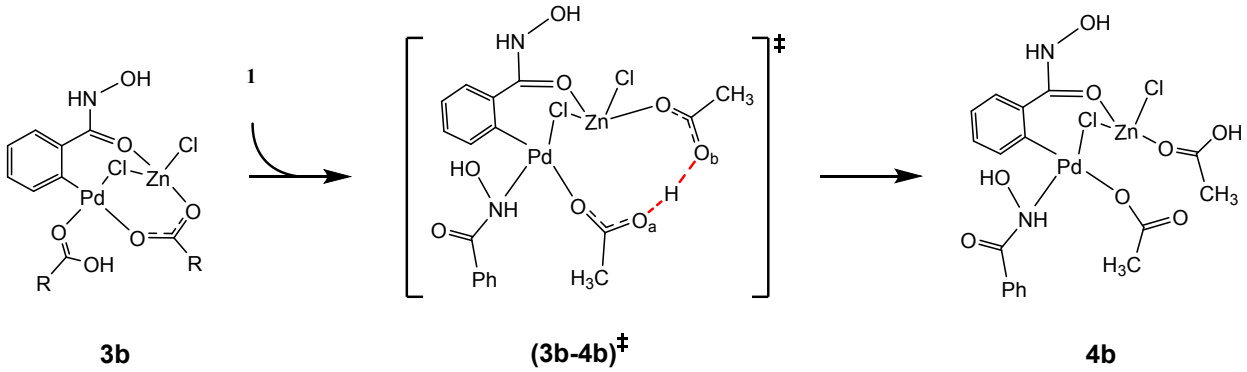



**Figure S8**. Scheme for the ligand exchange process for the formation of intermediate **4b** from **3b**.

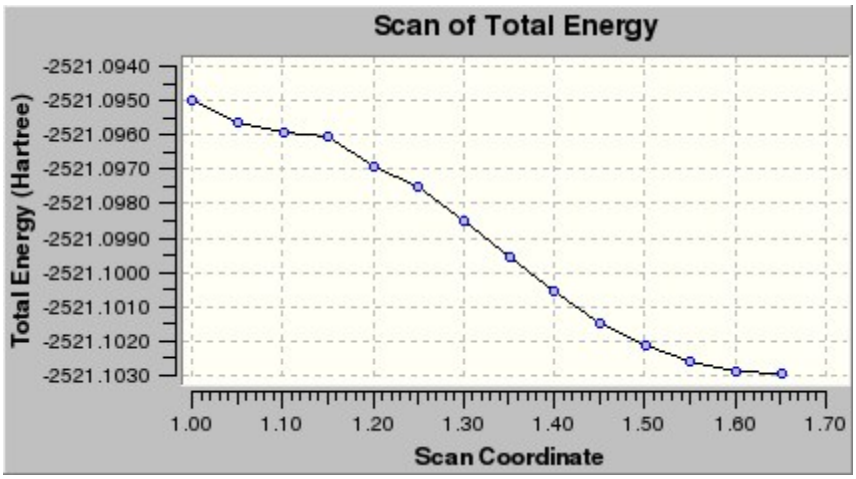



**Figure S9**. Potentail energy surface scan for ligand exchange process for the formation of **4b** from **3b**. The X-axis (in Å) represents $O_a$–H to $O_b$–H proton transfrer as the scan coordinate and Y-axis represents the total energy in hartree.

## 2.5. N–H Activation or N–H deprotonation

The involvement of Pd-Zn hetero-bimetallic species in the second N-H deprotonation is shown in Figure S10.

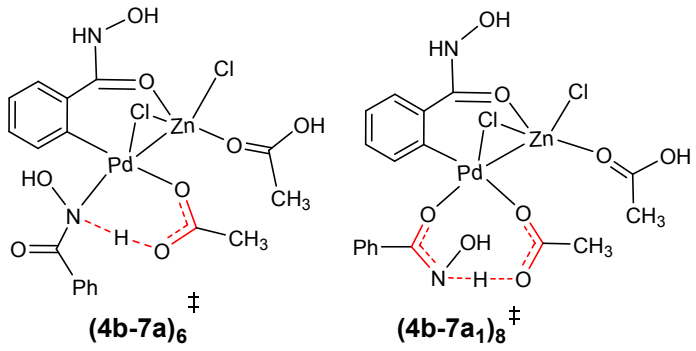



**Figure S10**. Different modes of N–H bond activation and N–H deprotonation of second hydroxamic acid via Pd-Zn hetero-bimetallic species.

**Table S15**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for N–H Deprotonation of Second Hydroxamic Acid via Pd-Zn Hetero-bimetallic Species (with Acetate Ligand)

| | **L1** | | **L2** | | **L3** | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | |
| **(4b-7a)$_6$**‡ | -31.4 | -14.7 | -15.7 | 0.01 | -16.1 | -0.3 | 2.99 |
| **(4b-7a)$_8$**‡ | -20.6 | -7.7 | -5.2 | 4.0 | -6.1 | 3.1 | 2.88 |

L1-M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S16**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for N–H Deprotonation of Second Hydroxamic Acid via Pd-Zn Hetero-bimetallic Species (with Pivalate Ligand)

| | **L1** | | **L2** | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | |
| **(4b-7a)$_6$**‡ | -[a] | -[a] | -[a] | -[a] | -[a] |
| **(4b-7a)$_8$**‡ | -21.9 | -4.9 | -8.6 | 5.6 | 2.75 |

[a] The transition states could not be located even after several attempts. L1-M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 2.6. Reductive Elimination via Pd-Zn Heterobimetallic Species

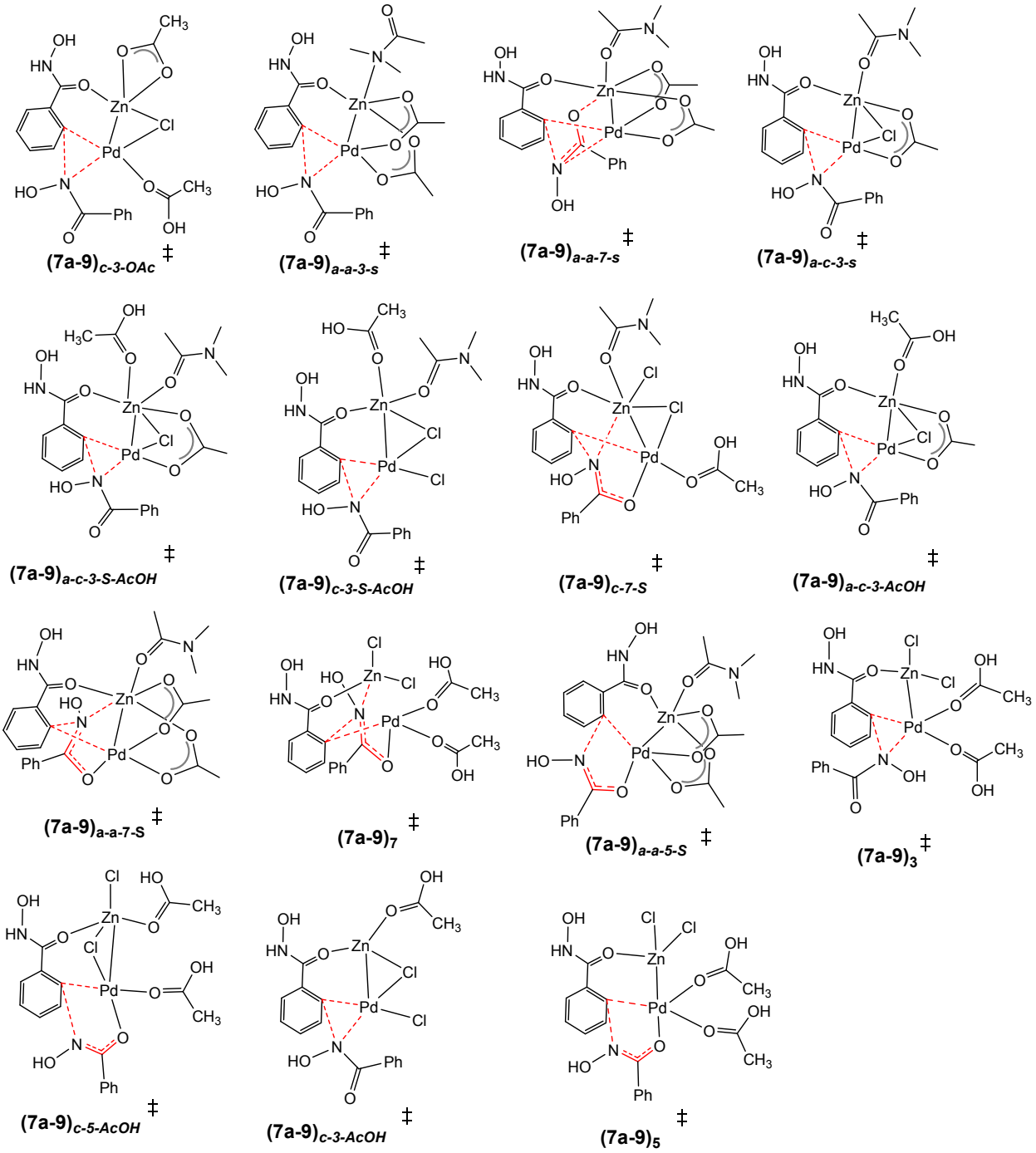



**Figure S11**. $C_{aryl}$–N bond formation transition states with Pd-Zn hetero-bimetallic interaction.

**Table S17**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for $C_{aryl}$–N Bond Formation invovling Pd-Zn Hetero-bimetallic Interaction (with Acetate as Ligand)

| | L1 | | L2 | | L3 | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | |
| **(7a-9)$_3$**‡ | -7.1 | 8.2 | 6.1 | 21.0 | 5.9 | 20.7 | 2.62 |
| **(7a-9)$_7$**‡ | -9.6 | 6.8 | 4.0 | 20.6 | 6.2 | 22.8 | 3.06 |
| **(7a-9)$_{c\text{-}5\text{-}AcOH}$**‡ | -4.2 | 9.2 | 8.0 | 20.5 | 9.0 | 21.5 | 2.78 |
| **(7a-9)$_{a\text{-}a\text{-}3\text{-}s\text{-}(N\text{-}cordn)}$**‡ | 19.1 | 31.5 | 39.3 | 45.9 | 52.9 | 59.9 | 2.59 |
| **(7a-9)$_{a\text{-}c\text{-}3\text{-}S\text{-}AcOH}$**‡ | -1.4 | 20.5 | 14.6 | 34.4 | 25.6 | 45.4 | 2.66 |
| **(7a-9)$_{a\text{-}a\text{-}7\text{-}s}$**‡ | 19.2 | 33.1 | 38.6 | 46.9 | 52.6 | 61.0 | 2.61 |
| **(7a-9)$_{c\text{-}3\text{-}AcOH}$**‡ | -0.9 | 13.1 | 11.2 | 24.0 | 13.5 | 26.4 | 2.88 |
| **(7a-9)$_{c\text{-}3\text{-}OAc}$**‡ | 26.2 | 29.6 | 39.9 | 37.8 | 45.1 | 42.9 | 2.68 |
| **(7a-9)$_{a\text{-}c\text{-}3\text{-}AcOH}$**‡ | 14.3 | 18.7 | 29.8 | 29.3 | 35.2 | 34.7 | 2.65 |
| **(7a-9)$_{a\text{-}c\text{-}3\text{-}s}$**‡ | 18.2 | 24.6 | 30.7 | 32.9 | 35.9 | 38.2 | 2.66 |
| **(7a-9)$_{c\text{-}7\text{-}S}$**‡ | -8.2 | 10.5 | 3.7 | 23.6 | 9.4 | 29.3 | 2.86 |
| **(7a-9)$_{c\text{-}3\text{-}S\text{-}AcOH}$**‡ | 1.1 | 18.1 | 7.5 | 25.0 | 10.7 | 28.4 | 2.63 |
| **(7a-9)$_5$**‡ | 0.0 | 16.2 | 7.8 | 22.9 | 10.3 | 26.6 | 2.73 |
| **(7a-9)$_{a\text{-}a\text{-}5\text{-}s}$**‡ | 21.2 | 31.0 | 37.2 | 42.6 | 52.1 | 53.7 | 2.60 |

L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**, L3- SMD$_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G**.

**Table S18**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for $C_{aryl}$–N Bond Formation invovling Pd-Zn Hetero-bimetallic Interaction (with Pivalate as Ligand)

| | L1 | | L2 | | Pd-Zn distance (Å) |
|---|---|---|---|---|---|
| | ΔE | ΔG | ΔE | ΔG | |
| **(7a-9)$_3$**‡ | -8.1 | 9.6 | 4.8 | 22.6 | 2.62 |
| **(7a-9)$_7$**‡ | -9.0 | 10.1 | 2.7 | 22.2 | 3.09 |
| **(7a-9)$_{c\text{-}5\text{-}PivOH}$**‡ | -3.7 | 12.8 | 7.5 | 24.0 | 2.76 |
| **(7a-9)$_{a\text{-}a\text{-}3\text{-}s\text{-}(N\text{-}cordn)}$**‡ | -[a] | -[a] | -[a] | -[a] | -[a] |
| **(7a-9)$_{a\text{-}c\text{-}3\text{-}S\text{-}PivOH}$**‡ | -5.5 | 19.3 | 11.5 | 34.5 | 2.69 |
| **(7a-9)$_{p\text{-}p\text{-}7\text{-}s}$**‡ | 17.6 | 34.7 | 36.7 | 49.2 | 2.61 |
| **(7a-9)$_{c\text{-}3\text{-}PivOH}$**‡ | -5.3 | 13.8 | 6.8 | 25.8 | 2.91 |
| **(7a-9)$_{c\text{-}\text{-}3\text{-}OPv}$**‡ | -[a] | -[a] | -[a] | -[a] | -[a] |
| **(7a-9)$_{p\text{-}c\text{-}3\text{-}PivOH}$**‡ | 17.4 | 26.1 | 31.3 | 36.3 | 2.65 |
| **(7a-9)$_{p\text{-}c\text{-}3\text{-}s}$**‡ | 17.8 | 26.2 | 29.8 | 34.3 | 2.65 |
| **(7a-9)$_{c\text{-}7\text{-}S}$**‡ | -8.3 | 11.6 | 3.9 | 25.3 | 2.87 |
| **(7a-9)$_{c\text{-}3\text{-}S\text{-}PivOH}$**‡ | 0.6 | 18.1 | 7.3 | 25.1 | 2.62 |
| **(7a-9)$_5$**‡ | -a | -a | -a | -a | -a |
| **(7a-9)$_{p\text{-}p\text{-}5\text{-}s}$**‡ | -a | -a | -a | -a | -a |

[a] The transition states could not be located even after several attempts. L1-M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

**3. Natural Bond Orbital (NBO) Analysis for $C_{aryl}$–N bond Formation via Pd-Zn Heterobimetallic Pathway**

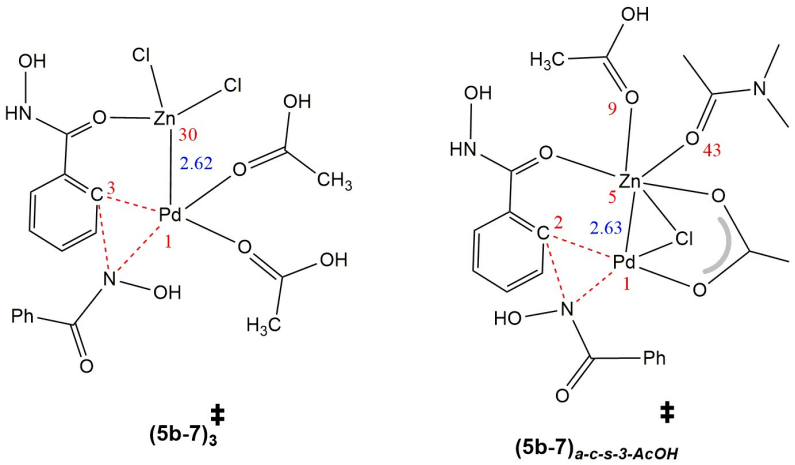



**Figure S12**. Schematic representations for NBO analysis of $C_{aryl}$–N bond formation via Pd-Zn heterobimetallic species.

**Table S19**. Natural Bond Orbital Analysis of $C_{aryl}$–N Bond Formation Transition States with Pd-Zn Hetero-bimetallic Interaction

| **(7a-9)$_3$‡** | | |
|---|---|---|
| Donor | Acceptor | E(2) kcal/mol |
| LP (4)Pd1 | LP*(6)Zn30 | 32.07 |
| BD (1)Pd1- C3 | LP*(6)Zn30 | 3.43 |
| BD (1)Pd1- C3 | LP*(7)Zn30 | 1.87 |
| LP (4)Pd1 | LP*(7)Zn30 | 6.37 |
| LP (4)Pd1 | LP*(8)Zn30 | 4.06 |
| **(7a-9)$_{a\text{-}c\text{-}s\text{-}AcOH}$‡** | | |
| Donor | Acceptor | E(2) kcal/mol |
| BD (1)Pd1-C26 | LP*(6)Zn5 | 1.58 |
| LP (4)Pd1 | LP*(6)Zn5 | 8.77 |
| LP (4)Pd1 | LP*(7)Zn5 | 3.01 |
| BD (1)O9 - C10 | LP*(7)Zn5 | 6.98 |
| LP (1) O9 | LP*(6)Zn5 | 4.08 |
| LP (1) O9 | LP*(7)Zn5 | 31.22 |
| LP (3) O9 | LP*(6)Zn5 | 7.88 |
| LP (3) O9 | LP*(7)Zn5 | 6.38 |
| BD (1) O43 - C 44 | LP*( 8)Zn5 | 5.40 |
| LP (1) O43 | LP*( 8)Zn5 | 24.18 |
| LP (1) O43 | LP*(6)Zn5 | 6.79 |

## 4. Nucleophilic Addition and Elimination

This step involves the conversion of intermediate **7** to Isoxazolone. The formation of Isoxazolone can takes place either concerted manner (Figure S14) or stepwise manner.

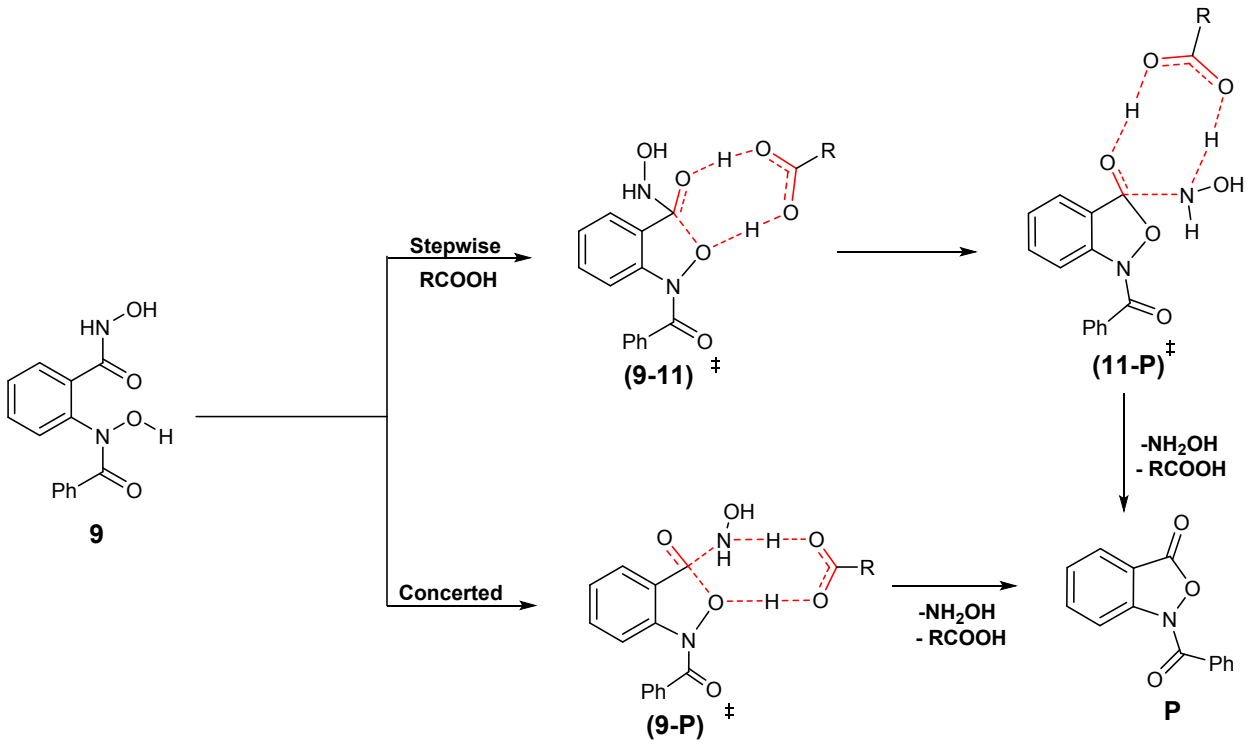



**Figure S13**. Nucleophilic addition and elimination for the formation of Isoxazolone in stepwise and concerted manner.

### 4.1. Concerted pathway

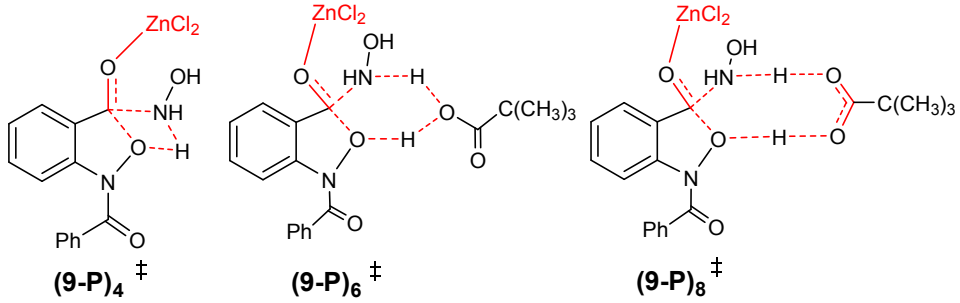



**Figure S14**. Protic additive unassisted and assisted nucleophilic addition elimination via concerted manner.

**Table S20**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Nucleophilic Addition Elimination via Concerted Pathway (Acetate as Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(9-P)$_4$‡** | 24.9 | 37.1 | 24.0 | 36.6 | 46.7 | 46.8 | 48.3 | 45.5 | 20.0 | 33.6 | 26.5 | 39.2 |
| **(9-P)$_6$‡** | 2.6 | 29.3 | 5.4 | 33.5 | 37.6 | 51.4 | 41.6 | 52.9 | 8.5 | 37.1 | 19.4 | 47.1 |
| **(9-P)$_8$‡** | -8.2 | 19.8 | -4.3 | 24.1 | 16.7 | 32.1 | 24.0 | 38.1 | -8.8 | 20.5 | 2.5 | 32.9 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S21**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Nucleophilic Addition Elimination via Concerted Pathway (Pivalate as Ligand)

| | LA=0 | | | | LA=1 | | | | LA=1, S=1 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **L1** | | **L2** | | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(9-P)$_4$‡** | 25.8 | 39.6 | 24.3 | 38.9 | 47.7 | 49.3 | 48.6 | 47.8 | 21.0 | 36.1 | 26.8 | 41.6 |
| **(9-P)$_6$‡** | 5.2 | 31.8 | 7.3 | 35.2 | 37.5 | 50.7 | 40.6 | 51.9 | 11.0 | 40.0 | 21.8 | 50.9 |
| **(9-P)$_8$‡** | -6.1 | 21.3 | -2.9 | 24.8 | 19.5 | 35.1 | 26.1 | 40.9 | -6.1 | 23.3 | 4.6 | 35.6 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-SMD$_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

In stepwise pathway (Figure S15 and Figure S16), the first step involves the activation of carbonyl oxygen using carboxylic acid followed by C–O bond formation and in second step the elimination of hydroxylamine takes place. In the activation of carbonyl oxygen, two molecules of carboxylic acids act as a proton shuttle.

### 4.2. C–O bond formation via stepwise pathway

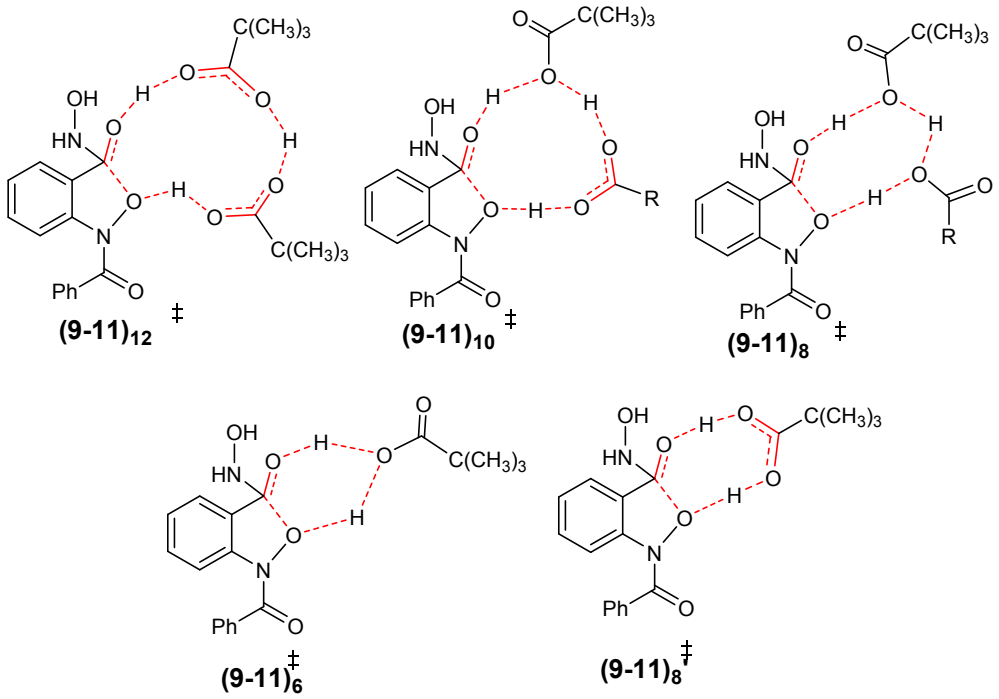



**Figure S15**. Transition states for C–O bond formation and protonation of carbonyl oxygen.

**Table S22**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Nucleophilic Addition via Stepwise Pathway

| | LA=0 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $Pd(OAc)_2$ | | | | $Pd(OPiv)_2$ | | | |
| | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(9-11)$_{12}$‡** | -23.2 | 16.5 | -16.3 | 28.5 | -0.04 | 0.02 | -14.5 | 26.8 |
| **(9-11)$_{10}$‡** | -25.5 | 18.0 | -15.6 | 29.5 | -0.03 | 0.02 | -13.6 | 26.7 |
| **(9-11)$_{8}$‡** | -21.3 | 20.8 | -13.7 | 31.1 | *-a* | *-a* | *-a* | *-a* |
| **(9-11)$_{8'}$‡** | -2.7 | 23.0 | 5.6 | 30.4 | -0.0 | 0.03 | 5.9 | 31.7 |
| **(9-11)$_{6}$‡** | 10.4 | 37.3 | 19.4 | 45.7 | 0.02 | 0.1 | 20.3 | 46.3 |

[a] The transition states could not be located even after several attempts. L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S23**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Nucleophilic Addition via Stepwise Pathway

| | LA=1, S=1 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $Pd(OAc)_2$ | | | | $Pd(OPiv)_2$ | | | |
| | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(9a'-11a')$_{12\text{-}s}^{‡}$** | -38.3 | 7.8 | -21.5 | 27.4 | -35.3 | 8.2 | -18.4 | 27.3 |
| **(9a'-11a')$_{10\text{-}s}^{‡}$** | -22.2 | 20.1 | -10.1 | 33.8 | -22.1 | 21.8 | -9.3 | 38.1 |
| **(9a'-11a')$_{8\text{-}s}^{‡}$** | 1.0 | 45.7 | 14.8 | 61.1 | -1.9 | 35.7 | 4.9 | 40.6 |
| **(9a'-11a')$_{8'\text{-}s}^{‡}$** | -22.8 | 6.7 | -10.2 | 19.7 | -20.7 | 8.3 | -8.6 | 20.6 |
| **(9a'-11a')$_{6\text{-}s}^{‡}$** | 7.8 | 36.9 | 26.5 | 39.2 | 9.1 | 38.2 | 19.6 | 49.5 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

### 4.3. $NH_2OH$ Elimination via Stepwise Pathway

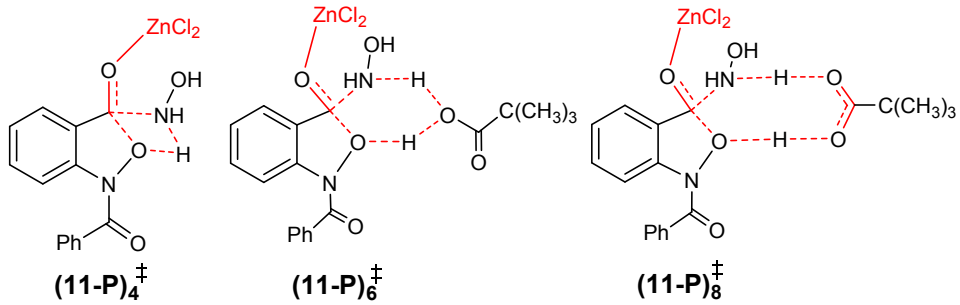



**Figure S16**. Elimination of hydroxylamine unassisted and assisted by carboxylic acid.

**Table S24**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Elimination of Hydroxylamine via Stepwise Pathway

| | LA=0 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $Pd(OAc)_2$ | | | | $Pd(OPiv)_2$ | | | |
| | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **(11-P)$_4^{‡}$** | 28.3 | 40.6 | 31.1 | 42.3 | -0.03 | 0.02 | 31.4 | 44.6 |
| **(11-P)$_6^{‡}$** | -1.1 | 24.8 | -2.5 | 25.8 | 0.0 | 0.04 | -0.8 | 27.2 |
| **(11-P)$_8^{‡}$** | -12.6 | 13.6 | -10.5 | 18.5 | -0.3 | 0.02 | -9.4 | 19.3 |

L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

**Table S25**. Relative Energies (in kcal/mol) of Transition States Computed with Respect to the Infinitely Separated Reactants for Elimination of Hydroxylamine via Stepwise Pathway

| | LA=1,S=1 | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | $Pd(OAc)_2$ | | | | $Pd(OPiv)_2$ | | | |
| | **L1** | | **L2** | | **L1** | | **L2** | |
| | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG | ΔE | ΔG |
| **$(11a'\text{-}P)_{4s}$‡** | 25.7 | 38.8 | 30.2 | 42.0 | 26.7 | 41.4 | 30.4 | 44.6 |
| **$(11a'\text{-}P)_{6s}$‡** | -8.5 | 21.9 | -0.3 | 33.5 | -7.4 | 20.6 | 1.1 | 30.9 |
| **$(11a'\text{-}P)_{8s}$‡** | -24.8 | 6.2 | -11.9 | 20.3 | -24.1 | 6.1 | -11.2 | 19.6 |

Binding of $ZnCl_2$ to the carbonyl oxygen of the substrate is denoted as LA=1. S=1 refers to the coordination of a molecule of solvent (DMA) to $ZnCl_2$.
L1- M06/LANL2DZ(Pd,Zn),6-31G**, L2-$SMD_{(DMA)}$/M06/LANL2DZ(Pd,Zn),6-31G**//M06/LANL2DZ(Pd,Zn),6-31G**

## 5. Free Energy Profile Diagram For the Formation of Isoxazolone Under Different Conditions

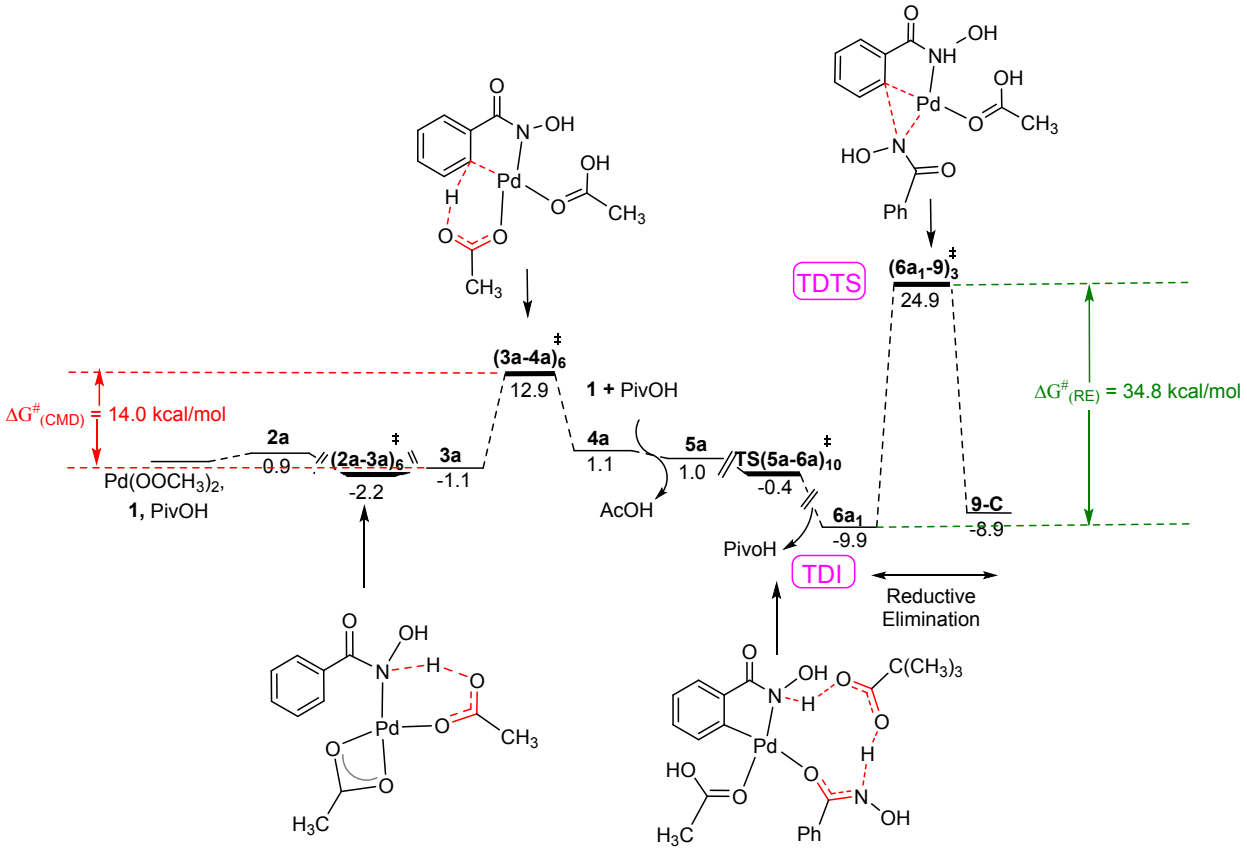



**Figure S17**. Free energy profile for the formation Isoxazolone without $ZnCl_2$ participation at the $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** level of theory. As per the Murdoch recommendations, the activation energy for CMD process (**$(3a\text{-}4a)_6$**‡) is calculated with respect to the preceding exoergic intermediate (**3a**) which is found to be 14.0

kcal/mol.[1] Similarly, the activation barrier for the reductive elimination step (**((6a-9)$_3$**$^‡$) is (calculated with respect to intermediate **6a**) found to be 34.8 kcal/mol.

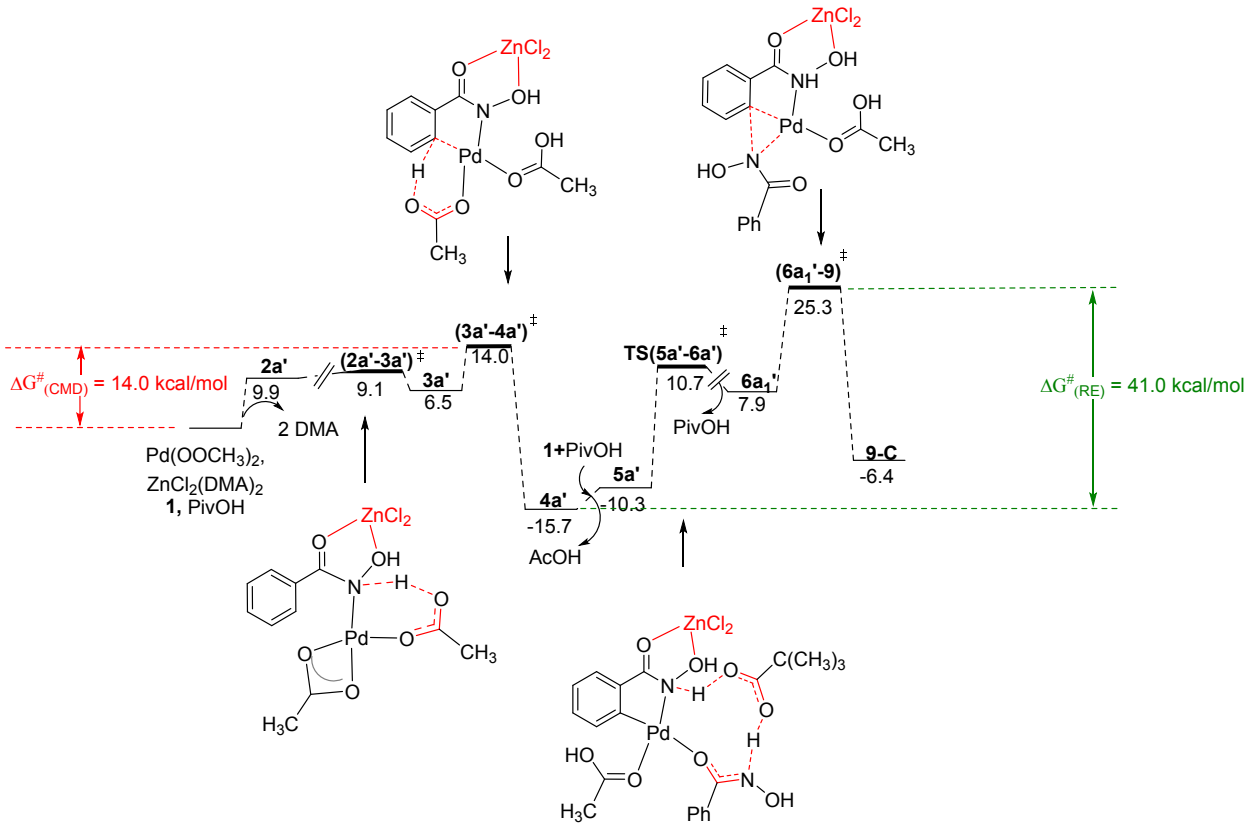



**Figure S18**. Free energy profile for the formation Isoxazolone with $ZnCl_2$ participation at the $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** level of theory. Note that both the activation energy and the relative energy for the $C_{aryl}$–N bond formation are higher than in the absence of Lewis acid additive in the transition states.

(1) Murdoch, J. R.*J. Chem. Educ*. **1981**, *58*, 32.

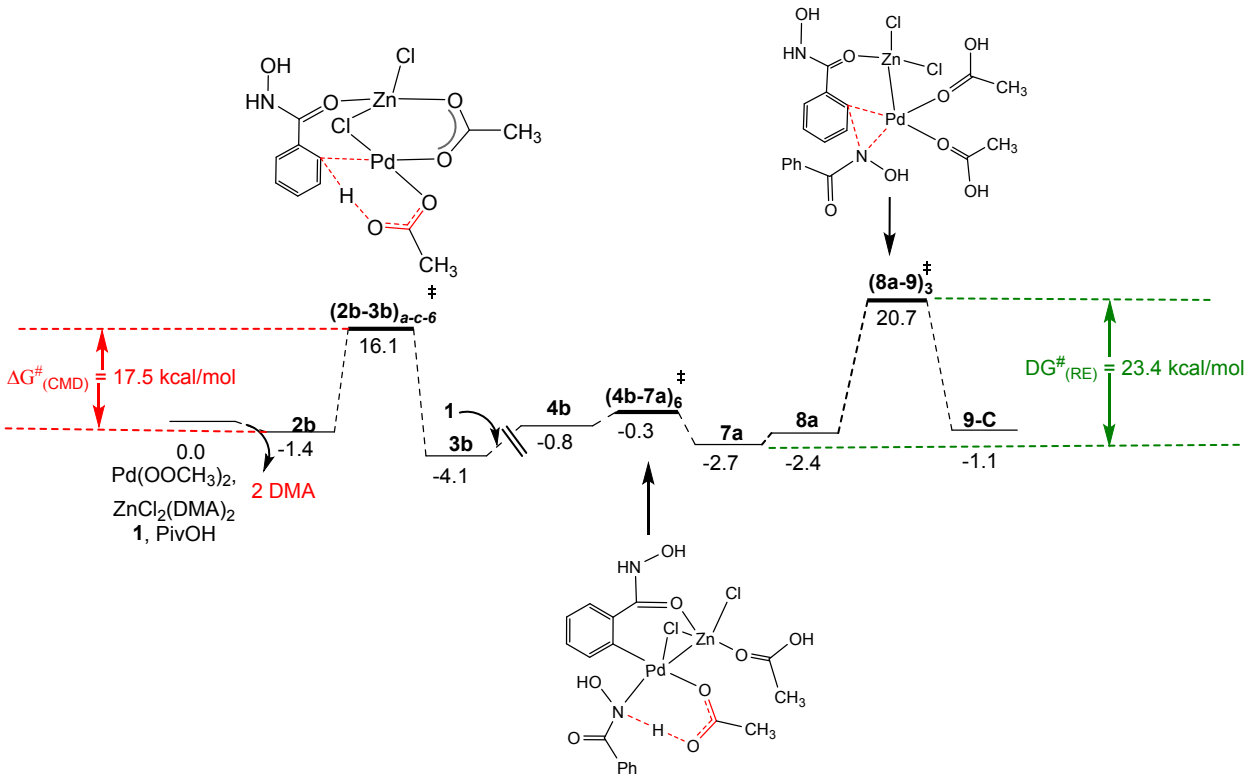



**Figure S19**. Free energy profile for the formation Isoxazolone via Pd-Zn hetero-bimetallic pathway at the $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** level of theory. Here, both the activation energy and relative free energy for the $C_{aryl}$–N is found to be lower as compared to all other possibilities.

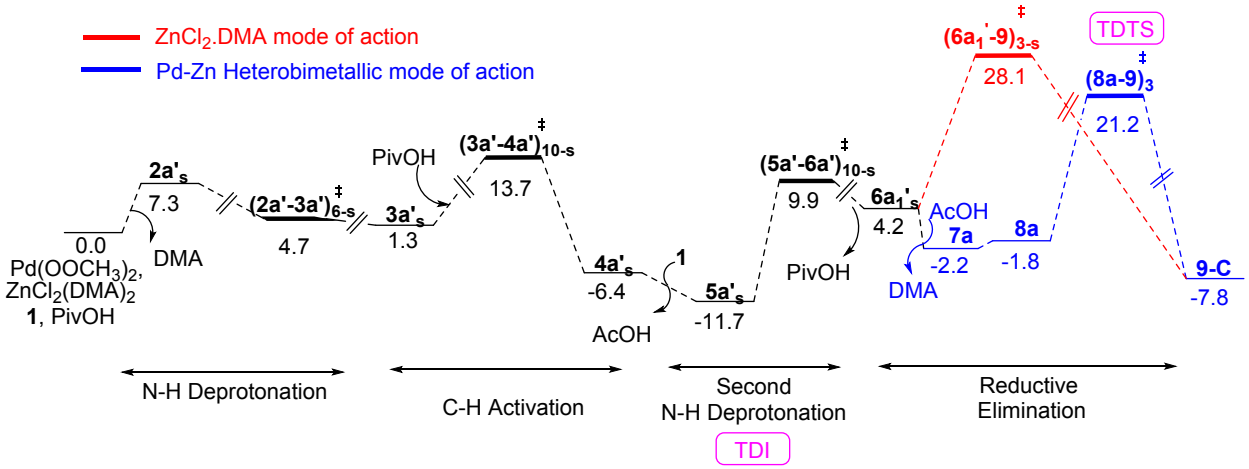



**Figure S20**. Free energy profile for the formation isoxazolone via Pd-Zn hetero-bimetallic pathway at the $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** level of theory. Standard state correction per solvent molecule (10.75M, *N,N*-dimethyl acetamide) is added to the electronic energy to obtain Gibbs Free Energies.

**Table S26.** Comparison of the Effect of Lewis Acid Additive on the Relative Free Energy and on Activation Energy (in kcal/mol) for the Formation of the Product Precursor **9** Computed at the $SMD_{(DMA)}$/M06/SDD(Pd,Zn),6-311+G**//M06/LANL2DZ(Pd,Zn),6-31G** Level of Theory

| | $ZnCl_2$·DMA | Pd-Zn hetero-bimetallic interaction | Without $ZnCl_2$ |
|---|---|---|---|
| C–H activation | | | |
| Relative free energy | 10.7 | 16.1 | 12.9 |
| Activation barrier | 9.9 | 17.5 | 14.0 |
| $C_{aryl}$–N bond formation | | | |
| Relative free energy | 27.6 | 20.7 | 24.9 |
| Activation barrier | 40.2 | 23.4 (33.4)[a] | 34.8 |

[a] With respect to **5a's**

## 6. Energetic Span Model

According to energetic span model, the turn over frequency (TOF) determines the efficiency of the catalytic cycle. The TOF is related to the energetic span (δE) as in equation (a) shown below.

The energetic span (δE) can be calculated from TOF-determining transition state (TDTS) and TOF-determining intermediate (TDI) as shown in equations (b) and (c).

$$TOF = \frac{k_B T}{h}\, e^{\frac{-\delta E}{RT}} \qquad \text{(a)}$$

where δE is the energetic span, which can be defined as

$\delta E = TDTS - TDI$ when TDTS appear after TDI or (b)

$\delta E = TDTS - TDI + \Delta G_r$ when TDTS appear before TDI (c)

$\Delta G_r$ is the Gibbs free energy of the reaction.

**Table S27**. Calculation of Energetic Span (δE) in kcal/mol using TDI and TDTS in the Lewis acid Assisted and Unassisted Pathways [a]

| LA=1, S=1 | | | LA=0 | | |
|---|---|---|---|---|---|
| TDI | TDTS | δE | TDI | TDTS | δE |
| **5a's** | **(3a'-4a')‡$_{10\text{-}s}$** | 15.0 | **6a1** | **(3a-4a)‡$_6$** | 13.9 |
| | **(5a'-6a')‡$_{10\text{-}s}$** | 13.2 | | **(5a-6a)‡$_{10}$** | 0.6 |
| | **(8a-9)‡$_3$** | 33.4 | | **(6a-9)‡$_3$** | 34.8 |

*a Figure 7 in the main text shows the Gibbs free energy profile for the LA=1,S=1 and Figure S17 shows the Gibbs free energy profile for LA=0.*

Optimized Gas phase Cartesian Coordinates at the M06/LANL2DZ(Pd,Zn), 6-31G** Level of Theory.

# I. Palladium Acetate as Ligand

## Pathway A (LA=0)

---

**2a**

---

Number of imaginary frequencies: 0
Electronic energy =-1059.307829
Zero-point correction= 0.236611
Thermal correction to Energy= 0.257055
Thermal correction to Enthalpy= 0.257999
Thermal correction to Gibbs Free Energy= 0.185296
Sum of electronic and zero-point Energies= -1059.071218
Sum of electronic and thermal Energies= -1059.050774
Sum of electronic and thermal Enthalpies= -1059.049830
Sum of electronic and thermal Free Energies= -1059.122533

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.417084 | -1.621417 | -1.055941 |
| 6 | -1.580332 | -1.544229 | 0.077807 |
| 6 | -1.806462 | -0.535736 | 1.058712 |
| 6 | -2.868183 | 0.376127 | 0.874376 |
| 6 | -3.653143 | 0.300255 | -0.252650 |
| 6 | -3.429659 | -0.704565 | -1.215792 |
| 1 | -2.227798 | -2.406026 | -1.783809 |
| 1 | -1.303315 | -0.583305 | 2.023021 |
| 1 | -3.040731 | 1.137749 | 1.629452 |
| 1 | -4.463274 | 1.010224 | -0.399273 |
| 1 | -4.064942 | -0.750584 | -2.096805 |
| 6 | -0.429400 | -2.477432 | 0.188041 |
| 8 | -0.310134 | -3.561288 | -0.375247 |
| 7 | 0.590945 | -1.828136 | 0.849962 |
| 8 | 1.781749 | -2.501230 | 0.612686 |
| 1 | 1.525179 | -3.231048 | -0.002310 |
| 46 | 0.170819 | 0.035094 | 0.034144 |
| 8 | -0.532840 | 1.786423 | -0.727481 |
| 8 | -0.386508 | 2.417338 | 1.412617 |
| 8 | 2.112108 | 0.760856 | -0.598391 |
| 6 | -0.650002 | 2.652114 | 0.235702 |

| | | | |
|---|---|---|---|
| 6 | 3.280107 | 0.458991 | -0.354031 |
| 8 | 3.679892 | -0.659175 | 0.191996 |
| 1 | 2.938764 | -1.299360 | 0.356307 |
| 6 | -1.201059 | 3.982217 | -0.219833 |
| 1 | -1.062626 | 4.732551 | 0.561469 |
| 1 | -0.725787 | 4.303606 | -1.150569 |
| 1 | -2.272817 | 3.871144 | -0.423609 |
| 6 | 4.401766 | 1.387135 | -0.684522 |
| 1 | 4.969260 | 1.605935 | 0.225171 |
| 1 | 5.087464 | 0.898709 | -1.383462 |
| 1 | 4.012898 | 2.308894 | -1.116566 |

---

**$(2a\text{-}3a)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy=-1059.3154521
Zero-point correction= 0.232833
Thermal correction to Energy= 0.252759
Thermal correction to Enthalpy= 0.253704
Thermal correction to Gibbs Free Energy= 0.180798
Sum of electronic and zero-point Energies= -1059.082619
Sum of electronic and thermal Energies= -1059.062693
Sum of electronic and thermal Enthalpies= -1059.061748
Sum of electronic and thermal Free Energies= -1059.134654

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 4.041488 | -0.834370 | -1.589375 |
| 6 | 3.727303 | -1.934071 | -0.794589 |
| 6 | 2.775636 | -1.813237 | 0.206850 |
| 6 | 2.123028 | -0.592802 | 0.408427 |
| 6 | 2.443345 | 0.512143 | -0.387184 |
| 6 | 3.404861 | 0.385918 | -1.380977 |
| 1 | 4.790106 | -0.928022 | -2.372666 |
| 1 | 4.226965 | -2.885892 | -0.955795 |
| 1 | 2.515630 | -2.652821 | 0.846103 |
| 1 | 1.964612 | 1.474596 | -0.220727 |
| 1 | 3.660983 | 1.246256 | -1.993834 |
| 6 | 1.134623 | -0.542368 | 1.500362 |
| 8 | 1.052994 | -1.364662 | 2.393453 |
| 7 | 0.168097 | 0.516047 | 1.472440 |
| 1 | 0.395451 | 1.623202 | 1.172583 |
| 8 | -0.579229 | 0.528918 | 2.638804 |
| 46 | -1.125003 | 0.060871 | -0.082393 |
| 8 | 0.394646 | 2.863464 | 0.662773 |

| | | | |
|---|---|---|---|
| 8 | -1.083134 | 1.990560 | -0.794057 |
| 8 | -2.508682 | -0.909789 | -1.373718 |
| 8 | -1.503545 | -1.943839 | 0.267031 |
| 6 | -0.416971 | 2.950231 | -0.298489 |
| 6 | -2.329917 | -1.974087 | -0.710513 |
| 6 | -0.637910 | 4.300645 | -0.917185 |
| 1 | -1.299099 | 4.878543 | -0.262750 |
| 1 | 0.312120 | 4.836864 | -0.981058 |
| 1 | -1.103659 | 4.210850 | -1.899738 |
| 6 | -3.073819 | -3.222346 | -1.026630 |
| 1 | -4.000275 | -3.241458 | -0.442695 |
| 1 | -3.335754 | -3.244878 | -2.086792 |
| 1 | -2.479632 | -4.097078 | -0.752196 |
| 1 | -0.408376 | -0.363675 | 3.014103 |

---

**$(2a\text{-}3a)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1406.1323562
Zero-point correction= 0.379473
Thermal correction to Energy= 0.408007
Thermal correction to Enthalpy= 0.408951
Thermal correction to Gibbs Free Energy= 0.319387
Sum of electronic and zero-point Energies= -1405.752883
Sum of electronic and thermal Energies= -1405.724349
Sum of electronic and thermal Enthalpies= -1405.723405
Sum of electronic and thermal Free Energies= -1405.812970

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.266989 | 4.374866 | -0.466512 |
| 6 | 0.248869 | 4.282683 | -1.413067 |
| 6 | -0.137824 | 3.040870 | -1.896345 |
| 6 | 0.477636 | 1.882587 | -1.414516 |
| 6 | 1.507399 | 1.978085 | -0.475106 |
| 6 | 1.901672 | 3.224332 | -0.006008 |
| 1 | 1.571455 | 5.348861 | -0.090386 |
| 1 | -0.242674 | 5.182015 | -1.775218 |
| 1 | -0.925711 | 2.945436 | -2.639488 |
| 1 | 2.001801 | 1.087599 | -0.096333 |
| 1 | 2.702743 | 3.291617 | 0.726060 |
| 6 | 0.004059 | 0.592433 | -1.948420 |
| 8 | -0.429228 | 0.426007 | -3.073594 |
| 7 | 0.012849 | -0.527886 | -1.051600 |
| 1 | 0.841946 | -0.753565 | -0.198024 |

| | | | |
|---|---|---|---|
| 8 | -0.138571 | -1.710662 | -1.754115 |
| 46 | -1.684071 | -0.331418 | 0.135920 |
| 8 | 0.690893 | 0.696778 | 2.423602 |
| 8 | -1.076895 | 1.345259 | 1.166057 |
| 8 | -3.565142 | -0.656909 | 1.045880 |
| 8 | -2.891347 | -1.832587 | -0.661000 |
| 6 | -0.231009 | 1.499164 | 2.087140 |
| 6 | -3.789509 | -1.588403 | 0.212400 |
| 6 | 2.781254 | -1.248758 | 1.005909 |
| 8 | 1.467037 | -0.980338 | 0.879725 |
| 1 | 1.023746 | -0.147644 | 1.726652 |
| 8 | 3.432639 | -0.758135 | 1.897884 |
| 6 | 3.349208 | -2.183037 | -0.057364 |
| 1 | -0.589358 | -1.430846 | -2.580636 |
| 6 | -5.039507 | -2.390910 | 0.265039 |
| 1 | -4.929567 | -3.169858 | 1.027068 |
| 1 | -5.880829 | -1.755587 | 0.552586 |
| 1 | -5.224786 | -2.868744 | -0.699355 |
| 6 | -0.334360 | 2.772763 | 2.871597 |
| 1 | -1.056801 | 2.630250 | 3.682405 |
| 1 | 0.634142 | 3.029088 | 3.305710 |
| 1 | -0.702163 | 3.574889 | 2.227537 |
| 6 | 3.362560 | -1.442037 | -1.401251 |
| 1 | 3.889561 | -2.052194 | -2.145255 |
| 1 | 2.353424 | -1.266928 | -1.792753 |
| 1 | 3.892102 | -0.482818 | -1.325285 |
| 6 | 2.493084 | -3.445891 | -0.170165 |
| 1 | 1.469375 | -3.223084 | -0.488161 |
| 1 | 2.937228 | -4.122096 | -0.911694 |
| 1 | 2.450208 | -3.980707 | 0.786545 |
| 6 | 4.777223 | -2.548635 | 0.329738 |
| 1 | 5.408909 | -1.657361 | 0.403527 |
| 1 | 4.805745 | -3.051676 | 1.302456 |
| 1 | 5.205283 | -3.222197 | -0.422970 |

---

**$(2a\text{-}3a)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1406.1432049
Zero-point correction= 0.379662
Thermal correction to Energy= 0.408192
Thermal correction to Enthalpy= 0.409136
Thermal correction to Gibbs Free Energy= 0.319374
Sum of electronic and zero-point Energies= -1405.763543
Sum of electronic and thermal Energies= -1405.735013

Sum of electronic and thermal Enthalpies= -1405.734068
Sum of electronic and thermal Free Energies= -1405.823831

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.640003 | 4.488981 | 1.504810 |
| 6 | -0.122238 | 3.258589 | 1.899681 |
| 6 | -0.118158 | 2.186723 | 1.016946 |
| 6 | -0.638279 | 2.344375 | -0.272037 |
| 6 | -1.156731 | 3.582718 | -0.663043 |
| 6 | -1.158851 | 4.650043 | 0.222768 |
| 1 | -0.639784 | 5.325529 | 2.199891 |
| 1 | 0.280429 | 3.132323 | 2.901532 |
| 1 | 0.279870 | 1.227851 | 1.338198 |
| 1 | -1.550896 | 3.682901 | -1.670833 |
| 1 | -1.563820 | 5.610485 | -0.086212 |
| 6 | -0.640003 | 1.268389 | -1.285570 |
| 8 | -0.999117 | 1.428048 | -2.441027 |
| 7 | -0.163450 | -0.012929 | -0.869144 |
| 8 | -0.058951 | -0.842403 | -1.979541 |
| 46 | -1.732216 | -0.812218 | 0.216812 |
| 8 | 0.730816 | -2.343854 | 0.655971 |
| 8 | -0.496857 | -1.014152 | 1.919575 |
| 8 | -3.631993 | -1.632523 | 0.740507 |
| 8 | -3.244825 | -0.713804 | -1.204198 |
| 6 | 0.556248 | -1.653406 | 1.723175 |
| 6 | -4.050726 | -1.311084 | -0.410853 |
| 1 | -0.580137 | -0.369171 | -2.667552 |
| 1 | 1.160525 | -0.012466 | -0.425667 |
| 8 | 2.254348 | 0.186049 | -0.286662 |
| 6 | 3.152316 | -0.733246 | -0.376082 |
| 6 | 4.573829 | -0.243589 | -0.600727 |
| 8 | 2.951740 | -1.953256 | -0.203819 |
| 1 | 1.745381 | -2.292762 | 0.269536 |
| 6 | -5.432761 | -1.639975 | -0.854301 |
| 1 | -5.776903 | -0.913768 | -1.594334 |
| 1 | -5.430776 | -2.630971 | -1.320731 |
| 1 | -6.105364 | -1.667730 | 0.006018 |
| 6 | 1.652434 | -1.555144 | 2.740874 |
| 1 | 2.338629 | -2.402739 | 2.680305 |
| 1 | 2.215118 | -0.633044 | 2.545897 |
| 1 | 1.222798 | -1.472936 | 3.741263 |
| 6 | 5.411005 | -1.338904 | -1.253793 |
| 1 | 5.021807 | -1.598213 | -2.245247 |
| 1 | 6.442946 | -0.987709 | -1.374908 |

| | | | |
|---|---|---|---|
| 1 | 5.420143 | -2.250296 | -0.648836 |
| 6 | 4.594508 | 1.021787 | -1.452452 |
| 1 | 4.026099 | 1.831173 | -0.984930 |
| 1 | 5.630766 | 1.355772 | -1.585802 |
| 1 | 4.168591 | 0.840149 | -2.446290 |
| 6 | 5.126616 | 0.063399 | 0.799204 |
| 1 | 6.164668 | 0.408349 | 0.717661 |
| 1 | 4.543963 | 0.852111 | 1.291218 |
| 1 | 5.115518 | -0.833093 | 1.432412 |

---

**3a**

---

Number of imaginary frequencies : 0
Electronic energy =-1059.3306767
Zero-point correction= 0.236737
Thermal correction to Energy= 0.257433
Thermal correction to Enthalpy= 0.258377
Thermal correction to Gibbs Free Energy= 0.184811
Sum of electronic and zero-point Energies= -1059.093940
Sum of electronic and thermal Energies= -1059.073244
Sum of electronic and thermal Enthalpies= -1059.072300
Sum of electronic and thermal Free Energies= -1059.145866

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.417084 | -1.621417 | -1.055941 |
| 6 | -1.580332 | -1.544229 | 0.077807 |
| 6 | -1.806462 | -0.535736 | 1.058712 |
| 6 | -2.868183 | 0.376127 | 0.874376 |
| 6 | -3.653143 | 0.300255 | -0.252650 |
| 6 | -3.429659 | -0.704565 | -1.215792 |
| 1 | -2.227798 | -2.406026 | -1.783809 |
| 1 | -1.303315 | -0.583305 | 2.023021 |
| 1 | -3.040731 | 1.137749 | 1.629452 |
| 1 | -4.463274 | 1.010224 | -0.399273 |
| 1 | -4.064942 | -0.750584 | -2.096805 |
| 6 | -0.429400 | -2.477432 | 0.188041 |
| 8 | -0.310134 | -3.561288 | -0.375247 |
| 7 | 0.590945 | -1.828136 | 0.849962 |
| 8 | 1.781749 | -2.501230 | 0.612686 |
| 1 | 1.525179 | -3.231048 | -0.002310 |
| 46 | 0.170819 | 0.035094 | 0.034144 |
| 8 | -0.532840 | 1.786423 | -0.727481 |
| 8 | -0.386508 | 2.417338 | 1.412617 |
| 8 | 2.112108 | 0.760856 | -0.598391 |

| | | | |
|---|---|---|---|
| 6 | -0.650002 | 2.652114 | 0.235702 |
| 6 | 3.280107 | 0.458991 | -0.354031 |
| 8 | 3.679892 | -0.659175 | 0.191996 |
| 1 | 2.938764 | -1.299360 | 0.356307 |
| 6 | -1.201059 | 3.982217 | -0.219833 |
| 1 | -1.062626 | 4.732551 | 0.561469 |
| 1 | -0.725787 | 4.303606 | -1.150569 |
| 1 | -2.272817 | 3.871144 | -0.423609 |
| 6 | 4.401766 | 1.387135 | -0.684522 |
| 1 | 4.969260 | 1.605935 | 0.225171 |
| 1 | 5.087464 | 0.898709 | -1.383462 |
| 1 | 4.012898 | 2.308894 | -1.116566 |

---

**$(3a\text{-}4a)_6^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1059.2906296
Zero-point correction= 0.231669
Thermal correction to Energy= 0.251461
Thermal correction to Enthalpy= 0.252405
Thermal correction to Gibbs Free Energy= 0.182200
Sum of electronic and zero-point Energies= -1059.058961
Sum of electronic and thermal Energies= -1059.039169
Sum of electronic and thermal Enthalpies= -1059.038224
Sum of electronic and thermal Free Energies= -1059.108430

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.276411 | -1.718376 | 0.295136 |
| 6 | 2.064587 | -1.221947 | -0.168996 |
| 6 | 1.709329 | 0.134330 | 0.030272 |
| 6 | 2.559246 | 0.923064 | 0.827291 |
| 6 | 3.771811 | 0.426287 | 1.285708 |
| 6 | 4.138922 | -0.888489 | 1.000640 |
| 1 | 3.489878 | -2.773266 | 0.137787 |
| 1 | 1.277410 | 1.001496 | -0.827230 |
| 1 | 2.293434 | 1.959308 | 1.020819 |
| 1 | 4.436654 | 1.066200 | 1.860674 |
| 1 | 5.089017 | -1.275640 | 1.361817 |
| 6 | 1.049519 | -2.188158 | -0.637718 |
| 8 | 1.211835 | -3.405542 | -0.772636 |
| 7 | -0.158047 | -1.592293 | -0.793719 |
| 8 | -1.166849 | -2.540750 | -0.955545 |
| 1 | -0.672371 | -3.389083 | -0.837569 |
| 46 | -0.415941 | 0.243023 | 0.001074 |

| | | | |
|---|---|---|---|
| 8 | -0.450229 | 2.301238 | 0.336398 |
| 8 | 1.058209 | 2.347489 | -1.326123 |
| 8 | -2.558694 | 0.329294 | 0.263933 |
| 6 | 0.244105 | 2.904102 | -0.544072 |
| 6 | -3.432780 | -0.497200 | 0.527850 |
| 8 | -3.310608 | -1.791733 | 0.411885 |
| 1 | -2.458324 | -2.060334 | -0.032164 |
| 6 | 0.048223 | 4.391649 | -0.650974 |
| 1 | 0.975238 | 4.873192 | -0.969008 |
| 1 | -0.711028 | 4.583065 | -1.416792 |
| 1 | -0.307799 | 4.805916 | 0.294076 |
| 6 | -4.777675 | -0.067573 | 1.013820 |
| 1 | -5.521584 | -0.271968 | 0.237021 |
| 1 | -5.058636 | -0.654885 | 1.892543 |
| 1 | -4.771775 | 0.996909 | 1.247600 |

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**$(3a\text{-}4a)_8^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1406.1194147
Zero-point correction= 0.377015
Thermal correction to Energy= 0.406429
Thermal correction to Enthalpy= 0.407373
Thermal correction to Gibbs Free Energy= 0.314624
Sum of electronic and zero-point Energies= -1405.742400
Sum of electronic and thermal Energies= -1405.712986
Sum of electronic and thermal Enthalpies= -1405.712042
Sum of electronic and thermal Free Energies= -1405.804791

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.745625 | -2.871560 | 1.728722 |
| 6 | 2.378036 | -2.288649 | 2.819883 |
| 6 | 2.213330 | -0.927886 | 3.099476 |
| 6 | 1.420571 | -0.141066 | 2.278953 |
| 6 | 0.827028 | -0.688085 | 1.124419 |
| 6 | 0.972077 | -2.076476 | 0.891611 |
| 1 | 1.807217 | -3.938633 | 1.528689 |
| 1 | 2.993361 | -2.900189 | 3.475977 |
| 1 | 2.713162 | -0.487596 | 3.958811 |
| 1 | 1.319036 | 0.925585 | 2.470519 |
| 6 | 0.151447 | -2.689380 | -0.168149 |
| 8 | 0.064658 | -3.891914 | -0.422712 |
| 7 | -0.594897 | -1.742540 | -0.820572 |
| 8 | -1.533609 | -2.364737 | -1.631515 |

| | | | |
|---|---|---|---|
| 1 | -1.420626 | -3.322233 | -1.412623 |
| 46 | -1.070477 | -0.164686 | 0.359356 |
| 8 | -3.102643 | 0.323865 | -0.269909 |
| 1 | 1.035967 | 0.189971 | 0.195961 |
| 6 | -3.915442 | 0.002181 | -1.135647 |
| 6 | -5.214059 | 0.723252 | -1.289513 |
| 1 | -5.265976 | 1.164903 | -2.289536 |
| 1 | -6.039853 | 0.010044 | -1.209637 |
| 1 | -5.308681 | 1.500000 | -0.530986 |
| 8 | -3.759140 | -0.967344 | -1.997053 |
| 1 | -2.905249 | -1.457261 | -1.857368 |
| 8 | 1.314998 | 1.380800 | -0.421409 |
| 6 | 2.302866 | 1.833752 | -1.203612 |
| 6 | 3.224321 | 0.753126 | -1.760820 |
| 8 | 2.427383 | 3.015338 | -1.432483 |
| 8 | -1.385724 | 1.465435 | 1.640079 |
| 6 | -0.966983 | 2.639929 | 1.478627 |
| 6 | -1.606770 | 3.722917 | 2.298533 |
| 1 | -2.307563 | 3.306005 | 3.022708 |
| 1 | -0.832270 | 4.307816 | 2.802408 |
| 1 | -2.135009 | 4.405253 | 1.624879 |
| 8 | -0.047438 | 3.020950 | 0.690012 |
| 1 | 0.591441 | 2.246176 | 0.109048 |
| 6 | 3.952441 | 0.067025 | -0.600153 |
| 1 | 3.267909 | -0.476472 | 0.061831 |
| 1 | 4.673849 | -0.658585 | -0.997092 |
| 1 | 4.508248 | 0.795523 | 0.003855 |
| 6 | 4.246574 | 1.407977 | -2.681966 |
| 1 | 4.919859 | 0.646578 | -3.095624 |
| 1 | 3.754346 | 1.926640 | -3.511568 |
| 1 | 4.845337 | 2.150173 | -2.143551 |
| 6 | 2.399089 | -0.270306 | -2.543102 |
| 1 | 1.882692 | 0.204976 | -3.386302 |
| 1 | 3.060632 | -1.046438 | -2.948893 |
| 1 | 1.639602 | -0.758549 | -1.921538 |

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**$(3a\text{-}4a)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1406.1351928
Zero-point correction= 0.378256
Thermal correction to Energy= 0.407609
Thermal correction to Enthalpy= 0.408553
Thermal correction to Gibbs Free Energy= 0.316879
Sum of electronic and zero-point Energies= -1405.756937

Sum of electronic and thermal Energies= -1405.727584
Sum of electronic and thermal Enthalpies= -1405.726640
Sum of electronic and thermal Free Energies= -1405.818314

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.520100 | -1.676065 | -1.129994 |
| 6 | -2.224093 | -1.230778 | -0.905320 |
| 6 | -1.932580 | -0.276517 | 0.100782 |
| 6 | -3.002874 | 0.255636 | 0.845209 |
| 6 | -4.293247 | -0.208524 | 0.641269 |
| 6 | -4.548177 | -1.166969 | -0.345524 |
| 1 | -3.700906 | -2.390873 | -1.929468 |
| 1 | -1.010786 | -0.712201 | 0.946766 |
| 1 | -2.791616 | 0.977525 | 1.631749 |
| 1 | -5.111593 | 0.169420 | 1.249518 |
| 1 | -5.567868 | -1.510765 | -0.505691 |
| 6 | -1.112503 | -1.651842 | -1.779637 |
| 8 | -1.193121 | -2.395936 | -2.760656 |
| 7 | 0.054750 | -1.045164 | -1.405064 |
| 8 | 1.030356 | -1.271876 | -2.373541 |
| 46 | -0.267062 | 0.794757 | -0.582375 |
| 8 | 1.480079 | 1.918362 | -1.298478 |
| 6 | 2.611667 | 1.659842 | -1.699005 |
| 8 | 2.997271 | 0.506516 | -2.185751 |
| 1 | 2.243065 | -0.136547 | -2.254057 |
| 8 | -0.254872 | -1.511182 | 1.670068 |
| 6 | 0.941637 | -1.180599 | 1.808574 |
| 8 | 1.330620 | 0.039780 | 1.970205 |
| 1 | 0.550517 | 0.728944 | 2.084486 |
| 1 | 0.534055 | -1.743522 | -3.086448 |
| 8 | -0.796262 | 2.578260 | 0.316877 |
| 6 | -0.778973 | 2.671179 | 1.585158 |
| 8 | -0.410794 | 1.781746 | 2.385950 |
| 6 | 2.049742 | -2.211253 | 1.761213 |
| 6 | 3.702445 | 2.680666 | -1.676545 |
| 1 | 4.536900 | 2.305871 | -1.075693 |
| 1 | 4.081404 | 2.836864 | -2.691069 |
| 1 | 3.331754 | 3.617907 | -1.261913 |
| 6 | -1.319501 | 3.963083 | 2.142302 |
| 1 | -2.409718 | 3.877958 | 2.223178 |
| 1 | -0.914080 | 4.147705 | 3.139175 |
| 1 | -1.102089 | 4.796236 | 1.470353 |
| 6 | 1.468569 | -3.600150 | 1.534729 |
| 1 | 2.282819 | -4.332330 | 1.476211 |

| | | | |
|---|---|---|---|
| 1 | 0.798502 | -3.893112 | 2.350311 |
| 1 | 0.897187 | -3.640213 | 0.600719 |
| 6 | 2.830374 | -2.160566 | 3.077351 |
| 1 | 2.190725 | -2.414233 | 3.931580 |
| 1 | 3.648244 | -2.890394 | 3.042441 |
| 1 | 3.258563 | -1.167659 | 3.248828 |
| 6 | 2.971762 | -1.832367 | 0.594254 |
| 1 | 2.433708 | -1.859327 | -0.362101 |
| 1 | 3.394349 | -0.831199 | 0.730462 |
| 1 | 3.797320 | -2.552737 | 0.539063 |

---

**4a**

---

Number of imaginary frequencies : 0
Electronic energy =-1059.3306767
Zero-point correction= 0.236737
Thermal correction to Energy= 0.257433
Thermal correction to Enthalpy= 0.258377
Thermal correction to Gibbs Free Energy= 0.184811
Sum of electronic and zero-point Energies= -1059.093940
Sum of electronic and thermal Energies= -1059.073244
Sum of electronic and thermal Enthalpies= -1059.072300
Sum of electronic and thermal Free Energies= -1059.145866

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.745571 | -1.044732 | -0.063086 |
| 6 | -2.362999 | -0.974635 | 0.049553 |
| 6 | -1.681427 | 0.224378 | -0.175250 |
| 6 | -2.387554 | 1.365053 | -0.533382 |
| 6 | -3.782217 | 1.300797 | -0.615577 |
| 6 | -4.458841 | 0.106842 | -0.382395 |
| 1 | -4.234084 | -2.006554 | 0.082557 |
| 1 | 0.048078 | 1.769106 | 1.582311 |
| 1 | -1.877495 | 2.298572 | -0.763398 |
| 1 | -4.342396 | 2.197562 | -0.874501 |
| 1 | -5.542460 | 0.072526 | -0.465661 |
| 6 | -1.511247 | -2.152571 | 0.306833 |
| 8 | -1.827603 | -3.341301 | 0.219358 |
| 7 | -0.248260 | -1.747279 | 0.619592 |
| 8 | 0.643597 | -2.833843 | 0.623927 |
| 1 | 0.062849 | -3.574527 | 0.328213 |
| 46 | 0.307442 | 0.068269 | -0.055523 |
| 8 | 0.713997 | 2.140444 | -0.597313 |
| 8 | 0.297204 | 2.719677 | 1.530862 |

| | | | |
|---|---|---|---|
| 8 | 2.544400 | -0.060918 | 0.000418 |
| 6 | 0.679664 | 2.982654 | 0.296529 |
| 6 | 3.328275 | -0.965872 | -0.279417 |
| 8 | 3.013359 | -2.230492 | -0.375561 |
| 1 | 2.075740 | -2.416438 | -0.079138 |
| 6 | 1.056669 | 4.407005 | 0.083281 |
| 1 | 0.216393 | 5.053230 | 0.354494 |
| 1 | 1.889289 | 4.666062 | 0.744316 |
| 1 | 1.338627 | 4.567614 | -0.956967 |
| 6 | 4.776344 | -0.702096 | -0.542421 |
| 1 | 5.379257 | -1.192913 | 0.228061 |
| 1 | 5.062330 | -1.143090 | -1.501860 |
| 1 | 4.973124 | 0.369981 | -0.543059 |

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**5a**

---

Number of imaginary frequencies : 0
Electronic energy =-1653.0263183
Zero-point correction= 0.456959
Thermal correction to Energy= 0.490524
Thermal correction to Enthalpy= 0.491468
Thermal correction to Gibbs Free Energy= 0.390436
Sum of electronic and zero-point Energies= -1652.569359
Sum of electronic and thermal Energies= -1652.535795
Sum of electronic and thermal Enthalpies= -1652.534851
Sum of electronic and thermal Free Energies= -1652.635882

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 2.662920 | -2.151367 | -2.783949 |
| 6 | 1.680532 | -1.514998 | -2.031209 |
| 6 | 1.683120 | -1.589485 | -0.637687 |
| 6 | 2.673584 | -2.301065 | 0.025828 |
| 6 | 3.680380 | -2.904978 | -0.731298 |
| 6 | 3.675796 | -2.837715 | -2.124469 |
| 1 | 2.609317 | -2.106822 | -3.870014 |
| 1 | 2.673879 | -2.372952 | 1.111296 |
| 1 | 4.480345 | -3.439718 | -0.221799 |
| 1 | 4.461402 | -3.330608 | -2.692091 |
| 6 | 0.536740 | -0.797503 | -2.617569 |
| 8 | 0.067871 | -0.936373 | -3.745681 |
| 7 | -0.023795 | 0.064291 | -1.688526 |
| 8 | -1.290294 | 0.485011 | -2.146145 |
| 46 | 0.175794 | -0.648577 | 0.241564 |
| 8 | 0.589875 | -1.538964 | 2.175298 |

| | | | |
|---|---|---|---|
| 6 | -0.236614 | -1.866930 | 3.029875 |
| 8 | -1.498914 | -1.525344 | 3.025384 |
| 1 | -1.691803 | -0.843591 | 2.321545 |
| 1 | -1.359029 | 0.018599 | -3.011690 |
| 8 | -1.601259 | 0.383341 | 1.252940 |
| 6 | -2.309163 | 1.069068 | 0.464216 |
| 7 | -1.798991 | 2.217158 | 0.016331 |
| 6 | -3.654199 | 0.609334 | 0.070987 |
| 6 | -3.872908 | -0.771449 | 0.057726 |
| 6 | -4.702012 | 1.484383 | -0.229063 |
| 6 | -5.123748 | -1.275993 | -0.267426 |
| 1 | -3.044545 | -1.439409 | 0.289716 |
| 6 | -5.957335 | 0.974010 | -0.532791 |
| 1 | -4.529196 | 2.556120 | -0.220454 |
| 6 | -6.167735 | -0.402004 | -0.558396 |
| 1 | -5.285962 | -2.350502 | -0.292458 |
| 1 | -6.775761 | 1.654259 | -0.754598 |
| 1 | -7.150652 | -0.795533 | -0.807238 |
| 1 | 1.281872 | 1.405150 | -1.372594 |
| 8 | -2.281864 | 2.811953 | -1.124061 |
| 1 | -1.968502 | 2.199970 | -1.826951 |
| 1 | -0.814415 | 2.427580 | 0.245558 |
| 8 | 0.960904 | 2.543875 | 0.650507 |
| 6 | 2.035823 | 2.314644 | 0.117902 |
| 8 | 2.155952 | 1.771780 | -1.082939 |
| 6 | 3.369249 | 2.545036 | 0.804047 |
| 6 | 0.141501 | -2.719668 | 4.195172 |
| 1 | -0.035590 | -2.166557 | 5.122657 |
| 1 | -0.501224 | -3.604824 | 4.222108 |
| 1 | 1.188296 | -3.015343 | 4.128246 |
| 6 | 3.189883 | 3.519077 | 1.961660 |
| 1 | 2.460950 | 3.143983 | 2.686742 |
| 1 | 4.149534 | 3.666016 | 2.472177 |
| 1 | 2.836434 | 4.494933 | 1.608544 |
| 6 | 4.415178 | 3.067578 | -0.178388 |
| 1 | 4.121300 | 4.038886 | -0.594751 |
| 1 | 5.371540 | 3.201076 | 0.342552 |
| 1 | 4.567795 | 2.372340 | -1.009036 |
| 6 | 3.794733 | 1.168538 | 1.338330 |
| 1 | 3.029235 | 0.753765 | 2.008763 |
| 1 | 3.955118 | 0.456026 | 0.520250 |
| 1 | 4.730119 | 1.268236 | 1.903514 |

---

**(5a-6a)$_4$‡**

---

Number of imaginary frequencies : 1
Electronic energy =-1306.1100468
Zero-point correction= 0.301723
Thermal correction to Energy= 0.325985
Thermal correction to Enthalpy= 0.326930
Thermal correction to Gibbs Free Energy= 0.246411
Sum of electronic and zero-point Energies= -1305.808324
Sum of electronic and thermal Energies= -1305.784061
Sum of electronic and thermal Enthalpies= -1305.783117
Sum of electronic and thermal Free Energies= -1305.863636

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 4.548347 | 0.023791 | -0.346300 |
| 6 | 3.180434 | -0.252002 | -0.261048 |
| 6 | 2.243268 | 0.786486 | -0.120867 |
| 6 | 2.681387 | 2.104713 | -0.079310 |
| 6 | 4.047269 | 2.371801 | -0.171747 |
| 6 | 4.979615 | 1.339517 | -0.299858 |
| 1 | 5.243242 | -0.806628 | -0.458031 |
| 1 | 1.975764 | 2.924367 | 0.042623 |
| 1 | 4.391869 | 3.403823 | -0.136231 |
| 1 | 6.039418 | 1.571717 | -0.365976 |
| 6 | 2.679274 | -1.622521 | -0.403026 |
| 8 | 3.307776 | -2.627114 | -0.624730 |
| 7 | 1.205824 | -1.668330 | -0.386311 |
| 8 | 0.814863 | -1.976431 | -1.720472 |
| 46 | 0.436647 | 0.068710 | 0.309337 |
| 7 | -0.728508 | -1.786086 | 1.172061 |
| 8 | -0.543531 | 1.850600 | 1.035095 |
| 6 | -1.334122 | 2.435028 | 0.294708 |
| 6 | -2.174511 | 3.574915 | 0.749850 |
| 1 | -2.074512 | 4.416216 | 0.058443 |
| 1 | -3.223318 | 3.259494 | 0.729100 |
| 1 | -1.896177 | 3.868305 | 1.761665 |
| 8 | -1.535034 | 2.109710 | -0.965613 |
| 1 | -0.993082 | 1.322364 | -1.190478 |
| 6 | -2.032032 | -1.378450 | 1.282532 |
| 6 | -2.726095 | -0.936942 | 0.040422 |
| 6 | -2.296730 | -1.260409 | -1.250166 |
| 6 | -3.845549 | -0.117142 | 0.207495 |
| 6 | -2.965812 | -0.742585 | -2.354729 |
| 1 | -1.436453 | -1.908156 | -1.396747 |
| 6 | -4.508815 | 0.399912 | -0.898722 |
| 1 | -4.172779 | 0.097982 | 1.222302 |

| | | | |
|---|---|---|---|
| 6 | -4.066695 | 0.093084 | -2.182550 |
| 1 | -2.627699 | -1.000204 | -3.355844 |
| 1 | -5.377631 | 1.039987 | -0.760228 |
| 1 | -4.584445 | 0.496875 | -3.049590 |
| 8 | -2.567753 | -1.284556 | 2.392594 |
| 8 | -0.176186 | -2.044523 | 2.426766 |
| 1 | -0.910454 | -1.788637 | 3.029824 |
| 1 | 1.063354 | -2.910839 | -1.815704 |
| 1 | 0.299449 | -2.103095 | 0.365920 |

---

**(5a-6a)$_6^‡$**

---

Number of imaginary frequencies : 1
Electronic energy =-1306.1472651
Zero-point correction= 0.301020
Thermal correction to Energy= 0.325493
Thermal correction to Enthalpy= 0.326437
Thermal correction to Gibbs Free Energy= 0.245127
Sum of electronic and zero-point Energies= -1305.846245
Sum of electronic and thermal Energies= -1305.821772
Sum of electronic and thermal Enthalpies= -1305.820828
Sum of electronic and thermal Free Energies= -1305.902138

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.488682 | -1.247980 | 0.910006 |
| 6 | -3.235569 | -1.009964 | 0.337952 |
| 6 | -2.713196 | 0.288111 | 0.241624 |
| 6 | -3.457101 | 1.361376 | 0.722440 |
| 6 | -4.693333 | 1.116617 | 1.316692 |
| 6 | -5.210393 | -0.178842 | 1.414207 |
| 1 | -4.876807 | -2.264505 | 0.931173 |
| 1 | -3.067037 | 2.373762 | 0.647064 |
| 1 | -5.269168 | 1.952174 | 1.711167 |
| 1 | -6.182647 | -0.341049 | 1.872639 |
| 6 | -2.484132 | -2.056340 | -0.347379 |
| 8 | -2.897848 | -3.113180 | -0.784401 |
| 7 | -1.130149 | -1.651773 | -0.628294 |
| 8 | -0.663743 | -2.261785 | -1.804492 |
| 46 | -0.863740 | 0.380944 | -0.452448 |
| 8 | -0.717583 | 2.499958 | -0.190868 |
| 6 | 0.292842 | 3.190871 | -0.374089 |
| 6 | 0.231852 | 4.678110 | -0.253381 |
| 1 | -0.761821 | 4.996119 | 0.061780 |
| 1 | 0.986727 | 5.020789 | 0.460278 |

| | | | |
|---|---|---|---|
| 1 | 0.478070 | 5.126490 | -1.221055 |
| 8 | 1.470899 | 2.737939 | -0.687569 |
| 1 | 1.509556 | 1.722659 | -0.735628 |
| 1 | -1.317220 | -2.974723 | -1.949491 |
| 8 | 1.328426 | 0.191107 | -0.683779 |
| 6 | 1.903171 | -0.743870 | 0.002831 |
| 7 | 1.188970 | -1.751410 | 0.440335 |
| 6 | 3.361524 | -0.592003 | 0.255516 |
| 6 | 3.845350 | 0.657789 | 0.646561 |
| 6 | 4.260781 | -1.639805 | 0.046383 |
| 6 | 5.206398 | 0.853932 | 0.845416 |
| 1 | 3.148058 | 1.477911 | 0.803659 |
| 6 | 5.622846 | -1.435303 | 0.222720 |
| 1 | 3.886147 | -2.611717 | -0.259817 |
| 6 | 6.097886 | -0.191584 | 0.629535 |
| 1 | 5.572012 | 1.827350 | 1.163771 |
| 1 | 6.318284 | -2.252284 | 0.045143 |
| 1 | 7.164593 | -0.037661 | 0.776207 |
| 1 | -0.229769 | -1.839603 | 0.088935 |
| 8 | 1.880713 | -2.639571 | 1.275158 |
| 1 | 1.512947 | -3.499290 | 1.037903 |

---

**$(5a\text{-}6a)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1652.9910612
Zero-point correction= 0.450174
Thermal correction to Energy= 0.483953
Thermal correction to Enthalpy= 0.484897
Thermal correction to Gibbs Free Energy= 0.383521
Sum of electronic and zero-point Energies= -1652.540887
Sum of electronic and thermal Energies= -1652.507108
Sum of electronic and thermal Enthalpies= -1652.506164
Sum of electronic and thermal Free Energies= -1652.607540

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 4.584574 | -0.526221 | -1.662942 |
| 6 | 3.202631 | -0.463872 | -1.473800 |
| 6 | 2.602117 | -0.948227 | -0.305632 |
| 6 | 3.392789 | -1.498356 | 0.695094 |
| 6 | 4.775597 | -1.527991 | 0.517837 |
| 6 | 5.372283 | -1.052664 | -0.652341 |
| 1 | 5.012340 | -0.160493 | -2.593991 |
| 1 | 2.943908 | -1.888472 | 1.605138 |

| | | | |
|---|---|---|---|
| 1 | 5.402911 | -1.931834 | 1.310469 |
| 1 | 6.451968 | -1.098032 | -0.767330 |
| 6 | 2.289614 | 0.043332 | -2.484851 |
| 8 | 2.416827 | 0.133367 | -3.685223 |
| 7 | 1.014656 | 0.411883 | -1.876559 |
| 8 | 0.005759 | 0.539979 | -2.827945 |
| 46 | 0.624849 | -0.829877 | -0.253344 |
| 8 | 0.516910 | -2.162301 | 1.438211 |
| 6 | -0.419124 | -2.907277 | 1.746754 |
| 8 | -1.596206 | -2.899111 | 1.185432 |
| 1 | -1.687956 | -2.132395 | 0.538273 |
| 8 | -1.597643 | -0.749870 | -0.227115 |
| 6 | -2.367267 | 0.272025 | -0.282793 |
| 7 | -1.836948 | 1.468715 | -0.214033 |
| 6 | -3.829843 | 0.047689 | -0.404390 |
| 6 | -4.400106 | -1.021071 | 0.292240 |
| 6 | -4.630758 | 0.828686 | -1.241536 |
| 6 | -5.756238 | -1.292907 | 0.170411 |
| 1 | -3.782544 | -1.634737 | 0.944223 |
| 6 | -5.982191 | 0.538948 | -1.377769 |
| 1 | -4.188563 | 1.659511 | -1.781670 |
| 6 | -6.548705 | -0.515571 | -0.668318 |
| 1 | -6.194422 | -2.117505 | 0.727309 |
| 1 | -6.597559 | 1.143764 | -2.039385 |
| 1 | -7.609468 | -0.732743 | -0.770566 |
| 1 | 1.064294 | 1.344754 | -1.371519 |
| 8 | -2.677594 | 2.576867 | -0.192987 |
| 1 | -2.085192 | 3.289661 | -0.478093 |
| 1 | -0.717588 | 1.813130 | -0.130187 |
| 8 | 0.405826 | 2.446536 | -0.278125 |
| 6 | 1.384589 | 2.500249 | 0.596366 |
| 8 | 2.550914 | 2.338125 | 0.268456 |
| 6 | 0.982547 | 2.705529 | 2.062534 |
| 6 | -0.269298 | -3.929399 | 2.823402 |
| 1 | -0.416643 | -4.925603 | 2.394316 |
| 1 | 0.719178 | -3.862020 | 3.277413 |
| 1 | -1.046898 | -3.786173 | 3.579254 |
| 6 | -0.142467 | 3.730976 | 2.191824 |
| 1 | -0.388916 | 3.884084 | 3.250878 |
| 1 | 0.158589 | 4.700991 | 1.776281 |
| 1 | -1.058003 | 3.409332 | 1.681961 |
| 6 | 2.196509 | 3.158228 | 2.864646 |
| 1 | 2.571320 | 4.122360 | 2.501310 |
| 1 | 1.931816 | 3.268051 | 3.924626 |
| 1 | 3.013139 | 2.435413 | 2.774343 |

| | | | |
|---|---|---|---|
| 6 | 0.506849 | 1.344879 | 2.588593 |
| 1 | -0.395511 | 0.998941 | 2.065675 |
| 1 | 1.288673 | 0.581103 | 2.468995 |
| 1 | 0.263612 | 1.420150 | 3.657100 |
| 1 | 0.497566 | 0.498270 | -3.674478 |

---

**$(5a\text{-}6a)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1653.0113308
Zero-point correction= 0.451305
Thermal correction to Energy= 0.484493
Thermal correction to Enthalpy= 0.485437
Thermal correction to Gibbs Free Energy= 0.385293
Sum of electronic and zero-point Energies= -1652.560026
Sum of electronic and thermal Energies= -1652.526838
Sum of electronic and thermal Enthalpies= -1652.525894
Sum of electronic and thermal Free Energies= -1652.626038

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.411358 | -0.194229 | 2.716314 |
| 6 | 2.189456 | 0.003016 | 2.071680 |
| 6 | 2.061526 | 0.918075 | 1.019902 |
| 6 | 3.168738 | 1.638067 | 0.588965 |
| 6 | 4.397247 | 1.408953 | 1.209131 |
| 6 | 4.521540 | 0.506830 | 2.269353 |
| 1 | 3.468260 | -0.887634 | 3.552944 |
| 1 | 3.077030 | 2.361903 | -0.216623 |
| 1 | 5.276189 | 1.949290 | 0.862010 |
| 1 | 5.488401 | 0.360185 | 2.743989 |
| 6 | 0.951699 | -0.669352 | 2.467820 |
| 8 | 0.636228 | -1.142076 | 3.541704 |
| 7 | 0.033170 | -0.679717 | 1.370004 |
| 8 | -1.243815 | -1.078109 | 1.766062 |
| 46 | 0.221689 | 1.104850 | 0.314130 |
| 8 | 0.711808 | 2.905841 | -0.758432 |
| 6 | 0.011947 | 3.509920 | -1.576730 |
| 8 | -1.226196 | 3.218172 | -1.866587 |
| 1 | -1.556338 | 2.432290 | -1.348684 |
| 1 | -1.124212 | -1.290001 | 2.715779 |
| 8 | -1.939555 | 1.159555 | -0.383577 |
| 6 | -2.426627 | 0.002913 | -0.604909 |
| 7 | -1.704913 | -0.845293 | -1.325438 |
| 6 | -3.764121 | -0.338321 | -0.094666 |

| | | | |
|---|---|---|---|
| 6 | -4.233187 | 0.387047 | 1.005379 |
| 6 | -4.577650 | -1.309241 | -0.687367 |
| 6 | -5.495060 | 0.132053 | 1.520831 |
| 1 | -3.586804 | 1.140701 | 1.446922 |
| 6 | -5.846514 | -1.548482 | -0.175770 |
| 1 | -4.215697 | -1.869966 | -1.542988 |
| 6 | -6.303081 | -0.835647 | 0.928921 |
| 1 | -5.851220 | 0.688919 | 2.383981 |
| 1 | -6.482114 | -2.297603 | -0.641227 |
| 1 | -7.294771 | -1.033110 | 1.329991 |
| 1 | 0.355522 | -1.450406 | 0.548324 |
| 8 | -1.948648 | -2.196697 | -1.365755 |
| 1 | -1.148043 | -2.558833 | -0.916629 |
| 1 | -0.747111 | -0.594574 | -1.651208 |
| 8 | 0.950598 | -0.820572 | -1.995459 |
| 6 | 1.342809 | -1.813078 | -1.361528 |
| 8 | 0.676056 | -2.354041 | -0.387431 |
| 6 | 2.680184 | -2.474864 | -1.691296 |
| 6 | 0.545785 | 4.672846 | -2.343874 |
| 1 | 0.580467 | 4.411835 | -3.406465 |
| 1 | -0.131494 | 5.525462 | -2.242718 |
| 1 | 1.544662 | 4.932833 | -1.994180 |
| 6 | 3.374507 | -1.741913 | -2.830049 |
| 1 | 3.576929 | -0.698943 | -2.559542 |
| 1 | 4.328126 | -2.232261 | -3.065702 |
| 1 | 2.754051 | -1.733402 | -3.732771 |
| 6 | 2.411140 | -3.930222 | -2.081805 |
| 1 | 1.784003 | -3.990056 | -2.980604 |
| 1 | 3.358588 | -4.440136 | -2.299902 |
| 1 | 1.905153 | -4.466312 | -1.272263 |
| 6 | 3.555085 | -2.435688 | -0.435716 |
| 1 | 3.773061 | -1.400543 | -0.137641 |
| 1 | 3.066089 | -2.942108 | 0.403804 |
| 1 | 4.513296 | -2.934252 | -0.632271 |

---

**6a**

---

Number of imaginary frequencies : 0
Electronic energy =-1306.1708775
Zero-point correction= 0.306866
Thermal correction to Energy= 0.331277
Thermal correction to Enthalpy= 0.332221
Thermal correction to Gibbs Free Energy= 0.251232
Sum of electronic and zero-point Energies= -1305.864012
Sum of electronic and thermal Energies= -1305.839600

Sum of electronic and thermal Enthalpies= -1305.838656
Sum of electronic and thermal Free Energies= -1305.919645

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.917760 | -0.297223 | 0.595746 |
| 6 | 2.384656 | 1.936204 | -0.422681 |
| 6 | 1.192014 | 1.646187 | 0.267169 |
| 6 | 2.710705 | 3.234976 | -0.833395 |
| 6 | 0.331248 | 2.700422 | 0.568519 |
| 6 | 1.852809 | 4.270120 | -0.510286 |
| 1 | 3.628985 | 3.402600 | -1.392734 |
| 6 | 0.676314 | 3.996944 | 0.195837 |
| 1 | -0.593787 | 2.505936 | 1.107987 |
| 1 | 2.087507 | 5.289900 | -0.803893 |
| 1 | 0.008826 | 4.817711 | 0.452748 |
| 8 | -1.450971 | -1.138859 | -1.133514 |
| 6 | -1.899943 | -0.444970 | -0.190633 |
| 7 | -1.096389 | -0.100386 | 0.822338 |
| 8 | -1.650377 | 0.683058 | 1.838782 |
| 1 | -1.506257 | 0.157926 | 2.636949 |
| 6 | -3.338821 | -0.050461 | -0.234936 |
| 6 | -4.231819 | -0.984470 | -0.765353 |
| 6 | -3.804983 | 1.216533 | 0.122763 |
| 6 | -5.578576 | -0.674723 | -0.897341 |
| 1 | -3.845308 | -1.950165 | -1.081453 |
| 6 | -5.148790 | 1.533931 | -0.035504 |
| 1 | -3.111187 | 1.956381 | 0.511018 |
| 6 | -6.039295 | 0.587307 | -0.532660 |
| 1 | -6.268963 | -1.413688 | -1.297659 |
| 1 | -5.502960 | 2.526943 | 0.232198 |
| 1 | -7.092346 | 0.836509 | -0.644568 |
| 6 | 3.248536 | 0.812175 | -0.734860 |
| 8 | 4.063750 | 0.662030 | -1.616260 |
| 8 | 0.910628 | -2.482119 | 0.950628 |
| 6 | 0.834310 | -3.292676 | 0.020465 |
| 6 | 1.536839 | -4.610191 | 0.098342 |
| 1 | 1.010339 | -5.375494 | -0.475214 |
| 1 | 2.536046 | -4.482117 | -0.333663 |
| 1 | 1.654950 | -4.909580 | 1.141035 |
| 8 | 0.194686 | -3.090244 | -1.091397 |
| 1 | -0.365311 | -2.234226 | -1.074795 |
| 7 | 3.017222 | -0.306360 | 0.199550 |
| 8 | 3.646941 | -1.467774 | -0.241495 |
| 1 | 4.197781 | -1.144188 | -0.986795 |

| | | | |
|---|---|---|---|
| 1 | 3.430428 | -0.057532 | 1.104663 |

---

**6a1**

---

Number of imaginary frequencies : 0
Electronic energy = -1306.1708775
Zero-point correction= 0.306866 (Hartree/Particle)
Thermal correction to Energy= 0.331277
Thermal correction to Enthalpy= 0.332221
Thermal correction to Gibbs Free Energy= 0.251232
Sum of electronic and zero-point Energies= -1305.864012
Sum of electronic and thermal Energies= -1305.839600
Sum of electronic and thermal Enthalpies= -1305.838656
Sum of electronic and thermal Free Energies= -1305.919645

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 0.917760 | -0.297223 | 0.595746 |
| 6 | 2.384656 | 1.936204 | -0.422681 |
| 6 | 1.192014 | 1.646187 | 0.267169 |
| 6 | 2.710705 | 3.234976 | -0.833395 |
| 6 | 0.331248 | 2.700422 | 0.568519 |
| 6 | 1.852809 | 4.270120 | -0.510286 |
| 1 | 3.628985 | 3.402600 | -1.392734 |
| 6 | 0.676314 | 3.996944 | 0.195837 |
| 1 | -0.593787 | 2.505936 | 1.107987 |
| 1 | 2.087507 | 5.289900 | -0.803893 |
| 1 | 0.008826 | 4.817711 | 0.452748 |
| 8 | -1.450971 | -1.138859 | -1.133514 |
| 6 | -1.899943 | -0.444970 | -0.190633 |
| 7 | -1.096389 | -0.100386 | 0.822338 |
| 8 | -1.650377 | 0.683058 | 1.838782 |
| 1 | -1.506257 | 0.157926 | 2.636949 |
| 6 | -3.338821 | -0.050461 | -0.234936 |
| 6 | -4.231819 | -0.984470 | -0.765353 |
| 6 | -3.804983 | 1.216533 | 0.122763 |
| 6 | -5.578576 | -0.674723 | -0.897341 |
| 1 | -3.845308 | -1.950165 | -1.081453 |
| 6 | -5.148790 | 1.533931 | -0.035504 |
| 1 | -3.111187 | 1.956381 | 0.511018 |
| 6 | -6.039295 | 0.587307 | -0.532660 |
| 1 | -6.268963 | -1.413688 | -1.297659 |
| 1 | -5.502960 | 2.526943 | 0.232198 |
| 1 | -7.092346 | 0.836509 | -0.644568 |
| 6 | 3.248536 | 0.812175 | -0.734860 |

| | | | |
|---|---|---|---|
| 8 | 4.063750 | 0.662030 | -1.616260 |
| 8 | 0.910628 | -2.482119 | 0.950628 |
| 6 | 0.834310 | -3.292676 | 0.020465 |
| 6 | 1.536839 | -4.610191 | 0.098342 |
| 1 | 1.010339 | -5.375494 | -0.475214 |
| 1 | 2.536046 | -4.482117 | -0.333663 |
| 1 | 1.654950 | -4.909580 | 1.141035 |
| 8 | 0.194686 | -3.090244 | -1.091397 |
| 1 | -0.365311 | -2.234226 | -1.074795 |
| 7 | 3.017222 | -0.306360 | 0.199550 |
| 8 | 3.646941 | -1.467774 | -0.241495 |
| 1 | 4.197781 | -1.144188 | -0.986795 |
| 1 | 3.430428 | -0.057532 | 1.104663 |

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**$(6a_1\text{-}9)_3^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1306.1227973
Zero-point correction= 0.304825
Thermal correction to Energy= 0.329425
Thermal correction to Enthalpy= 0.330369
Thermal correction to Gibbs Free Energy= 0.247445
Sum of electronic and zero-point Energies= -1305.817972
Sum of electronic and thermal Energies= -1305.793372
Sum of electronic and thermal Enthalpies= -1305.792428
Sum of electronic and thermal Free Energies= -1305.875352

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.106871 | 1.085616 | 0.173749 |
| 6 | -1.933299 | -1.774366 | 0.392779 |
| 6 | -1.056386 | -0.782449 | 0.878145 |
| 6 | -2.400626 | -2.733892 | 1.302728 |
| 6 | -0.624516 | -0.795986 | 2.210124 |
| 6 | -2.011375 | -2.725399 | 2.631645 |
| 1 | -3.089783 | -3.483581 | 0.921484 |
| 6 | -1.124876 | -1.749539 | 3.086310 |
| 1 | 0.116999 | -0.069486 | 2.536121 |
| 1 | -2.389867 | -3.482909 | 3.312707 |
| 1 | -0.802207 | -1.741573 | 4.125035 |
| 8 | 1.600319 | 1.009852 | 0.928587 |
| 6 | 1.603640 | 0.030472 | 0.152295 |
| 7 | 0.419855 | -0.367203 | -0.376493 |
| 8 | 0.433774 | -1.399698 | -1.291374 |

| | | | |
|---|---|---|---|
| 1 | -0.212840 | -1.118333 | -1.966026 |
| 6 | 2.880373 | -0.661264 | -0.159735 |
| 6 | 4.040535 | 0.118293 | -0.103737 |
| 6 | 2.985191 | -2.033457 | -0.408802 |
| 6 | 5.283924 | -0.455406 | -0.325708 |
| 1 | 3.945847 | 1.176841 | 0.123611 |
| 6 | 4.235064 | -2.607306 | -0.606230 |
| 1 | 2.092627 | -2.649050 | -0.438284 |
| 6 | 5.382724 | -1.821485 | -0.576247 |
| 1 | 6.178917 | 0.161377 | -0.295134 |
| 1 | 4.311887 | -3.676765 | -0.787122 |
| 1 | 6.357243 | -2.275420 | -0.742468 |
| 6 | -2.474628 | -1.903538 | -0.982116 |
| 8 | -3.090196 | -2.891152 | -1.367598 |
| 8 | -1.158211 | 3.265686 | -0.229609 |
| 6 | -0.177786 | 3.983268 | -0.036143 |
| 6 | -0.222187 | 5.459399 | -0.264510 |
| 1 | 0.029960 | 5.981716 | 0.663394 |
| 1 | 0.534796 | 5.737850 | -1.003975 |
| 1 | -1.212124 | 5.758930 | -0.608502 |
| 8 | 0.993040 | 3.567694 | 0.376886 |
| 1 | 1.043626 | 2.585149 | 0.553863 |
| 7 | -2.257901 | -0.874449 | -1.891124 |
| 8 | -2.986600 | -1.007899 | -3.067493 |
| 1 | -3.431666 | -1.870781 | -2.924732 |
| 1 | -2.342640 | 0.079309 | -1.529101 |

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**(6a-9)$_5^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-1306.1218802
Zero-point correction= 0.305297
Thermal correction to Energy= 0.329528
Thermal correction to Enthalpy= 0.330472
Thermal correction to Gibbs Free Energy= 0.249428
Sum of electronic and zero-point Energies= -1305.816583
Sum of electronic and thermal Energies= -1305.792352
Sum of electronic and thermal Enthalpies= -1305.791408
Sum of electronic and thermal Free Energies= -1305.872453

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.993245 | -3.315264 | -1.806054 |
| 6 | 0.576828 | -2.014398 | -1.647028 |
| 6 | 1.025039 | -1.253117 | -0.528026 |

| | | | |
|---|---|---|---|
| 6 | 2.065289 | -1.834764 | 0.264666 |
| 6 | 2.417820 | -3.194833 | 0.126885 |
| 6 | 1.873295 | -3.939990 | -0.892519 |
| 1 | 0.620771 | -3.885468 | -2.655676 |
| 1 | -0.151455 | -1.578598 | -2.329268 |
| 1 | 3.172615 | -3.607179 | 0.795379 |
| 1 | 2.152406 | -4.980891 | -1.029909 |
| 6 | 2.851205 | -0.938816 | 1.070243 |
| 8 | 3.434788 | -1.076884 | 2.129546 |
| 7 | 2.983303 | 0.365809 | 0.380711 |
| 46 | 1.059370 | 0.760597 | -0.461756 |
| 8 | 3.625724 | 1.302830 | 1.182810 |
| 1 | 3.914167 | 0.755894 | 1.946862 |
| 8 | 1.055395 | 3.022839 | -0.320015 |
| 8 | -1.110501 | 0.676780 | -0.698760 |
| 6 | -1.502840 | -0.327396 | 0.004387 |
| 7 | -0.553970 | -1.105566 | 0.499201 |
| 8 | -0.932112 | -2.311078 | 1.067578 |
| 1 | -0.175929 | -2.524070 | 1.633455 |
| 6 | -2.955036 | -0.512264 | 0.213322 |
| 6 | -3.558353 | -1.772005 | 0.293515 |
| 6 | -3.752969 | 0.636071 | 0.285712 |
| 6 | -4.936419 | -1.871588 | 0.446270 |
| 1 | -2.949357 | -2.666931 | 0.228026 |
| 6 | -5.124648 | 0.529321 | 0.460345 |
| 1 | -3.289510 | 1.616666 | 0.212958 |
| 6 | -5.720377 | -0.726720 | 0.537908 |
| 1 | -5.399549 | -2.854192 | 0.496676 |
| 1 | -5.731922 | 1.428658 | 0.527798 |
| 1 | -6.796994 | -0.812456 | 0.666195 |
| 6 | 0.065279 | 3.742070 | -0.245414 |
| 6 | 0.160062 | 5.218296 | -0.035094 |
| 1 | -0.356445 | 5.488569 | 0.891206 |
| 1 | 1.205046 | 5.523668 | 0.016461 |
| 1 | -0.349081 | 5.740274 | -0.850947 |
| 8 | -1.176542 | 3.316319 | -0.339222 |
| 1 | -1.206180 | 2.332979 | -0.489310 |
| 1 | 3.566545 | 0.219839 | -0.448727 |

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**9**

---

Number of imaginary frequencies : 0
Electronic energy = -950.4240544
Zero-point correction= 0.243994
Thermal correction to Energy= 0.260863

Thermal correction to Enthalpy= 0.261807
Thermal correction to Gibbs Free Energy= 0.198602
Sum of electronic and zero-point Energies= -950.180061
Sum of electronic and thermal Energies= -950.163191
Sum of electronic and thermal Enthalpies= -950.162247
Sum of electronic and thermal Free Energies= -950.225452

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -1.631679 | 3.115589 | -0.544721 |
| 6 | -2.265149 | 2.065574 | 0.103803 |
| 6 | -1.800716 | 0.753565 | -0.013389 |
| 6 | -0.668906 | 0.519342 | -0.813118 |
| 6 | -0.036165 | 1.573962 | -1.467171 |
| 6 | -0.509025 | 2.871726 | -1.329140 |
| 1 | -2.013239 | 4.127458 | -0.435045 |
| 1 | -3.131319 | 2.231464 | 0.738537 |
| 1 | 0.834458 | 1.359290 | -2.082746 |
| 1 | -0.005645 | 3.687668 | -1.841427 |
| 6 | -2.551518 | -0.256452 | 0.790337 |
| 8 | -3.356678 | 0.080136 | 1.663175 |
| 7 | -2.316155 | -1.570853 | 0.577088 |
| 1 | -2.004870 | -1.951559 | -0.315264 |
| 8 | -3.134906 | -2.436269 | 1.272260 |
| 7 | -0.153256 | -0.794378 | -0.979175 |
| 8 | -0.937850 | -1.571367 | -1.846585 |
| 1 | -0.255888 | -2.199945 | -2.186070 |
| 6 | 1.155186 | -1.217483 | -0.926843 |
| 8 | 1.481921 | -2.184513 | -1.612918 |
| 6 | 2.079285 | -0.524631 | -0.003013 |
| 6 | 1.654777 | 0.057353 | 1.194351 |
| 6 | 3.436784 | -0.536086 | -0.330943 |
| 6 | 2.583647 | 0.644920 | 2.043034 |
| 1 | 0.604242 | 0.022746 | 1.475016 |
| 6 | 4.359495 | 0.064451 | 0.514376 |
| 1 | 3.747842 | -1.027680 | -1.249530 |
| 6 | 3.932906 | 0.657671 | 1.699614 |
| 1 | 2.253641 | 1.086863 | 2.979702 |
| 1 | 5.414864 | 0.063369 | 0.253522 |
| 1 | 4.656781 | 1.121593 | 2.365578 |
| 1 | -3.668421 | -1.805548 | 1.801811 |

**Lewis acid Participation in Pathway A (LA=1)**

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**2a'**

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Number of imaginary frequencies : 0
Electronic energy =-2045.2406747
Zero-point correction= 0.240733
Thermal correction to Energy= 0.266526
Thermal correction to Enthalpy= 0.267470
Thermal correction to Gibbs Free Energy= 0.180221
Sum of electronic and zero-point Energies= -2044.999941
Sum of electronic and thermal Energies= -2044.974149
Sum of electronic and thermal Enthalpies= -2044.973204
Sum of electronic and thermal Free Energies= -2045.060453

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.635573 | 4.341442 | 0.345528 |
| 6 | -2.932972 | 3.294462 | -0.523647 |
| 6 | -1.992999 | 2.306099 | -0.775862 |
| 6 | -0.739820 | 2.373911 | -0.147954 |
| 6 | -0.444330 | 3.429788 | 0.724937 |
| 6 | -1.391651 | 4.410110 | 0.969103 |
| 1 | -3.379722 | 5.110974 | 0.536552 |
| 1 | -3.903387 | 3.247269 | -1.009811 |
| 1 | -2.247242 | 1.497288 | -1.459701 |
| 1 | 0.532775 | 3.460738 | 1.198619 |
| 1 | -1.162861 | 5.228836 | 1.645649 |
| 6 | 0.316382 | 1.383287 | -0.353173 |
| 8 | 1.447403 | 1.505369 | 0.110226 |
| 7 | -0.020458 | 0.207178 | -1.074732 |
| 8 | 1.113469 | -0.434168 | -1.600579 |
| 46 | -1.079284 | -1.028883 | 0.307062 |
| 1 | -0.760721 | 0.233056 | -1.838904 |
| 8 | -1.817670 | -2.102894 | -1.248496 |
| 8 | -1.873112 | -2.040169 | 1.934389 |
| 8 | -0.584158 | -0.304730 | 2.184943 |
| 6 | -1.233029 | -1.266273 | 2.719225 |
| 6 | -2.169946 | -1.565733 | -2.364333 |
| 8 | -1.965048 | -0.386864 | -2.707465 |
| 30 | 2.903821 | 0.030706 | -0.127662 |
| 1 | 1.115928 | -1.335284 | -1.203262 |
| 17 | 2.207001 | -1.905857 | 0.791847 |
| 17 | 4.765991 | 0.852931 | -0.898985 |
| 6 | -1.206769 | -1.492204 | 4.182859 |
| 1 | -1.132135 | -0.537718 | 4.709405 |
| 1 | -2.093808 | -2.045966 | 4.497929 |
| 1 | -0.318263 | -2.085366 | 4.425840 |

| | | | |
|---|---|---|---|
| 6 | -2.884398 | -2.497222 | -3.305805 |
| 1 | -2.992859 | -3.497223 | -2.884386 |
| 1 | -3.869570 | -2.076785 | -3.530052 |
| 1 | -2.329805 | -2.541232 | -4.247777 |

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**$(2a'\text{-}3a')_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2045.2394581
Zero-point correction= 0.236772
Thermal correction to Energy= 0.262161
Thermal correction to Enthalpy= 0.263105
Thermal correction to Gibbs Free Energy= 0.176961
Sum of electronic and zero-point Energies= -2045.002687
Sum of electronic and thermal Energies= -2044.977297
Sum of electronic and thermal Enthalpies= -2044.976353
Sum of electronic and thermal Free Energies= -2045.062497

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.806222 | 4.175960 | 0.345614 |
| 6 | -3.021796 | 3.179077 | -0.602957 |
| 6 | -2.035194 | 2.239588 | -0.864560 |
| 6 | -0.818276 | 2.305717 | -0.171364 |
| 6 | -0.604485 | 3.312040 | 0.778723 |
| 6 | -1.598445 | 4.242488 | 1.036007 |
| 1 | -3.584933 | 4.908170 | 0.545349 |
| 1 | -3.962508 | 3.135452 | -1.144941 |
| 1 | -2.218522 | 1.473008 | -1.614844 |
| 1 | 0.345956 | 3.342387 | 1.304048 |
| 1 | -1.433747 | 5.021102 | 1.775800 |
| 6 | 0.281853 | 1.361040 | -0.389410 |
| 8 | 1.414476 | 1.557686 | 0.051666 |
| 7 | -0.022535 | 0.171416 | -1.080780 |
| 8 | 1.140006 | -0.472266 | -1.553849 |
| 46 | -1.068437 | -1.037075 | 0.315582 |
| 1 | -0.805622 | 0.069887 | -1.917053 |
| 8 | -1.845805 | -2.104966 | -1.244860 |
| 8 | -1.842235 | -2.029116 | 1.964968 |
| 8 | -0.563591 | -0.281589 | 2.170810 |
| 6 | -1.199056 | -1.238607 | 2.730380 |
| 6 | -2.071972 | -1.607919 | -2.397766 |
| 8 | -1.712171 | -0.467451 | -2.787712 |
| 30 | 2.902031 | 0.112611 | -0.129006 |
| 1 | 1.159675 | -1.349893 | -1.109168 |

| | | | |
|---|---|---|---|
| 17 | 2.279973 | -1.805980 | 0.892512 |
| 17 | 4.759921 | 0.929314 | -0.922392 |
| 6 | -1.152124 | -1.437158 | 4.196812 |
| 1 | -1.067800 | -0.473184 | 4.704246 |
| 1 | -2.035454 | -1.983254 | 4.534885 |
| 1 | -0.260982 | -2.027399 | 4.437475 |
| 6 | -2.839290 | -2.479489 | -3.347560 |
| 1 | -2.991375 | -3.477892 | -2.936308 |
| 1 | -3.809045 | -2.011141 | -3.544629 |
| 1 | -2.304345 | -2.531511 | -4.299738 |

---

**$(2a'\text{-}3a')_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2392.0409889
Zero-point correction= 0.383193
Thermal correction to Energy= 0.417636
Thermal correction to Enthalpy= 0.418580
Thermal correction to Gibbs Free Energy= 0.313202
Sum of electronic and zero-point Energies= -2391.657795
Sum of electronic and thermal Energies= -2391.623353
Sum of electronic and thermal Enthalpies= -2391.622409
Sum of electronic and thermal Free Energies= -2391.727787

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.682864 | -2.059899 | 3.689356 |
| 6 | 2.587067 | -1.318214 | 2.931321 |
| 6 | 2.234120 | -0.894131 | 1.660934 |
| 6 | 0.964074 | -1.197414 | 1.151043 |
| 6 | 0.053504 | -1.938157 | 1.913261 |
| 6 | 0.426120 | -2.371137 | 3.179929 |
| 1 | 1.964144 | -2.401522 | 4.682584 |
| 1 | 3.565831 | -1.069233 | 3.331593 |
| 1 | 2.913563 | -0.254778 | 1.094995 |
| 1 | -0.905253 | -2.236962 | 1.489677 |
| 1 | -0.266483 | -2.968477 | 3.766828 |
| 6 | 0.648086 | -0.802477 | -0.227134 |
| 8 | 1.450735 | -0.829629 | -1.159026 |
| 7 | -0.647031 | -0.291267 | -0.441087 |
| 8 | -0.993358 | -0.372041 | -1.786724 |
| 1 | -1.759521 | 0.234012 | -1.838977 |
| 46 | -0.337009 | 1.752707 | -0.075849 |
| 8 | -3.942231 | 1.486195 | 0.452781 |
| 8 | -2.263102 | 1.874680 | -0.954075 |

| | | | |
|---|---|---|---|
| 8 | 0.363109 | 3.699688 | 0.285136 |
| 8 | 1.510278 | 1.926100 | 0.790066 |
| 6 | -3.175436 | 2.285137 | -0.167179 |
| 6 | 1.457472 | 3.203069 | 0.704891 |
| 6 | -3.363176 | 3.751658 | 0.021286 |
| 6 | 2.638940 | 4.023093 | 1.047216 |
| 30 | 3.499529 | -1.054238 | -1.139380 |
| 17 | 4.143478 | -3.136411 | -1.110258 |
| 17 | 4.322628 | 0.991417 | -1.058690 |
| 1 | -1.662704 | -0.566207 | 0.186090 |
| 8 | -2.901061 | -0.676486 | 0.457016 |
| 1 | -3.532538 | 0.404580 | 0.407924 |
| 6 | -3.325011 | -1.895495 | 0.080436 |
| 8 | -2.567187 | -2.839094 | 0.136937 |
| 6 | -4.746097 | -1.964478 | -0.455620 |
| 1 | 3.041600 | 3.707170 | 2.013631 |
| 1 | 3.413861 | 3.832403 | 0.295410 |
| 1 | 2.381748 | 5.083848 | 1.061972 |
| 1 | -4.168135 | 3.967663 | 0.724272 |
| 1 | -2.418035 | 4.179831 | 0.377220 |
| 1 | -3.568320 | 4.213704 | -0.949451 |
| 6 | -5.083966 | -3.415500 | -0.774404 |
| 1 | -6.097110 | -3.477970 | -1.189625 |
| 1 | -4.380515 | -3.835046 | -1.500626 |
| 1 | -5.038810 | -4.038907 | 0.125093 |
| 6 | -4.789708 | -1.129160 | -1.742232 |
| 1 | -5.779874 | -1.216636 | -2.205626 |
| 1 | -4.605786 | -0.065063 | -1.550540 |
| 1 | -4.046524 | -1.487432 | -2.466879 |
| 6 | -5.737272 | -1.412461 | 0.572169 |
| 1 | -6.754815 | -1.494256 | 0.170535 |
| 1 | -5.700630 | -1.987990 | 1.504878 |
| 1 | -5.560659 | -0.358297 | 0.810699 |

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**$(2a'\text{-}3a')_{10}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2392.063409
Zero-point correction= 0.383221
Thermal correction to Energy= 0.417301
Thermal correction to Enthalpy= 0.418245
Thermal correction to Gibbs Free Energy= 0.315009
Sum of electronic and zero-point Energies= -2391.680188
Sum of electronic and thermal Energies= -2391.646108
Sum of electronic and thermal Enthalpies= -2391.645164

Sum of electronic and thermal Free Energies= -2391.748400

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.790345 | 4.916193 | -0.151114 |
| 6 | -1.688180 | 4.254060 | -0.985213 |
| 6 | -1.468012 | 2.928367 | -1.319290 |
| 6 | -0.343871 | 2.254705 | -0.819067 |
| 6 | 0.556541 | 2.925340 | 0.020709 |
| 6 | 0.328989 | 4.253758 | 0.346552 |
| 1 | -0.964663 | 5.956632 | 0.113738 |
| 1 | -2.564883 | 4.770350 | -1.366705 |
| 1 | -2.168668 | 2.387411 | -1.949818 |
| 1 | 1.440646 | 2.429166 | 0.408253 |
| 1 | 1.029542 | 4.776681 | 0.992072 |
| 6 | -0.213716 | 0.843005 | -1.174711 |
| 8 | -0.884590 | 0.333634 | -2.090395 |
| 7 | 0.627081 | 0.021014 | -0.389943 |
| 1 | 1.749536 | 0.428754 | 0.043886 |
| 8 | 1.117336 | -1.074013 | -1.110005 |
| 1 | 0.363176 | -1.596567 | -1.460379 |
| 46 | -0.801272 | -0.494873 | 1.127008 |
| 8 | 1.819501 | -1.520738 | 1.779594 |
| 8 | -0.085185 | -2.409629 | 1.098453 |
| 8 | -2.392963 | -0.634412 | 2.471726 |
| 8 | -1.931394 | 1.221333 | 1.434666 |
| 6 | 1.160079 | -2.486039 | 1.292440 |
| 6 | -2.700896 | 0.575187 | 2.226381 |
| 6 | 3.929938 | 0.090788 | 0.257721 |
| 8 | 3.947316 | -1.033477 | 0.841655 |
| 1 | 2.937366 | -1.330113 | 1.343043 |
| 8 | 2.901829 | 0.815056 | 0.107675 |
| 6 | 5.226588 | 0.572540 | -0.365654 |
| 30 | -2.323090 | -1.074083 | -1.518288 |
| 17 | -1.373126 | -3.001802 | -2.022457 |
| 17 | -4.146609 | -0.025737 | -0.919895 |
| 6 | -3.919474 | 1.199119 | 2.789210 |
| 1 | -4.171029 | 0.744361 | 3.749978 |
| 1 | -3.783547 | 2.278619 | 2.887261 |
| 1 | -4.742225 | 1.015391 | 2.088173 |
| 6 | 1.851538 | -3.743710 | 0.876721 |
| 1 | 2.508660 | -4.104877 | 1.672500 |
| 1 | 1.132436 | -4.509495 | 0.582990 |
| 1 | 2.478947 | -3.489377 | 0.012724 |
| 6 | 5.249189 | 2.094318 | -0.467879 |

| | | | |
|---|---|---|---|
| 1 | 6.186530 | 2.413489 | -0.939148 |
| 1 | 4.415276 | 2.470014 | -1.068346 |
| 1 | 5.192460 | 2.562386 | 0.522240 |
| 6 | 5.235044 | -0.042698 | -1.774429 |
| 1 | 5.246710 | -1.137694 | -1.725980 |
| 1 | 4.354032 | 0.269798 | -2.348265 |
| 1 | 6.131709 | 0.287792 | -2.312714 |
| 6 | 6.430602 | 0.072905 | 0.426060 |
| 1 | 7.354231 | 0.389116 | -0.073583 |
| 1 | 6.438388 | 0.484856 | 1.442317 |
| 1 | 6.433632 | -1.018054 | 0.504058 |

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**3a**

---

Number of imaginary frequencies : 0
Electronic energy =-2045.248489
Zero-point correction= 0.240889
Thermal correction to Energy= 0.266723
Thermal correction to Enthalpy= 0.267667
Thermal correction to Gibbs Free Energy= 0.180489
Sum of electronic and zero-point Energies= -2045.007600
Sum of electronic and thermal Energies= -2044.981766
Sum of electronic and thermal Enthalpies= -2044.980822
Sum of electronic and thermal Free Energies= -2045.068000

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.554276 | 3.639840 | -1.941486 |
| 6 | -2.617762 | 2.307279 | -2.341410 |
| 6 | -1.606504 | 1.426265 | -1.983846 |
| 6 | -0.521206 | 1.879898 | -1.226035 |
| 6 | -0.452386 | 3.221761 | -0.844105 |
| 6 | -1.470767 | 4.096061 | -1.195694 |
| 1 | -3.349446 | 4.327050 | -2.220458 |
| 1 | -3.453095 | 1.956443 | -2.941777 |
| 1 | -1.649493 | 0.392665 | -2.320804 |
| 1 | 0.402940 | 3.556153 | -0.263549 |
| 1 | -1.419789 | 5.137354 | -0.888514 |
| 6 | 0.576187 | 0.994486 | -0.788949 |
| 8 | 1.713260 | 1.453884 | -0.583697 |
| 7 | 0.253504 | -0.330990 | -0.659422 |
| 8 | 1.361717 | -1.139512 | -0.305727 |
| 46 | -1.393647 | -0.812554 | 0.471744 |
| 1 | -0.259354 | -1.409898 | -1.940103 |
| 8 | -1.516532 | -2.702508 | -0.424475 |

| | | | |
|---|---|---|---|
| 8 | -2.942517 | -0.872837 | 1.870519 |
| 8 | -1.648043 | 0.859594 | 1.632879 |
| 6 | -2.612456 | 0.293744 | 2.255981 |
| 6 | -1.173879 | -3.026720 | -1.571067 |
| 8 | -0.543353 | -2.247837 | -2.403438 |
| 30 | 3.108638 | 0.275901 | 0.341239 |
| 1 | 1.300561 | -1.261354 | 0.672881 |
| 17 | 2.245557 | -0.176027 | 2.394548 |
| 17 | 5.052720 | 0.070801 | -0.629276 |
| 6 | -3.283346 | 0.966860 | 3.392398 |
| 1 | -3.313259 | 2.046259 | 3.226036 |
| 1 | -4.288815 | 0.562886 | 3.528874 |
| 1 | -2.703667 | 0.780206 | 4.302859 |
| 6 | -1.466473 | -4.386943 | -2.098126 |
| 1 | -2.120755 | -4.927406 | -1.414747 |
| 1 | -1.919411 | -4.307223 | -3.090318 |
| 1 | -0.522076 | -4.928351 | -2.215893 |

---

**$(3a'\text{-}4a')_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2045.2267625
Zero-point correction= 0.235851
Thermal correction to Energy= 0.261229
Thermal correction to Enthalpy= 0.262173
Thermal correction to Gibbs Free Energy= 0.176896
Sum of electronic and zero-point Energies= -2044.990911
Sum of electronic and thermal Energies= -2044.965534
Sum of electronic and thermal Enthalpies= -2044.964590
Sum of electronic and thermal Free Energies= -2045.049866

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.002430 | -3.534297 | -0.340423 |
| 6 | -0.270280 | -2.211759 | -0.031372 |
| 6 | -1.599189 | -1.724786 | -0.010750 |
| 6 | -2.625002 | -2.586487 | -0.432773 |
| 6 | -2.349373 | -3.908637 | -0.762428 |
| 6 | -1.043652 | -4.385642 | -0.693481 |
| 1 | 1.036296 | -3.870342 | -0.341711 |
| 1 | -2.146678 | -1.083093 | 0.941603 |
| 1 | -3.651481 | -2.228753 | -0.431217 |
| 1 | -3.157030 | -4.571440 | -1.061708 |
| 1 | -0.832240 | -5.422847 | -0.941555 |
| 6 | 0.849468 | -1.250865 | 0.080848 |

| | | | |
|---|---|---|---|
| 8 | 2.020941 | -1.605319 | 0.344211 |
| 7 | 0.435382 | -0.017355 | -0.217758 |
| 8 | 1.412211 | 0.980733 | -0.122570 |
| 1 | 1.811976 | 1.072160 | -1.025486 |
| 46 | -1.547527 | 0.372446 | -0.336332 |
| 8 | -3.575802 | 0.633993 | -0.089797 |
| 8 | -3.315772 | -0.629153 | 1.747629 |
| 8 | -1.506609 | 2.459649 | -0.860242 |
| 6 | -3.988500 | 0.128593 | 1.009082 |
| 6 | -5.389393 | 0.485055 | 1.423763 |
| 6 | -0.920568 | 3.426875 | -0.369973 |
| 8 | 0.147540 | 3.354714 | 0.382917 |
| 1 | 0.536006 | 2.447354 | 0.384605 |
| 6 | -1.389934 | 4.821984 | -0.601654 |
| 1 | -1.547282 | 5.314475 | 0.362833 |
| 1 | -0.610979 | 5.384614 | -1.125288 |
| 1 | -2.311435 | 4.819596 | -1.182985 |
| 1 | -5.337367 | 1.123470 | 2.311334 |
| 1 | -5.918885 | 1.010463 | 0.628200 |
| 1 | -5.925222 | -0.423316 | 1.711432 |
| 30 | 3.515070 | -0.237488 | 0.247776 |
| 17 | 3.705535 | 0.358477 | -1.929834 |
| 17 | 4.625329 | 0.195883 | 2.076306 |

---

**$(3a'\text{-}4a')_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2392.0732548
Zero-point correction= 0.384015
Thermal correction to Energy= 0.418097
Thermal correction to Enthalpy= 0.419041
Thermal correction to Gibbs Free Energy= 0.317745
Sum of electronic and zero-point Energies= -2391.689240
Sum of electronic and thermal Energies= -2391.655158
Sum of electronic and thermal Enthalpies= -2391.654214
Sum of electronic and thermal Free Energies= -2391.755510

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.053709 | 3.697896 | -0.974281 |
| 6 | 1.067500 | 4.518327 | -1.092136 |
| 6 | 2.351134 | 4.008870 | -0.898834 |
| 6 | 2.525741 | 2.670474 | -0.568445 |
| 6 | 1.413469 | 1.825462 | -0.409128 |
| 6 | 0.126045 | 2.362140 | -0.659779 |

| | | | |
|---|---|---|---|
| 1 | -1.058850 | 4.075541 | -1.144855 |
| 1 | 0.939176 | 5.567894 | -1.345688 |
| 1 | 3.213674 | 4.663399 | -0.993553 |
| 1 | 3.523802 | 2.288379 | -0.360143 |
| 6 | -1.015743 | 1.424254 | -0.634938 |
| 8 | -2.209248 | 1.789412 | -0.559720 |
| 7 | -0.581821 | 0.160612 | -0.697038 |
| 8 | -1.551827 | -0.825971 | -0.637131 |
| 1 | -1.852283 | -1.003936 | -1.558791 |
| 46 | 1.358892 | -0.231754 | -0.910322 |
| 8 | 0.967076 | -2.218481 | -1.645118 |
| 1 | 1.557292 | 1.210170 | 0.712040 |
| 6 | 0.471851 | -3.188363 | -1.053483 |
| 8 | 0.366204 | -3.324933 | 0.232744 |
| 1 | 0.748107 | -2.567299 | 0.770125 |
| 8 | 1.880745 | 0.716864 | 1.963010 |
| 6 | 1.191451 | -0.372140 | 2.156072 |
| 8 | 1.524145 | -1.431321 | 1.597136 |
| 8 | 3.426208 | -0.584366 | -1.091760 |
| 6 | 4.326385 | -0.513981 | -0.242376 |
| 8 | 4.214831 | -0.040613 | 0.960725 |
| 1 | 3.280173 | 0.188578 | 1.275824 |
| 30 | -3.600210 | 0.292945 | -0.315795 |
| 17 | -4.048012 | -0.596562 | -2.337013 |
| 17 | -4.403305 | 0.172153 | 1.721443 |
| 6 | -0.009099 | -0.287416 | 3.085530 |
| 6 | -0.107365 | -4.324507 | -1.828705 |
| 1 | 0.118581 | -5.276850 | -1.343719 |
| 1 | -1.197949 | -4.209870 | -1.835553 |
| 1 | 0.255386 | -4.308083 | -2.856726 |
| 6 | 5.699018 | -0.997439 | -0.574936 |
| 1 | 5.809665 | -1.119181 | -1.652637 |
| 1 | 6.449110 | -0.309706 | -0.176826 |
| 1 | 5.852394 | -1.965919 | -0.086572 |
| 6 | 0.555766 | -0.303932 | 4.513026 |
| 1 | -0.270518 | -0.257204 | 5.232782 |
| 1 | 1.121494 | -1.224401 | 4.704199 |
| 1 | 1.215417 | 0.553868 | 4.687660 |
| 6 | -0.930457 | -1.482718 | 2.869626 |
| 1 | -0.420044 | -2.426446 | 3.094548 |
| 1 | -1.811072 | -1.398426 | 3.516873 |
| 1 | -1.291938 | -1.527982 | 1.833319 |
| 6 | -0.769952 | 1.018038 | 2.855539 |
| 1 | -0.111962 | 1.887186 | 2.961534 |
| 1 | -1.237386 | 1.046344 | 1.861967 |

| | | | |
|---|---|---|---|
| 1 | -1.587153 | 1.102426 | 3.581207 |

---

**$(3a'\text{-}4a')_{10}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2392.0719131
Zero-point correction= 0.383033
Thermal correction to Energy= 0.417941
Thermal correction to Enthalpy= 0.418885
Thermal correction to Gibbs Free Energy= 0.313255
Sum of electronic and zero-point Energies= -2391.688880
Sum of electronic and thermal Energies= -2391.653972
Sum of electronic and thermal Enthalpies= -2391.653028
Sum of electronic and thermal Free Energies= -2391.758658

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 0.228846 | -0.468109 | 3.699222 |
| 6 | -0.005975 | -0.280793 | 2.347520 |
| 6 | -1.321624 | -0.271051 | 1.815080 |
| 6 | -2.395274 | -0.509135 | 2.691212 |
| 6 | -2.161719 | -0.691921 | 4.048409 |
| 6 | -0.858548 | -0.674590 | 4.546157 |
| 1 | 1.251623 | -0.472417 | 4.067455 |
| 1 | -1.550199 | 0.830633 | 1.168885 |
| 1 | -3.410703 | -0.470787 | 2.305101 |
| 1 | -2.996950 | -0.843148 | 4.727493 |
| 1 | -0.688183 | -0.827294 | 5.609300 |
| 6 | 1.117271 | -0.147777 | 1.396864 |
| 8 | 2.306422 | -0.034700 | 1.765307 |
| 7 | 0.674824 | -0.185663 | 0.128327 |
| 8 | 1.710664 | -0.286746 | -0.815206 |
| 46 | -1.194577 | -0.933180 | -0.168179 |
| 8 | -1.026430 | -1.738932 | -2.187119 |
| 6 | -0.167842 | -2.360026 | -2.812192 |
| 8 | 1.112262 | -2.360637 | -2.531790 |
| 1 | 1.330143 | -1.711862 | -1.824249 |
| 8 | -1.483219 | 2.150259 | 0.818528 |
| 6 | -1.749554 | 2.502465 | -0.347365 |
| 8 | -2.608200 | 1.898586 | -1.102793 |
| 1 | -3.140352 | 1.167545 | -0.616884 |
| 8 | -3.051762 | -1.780829 | -0.252872 |
| 6 | -4.100853 | -1.056468 | -0.169535 |
| 8 | -4.120410 | 0.180525 | -0.011501 |
| 6 | -0.983793 | 3.639295 | -0.987482 |

| | | | |
|---|---|---|---|
| 1 | 1.811221 | 0.601244 | -1.227725 |
| 6 | -0.510967 | -3.206708 | -3.990347 |
| 1 | -0.250569 | -4.246523 | -3.767331 |
| 1 | -1.574765 | -3.129676 | -4.213003 |
| 1 | 0.088867 | -2.903928 | -4.853295 |
| 6 | -5.401701 | -1.806643 | -0.283043 |
| 1 | -5.298814 | -2.835958 | 0.066394 |
| 1 | -6.184538 | -1.281439 | 0.268650 |
| 1 | -5.694291 | -1.833364 | -1.338414 |
| 6 | -0.739407 | 4.743565 | 0.038316 |
| 1 | -0.233320 | 4.357057 | 0.927611 |
| 1 | -0.109406 | 5.521108 | -0.408735 |
| 1 | -1.680905 | 5.209670 | 0.352644 |
| 6 | -1.706024 | 4.191992 | -2.210689 |
| 1 | -1.115118 | 5.010309 | -2.638572 |
| 1 | -1.844063 | 3.427507 | -2.981569 |
| 1 | -2.694029 | 4.587101 | -1.947707 |
| 6 | 0.357936 | 3.013940 | -1.401331 |
| 1 | 0.199771 | 2.176599 | -2.097890 |
| 1 | 0.980046 | 3.761238 | -1.907347 |
| 1 | 0.913568 | 2.662339 | -0.523123 |
| 30 | 3.755738 | -0.022743 | 0.327400 |
| 17 | 5.000833 | -1.825359 | 0.286452 |
| 17 | 3.771304 | 1.956173 | -0.749801 |

---

**4a'**

---

Number of imaginary frequencies : 0
Electronic energy =-2045.2722508
Zero-point correction= 0.241292
Thermal correction to Energy= 0.267637
Thermal correction to Enthalpy= 0.268581
Thermal correction to Gibbs Free Energy= 0.179531
Sum of electronic and zero-point Energies= -2045.030959
Sum of electronic and thermal Energies= -2045.004614
Sum of electronic and thermal Enthalpies= -2045.003669
Sum of electronic and thermal Free Energies= -2045.092720

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.005046 | 3.644350 | 0.086201 |
| 6 | 0.182939 | 2.274399 | -0.066231 |
| 6 | 1.454301 | 1.734610 | -0.284587 |
| 6 | 2.558710 | 2.568942 | -0.371493 |
| 6 | 2.375396 | 3.948300 | -0.223854 |

| | | | |
|---|---|---|---|
| 6 | 1.112447 | 4.483035 | 0.010093 |
| 1 | -0.997725 | 4.029782 | 0.257981 |
| 1 | 2.725223 | 0.099087 | 1.648338 |
| 1 | 3.551035 | 2.171420 | -0.574385 |
| 1 | 3.236614 | 4.609227 | -0.298004 |
| 1 | 0.990674 | 5.556784 | 0.125658 |
| 6 | -0.938945 | 1.323034 | -0.042749 |
| 8 | -2.119827 | 1.643369 | 0.219517 |
| 7 | -0.502465 | 0.094338 | -0.363446 |
| 8 | -1.470090 | -0.917934 | -0.274229 |
| 1 | -1.861630 | -1.018532 | -1.177347 |
| 46 | 1.487050 | -0.252845 | -0.429949 |
| 8 | 3.633520 | -0.394677 | -0.421110 |
| 8 | 3.681945 | -0.059949 | 1.797828 |
| 8 | 1.594747 | -2.490455 | -0.487902 |
| 6 | 4.251435 | -0.330064 | 0.640983 |
| 6 | 5.721301 | -0.536496 | 0.732174 |
| 6 | 0.906856 | -3.424584 | -0.081985 |
| 8 | -0.320300 | -3.312816 | 0.363907 |
| 1 | -0.676086 | -2.398302 | 0.247560 |
| 6 | 1.407843 | -4.830288 | -0.055109 |
| 1 | 1.289223 | -5.245035 | 0.950304 |
| 1 | 0.797588 | -5.443307 | -0.725819 |
| 1 | 2.452252 | -4.866852 | -0.364224 |
| 1 | 5.937436 | -1.313637 | 1.471013 |
| 1 | 6.121993 | -0.814216 | -0.242230 |
| 1 | 6.194629 | 0.384747 | 1.086469 |
| 30 | -3.547854 | 0.205452 | 0.193025 |
| 17 | -3.892301 | -0.399340 | -1.960833 |
| 17 | -4.486323 | -0.295715 | 2.106772 |

---

**5a'**

---

Number of imaginary frequencies : 0
Electronic energy =-2638.9860756
Zero-point correction= 0.462884
Thermal correction to Energy= 0.501120
Thermal correction to Enthalpy= 0.502064
Thermal correction to Gibbs Free Energy= 0.392220
Sum of electronic and zero-point Energies= -2638.523192
Sum of electronic and thermal Energies= -2638.484955
Sum of electronic and thermal Enthalpies= -2638.484011
Sum of electronic and thermal Free Energies= -2638.593855
.....
Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.844232 | -3.325204 | -1.941708 |
| 6 | -1.202356 | -2.120870 | -1.669709 |
| 6 | -1.854105 | -0.898961 | -1.869672 |
| 6 | -3.141603 | -0.864133 | -2.379672 |
| 6 | -3.768494 | -2.074585 | -2.688662 |
| 6 | -3.134830 | -3.295133 | -2.458931 |
| 1 | -1.324210 | -4.260749 | -1.746146 |
| 1 | -3.653798 | 0.084153 | -2.526913 |
| 1 | -4.772555 | -2.061375 | -3.108664 |
| 1 | -3.649912 | -4.224370 | -2.688824 |
| 6 | 0.176463 | -2.026348 | -1.169893 |
| 8 | 0.826653 | -2.979577 | -0.668276 |
| 7 | 0.635415 | -0.769941 | -1.331339 |
| 8 | 1.882422 | -0.561559 | -0.710408 |
| 46 | -0.805985 | 0.666751 | -1.260044 |
| 8 | -2.563096 | 1.899215 | -1.154095 |
| 6 | -2.690004 | 2.953067 | -0.518809 |
| 8 | -1.719474 | 3.591587 | 0.068030 |
| 1 | -0.843582 | 3.129041 | -0.071196 |
| 1 | 2.511816 | -0.356228 | -1.420763 |
| 8 | 0.550273 | 2.351321 | -0.486301 |
| 6 | 1.445559 | 2.066640 | 0.371278 |
| 7 | 1.058732 | 1.605940 | 1.552463 |
| 6 | 2.868447 | 2.258164 | 0.025042 |
| 6 | 3.171280 | 3.266004 | -0.895497 |
| 6 | 3.884015 | 1.409283 | 0.482200 |
| 6 | 4.478120 | 3.447283 | -1.327093 |
| 1 | 2.368662 | 3.898676 | -1.265158 |
| 6 | 5.182771 | 1.572709 | 0.020174 |
| 1 | 3.660187 | 0.600002 | 1.170463 |
| 6 | 5.483433 | 2.598341 | -0.872699 |
| 1 | 4.710270 | 4.242840 | -2.030613 |
| 1 | 5.957352 | 0.888464 | 0.356512 |
| 1 | 6.504217 | 2.728679 | -1.224305 |
| 1 | -0.778984 | -1.268657 | 1.976087 |
| 8 | 1.910477 | 1.477955 | 2.614707 |
| 1 | 1.949706 | 0.509679 | 2.775928 |
| 30 | 2.354023 | -2.314495 | 0.489580 |
| 17 | 4.509384 | -2.578911 | 0.115481 |
| 17 | 1.373228 | -1.599986 | 2.445105 |
| 1 | 0.062122 | 1.412711 | 1.731368 |
| 8 | -1.687487 | 0.907204 | 1.844084 |
| 6 | -2.316599 | -0.131741 | 1.990289 |
| 8 | -1.760265 | -1.330629 | 2.000882 |

| | | | |
|---|---|---|---|
| 6 | -3.827908 | -0.179720 | 2.136879 |
| 6 | -4.018056 | 3.625383 | -0.407158 |
| 1 | -4.080317 | 4.410016 | -1.169291 |
| 1 | -4.820575 | 2.905725 | -0.578980 |
| 1 | -4.123412 | 4.102785 | 0.570142 |
| 6 | -4.392023 | -0.556276 | 0.761536 |
| 1 | -4.110243 | 0.188061 | 0.004771 |
| 1 | -4.021968 | -1.534341 | 0.429806 |
| 1 | -5.487121 | -0.601740 | 0.816404 |
| 6 | -4.341641 | 1.194278 | 2.549262 |
| 1 | -5.435579 | 1.171650 | 2.621783 |
| 1 | -3.938839 | 1.497484 | 3.522479 |
| 1 | -4.056927 | 1.961399 | 1.821194 |
| 6 | -4.239681 | -1.226550 | 3.171831 |
| 1 | -3.814159 | -1.005317 | 4.158109 |
| 1 | -5.332228 | -1.229286 | 3.269640 |
| 1 | -3.916102 | -2.229670 | 2.880045 |

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**(5a'-6a')$_4$‡**

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Number of imaginary frequencies : 1
Electronic energy =-2292.0574595
Zero-point correction= 0.304609
Thermal correction to Energy= 0.334408
Thermal correction to Enthalpy= 0.335353
Thermal correction to Gibbs Free Energy= 0.240245
Sum of electronic and zero-point Energies= -2291.752850
Sum of electronic and thermal Energies= -2291.723051
Sum of electronic and thermal Enthalpies= -2291.722107
Sum of electronic and thermal Free Energies= -2291.817215

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.547276 | 3.888060 | 0.446567 |
| 6 | -1.268613 | 2.553382 | 0.124191 |
| 6 | -2.263246 | 1.729609 | -0.438306 |
| 6 | -3.524855 | 2.241156 | -0.699128 |
| 6 | -3.791584 | 3.569438 | -0.365914 |
| 6 | -2.814922 | 4.388711 | 0.207732 |
| 1 | -0.752846 | 4.507124 | 0.858058 |
| 1 | -4.296699 | 1.614533 | -1.138653 |
| 1 | -4.784378 | 3.973890 | -0.553506 |
| 1 | -3.049658 | 5.420580 | 0.453710 |
| 6 | 0.077081 | 2.018625 | 0.213057 |
| 8 | 1.111537 | 2.647940 | 0.409290 |

| | | | |
|---|---|---|---|
| 7 | 0.124903 | 0.616335 | -0.088420 |
| 8 | 1.296810 | 0.399920 | -0.859694 |
| 1 | 1.399165 | -0.575484 | -0.910792 |
| 46 | -1.713757 | -0.168230 | -0.548665 |
| 7 | -0.469615 | -1.646711 | 0.867847 |
| 6 | 0.451950 | -2.653108 | 1.011431 |
| 8 | 0.476923 | -3.380079 | 2.002982 |
| 8 | -1.349334 | -1.667568 | 1.986282 |
| 1 | -0.934368 | -2.362887 | 2.557852 |
| 6 | 1.454000 | -2.701985 | -0.085387 |
| 6 | 1.067919 | -2.654040 | -1.431369 |
| 6 | 2.810955 | -2.736294 | 0.248917 |
| 6 | 2.036633 | -2.613271 | -2.433293 |
| 1 | 0.008610 | -2.659283 | -1.686290 |
| 6 | 3.770456 | -2.677900 | -0.753952 |
| 1 | 3.092662 | -2.761902 | 1.298445 |
| 6 | 3.385987 | -2.611079 | -2.092622 |
| 1 | 1.735648 | -2.577737 | -3.477152 |
| 1 | 4.824802 | -2.667668 | -0.490635 |
| 1 | 4.142031 | -2.555362 | -2.871507 |
| 1 | 0.093407 | -0.257566 | 0.711533 |
| 8 | -3.671823 | -0.928675 | -0.767937 |
| 6 | -4.218424 | -1.759797 | -0.025557 |
| 6 | -5.592286 | -2.253096 | -0.337186 |
| 1 | -5.577835 | -3.344480 | -0.410664 |
| 1 | -6.263486 | -1.997290 | 0.488446 |
| 1 | -5.955425 | -1.816265 | -1.267281 |
| 8 | -3.712246 | -2.280904 | 1.047487 |
| 1 | -2.792660 | -1.977729 | 1.340815 |
| 30 | 2.881470 | 1.414127 | 0.386982 |
| 17 | 4.474695 | 2.066685 | -0.961019 |
| 17 | 2.613255 | 0.160928 | 2.207398 |

---

**(5a'-6a')$_6^‡$**

---

Number of imaginary frequencies : 1
Electronic energy =-2292.0909658
Zero-point correction= 0.307027
Thermal correction to Energy= 0.336253
Thermal correction to Enthalpy= 0.337197
Thermal correction to Gibbs Free Energy= 0.243988
Sum of electronic and zero-point Energies= -2291.783939
Sum of electronic and thermal Energies= -2291.754713
Sum of electronic and thermal Enthalpies= -2291.753769
Sum of electronic and thermal Free Energies= -2291.846978

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.045321 | 2.870952 | -1.459569 |
| 6 | 2.039910 | 2.120247 | -0.833419 |
| 6 | 0.833495 | 2.714485 | -0.417650 |
| 6 | 0.640449 | 4.075463 | -0.618703 |
| 6 | 1.635547 | 4.811736 | -1.258525 |
| 6 | 2.830993 | 4.218600 | -1.680378 |
| 1 | 3.974901 | 2.382115 | -1.742940 |
| 1 | -0.282872 | 4.549918 | -0.296050 |
| 1 | 1.478337 | 5.874151 | -1.435335 |
| 1 | 3.591916 | 4.820467 | -2.169234 |
| 6 | 2.242550 | 0.738717 | -0.463733 |
| 8 | 3.309459 | 0.132444 | -0.422808 |
| 7 | 1.019983 | 0.115930 | -0.029051 |
| 8 | 1.305401 | -0.836579 | 0.978224 |
| 46 | -0.504927 | 1.451249 | 0.300905 |
| 8 | -1.979475 | 2.956207 | 0.565461 |
| 6 | -3.132009 | 2.779084 | 0.989348 |
| 6 | -4.032223 | 3.940621 | 1.244708 |
| 1 | -4.226350 | 4.008861 | 2.320032 |
| 1 | -3.574469 | 4.865524 | 0.894238 |
| 1 | -4.995765 | 3.777458 | 0.754029 |
| 8 | -3.663968 | 1.626354 | 1.262221 |
| 1 | -3.055774 | 0.840341 | 1.058728 |
| 1 | 0.592807 | -1.503412 | 0.818954 |
| 8 | -1.953620 | -0.168645 | 0.622303 |
| 6 | -1.915329 | -1.225210 | -0.132720 |
| 7 | -0.766490 | -1.562938 | -0.678664 |
| 6 | -3.177416 | -1.986693 | -0.298462 |
| 6 | -4.381971 | -1.281193 | -0.372675 |
| 6 | -3.200511 | -3.384796 | -0.309807 |
| 6 | -5.589425 | -1.959880 | -0.469797 |
| 1 | -4.372108 | -0.194111 | -0.368016 |
| 6 | -4.411737 | -4.059514 | -0.383195 |
| 1 | -2.266218 | -3.934124 | -0.265468 |
| 6 | -5.606429 | -3.350846 | -0.468776 |
| 1 | -6.519511 | -1.401179 | -0.540628 |
| 1 | -4.421842 | -5.146547 | -0.378672 |
| 1 | -6.552249 | -3.883508 | -0.536203 |
| 1 | 0.378329 | -0.524766 | -0.715202 |
| 8 | -0.817759 | -2.634825 | -1.562201 |
| 1 | 0.116821 | -2.909613 | -1.623590 |
| 30 | 3.258675 | -1.818852 | 0.370186 |

| | | | |
|---|---|---|---|
| 17 | 4.551717 | -2.129110 | 2.098554 |
| 17 | 2.348190 | -3.071754 | -1.258162 |

---

**$(5a'\text{-}6a')_{10}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2638.931953
Zero-point correction= 0.452902
Thermal correction to Energy= 0.491340
Thermal correction to Enthalpy= 0.492284
Thermal correction to Gibbs Free Energy= 0.380017
Sum of electronic and zero-point Energies= -2638.479051
Sum of electronic and thermal Energies= -2638.440613
Sum of electronic and thermal Enthalpies= -2638.439669
Sum of electronic and thermal Free Energies= -2638.551936

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -1.937707 | -3.297995 | -1.877029 |
| 6 | -1.345441 | -2.083060 | -1.505239 |
| 6 | -2.026493 | -0.859215 | -1.659865 |
| 6 | -3.297645 | -0.855061 | -2.219348 |
| 6 | -3.882316 | -2.067678 | -2.580605 |
| 6 | -3.214119 | -3.284867 | -2.408593 |
| 1 | -1.377134 | -4.221345 | -1.748370 |
| 1 | -3.835241 | 0.080690 | -2.349490 |
| 1 | -4.886187 | -2.066513 | -3.000958 |
| 1 | -3.695463 | -4.214105 | -2.700279 |
| 6 | 0.001668 | -2.018279 | -0.991496 |
| 8 | 0.864273 | -2.888015 | -0.963742 |
| 7 | 0.275882 | -0.705033 | -0.443403 |
| 8 | 1.657743 | -0.438638 | -0.439725 |
| 46 | -1.062282 | 0.755786 | -1.036689 |
| 8 | -2.705180 | 2.033192 | -1.453942 |
| 6 | -2.897258 | 3.111687 | -0.865868 |
| 8 | -2.027056 | 3.729086 | -0.131244 |
| 1 | -1.139300 | 3.249832 | -0.095998 |
| 1 | 1.864743 | -0.005507 | -1.286516 |
| 8 | 0.211608 | 2.438142 | -0.326748 |
| 6 | 1.098928 | 2.139165 | 0.575006 |
| 7 | 0.681879 | 1.500313 | 1.637937 |
| 6 | 2.503007 | 2.511550 | 0.285250 |
| 6 | 2.714231 | 3.619086 | -0.544195 |
| 6 | 3.602068 | 1.756270 | 0.715576 |
| 6 | 4.000815 | 3.986317 | -0.912800 |

| | | | |
|---|---|---|---|
| 1 | 1.854703 | 4.184593 | -0.893756 |
| 6 | 4.884279 | 2.109871 | 0.315328 |
| 1 | 3.451106 | 0.892708 | 1.354747 |
| 6 | 5.087824 | 3.227610 | -0.488530 |
| 1 | 4.155088 | 4.858256 | -1.543678 |
| 1 | 5.728472 | 1.503374 | 0.633245 |
| 1 | 6.095661 | 3.503527 | -0.789848 |
| 1 | -0.081036 | -0.774047 | 0.622561 |
| 8 | 1.577494 | 1.213940 | 2.652731 |
| 1 | 1.604649 | 0.237186 | 2.696433 |
| 30 | 2.712950 | -2.317738 | 0.037188 |
| 17 | 4.367307 | -2.346658 | -1.400976 |
| 17 | 2.349216 | -2.101760 | 2.220282 |
| 1 | -0.509078 | 1.261254 | 1.832579 |
| 8 | -1.714485 | 0.970145 | 2.027433 |
| 6 | -1.861664 | -0.296704 | 2.086130 |
| 8 | -0.988120 | -1.118390 | 1.711380 |
| 6 | -3.211792 | -0.819373 | 2.561938 |
| 6 | -4.217663 | 3.797961 | -0.959174 |
| 1 | -4.074383 | 4.866707 | -1.136569 |
| 1 | -4.827691 | 3.351470 | -1.744374 |
| 1 | -4.729531 | 3.693153 | 0.003741 |
| 6 | -4.088494 | -0.889522 | 1.303585 |
| 1 | -4.175358 | 0.095255 | 0.822891 |
| 1 | -3.667546 | -1.590447 | 0.570426 |
| 1 | -5.096061 | -1.233962 | 1.569707 |
| 6 | -3.839362 | 0.132121 | 3.575218 |
| 1 | -4.820699 | -0.249800 | 3.884395 |
| 1 | -3.215550 | 0.224311 | 4.472242 |
| 1 | -3.969984 | 1.133965 | 3.154977 |
| 6 | -3.067428 | -2.214333 | 3.160514 |
| 1 | -2.419791 | -2.203012 | 4.044926 |
| 1 | -4.052475 | -2.590331 | 3.465113 |
| 1 | -2.633522 | -2.914105 | 2.439976 |

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**6a'**

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Number of imaginary frequencies : 0
Electronic energy =-2292.0871755
Zero-point correction= 0.310757
Thermal correction to Energy= 0.340955
Thermal correction to Enthalpy= 0.341899
Thermal correction to Gibbs Free Energy= 0.245414
Sum of electronic and zero-point Energies= -2291.776419
Sum of electronic and thermal Energies= -2291.746220

Sum of electronic and thermal Enthalpies= -2291.745276
Sum of electronic and thermal Free Energies= -2291.841761

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.652047 | -3.726712 | -0.085620 |
| 6 | 1.726491 | -2.369137 | 0.216201 |
| 6 | 0.570718 | -1.600628 | 0.156070 |
| 6 | -0.646017 | -2.217871 | -0.215955 |
| 6 | -0.706004 | -3.583315 | -0.541272 |
| 6 | 0.449535 | -4.335047 | -0.469045 |
| 1 | 2.556165 | -4.329384 | -0.026067 |
| 1 | 2.674260 | -1.918690 | 0.499742 |
| 1 | -1.658445 | -4.016550 | -0.838828 |
| 1 | 0.429756 | -5.394626 | -0.707605 |
| 6 | -1.817197 | -1.384755 | -0.263587 |
| 8 | -2.904480 | -1.586731 | -0.782726 |
| 7 | -1.601722 | -0.127480 | 0.476547 |
| 46 | 0.425473 | 0.344534 | 0.392996 |
| 8 | -2.483906 | 0.843810 | -0.037646 |
| 8 | -0.286698 | 2.514617 | 0.540358 |
| 8 | 2.448092 | 0.664071 | 0.532209 |
| 6 | 3.258213 | 0.561032 | -0.475473 |
| 7 | 3.017803 | 0.825097 | -1.729476 |
| 8 | 1.671952 | 1.299198 | -1.864608 |
| 1 | 1.574477 | 1.353329 | -2.822353 |
| 6 | 4.642370 | 0.101669 | -0.177701 |
| 6 | 5.624925 | 0.045208 | -1.171723 |
| 6 | 4.963775 | -0.283300 | 1.125509 |
| 6 | 6.902347 | -0.399890 | -0.864114 |
| 1 | 5.371375 | 0.354181 | -2.182090 |
| 6 | 6.246953 | -0.726053 | 1.430320 |
| 1 | 4.195522 | -0.220127 | 1.892174 |
| 6 | 7.217789 | -0.787247 | 0.437274 |
| 1 | 7.660115 | -0.444055 | -1.643235 |
| 1 | 6.488575 | -1.020889 | 2.449100 |
| 1 | 8.221583 | -1.132437 | 0.674934 |
| 6 | 0.335684 | 3.549763 | 0.264656 |
| 6 | -0.019204 | 4.870284 | 0.859327 |
| 1 | -0.126842 | 5.621227 | 0.071865 |
| 1 | -0.933201 | 4.794072 | 1.448382 |
| 1 | 0.804691 | 5.196183 | 1.502855 |
| 8 | 1.347430 | 3.593957 | -0.550124 |
| 1 | 1.513448 | 2.709261 | -0.990595 |
| 1 | -1.921643 | -0.308495 | 1.446898 |

| | | | |
|---|---|---|---|
| 30 | -4.461913 | -0.229921 | -0.083176 |
| 17 | -5.753667 | 0.617880 | -1.612705 |
| 1 | -2.040063 | 1.695305 | 0.156716 |
| 17 | -4.316355 | -0.717169 | 2.095478 |

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**6a'1**

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Number of imaginary frequencies : 0
Electronic energy =-2292.0833433
Zero-point correction= 0.309723 (Hartree/Particle)
Thermal correction to Energy= 0.340053
Thermal correction to Enthalpy= 0.340997
Thermal correction to Gibbs Free Energy= 0.244457
Sum of electronic and zero-point Energies= -2291.773621
Sum of electronic and thermal Energies= -2291.743291
Sum of electronic and thermal Enthalpies= -2291.742346
Sum of electronic and thermal Free Energies= -2291.838886

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.385098 | -1.489094 | 0.895443 |
| 6 | 0.547589 | 0.579035 | 2.053323 |
| 6 | -0.746846 | 0.034013 | 2.015731 |
| 6 | 0.813881 | 1.700778 | 2.847884 |
| 6 | -1.756981 | 0.646745 | 2.756482 |
| 6 | -0.192252 | 2.277261 | 3.608564 |
| 1 | 1.823410 | 2.105853 | 2.853580 |
| 6 | -1.478791 | 1.748066 | 3.564199 |
| 1 | -2.783356 | 0.286266 | 2.681315 |
| 1 | 0.022752 | 3.147904 | 4.222207 |
| 1 | -2.280149 | 2.210914 | 4.135682 |
| 8 | -3.351688 | 0.210034 | -0.525422 |
| 6 | -2.214963 | 0.683924 | -0.709799 |
| 7 | -1.146390 | -0.179857 | -0.669949 |
| 8 | 0.089638 | 0.402771 | -0.843280 |
| 1 | 0.519537 | -0.040294 | -1.602519 |
| 6 | -2.070197 | 2.125647 | -1.034172 |
| 6 | -3.101674 | 2.705562 | -1.779764 |
| 6 | -1.039262 | 2.931574 | -0.537651 |
| 6 | -3.086368 | 4.064139 | -2.060513 |
| 1 | -3.912661 | 2.072745 | -2.130637 |
| 6 | -1.045934 | 4.296113 | -0.797113 |
| 1 | -0.238993 | 2.497388 | 0.053870 |
| 6 | -2.057760 | 4.861852 | -1.566893 |

| | | | |
|---|---|---|---|
| 1 | -3.881935 | 4.503707 | -2.657080 |
| 1 | -0.248813 | 4.920272 | -0.401023 |
| 1 | -2.046453 | 5.928331 | -1.780176 |
| 6 | 1.674227 | 0.063701 | 1.252185 |
| 8 | 2.555200 | 0.799143 | 0.783114 |
| 8 | -2.215804 | -3.212209 | -0.171188 |
| 6 | -3.122859 | -3.240791 | -1.009341 |
| 6 | -3.515570 | -4.514568 | -1.683975 |
| 1 | -3.372803 | -4.409007 | -2.763840 |
| 1 | -2.919799 | -5.345915 | -1.307370 |
| 1 | -4.580547 | -4.703369 | -1.519354 |
| 8 | -3.823775 | -2.215703 | -1.395057 |
| 1 | -3.570847 | -1.340718 | -0.959982 |
| 7 | 1.766351 | -1.296889 | 1.159143 |
| 8 | 2.631847 | -1.772535 | 0.183176 |
| 1 | 3.410027 | -2.130017 | 0.652328 |
| 1 | 0.892708 | -1.831588 | 1.178946 |
| 30 | 3.665724 | -0.002086 | -0.785736 |
| 17 | 5.633027 | -0.740933 | -0.077637 |
| 17 | 2.593455 | 0.244189 | -2.714375 |

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**$(6a'\text{-}9)_5^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2292.0188586
Zero-point correction= 0.308544
Thermal correction to Energy= 0.338366
Thermal correction to Enthalpy= 0.339311
Thermal correction to Gibbs Free Energy= 0.244351
Sum of electronic and zero-point Energies= -2291.710315
Sum of electronic and thermal Energies= -2291.680492
Sum of electronic and thermal Enthalpies= -2291.679548
Sum of electronic and thermal Free Energies= -2291.774507

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.078417 | -3.191798 | -1.112377 |
| 6 | -2.028610 | -1.826050 | -1.194126 |
| 6 | -1.011233 | -1.112098 | -0.485489 |
| 6 | 0.089312 | -1.892291 | 0.012628 |
| 6 | -0.040502 | -3.301013 | 0.163697 |
| 6 | -1.120593 | -3.940910 | -0.374095 |
| 1 | -2.880536 | -3.720465 | -1.624723 |
| 1 | -2.803993 | -1.279175 | -1.728682 |

| | | | |
|---|---|---|---|
| 1 | 0.774026 | -3.844895 | 0.637976 |
| 1 | -1.217496 | -5.020418 | -0.303408 |
| 6 | 1.327272 | -1.262158 | 0.217091 |
| 8 | 2.319196 | -1.621138 | 0.874008 |
| 7 | 1.464071 | -0.057645 | -0.639371 |
| 46 | -0.436273 | 0.772538 | -0.949696 |
| 8 | 2.405694 | 0.804285 | 0.001612 |
| 8 | 0.321358 | 2.922906 | -1.025718 |
| 8 | -2.508643 | 1.338854 | -0.394939 |
| 6 | -2.848595 | 0.426245 | 0.392535 |
| 7 | -1.928115 | -0.376266 | 1.069489 |
| 8 | -0.928194 | 0.484550 | 1.633766 |
| 1 | -0.758599 | 0.066604 | 2.486933 |
| 6 | -4.256614 | 0.042511 | 0.519056 |
| 6 | -4.660458 | -0.936840 | 1.436171 |
| 6 | -5.204353 | 0.650718 | -0.316633 |
| 6 | -5.997581 | -1.300736 | 1.513307 |
| 1 | -3.912136 | -1.400838 | 2.071810 |
| 6 | -6.539217 | 0.292143 | -0.225115 |
| 1 | -4.866994 | 1.398874 | -1.029277 |
| 6 | -6.935120 | -0.685001 | 0.688522 |
| 1 | -6.312338 | -2.062907 | 2.221429 |
| 1 | -7.275362 | 0.764928 | -0.870177 |
| 1 | -7.982941 | -0.969096 | 0.754400 |
| 6 | 0.189952 | 3.629781 | -0.027369 |
| 6 | 0.578241 | 5.070561 | -0.007429 |
| 1 | 1.332777 | 5.237561 | 0.767510 |
| 1 | 0.962936 | 5.372212 | -0.981468 |
| 1 | -0.292582 | 5.677493 | 0.258314 |
| 8 | -0.289820 | 3.220494 | 1.126224 |
| 1 | -0.547527 | 2.268461 | 1.126863 |
| 1 | 1.947800 | -0.390599 | -1.496815 |
| 30 | 4.104420 | -0.677255 | 0.383239 |
| 17 | 5.406598 | -0.002181 | 2.001882 |
| 1 | 2.516820 | 1.542401 | -0.619776 |
| 17 | 4.250037 | -0.997811 | -1.849807 |

**Role of Explicit Solvent Coordination on Lewis Acid (Acetate as Ligand, LA=1,S=1)**

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**2a'$_s$**

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Number of imaginary frequencies : 0
Electronic energy =-2332.925386
Zero-point correction= 0.374165
Thermal correction to Energy= 0.408357

Thermal correction to Enthalpy= 0.409302
Thermal correction to Gibbs Free Energy= 0.305343
Sum of electronic and zero-point Energies= -2332.551221
Sum of electronic and thermal Energies= -2332.517029
Sum of electronic and thermal Enthalpies= -2332.516084
Sum of electronic and thermal Free Energies= -2332.620043

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -3.911649 | 3.399455 | 2.109077 |
| 6 | -4.296876 | 2.474133 | 1.142537 |
| 6 | -3.342188 | 1.840547 | 0.359935 |
| 6 | -1.985596 | 2.140922 | 0.551257 |
| 6 | -1.602364 | 3.069967 | 1.527339 |
| 6 | -2.564254 | 3.696854 | 2.302302 |
| 1 | -4.667314 | 3.893461 | 2.715331 |
| 1 | -5.348603 | 2.245949 | 0.993006 |
| 1 | -3.669214 | 1.119180 | -0.387661 |
| 1 | -0.545473 | 3.286155 | 1.656318 |
| 1 | -2.265975 | 4.419654 | 3.056892 |
| 6 | -0.908827 | 1.537997 | -0.241085 |
| 8 | 0.263466 | 1.875318 | -0.131650 |
| 7 | -1.259896 | 0.481955 | -1.126401 |
| 8 | -0.369351 | 0.360032 | -2.189170 |
| 46 | -1.406810 | -1.246606 | 0.107759 |
| 1 | -2.233473 | 0.455080 | -1.518386 |
| 8 | -2.370211 | -2.187506 | -1.394936 |
| 8 | -1.411602 | -2.709192 | 1.598789 |
| 8 | -0.464557 | -0.768985 | 1.915806 |
| 6 | -0.746620 | -1.933404 | 2.355054 |
| 6 | -3.285957 | -1.608313 | -2.098982 |
| 8 | -3.581834 | -0.405273 | -2.067079 |
| 1 | 0.087603 | -0.504425 | -2.064060 |
| 17 | 1.728087 | -1.350106 | -0.891681 |
| 17 | 2.915011 | 2.124774 | -2.620764 |
| 30 | 1.973017 | 0.987950 | -0.973702 |
| 8 | 3.002852 | 1.163833 | 0.804387 |
| 6 | 3.464223 | 0.133743 | 1.344176 |
| 6 | 2.797337 | -0.402030 | 2.575396 |
| 1 | 2.212529 | -1.289794 | 2.299311 |
| 1 | 3.499255 | -0.668401 | 3.371148 |
| 1 | 2.097526 | 0.356332 | 2.929861 |
| 7 | 4.532012 | -0.504295 | 0.839195 |
| 6 | 5.129318 | -0.042715 | -0.406527 |
| 1 | 6.215679 | -0.163957 | -0.346107 |

| | | | |
|---|---|---|---|
| 1 | 4.750378 | -0.631012 | -1.253689 |
| 1 | 4.889546 | 1.008317 | -0.573883 |
| 6 | 4.905748 | -1.852668 | 1.225023 |
| 1 | 4.421458 | -2.580344 | 0.558681 |
| 1 | 5.991396 | -1.963595 | 1.139189 |
| 1 | 4.621726 | -2.072939 | 2.254463 |
| 6 | -0.299246 | -2.381066 | 3.700516 |
| 1 | 0.467254 | -3.154906 | 3.585196 |
| 1 | 0.109399 | -1.541275 | 4.267404 |
| 1 | -1.138696 | -2.831286 | 4.237648 |
| 6 | -3.998776 | -2.558360 | -3.026007 |
| 1 | -4.420037 | -3.389271 | -2.453044 |
| 1 | -4.785540 | -2.031835 | -3.568592 |
| 1 | -3.279891 | -2.984882 | -3.732111 |

---

**$(2a'\text{-}3a')_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2332.9223143
Zero-point correction= 0.368132
Thermal correction to Energy= 0.402669
Thermal correction to Enthalpy= 0.403613
Thermal correction to Gibbs Free Energy= 0.297097
Sum of electronic and zero-point Energies= -2332.554182
Sum of electronic and thermal Energies= -2332.519645
Sum of electronic and thermal Enthalpies= -2332.518701
Sum of electronic and thermal Free Energies= -2332.625217

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.661785 | 1.310813 | 3.826745 |
| 6 | 4.119458 | 0.452679 | 2.830416 |
| 6 | 3.217174 | -0.207876 | 2.007982 |
| 6 | 1.842698 | -0.011038 | 2.192120 |
| 6 | 1.386754 | 0.848017 | 3.198514 |
| 6 | 2.295360 | 1.508799 | 4.010436 |
| 1 | 4.374890 | 1.826467 | 4.465672 |
| 1 | 5.185818 | 0.293377 | 2.694762 |
| 1 | 3.593395 | -0.879841 | 1.239746 |
| 1 | 0.315507 | 0.983093 | 3.321997 |
| 1 | 1.939901 | 2.178295 | 4.789284 |
| 6 | 0.816492 | -0.676008 | 1.372941 |
| 8 | -0.360019 | -0.720856 | 1.723793 |
| 7 | 1.232378 | -1.206342 | 0.137544 |
| 8 | 0.313086 | -2.122529 | -0.382874 |

| | | | |
|---|---|---|---|
| 46 | 1.542309 | 0.453041 | -1.122550 |
| 1 | 2.286146 | -1.674302 | -0.069769 |
| 8 | 2.712110 | -0.724289 | -2.311674 |
| 8 | 1.606633 | 2.295387 | -2.108353 |
| 8 | 0.496129 | 2.028613 | -0.250365 |
| 6 | 0.839691 | 2.784685 | -1.220780 |
| 6 | 3.402355 | -1.698589 | -1.868309 |
| 8 | 3.362817 | -2.149684 | -0.693560 |
| 1 | -0.126780 | -1.678257 | -1.145342 |
| 17 | -1.760829 | -0.331131 | -1.601826 |
| 17 | -2.965920 | -3.227027 | 0.964948 |
| 30 | -2.003549 | -1.277879 | 0.553591 |
| 8 | -3.093230 | 0.293028 | 1.345797 |
| 6 | -3.492496 | 1.192503 | 0.574374 |
| 6 | -2.747215 | 2.492491 | 0.517823 |
| 1 | -2.182951 | 2.527095 | -0.423321 |
| 1 | -3.396561 | 3.370883 | 0.582375 |
| 1 | -2.025910 | 2.498680 | 1.336912 |
| 7 | -4.561429 | 1.008117 | -0.216542 |
| 6 | -5.204072 | -0.298777 | -0.259196 |
| 1 | -6.279149 | -0.161671 | -0.412865 |
| 1 | -4.795207 | -0.896999 | -1.085558 |
| 1 | -5.032939 | -0.832200 | 0.676816 |
| 6 | -4.889409 | 1.883869 | -1.325506 |
| 1 | -4.438843 | 1.502289 | -2.252781 |
| 1 | -5.976673 | 1.918405 | -1.450268 |
| 1 | -4.533551 | 2.900155 | -1.153550 |
| 6 | 0.336981 | 4.179006 | -1.322925 |
| 1 | -0.474154 | 4.209854 | -2.058804 |
| 1 | -0.042979 | 4.518806 | -0.356410 |
| 1 | 1.133123 | 4.837917 | -1.678813 |
| 6 | 4.314036 | -2.363619 | -2.855964 |
| 1 | 5.279279 | -2.560013 | -2.382071 |
| 1 | 3.880645 | -3.331390 | -3.128883 |
| 1 | 4.437596 | -1.756994 | -3.753757 |

---

**$(2a'\text{-}3a')_{8s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2679.7374564
Zero-point correction= 0.516632
Thermal correction to Energy= 0.559038
Thermal correction to Enthalpy= 0.559982
Thermal correction to Gibbs Free Energy= 0.438737
Sum of electronic and zero-point Energies= -2679.220825

Sum of electronic and thermal Energies= -2679.178419
Sum of electronic and thermal Enthalpies= -2679.177474
Sum of electronic and thermal Free Energies= -2679.298719

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.009966 | -2.738594 | 3.817859 |
| 6 | -1.180216 | -1.704089 | 4.243576 |
| 6 | -0.505950 | -0.928815 | 3.311598 |
| 6 | -0.688891 | -1.164756 | 1.945572 |
| 6 | -1.514391 | -2.208791 | 1.520118 |
| 6 | -2.166191 | -2.997633 | 2.458816 |
| 1 | -2.532220 | -3.350560 | 4.549502 |
| 1 | -1.055099 | -1.505356 | 5.304740 |
| 1 | 0.154788 | -0.124125 | 3.624098 |
| 1 | -1.656287 | -2.413692 | 0.462546 |
| 1 | -2.801331 | -3.814227 | 2.124161 |
| 6 | 0.050367 | -0.296774 | 1.010622 |
| 8 | 1.183962 | 0.095732 | 1.265943 |
| 7 | -0.612738 | 0.082663 | -0.179107 |
| 1 | -1.252371 | -0.699712 | -0.841771 |
| 8 | 0.283204 | 0.672788 | -1.081782 |
| 46 | -2.181963 | 1.454203 | 0.174700 |
| 8 | -4.130952 | -1.172993 | -0.175998 |
| 8 | -3.358826 | 0.294612 | 1.362825 |
| 8 | -3.307426 | 3.237346 | 0.079222 |
| 8 | -1.362383 | 3.013899 | -0.863162 |
| 6 | -4.146126 | -0.614357 | 0.950345 |
| 6 | -2.374741 | 3.758909 | -0.604406 |
| 6 | -2.092981 | -2.358012 | -2.359873 |
| 8 | -2.157965 | -1.278227 | -1.533331 |
| 1 | -3.163241 | -1.180846 | -0.931077 |
| 8 | -3.071624 | -3.037617 | -2.538453 |
| 6 | -0.727578 | -2.595790 | -2.987461 |
| 1 | 0.179839 | 1.652252 | -1.040200 |
| 6 | -2.428280 | 5.150410 | -1.107329 |
| 1 | -1.451305 | 5.623310 | -0.974173 |
| 1 | -2.644947 | 5.133381 | -2.180684 |
| 1 | -3.209236 | 5.712086 | -0.591354 |
| 6 | -5.202559 | -1.035090 | 1.928316 |
| 1 | -6.065390 | -0.369419 | 1.817878 |
| 1 | -5.522610 | -2.057688 | 1.718569 |
| 1 | -4.828791 | -0.938292 | 2.950079 |
| 6 | 0.290866 | -2.899572 | -1.882789 |
| 1 | 1.257361 | -3.148168 | -2.336220 |

| | | | |
|---|---|---|---|
| 1 | 0.485925 | -2.036411 | -1.234839 |
| 1 | -0.026277 | -3.751828 | -1.266470 |
| 6 | -0.288044 | -1.357484 | -3.773145 |
| 1 | -0.202587 | -0.471173 | -3.137233 |
| 1 | 0.700773 | -1.541126 | -4.210815 |
| 1 | -0.988897 | -1.140878 | -4.588850 |
| 6 | -0.832017 | -3.796393 | -3.921320 |
| 1 | -1.132393 | -4.698629 | -3.377449 |
| 1 | -1.575710 | -3.623355 | -4.706485 |
| 1 | 0.140106 | -3.979307 | -4.394472 |
| 30 | 2.546801 | 0.900917 | -0.171109 |
| 17 | 3.352489 | -0.793132 | -1.466013 |
| 17 | 2.145358 | 3.075304 | -0.616678 |
| 8 | 4.025355 | 0.851783 | 1.300336 |
| 6 | 5.108655 | 0.345109 | 0.937228 |
| 6 | 6.079364 | 1.152136 | 0.126025 |
| 1 | 5.693134 | 2.171230 | 0.055518 |
| 1 | 7.081482 | 1.172378 | 0.566738 |
| 1 | 6.153068 | 0.733214 | -0.885174 |
| 7 | 5.415884 | -0.924451 | 1.256112 |
| 6 | 4.390918 | -1.759311 | 1.863176 |
| 1 | 3.854440 | -2.315479 | 1.081326 |
| 1 | 4.861286 | -2.461693 | 2.558960 |
| 1 | 3.678852 | -1.126549 | 2.393593 |
| 6 | 6.500547 | -1.645448 | 0.616624 |
| 1 | 6.829252 | -2.455218 | 1.275479 |
| 1 | 6.159620 | -2.076680 | -0.335939 |
| 1 | 7.356119 | -0.995231 | 0.427691 |

---

**$(2a'\text{-}3a')_{10s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2679.7530671
Zero-point correction= 0.517000
Thermal correction to Energy= 0.560522
Thermal correction to Enthalpy= 0.561466
Thermal correction to Gibbs Free Energy= 0.435227
Sum of electronic and zero-point Energies= -2679.236067
Sum of electronic and thermal Energies= -2679.192546
Sum of electronic and thermal Enthalpies= -2679.191601
Sum of electronic and thermal Free Energies= -2679.317840

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 2.122917 | -1.452441 | 4.766187 |

| | | | |
|---|---|---|---|
| 6 | 2.818862 | -0.776219 | 3.768063 |
| 6 | 2.218918 | -0.528253 | 2.540716 |
| 6 | 0.905450 | -0.958231 | 2.310656 |
| 6 | 0.207705 | -1.627304 | 3.321111 |
| 6 | 0.816601 | -1.878481 | 4.541598 |
| 1 | 2.600105 | -1.645228 | 5.724421 |
| 1 | 3.836682 | -0.438331 | 3.944804 |
| 1 | 2.778280 | 0.000555 | 1.771984 |
| 1 | -0.814011 | -1.940431 | 3.124739 |
| 1 | 0.271750 | -2.404246 | 5.321624 |
| 6 | 0.177578 | -0.706160 | 1.048266 |
| 8 | -1.042935 | -0.887718 | 0.978714 |
| 7 | 0.921467 | -0.197989 | -0.017434 |
| 8 | 0.079364 | 0.044290 | -1.127411 |
| 46 | 2.477732 | -1.438089 | -0.617388 |
| 8 | 2.709922 | 1.182675 | -1.884990 |
| 8 | 3.858295 | 0.060432 | -0.342903 |
| 8 | 3.554213 | -3.098641 | -1.365154 |
| 8 | 1.405812 | -3.163190 | -0.982420 |
| 6 | 3.650887 | 1.089242 | -1.069026 |
| 6 | 2.467158 | -3.751680 | -1.391631 |
| 1 | 0.031398 | -0.771768 | -1.666298 |
| 1 | 1.246086 | 1.236780 | 0.253420 |
| 8 | 1.220504 | 2.255542 | 0.589836 |
| 6 | 0.971592 | 3.190809 | -0.239949 |
| 6 | 0.612018 | 4.549909 | 0.298573 |
| 8 | 1.163733 | 3.089018 | -1.495555 |
| 1 | 1.714351 | 2.250225 | -1.764513 |
| 6 | 2.402879 | -5.144758 | -1.903675 |
| 1 | 1.625424 | -5.702767 | -1.376586 |
| 1 | 2.139918 | -5.119841 | -2.966640 |
| 1 | 3.375117 | -5.630842 | -1.797106 |
| 6 | 4.622137 | 2.226964 | -0.896607 |
| 1 | 5.248505 | 2.289945 | -1.792441 |
| 1 | 4.071807 | 3.172579 | -0.825338 |
| 1 | 5.258735 | 2.091215 | -0.021068 |
| 6 | -0.310943 | 5.287617 | -0.670641 |
| 1 | -1.263007 | 4.756628 | -0.782788 |
| 1 | -0.509455 | 6.289383 | -0.271443 |
| 1 | 0.145279 | 5.395088 | -1.659566 |
| 6 | -0.018334 | 4.449761 | 1.683420 |
| 1 | 0.661610 | 3.983736 | 2.404086 |
| 1 | -0.253593 | 5.460109 | 2.038153 |
| 1 | -0.944005 | 3.864873 | 1.649376 |
| 6 | 1.963579 | 5.285934 | 0.391444 |

| | | | |
|---|---|---|---|
| 1 | 1.794247 | 6.284050 | 0.811685 |
| 1 | 2.664202 | 4.755734 | 1.049749 |
| 1 | 2.422899 | 5.404276 | -0.597610 |
| 30 | -2.176344 | 0.029745 | -0.542246 |
| 17 | -2.146961 | 2.292012 | -0.201008 |
| 17 | -2.404591 | -1.158535 | -2.479167 |
| 8 | -3.915701 | -0.563248 | 0.441373 |
| 6 | -5.068056 | -0.417121 | -0.007251 |
| 6 | -5.332071 | 0.532675 | -1.136601 |
| 1 | -4.635702 | 1.373262 | -1.038416 |
| 1 | -5.101583 | 0.028985 | -2.084630 |
| 1 | -6.350956 | 0.922180 | -1.168138 |
| 7 | -6.090480 | -1.123234 | 0.521928 |
| 6 | -5.861166 | -1.987715 | 1.666067 |
| 1 | -6.049240 | -3.034468 | 1.397316 |
| 1 | -4.827466 | -1.881001 | 1.992977 |
| 1 | -6.537073 | -1.708729 | 2.483878 |
| 6 | -7.455604 | -1.075517 | 0.034119 |
| 1 | -8.061969 | -0.342813 | 0.584040 |
| 1 | -7.493220 | -0.844377 | -1.031490 |
| 1 | -7.909302 | -2.063006 | 0.169615 |

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**$(3a'\text{-}4a')_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2332.9089689
Zero-point correction= 0.368395
Thermal correction to Energy= 0.402405
Thermal correction to Enthalpy= 0.403349
Thermal correction to Gibbs Free Energy= 0.298472
Sum of electronic and zero-point Energies= -2332.540574
Sum of electronic and thermal Energies= -2332.506564
Sum of electronic and thermal Enthalpies= -2332.505620
Sum of electronic and thermal Free Energies= -2332.610496

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.553870 | 3.342350 | -0.656027 |
| 6 | 1.010803 | 2.109693 | -0.216085 |
| 6 | 2.394322 | 1.858192 | -0.067071 |
| 6 | 3.297196 | 2.845943 | -0.493427 |
| 6 | 2.839327 | 4.076201 | -0.949793 |
| 6 | 1.471515 | 4.329731 | -1.008606 |
| 1 | -0.517594 | 3.494940 | -0.760621 |
| 1 | 2.970415 | 1.377955 | 0.970514 |

| | | | |
|---|---|---|---|
| 1 | 4.364454 | 2.661621 | -0.398287 |
| 1 | 3.549843 | 4.841623 | -1.251214 |
| 1 | 1.114603 | 5.294737 | -1.360551 |
| 6 | 0.054920 | 0.982989 | -0.104043 |
| 8 | -1.176629 | 1.165037 | 0.026990 |
| 7 | 0.692287 | -0.179190 | -0.254719 |
| 8 | -0.082777 | -1.325436 | -0.174928 |
| 1 | -0.469389 | -1.483330 | -1.078029 |
| 46 | 2.708329 | -0.231527 | -0.224875 |
| 8 | 4.738671 | -0.128085 | 0.184830 |
| 8 | 4.116289 | 1.195435 | 1.887752 |
| 8 | 3.055405 | -2.322074 | -0.582686 |
| 6 | 4.963850 | 0.507023 | 1.268324 |
| 6 | 6.354361 | 0.386049 | 1.829238 |
| 6 | 2.571089 | -3.350012 | -0.102907 |
| 8 | 1.427843 | -3.426800 | 0.522632 |
| 1 | 0.890446 | -2.597362 | 0.423563 |
| 6 | 3.280952 | -4.658006 | -0.206415 |
| 1 | 3.368299 | -5.104500 | 0.788574 |
| 1 | 2.683457 | -5.344068 | -0.814875 |
| 1 | 4.265820 | -4.520509 | -0.652127 |
| 1 | 7.083214 | 0.240097 | 1.029647 |
| 1 | 6.599070 | 1.263826 | 2.430170 |
| 1 | 6.386363 | -0.494065 | 2.480335 |
| 30 | -2.609076 | -0.231836 | -0.307394 |
| 17 | -2.111623 | -1.135709 | -2.367928 |
| 17 | -3.376607 | -1.479081 | 1.423829 |
| 8 | -4.221003 | 1.045519 | -0.520046 |
| 6 | -5.302906 | 0.523681 | -0.164943 |
| 7 | -5.866095 | 0.846771 | 1.010018 |
| 6 | -5.109115 | 1.664362 | 1.946822 |
| 1 | -5.802540 | 2.271793 | 2.536867 |
| 1 | -4.521201 | 1.017204 | 2.612508 |
| 1 | -4.427496 | 2.309777 | 1.392771 |
| 6 | -6.936918 | 0.063929 | 1.599496 |
| 1 | -6.520295 | -0.785578 | 2.159763 |
| 1 | -7.506905 | 0.697415 | 2.286092 |
| 1 | -7.622909 | -0.312255 | 0.839142 |
| 6 | -5.972332 | -0.486684 | -1.049205 |
| 1 | -7.017778 | -0.237866 | -1.258214 |
| 1 | -5.414225 | -0.536356 | -1.986536 |
| 1 | -5.937931 | -1.472821 | -0.569332 |

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**$(3a'\text{-}4a')_{8s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2679.7337125
Zero-point correction= 0.513112
Thermal correction to Energy= 0.556975
Thermal correction to Enthalpy= 0.557920
Thermal correction to Gibbs Free Energy= 0.428735
Sum of electronic and zero-point Energies= -2679.220600
Sum of electronic and thermal Energies= -2679.176737
Sum of electronic and thermal Enthalpies= -2679.175793
Sum of electronic and thermal Free Energies= -2679.304977

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.264613 | -2.657973 | -1.394220 |
| 6 | -0.599494 | -3.430027 | -2.167933 |
| 6 | -1.909244 | -3.016512 | -2.415287 |
| 6 | -2.374464 | -1.831387 | -1.864978 |
| 6 | -1.541099 | -1.066761 | -1.030778 |
| 6 | -0.199871 | -1.473694 | -0.848357 |
| 1 | 1.299292 | -2.946926 | -1.227946 |
| 1 | -0.243353 | -4.363943 | -2.596597 |
| 1 | -2.565259 | -3.630413 | -3.027144 |
| 1 | -3.410466 | -1.523170 | -1.999947 |
| 6 | 0.710926 | -0.544912 | -0.143681 |
| 8 | 1.871843 | -0.871522 | 0.185585 |
| 7 | 0.117842 | 0.641447 | 0.029852 |
| 8 | 0.847810 | 1.629053 | 0.657508 |
| 1 | 1.489225 | 1.992257 | -0.012167 |
| 46 | -1.687495 | 0.996431 | -0.767631 |
| 8 | -1.832078 | 3.154143 | -0.518176 |
| 1 | -2.227799 | -0.871796 | 0.019419 |
| 6 | -1.575333 | 3.905589 | 0.425119 |
| 8 | -0.767286 | 3.628009 | 1.412523 |
| 1 | -0.246590 | 2.799074 | 1.243249 |
| 8 | -3.308510 | -0.906217 | 0.956812 |
| 6 | -3.608221 | -2.175376 | 1.270386 |
| 8 | -2.763342 | -3.039381 | 1.196437 |
| 8 | -3.577160 | 1.208969 | -1.643155 |
| 6 | -4.654329 | 1.222467 | -0.993815 |
| 8 | -4.827217 | 0.773096 | 0.183276 |
| 1 | -4.069748 | -0.067814 | 0.618257 |
| 30 | 3.463368 | 0.330709 | 0.554855 |
| 17 | 4.076075 | 0.847412 | 2.644203 |
| 17 | 3.266698 | 1.958048 | -1.100126 |

| | | | |
|---|---|---|---|
| 6 | -5.062765 | -2.450575 | 1.645766 |
| 6 | -2.184724 | 5.264157 | 0.524426 |
| 1 | -2.621631 | 5.397542 | 1.518347 |
| 1 | -1.399229 | 6.018499 | 0.414329 |
| 1 | -2.940331 | 5.399264 | -0.249338 |
| 6 | -5.866770 | 1.798457 | -1.664605 |
| 1 | -6.355712 | 2.501779 | -0.984594 |
| 1 | -5.604901 | 2.291222 | -2.601510 |
| 1 | -6.582552 | 0.991782 | -1.857755 |
| 6 | -5.605890 | -1.402765 | 2.617586 |
| 1 | -6.629700 | -1.673487 | 2.905492 |
| 1 | -5.002288 | -1.361901 | 3.532238 |
| 1 | -5.640900 | -0.399633 | 2.181721 |
| 6 | -5.152451 | -3.835845 | 2.275572 |
| 1 | -4.567127 | -3.886428 | 3.200574 |
| 1 | -6.197707 | -4.068418 | 2.514878 |
| 1 | -4.765506 | -4.603724 | 1.598951 |
| 6 | -5.865142 | -2.431396 | 0.337190 |
| 1 | -5.842779 | -1.442870 | -0.137564 |
| 1 | -5.471712 | -3.174280 | -0.369643 |
| 1 | -6.913775 | -2.681720 | 0.542028 |
| 8 | 4.902616 | -0.974789 | -0.124275 |
| 6 | 6.123425 | -0.713562 | -0.152705 |
| 6 | 6.595867 | 0.694542 | 0.026666 |
| 1 | 5.950324 | 1.345066 | -0.575539 |
| 1 | 6.431876 | 0.977725 | 1.075704 |
| 1 | 7.636882 | 0.872042 | -0.243849 |
| 7 | 7.020891 | -1.700691 | -0.338981 |
| 6 | 8.458928 | -1.479688 | -0.336036 |
| 1 | 8.953819 | -2.450903 | -0.257221 |
| 1 | 8.804615 | -0.995829 | -1.258022 |
| 1 | 8.772518 | -0.879953 | 0.523251 |
| 6 | 6.570364 | -3.068084 | -0.541082 |
| 1 | 6.912598 | -3.706730 | 0.281888 |
| 1 | 5.481894 | -3.083363 | -0.575860 |
| 1 | 6.972128 | -3.458964 | -1.483343 |

---

**3a'$_s$**

---

Number of imaginary frequencies : 0
Electronic energy =-2679.7715051
Zero-point correction= 0.521519
Thermal correction to Energy= 0.565915
Thermal correction to Enthalpy= 0.566859
Thermal correction to Gibbs Free Energy= 0.439095

Sum of electronic and zero-point Energies= -2679.249986
Sum of electronic and thermal Energies= -2679.205590
Sum of electronic and thermal Enthalpies= -2679.204646
Sum of electronic and thermal Free Energies= -2679.332410

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.068369 | -2.912336 | -2.000566 |
| 6 | 0.365615 | -1.626648 | -1.676266 |
| 6 | 1.725383 | -1.249995 | -1.873259 |
| 6 | 2.631341 | -2.220467 | -2.355739 |
| 6 | 2.197666 | -3.498104 | -2.647052 |
| 6 | 0.845414 | -3.834428 | -2.484419 |
| 1 | -1.110927 | -3.171209 | -1.836534 |
| 1 | 2.016078 | -0.190208 | -1.986406 |
| 1 | 3.664887 | -1.921402 | -2.510070 |
| 1 | 2.895618 | -4.240535 | -3.024929 |
| 1 | 0.512386 | -4.841221 | -2.725865 |
| 6 | -0.560213 | -0.713116 | -0.972431 |
| 8 | -1.794948 | -0.775249 | -1.075834 |
| 7 | 0.134462 | 0.121690 | -0.160290 |
| 8 | -0.645553 | 0.640007 | 0.836343 |
| 46 | 1.906424 | -0.723466 | 0.301853 |
| 8 | 1.765842 | -0.031737 | 2.328699 |
| 6 | 2.277740 | -0.534335 | 3.336262 |
| 8 | 3.170785 | -1.485757 | 3.321732 |
| 1 | 3.434631 | -1.708373 | 2.382175 |
| 8 | 2.546190 | 1.748542 | -2.197051 |
| 6 | 2.898986 | 2.376710 | -1.215500 |
| 8 | 3.758196 | 1.893805 | -0.320459 |
| 1 | 4.078272 | 1.006392 | -0.620412 |
| 8 | 3.685001 | -1.715780 | 0.771505 |
| 6 | 4.772690 | -1.398805 | 0.132577 |
| 8 | 4.826136 | -0.567575 | -0.773162 |
| 6 | 2.338484 | 3.738335 | -0.842157 |
| 1 | -0.574232 | 1.616606 | 0.769952 |
| 30 | -2.981228 | 0.508843 | 0.083226 |
| 17 | -3.787056 | -0.516589 | 1.953228 |
| 17 | -2.547983 | 2.742475 | -0.146323 |
| 8 | -4.639776 | 0.188185 | -1.157290 |
| 6 | -5.715793 | 0.089733 | -0.531064 |
| 7 | -6.283433 | -1.112630 | -0.322693 |
| 6 | -6.384148 | 1.318619 | 0.011850 |
| 1 | -5.825501 | 2.187732 | -0.341680 |
| 1 | -7.430410 | 1.402153 | -0.299729 |

| | | | |
|---|---|---|---|
| 1 | -6.346793 | 1.301030 | 1.108093 |
| 6 | -7.354212 | -1.311938 | 0.635077 |
| 1 | -7.921487 | -2.205949 | 0.356717 |
| 1 | -6.940227 | -1.451964 | 1.644282 |
| 1 | -8.043120 | -0.465944 | 0.646732 |
| 6 | -5.533171 | -2.310772 | -0.663522 |
| 1 | -5.021070 | -2.692577 | 0.230515 |
| 1 | -6.219786 | -3.071711 | -1.050141 |
| 1 | -4.785622 | -2.064069 | -1.418160 |
| 6 | 1.883600 | -0.081193 | 4.699761 |
| 1 | 1.380086 | -0.906799 | 5.213302 |
| 1 | 2.775309 | 0.169444 | 5.281051 |
| 1 | 1.209358 | 0.772326 | 4.634367 |
| 6 | 5.991182 | -2.160506 | 0.583421 |
| 1 | 6.861325 | -1.868399 | -0.006188 |
| 1 | 6.181224 | -1.957891 | 1.643242 |
| 1 | 5.815968 | -3.236688 | 0.489562 |
| 6 | 3.330828 | 4.571595 | -0.037188 |
| 1 | 4.257774 | 4.742470 | -0.597701 |
| 1 | 2.886078 | 5.549375 | 0.186281 |
| 1 | 3.592965 | 4.088929 | 0.909337 |
| 6 | 1.925421 | 4.477977 | -2.109905 |
| 1 | 1.425162 | 5.416883 | -1.843969 |
| 1 | 2.797963 | 4.719241 | -2.729181 |
| 1 | 1.239824 | 3.874418 | -2.711503 |
| 6 | 1.092770 | 3.441875 | 0.005361 |
| 1 | 0.355108 | 2.884026 | -0.587621 |
| 1 | 1.359210 | 2.868037 | 0.905429 |
| 1 | 0.617455 | 4.377782 | 0.323251 |

---

**$(3a'\text{-}4a')_{10s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2679.7555977
Zero-point correction= 0.515945
Thermal correction to Energy= 0.559601
Thermal correction to Enthalpy= 0.560546
Thermal correction to Gibbs Free Energy= 0.435376
Sum of electronic and zero-point Energies= -2679.239652
Sum of electronic and thermal Energies= -2679.195996
Sum of electronic and thermal Enthalpies= -2679.195052
Sum of electronic and thermal Free Energies= -2679.320222

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.100044 | -1.149581 | 3.364230 |
| 6 | -0.371514 | -0.707082 | 2.136973 |
| 6 | -1.759495 | -0.602894 | 1.871930 |
| 6 | -2.661504 | -1.015237 | 2.868532 |
| 6 | -2.190214 | -1.451615 | 4.099656 |
| 6 | -0.816939 | -1.518529 | 4.343410 |
| 1 | 1.173192 | -1.219422 | 3.524049 |
| 1 | -2.086822 | 0.616746 | 1.493454 |
| 1 | -3.729647 | -0.914645 | 2.690012 |
| 1 | -2.891904 | -1.733473 | 4.880994 |
| 1 | -0.459632 | -1.868485 | 5.309307 |
| 6 | 0.558817 | -0.401413 | 1.033414 |
| 8 | 1.798968 | -0.399937 | 1.173192 |
| 7 | -0.105134 | -0.144932 | -0.110774 |
| 8 | 0.692898 | -0.181714 | -1.229643 |
| 46 | -1.996977 | -0.818713 | -0.200340 |
| 8 | -1.890971 | -1.094514 | -2.353381 |
| 6 | -2.462777 | -1.941995 | -3.042705 |
| 8 | -3.442127 | -2.703397 | -2.623252 |
| 1 | -3.698471 | -2.454210 | -1.692364 |
| 8 | -2.109974 | 1.952498 | 1.407409 |
| 6 | -2.689674 | 2.517063 | 0.459864 |
| 8 | -3.735244 | 2.028657 | -0.133374 |
| 1 | -4.098068 | 1.186692 | 0.296171 |
| 8 | -3.908841 | -1.687363 | -0.241148 |
| 6 | -4.953738 | -1.143277 | 0.280782 |
| 8 | -4.971191 | -0.028527 | 0.821050 |
| 6 | -2.138589 | 3.791654 | -0.131921 |
| 1 | 0.691957 | 0.726541 | -1.602734 |
| 30 | 2.996058 | 0.215022 | -0.390000 |
| 17 | 4.034858 | -1.406135 | -1.605352 |
| 17 | 2.419429 | 2.284021 | -1.226163 |
| 8 | 4.575406 | 0.637303 | 0.927969 |
| 6 | 5.701306 | 0.370464 | 0.459556 |
| 7 | 6.349132 | -0.752547 | 0.822222 |
| 6 | 6.344725 | 1.301792 | -0.525997 |
| 1 | 5.711088 | 2.186893 | -0.611323 |
| 1 | 7.355320 | 1.599404 | -0.227313 |
| 1 | 6.400718 | 0.815683 | -1.507839 |
| 6 | 7.501431 | -1.252324 | 0.097901 |
| 1 | 8.104248 | -1.874745 | 0.767213 |
| 1 | 7.178409 | -1.860645 | -0.759459 |
| 1 | 8.128927 | -0.435504 | -0.262190 |
| 6 | 5.631589 | -1.749334 | 1.601805 |
| 1 | 5.180436 | -2.491272 | 0.928069 |

| | | | |
|---|---|---|---|
| 1 | 6.328134 | -2.243718 | 2.287208 |
| 1 | 4.835913 | -1.259798 | 2.164388 |
| 6 | -2.063809 | -2.192539 | -4.456955 |
| 1 | -1.613791 | -3.188532 | -4.524843 |
| 1 | -2.946210 | -2.189337 | -5.102568 |
| 1 | -1.339639 | -1.445877 | -4.782149 |
| 6 | -6.200556 | -1.983798 | 0.216663 |
| 1 | -7.038918 | -1.462928 | 0.681062 |
| 1 | -6.439767 | -2.210165 | -0.827998 |
| 1 | -6.027649 | -2.940691 | 0.719161 |
| 6 | -3.227274 | 4.610357 | -0.817591 |
| 1 | -4.006466 | 4.916297 | -0.109284 |
| 1 | -2.779897 | 5.517468 | -1.240614 |
| 1 | -3.705901 | 4.053253 | -1.628690 |
| 6 | -1.441461 | 4.615819 | 0.946240 |
| 1 | -0.976671 | 5.493941 | 0.483420 |
| 1 | -2.152646 | 4.966832 | 1.703791 |
| 1 | -0.659339 | 4.038617 | 1.447442 |
| 6 | -1.102499 | 3.310461 | -1.163235 |
| 1 | -0.280619 | 2.771964 | -0.675870 |
| 1 | -1.562311 | 2.662782 | -1.922426 |
| 1 | -0.664269 | 4.176779 | -1.672722 |

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**4a'$_s$**

---

Number of imaginary frequencies : 0
Electronic energy =-2679.7897263
Zero-point correction= 0.522871
Thermal correction to Energy= 0.567159
Thermal correction to Enthalpy= 0.568103
Thermal correction to Gibbs Free Energy= 0.441217
Sum of electronic and zero-point Energies= -2679.266856
Sum of electronic and thermal Energies= -2679.222567
Sum of electronic and thermal Enthalpies= -2679.221623
Sum of electronic and thermal Free Energies= -2679.348509

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.007557 | -2.838900 | -1.998604 |
| 6 | -0.380021 | -1.607211 | -1.487035 |
| 6 | -1.719740 | -1.196936 | -1.508737 |
| 6 | -2.679167 | -2.043734 | -2.055004 |
| 6 | -2.290797 | -3.293674 | -2.557159 |
| 6 | -0.956864 | -3.689714 | -2.531820 |
| 1 | 1.059946 | -3.112995 | -1.962777 |

| | | | |
|---|---|---|---|
| 1 | -2.330770 | -2.861426 | 0.244706 |
| 1 | -3.729745 | -1.760973 | -2.091702 |
| 1 | -3.045527 | -3.959520 | -2.971704 |
| 1 | -0.670590 | -4.661129 | -2.926744 |
| 6 | 0.574919 | -0.667858 | -0.871504 |
| 8 | 1.815968 | -0.829624 | -0.878223 |
| 7 | -0.082368 | 0.353776 | -0.305000 |
| 8 | 0.698364 | 1.433335 | 0.056452 |
| 46 | -2.051278 | 0.557548 | -0.617936 |
| 8 | -2.164124 | 2.528638 | 0.469238 |
| 6 | -2.612414 | 3.569709 | 0.005888 |
| 8 | -3.471684 | 3.613787 | -0.999704 |
| 1 | -3.714340 | 2.699793 | -1.258836 |
| 8 | -1.848333 | -2.791820 | 1.090353 |
| 6 | -2.389798 | -1.825690 | 1.814746 |
| 8 | -3.435737 | -1.269605 | 1.496511 |
| 1 | -4.473690 | -1.023331 | 0.286027 |
| 8 | -4.142729 | 0.880803 | -1.171057 |
| 6 | -5.192396 | 0.247958 | -0.992609 |
| 8 | -5.291704 | -0.820129 | -0.262491 |
| 6 | -1.634874 | -1.471085 | 3.076664 |
| 1 | 0.729384 | 1.435316 | 1.039770 |
| 30 | 2.978421 | 0.416062 | 0.269021 |
| 17 | 4.124312 | 2.080070 | -0.784129 |
| 17 | 2.262529 | 0.530548 | 2.464529 |
| 8 | 4.530361 | -0.998095 | 0.332020 |
| 6 | 5.673586 | -0.535029 | 0.144404 |
| 7 | 6.238806 | -0.567825 | -1.077364 |
| 6 | 6.429152 | 0.077691 | 1.286668 |
| 1 | 5.853891 | -0.099744 | 2.197512 |
| 1 | 7.437795 | -0.332698 | 1.400863 |
| 1 | 6.507045 | 1.160435 | 1.128283 |
| 6 | 7.415713 | 0.210070 | -1.412866 |
| 1 | 7.928214 | -0.263330 | -2.256655 |
| 1 | 7.129142 | 1.232849 | -1.698451 |
| 1 | 8.115147 | 0.257159 | -0.576589 |
| 6 | 5.418156 | -0.961330 | -2.212705 |
| 1 | 4.981008 | -0.067944 | -2.680921 |
| 1 | 6.039213 | -1.494663 | -2.940178 |
| 1 | 4.607778 | -1.604205 | -1.867393 |
| 6 | -2.218892 | 4.915668 | 0.508389 |
| 1 | -1.483567 | 5.340003 | -0.184158 |
| 1 | -3.078543 | 5.589237 | 0.535468 |
| 1 | -1.757497 | 4.822954 | 1.491803 |
| 6 | -6.470676 | 0.657965 | -1.642292 |

| | | | |
|---|---|---|---|
| 1 | -7.232151 | 0.831440 | -0.876180 |
| 1 | -6.329047 | 1.553833 | -2.246873 |
| 1 | -6.831737 | -0.162058 | -2.271008 |
| 6 | -2.498056 | -1.940862 | 4.254723 |
| 1 | -2.608586 | -3.032520 | 4.259132 |
| 1 | -2.014535 | -1.647469 | 5.193928 |
| 1 | -3.495064 | -1.487752 | 4.219663 |
| 6 | -0.260664 | -2.127780 | 3.131261 |
| 1 | 0.249193 | -1.822347 | 4.052074 |
| 1 | -0.334739 | -3.220593 | 3.118562 |
| 1 | 0.373458 | -1.809638 | 2.296032 |
| 6 | -1.499202 | 0.054315 | 3.111436 |
| 1 | -0.952719 | 0.418906 | 2.232140 |
| 1 | -2.479915 | 0.541764 | 3.130475 |
| 1 | -0.929829 | 0.349646 | 4.000055 |

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**$(5a'\text{-}6a')_{4s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2579.736287
Zero-point correction= 0.437598
Thermal correction to Energy= 0.476021
Thermal correction to Enthalpy= 0.476965
Thermal correction to Gibbs Free Energy= 0.363173
Sum of electronic and zero-point Energies= -2579.298689
Sum of electronic and thermal Energies= -2579.260266
Sum of electronic and thermal Enthalpies= -2579.259322
Sum of electronic and thermal Free Energies= -2579.373114

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.931103 | 4.065836 | 0.255578 |
| 6 | -1.167847 | 2.711205 | -0.008995 |
| 6 | -2.417384 | 2.280796 | -0.493417 |
| 6 | -3.422388 | 3.207403 | -0.733775 |
| 6 | -3.178541 | 4.552474 | -0.458073 |
| 6 | -1.944846 | 4.982953 | 0.038196 |
| 1 | 0.052974 | 4.368900 | 0.607316 |
| 1 | -4.389252 | 2.888106 | -1.114575 |
| 1 | -3.968350 | 5.281527 | -0.629837 |
| 1 | -1.780385 | 6.037734 | 0.241194 |
| 6 | -0.097509 | 1.729431 | 0.056201 |
| 8 | 1.101457 | 1.962723 | 0.165273 |
| 7 | -0.566105 | 0.395100 | -0.169769 |
| 8 | 0.397611 | -0.252548 | -0.965778 |

| | | | |
|---|---|---|---|
| 1 | 0.322516 | -1.207933 | -0.759191 |
| 46 | -2.583614 | 0.307921 | -0.521990 |
| 7 | -1.896915 | -1.467771 | 0.898412 |
| 6 | -1.409853 | -2.743440 | 1.041197 |
| 8 | -1.583741 | -3.392664 | 2.072353 |
| 8 | -2.634018 | -1.125964 | 2.068171 |
| 1 | -2.455048 | -1.907106 | 2.651709 |
| 6 | -0.591685 | -3.209929 | -0.106675 |
| 6 | -1.001551 | -3.023824 | -1.431791 |
| 6 | 0.643189 | -3.808769 | 0.163319 |
| 6 | -0.166572 | -3.406174 | -2.478183 |
| 1 | -1.974183 | -2.577610 | -1.636055 |
| 6 | 1.478238 | -4.170960 | -0.884385 |
| 1 | 0.943498 | -3.937643 | 1.199710 |
| 6 | 1.077458 | -3.964629 | -2.203067 |
| 1 | -0.483783 | -3.256198 | -3.506981 |
| 1 | 2.456237 | -4.596023 | -0.675066 |
| 1 | 1.743311 | -4.233252 | -3.019120 |
| 1 | -0.881501 | -0.386902 | 0.668830 |
| 8 | -4.702981 | 0.270671 | -0.624683 |
| 6 | -5.460231 | -0.276804 | 0.190384 |
| 6 | -6.936857 | -0.269539 | -0.034520 |
| 1 | -7.427573 | 0.240535 | 0.800159 |
| 1 | -7.178975 | 0.227022 | -0.974013 |
| 1 | -7.307672 | -1.298766 | -0.042699 |
| 8 | -5.108973 | -0.890713 | 1.276750 |
| 1 | -4.124529 | -0.925521 | 1.513481 |
| 30 | 2.407077 | 0.251795 | 0.285801 |
| 17 | 3.604449 | -0.698760 | -1.411299 |
| 17 | 1.546600 | -0.944054 | 2.015499 |
| 8 | 3.916764 | 1.505374 | 0.976833 |
| 6 | 5.055829 | 0.996867 | 0.876085 |
| 6 | 5.455270 | -0.140062 | 1.769500 |
| 1 | 5.505182 | -1.064855 | 1.180646 |
| 1 | 6.426334 | 0.019166 | 2.248899 |
| 1 | 4.684248 | -0.259893 | 2.533931 |
| 7 | 5.926560 | 1.455566 | -0.038433 |
| 6 | 7.112118 | 0.714392 | -0.427417 |
| 1 | 7.869056 | 1.413024 | -0.797620 |
| 1 | 7.537465 | 0.169385 | 0.416468 |
| 1 | 6.865458 | -0.000713 | -1.225444 |
| 6 | 5.453449 | 2.425653 | -1.015741 |
| 1 | 6.304571 | 3.012144 | -1.374711 |
| 1 | 4.976767 | 1.906362 | -1.859001 |
| 1 | 4.720895 | 3.085545 | -0.551257 |

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**(5a-6a')$_{6S}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2579.7709401
Zero-point correction= 0.439012
Thermal correction to Energy= 0.477141
Thermal correction to Enthalpy= 0.478085
Thermal correction to Gibbs Free Energy= 0.365238
Sum of electronic and zero-point Energies= -2579.331928
Sum of electronic and thermal Energies= -2579.293799
Sum of electronic and thermal Enthalpies= -2579.292855
Sum of electronic and thermal Free Energies= -2579.405703

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.738903 | 3.888789 | -1.554281 |
| 6 | 0.106429 | 2.825407 | -0.896708 |
| 6 | -1.204246 | 2.945117 | -0.402058 |
| 6 | -1.879953 | 4.151162 | -0.553899 |
| 6 | -1.253448 | 5.198865 | -1.224630 |
| 6 | 0.046404 | 5.073335 | -1.727723 |
| 1 | 1.762818 | 3.764074 | -1.900395 |
| 1 | -2.889837 | 4.262465 | -0.166415 |
| 1 | -1.787892 | 6.137287 | -1.361921 |
| 1 | 0.512441 | 5.909783 | -2.241537 |
| 6 | 0.812097 | 1.604525 | -0.565669 |
| 8 | 2.027373 | 1.440355 | -0.570974 |
| 7 | -0.077343 | 0.577509 | -0.098657 |
| 8 | 0.585614 | -0.200502 | 0.863330 |
| 46 | -1.959822 | 1.281113 | 0.347404 |
| 8 | -3.861215 | 2.156068 | 0.737070 |
| 6 | -4.854542 | 1.568558 | 1.191285 |
| 6 | -6.098208 | 2.325935 | 1.519669 |
| 1 | -5.996620 | 3.373345 | 1.236156 |
| 1 | -6.950758 | 1.871058 | 1.007135 |
| 1 | -6.290611 | 2.247421 | 2.594352 |
| 8 | -4.931917 | 0.295797 | 1.433039 |
| 1 | -4.089466 | -0.217130 | 1.175345 |
| 1 | 0.246873 | -1.106117 | 0.683026 |
| 8 | -2.738540 | -0.743987 | 0.676314 |
| 6 | -2.388186 | -1.686894 | -0.148940 |
| 7 | -1.248243 | -1.577657 | -0.787313 |
| 6 | -3.319093 | -2.834564 | -0.295188 |
| 6 | -4.691996 | -2.580811 | -0.345690 |

| | | | |
|---|---|---|---|
| 6 | -2.864781 | -4.155829 | -0.319193 |
| 6 | -5.598571 | -3.629409 | -0.434384 |
| 1 | -5.050110 | -1.554012 | -0.327787 |
| 6 | -3.775073 | -5.202397 | -0.383574 |
| 1 | -1.798505 | -4.354873 | -0.289969 |
| 6 | -5.141210 | -4.942795 | -0.447604 |
| 1 | -6.664370 | -3.420168 | -0.487076 |
| 1 | -3.414731 | -6.228285 | -0.389092 |
| 1 | -5.849845 | -5.765697 | -0.508220 |
| 1 | -0.493370 | -0.226920 | -0.780946 |
| 8 | -0.997490 | -2.569649 | -1.726909 |
| 1 | -0.026804 | -2.525598 | -1.821774 |
| 30 | 2.901260 | -0.385866 | 0.050160 |
| 17 | 3.629960 | -0.717392 | 2.169354 |
| 17 | 2.106090 | -1.982603 | -1.394453 |
| 8 | 4.722707 | 0.225218 | -0.755010 |
| 6 | 5.760219 | 0.092251 | -0.070376 |
| 6 | 6.381704 | 1.303648 | 0.557666 |
| 1 | 6.130237 | 1.311150 | 1.626056 |
| 1 | 7.469687 | 1.342025 | 0.452449 |
| 1 | 5.936745 | 2.184959 | 0.093807 |
| 7 | 6.326428 | -1.111529 | 0.119666 |
| 6 | 5.660048 | -2.297386 | -0.399429 |
| 1 | 6.416146 | -3.051996 | -0.637722 |
| 1 | 4.967499 | -2.702960 | 0.352405 |
| 1 | 5.094511 | -2.047852 | -1.298714 |
| 6 | 7.282888 | -1.372413 | 1.179841 |
| 1 | 6.751583 | -1.691270 | 2.087946 |
| 1 | 7.962034 | -2.171456 | 0.865431 |
| 1 | 7.878992 | -0.489786 | 1.413299 |

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**5a'$_s$**

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Number of imaginary frequencies : 0
Electronic energy = -2926.6521585
Zero-point correction= 0.593584
Thermal correction to Energy= 0.641607
Thermal correction to Enthalpy= 0.642551
Thermal correction to Gibbs Free Energy= 0.507950
Sum of electronic and zero-point Energies= -2926.058574
Sum of electronic and thermal Energies= -2926.010552
Sum of electronic and thermal Enthalpies= -2926.009608
Sum of electronic and thermal Free Energies= -2926.144208

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.774545 | -2.490665 | -3.371295 |
| 6 | -0.972995 | -1.478476 | -2.438890 |
| 6 | -2.261909 | -1.005912 | -2.160094 |
| 6 | -3.360153 | -1.540251 | -2.812347 |
| 6 | -3.153335 | -2.552705 | -3.755008 |
| 6 | -1.873936 | -3.026324 | -4.033813 |
| 1 | 0.238829 | -2.839667 | -3.559868 |
| 1 | -4.363540 | -1.184139 | -2.591441 |
| 1 | -4.010272 | -2.978109 | -4.274313 |
| 1 | -1.735602 | -3.816027 | -4.768046 |
| 6 | 0.130612 | -0.843867 | -1.701695 |
| 8 | 1.340712 | -1.151664 | -1.800133 |
| 7 | -0.356913 | 0.120420 | -0.900676 |
| 8 | 0.602130 | 0.819831 | -0.174206 |
| 46 | -2.355862 | 0.356916 | -0.713201 |
| 8 | -4.498245 | 0.538290 | -0.797643 |
| 6 | -5.167988 | 1.506488 | -0.424120 |
| 8 | -4.712938 | 2.513596 | 0.270861 |
| 1 | -3.774488 | 2.363133 | 0.582501 |
| 1 | 0.897334 | 1.580872 | -0.713293 |
| 8 | -2.361119 | 1.746541 | 1.071500 |
| 6 | -1.239101 | 2.062792 | 1.583394 |
| 7 | -0.705970 | 1.187570 | 2.421957 |
| 6 | -0.592056 | 3.340303 | 1.220835 |
| 6 | -1.008451 | 3.930145 | 0.019422 |
| 6 | 0.390639 | 3.972122 | 1.991352 |
| 6 | -0.433360 | 5.112584 | -0.420504 |
| 1 | -1.780342 | 3.439483 | -0.571296 |
| 6 | 0.951288 | 5.164747 | 1.551449 |
| 1 | 0.714430 | 3.527061 | 2.924466 |
| 6 | 0.551023 | 5.730865 | 0.346206 |
| 1 | -0.751603 | 5.551940 | -1.362506 |
| 1 | 1.714738 | 5.650296 | 2.153720 |
| 1 | 1.006080 | 6.656658 | 0.002049 |
| 1 | -0.917487 | -1.467799 | 0.594095 |
| 8 | 0.536505 | 1.323011 | 2.968840 |
| 1 | 1.091486 | 0.627920 | 2.535767 |
| 1 | -1.180844 | 0.285398 | 2.587156 |
| 8 | -1.616601 | -1.458061 | 2.801833 |
| 6 | -1.355431 | -2.452241 | 2.146257 |
| 8 | -0.995159 | -2.403180 | 0.868004 |
| 6 | -1.344984 | -3.859693 | 2.709607 |
| 6 | -6.620105 | 1.615352 | -0.750072 |
| 1 | -6.931269 | 0.787226 | -1.386541 |

| | | | |
|---|---|---|---|
| 1 | -7.199865 | 1.613520 | 0.178146 |
| 1 | -6.812167 | 2.571380 | -1.246324 |
| 6 | -1.859130 | -4.870249 | 1.685967 |
| 1 | -2.891023 | -4.648601 | 1.386867 |
| 1 | -1.238398 | -4.883510 | 0.785271 |
| 1 | -1.844920 | -5.873487 | 2.129811 |
| 6 | -2.191035 | -3.905062 | 3.976011 |
| 1 | -2.135625 | -4.906601 | 4.419585 |
| 1 | -1.838513 | -3.176430 | 4.712387 |
| 1 | -3.243472 | -3.683544 | 3.761520 |
| 6 | 0.122295 | -4.162145 | 3.049210 |
| 1 | 0.503928 | -3.462180 | 3.801947 |
| 1 | 0.197512 | -5.179564 | 3.453514 |
| 1 | 0.763281 | -4.084375 | 2.163769 |
| 30 | 2.584151 | -0.412810 | -0.321872 |
| 17 | 3.436855 | 1.704973 | -0.793992 |
| 17 | 2.089034 | -1.163244 | 1.802362 |
| 8 | 4.270103 | -1.474706 | -0.902920 |
| 6 | 5.307503 | -0.846955 | -1.206255 |
| 6 | 5.663388 | -0.665403 | -2.651670 |
| 1 | 6.707489 | -0.907034 | -2.872869 |
| 1 | 5.006204 | -1.306193 | -3.240959 |
| 1 | 5.476985 | 0.378387 | -2.934315 |
| 7 | 6.112347 | -0.328738 | -0.262778 |
| 6 | 7.121685 | 0.672533 | -0.552763 |
| 1 | 6.685974 | 1.678721 | -0.471472 |
| 1 | 7.938613 | 0.579665 | 0.170162 |
| 1 | 7.536868 | 0.547591 | -1.553557 |
| 6 | 5.703701 | -0.397190 | 1.132811 |
| 1 | 6.597451 | -0.453937 | 1.762153 |
| 1 | 5.124955 | 0.497816 | 1.403166 |
| 1 | 5.081222 | -1.277899 | 1.297270 |

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**$(5a'\text{-}6a')_{10s}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2926.6137532
Zero-point correction= 0.584481
Thermal correction to Energy= 0.631627
Thermal correction to Enthalpy= 0.632572
Thermal correction to Gibbs Free Energy= 0.500405
Sum of electronic and zero-point Energies= -2926.029272
Sum of electronic and thermal Energies= -2925.982126
Sum of electronic and thermal Enthalpies= -2925.981182
Sum of electronic and thermal Free Energies= -2926.113349

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.200260 | -3.070290 | -3.047350 |
| 6 | -0.587671 | -2.019394 | -2.205655 |
| 6 | -1.924590 | -1.587669 | -2.136413 |
| 6 | -2.877974 | -2.209492 | -2.935319 |
| 6 | -2.489680 | -3.262869 | -3.760186 |
| 6 | -1.160472 | -3.696094 | -3.820385 |
| 1 | 0.846752 | -3.364313 | -3.077558 |
| 1 | -3.915185 | -1.886048 | -2.901205 |
| 1 | -3.240154 | -3.762808 | -4.370048 |
| 1 | -0.887003 | -4.518669 | -4.475635 |
| 6 | 0.369945 | -1.276274 | -1.420319 |
| 8 | 1.593793 | -1.301782 | -1.492021 |
| 7 | -0.289321 | -0.415844 | -0.466230 |
| 8 | 0.527169 | 0.676078 | -0.138726 |
| 46 | -2.310841 | -0.163065 | -0.812920 |
| 8 | -4.359711 | -0.025977 | -1.379679 |
| 6 | -5.151715 | 0.875644 | -1.054265 |
| 8 | -4.904073 | 1.828866 | -0.216605 |
| 1 | -3.991086 | 1.719345 | 0.249206 |
| 1 | 0.498758 | 1.304127 | -0.884754 |
| 8 | -2.708870 | 1.232346 | 0.814043 |
| 6 | -1.716138 | 1.842604 | 1.404198 |
| 7 | -0.985166 | 1.135330 | 2.214678 |
| 6 | -1.482861 | 3.264178 | 1.060716 |
| 6 | -1.826799 | 3.685518 | -0.229847 |
| 6 | -0.967201 | 4.196082 | 1.967184 |
| 6 | -1.633482 | 5.004276 | -0.617705 |
| 1 | -2.244753 | 2.965031 | -0.932487 |
| 6 | -0.798258 | 5.520180 | 1.582159 |
| 1 | -0.700761 | 3.875999 | 2.968436 |
| 6 | -1.121044 | 5.925349 | 0.290814 |
| 1 | -1.887522 | 5.314921 | -1.628405 |
| 1 | -0.404180 | 6.239897 | 2.295714 |
| 1 | -0.973876 | 6.960738 | -0.008116 |
| 1 | -0.386318 | -1.050893 | 0.480544 |
| 8 | 0.115790 | 1.762670 | 2.773788 |
| 1 | 0.832582 | 1.101058 | 2.683969 |
| 1 | -1.187653 | -0.136780 | 2.677637 |
| 8 | -1.236887 | -1.132473 | 3.211813 |
| 6 | -0.859845 | -2.154601 | 2.543243 |
| 8 | -0.537264 | -2.138351 | 1.334328 |
| 6 | -0.738226 | -3.455575 | 3.321167 |

| | | | |
|---|---|---|---|
| 6 | -6.523363 | 0.918757 | -1.644428 |
| 1 | -6.646776 | 0.139072 | -2.396058 |
| 1 | -7.261434 | 0.789609 | -0.846727 |
| 1 | -6.697535 | 1.904581 | -2.085592 |
| 6 | -0.906674 | -4.652621 | 2.392161 |
| 1 | -1.904800 | -4.667598 | 1.937141 |
| 1 | -0.168021 | -4.635689 | 1.585443 |
| 1 | -0.780102 | -5.581519 | 2.962306 |
| 6 | -1.758935 | -3.515319 | 4.453517 |
| 1 | -1.627068 | -4.448158 | 5.016215 |
| 1 | -1.641993 | -2.673586 | 5.142155 |
| 1 | -2.785684 | -3.495257 | 4.067720 |
| 6 | 0.683853 | -3.445619 | 3.901067 |
| 1 | 0.826231 | -2.595757 | 4.578722 |
| 1 | 0.857558 | -4.372065 | 4.463317 |
| 1 | 1.433785 | -3.371725 | 3.104392 |
| 30 | 2.730679 | -0.056615 | -0.121240 |
| 17 | 3.120938 | 1.890232 | -1.291944 |
| 17 | 2.434197 | -0.464506 | 2.097855 |
| 8 | 4.486664 | -1.028807 | -0.626288 |
| 6 | 5.368869 | -0.372638 | -1.222451 |
| 6 | 5.563781 | -0.572323 | -2.695712 |
| 1 | 6.605936 | -0.765176 | -2.968900 |
| 1 | 4.943060 | -1.416281 | -3.000006 |
| 1 | 5.221955 | 0.323817 | -3.228361 |
| 7 | 6.142389 | 0.511005 | -0.570734 |
| 6 | 6.946554 | 1.504044 | -1.259110 |
| 1 | 6.347370 | 2.403760 | -1.459549 |
| 1 | 7.796551 | 1.778115 | -0.626498 |
| 1 | 7.337764 | 1.120841 | -2.202695 |
| 6 | 5.866121 | 0.806404 | 0.828298 |
| 1 | 6.809551 | 1.020219 | 1.340469 |
| 1 | 5.205623 | 1.682024 | 0.905315 |
| 1 | 5.377595 | -0.046281 | 1.303431 |

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**6a'$_s$**

---

Number of imaginary frequencies : 0
Electronic energy = -2579.7717999
Zero-point correction= 0.443765
Thermal correction to Energy= 0.482361
Thermal correction to Enthalpy= 0.483305
Thermal correction to Gibbs Free Energy= 0.369605
Sum of electronic and zero-point Energies= -2579.328035
Sum of electronic and thermal Energies= -2579.289439

Sum of electronic and thermal Enthalpies= -2579.288495
Sum of electronic and thermal Free Energies= -2579.402195

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.401010 | -0.084880 | -0.456171 |
| 6 | 0.059774 | 2.401949 | -0.364754 |
| 6 | 1.370246 | 1.892741 | -0.257569 |
| 6 | -0.233372 | 3.752219 | -0.135491 |
| 6 | 2.401360 | 2.772473 | 0.058261 |
| 6 | 0.810095 | 4.616836 | 0.141507 |
| 1 | -1.264705 | 4.095769 | -0.181234 |
| 6 | 2.117464 | 4.124819 | 0.227125 |
| 1 | 3.417590 | 2.404877 | 0.178234 |
| 1 | 0.616817 | 5.674070 | 0.302232 |
| 1 | 2.930811 | 4.814590 | 0.444637 |
| 8 | 4.011978 | -1.216588 | -1.320782 |
| 6 | 4.236239 | -0.618825 | -0.269937 |
| 7 | 3.151858 | -0.416906 | 0.571156 |
| 8 | 3.406609 | 0.358519 | 1.716765 |
| 1 | 2.804256 | -0.008436 | 2.375537 |
| 6 | 5.638532 | -0.223367 | 0.081026 |
| 6 | 6.636007 | -0.939386 | -0.593178 |
| 6 | 6.018233 | 0.818288 | 0.935627 |
| 6 | 7.977210 | -0.644585 | -0.401823 |
| 1 | 6.326403 | -1.726223 | -1.275571 |
| 6 | 7.364117 | 1.124797 | 1.108653 |
| 1 | 5.267698 | 1.389208 | 1.469002 |
| 6 | 8.345532 | 0.392624 | 0.450856 |
| 1 | 8.738264 | -1.219267 | -0.924546 |
| 1 | 7.645106 | 1.942920 | 1.768081 |
| 1 | 9.396443 | 0.631428 | 0.599499 |
| 6 | -0.982690 | 1.418261 | -0.626819 |
| 8 | -2.134455 | 1.408913 | -0.227473 |
| 8 | 0.802841 | -2.227791 | -0.723188 |
| 7 | -0.462675 | 0.324233 | -1.424634 |
| 8 | -1.374110 | -0.711162 | -1.589764 |
| 1 | -0.190142 | 0.661253 | -2.352406 |
| 30 | -3.191376 | -0.467768 | 0.009626 |
| 17 | -4.728508 | -1.062344 | -1.547899 |
| 6 | 1.122658 | -3.122630 | 0.071942 |
| 8 | 2.147654 | -3.026941 | 0.871860 |
| 1 | 2.585438 | -2.132536 | 0.769903 |
| 6 | 0.325061 | -4.369945 | 0.199749 |
| 1 | 0.880904 | -5.151492 | 0.719090 |

| | | | |
|---|---|---|---|
| 1 | -0.577627 | -4.111934 | 0.771371 |
| 1 | 0.003399 | -4.706010 | -0.788518 |
| 1 | -0.895724 | -1.501948 | -1.240546 |
| 17 | -1.919145 | -1.796377 | 1.341942 |
| 8 | -4.467842 | 0.570778 | 1.285108 |
| 6 | -5.678153 | 0.277830 | 1.175159 |
| 6 | -6.215144 | -0.953596 | 1.842182 |
| 1 | -7.085635 | -0.746410 | 2.473090 |
| 1 | -6.505601 | -1.686097 | 1.079041 |
| 1 | -5.415941 | -1.380320 | 2.451608 |
| 7 | -6.509939 | 1.049774 | 0.455016 |
| 6 | -7.833388 | 0.606627 | 0.057460 |
| 1 | -8.454642 | 1.482484 | -0.153169 |
| 1 | -7.771631 | -0.011965 | -0.849594 |
| 1 | -8.317493 | 0.032115 | 0.848880 |
| 6 | -5.947901 | 2.120547 | -0.353796 |
| 1 | -5.776575 | 1.759704 | -1.377848 |
| 1 | -6.645110 | 2.964503 | -0.372352 |
| 1 | -4.994790 | 2.433924 | 0.073860 |

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**$6a_1$'s**

---

Number of imaginary frequencies : 0
Electronic energy = -2579.7717999
Zero-point correction= 0.443765 (Hartree/Particle)
Thermal correction to Energy= 0.482361
Thermal correction to Enthalpy= 0.483305
Thermal correction to Gibbs Free Energy= 0.369605
Sum of electronic and zero-point Energies= -2579.328035
Sum of electronic and thermal Energies= -2579.289439
Sum of electronic and thermal Enthalpies= -2579.288495
Sum of electronic and thermal Free Energies= -2579.402195

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.401010 | -0.084880 | -0.456171 |
| 6 | 0.059774 | 2.401949 | -0.364754 |
| 6 | 1.370246 | 1.892741 | -0.257569 |
| 6 | -0.233372 | 3.752219 | -0.135491 |
| 6 | 2.401360 | 2.772473 | 0.058261 |
| 6 | 0.810095 | 4.616836 | 0.141507 |
| 1 | -1.264705 | 4.095769 | -0.181234 |
| 6 | 2.117464 | 4.124819 | 0.227125 |
| 1 | 3.417590 | 2.404877 | 0.178234 |

| | | | |
|---|---|---|---|
| 1 | 0.616817 | 5.674070 | 0.302232 |
| 1 | 2.930811 | 4.814590 | 0.444637 |
| 8 | 4.011978 | -1.216588 | -1.320782 |
| 6 | 4.236239 | -0.618825 | -0.269937 |
| 7 | 3.151858 | -0.416906 | 0.571156 |
| 8 | 3.406609 | 0.358519 | 1.716765 |
| 1 | 2.804256 | -0.008436 | 2.375537 |
| 6 | 5.638532 | -0.223367 | 0.081026 |
| 6 | 6.636007 | -0.939386 | -0.593178 |
| 6 | 6.018233 | 0.818288 | 0.935627 |
| 6 | 7.977210 | -0.644585 | -0.401823 |
| 1 | 6.326403 | -1.726223 | -1.275571 |
| 6 | 7.364117 | 1.124797 | 1.108653 |
| 1 | 5.267698 | 1.389208 | 1.469002 |
| 6 | 8.345532 | 0.392624 | 0.450856 |
| 1 | 8.738264 | -1.219267 | -0.924546 |
| 1 | 7.645106 | 1.942920 | 1.768081 |
| 1 | 9.396443 | 0.631428 | 0.599499 |
| 6 | -0.982690 | 1.418261 | -0.626819 |
| 8 | -2.134455 | 1.408913 | -0.227473 |
| 8 | 0.802841 | -2.227791 | -0.723188 |
| 7 | -0.462675 | 0.324233 | -1.424634 |
| 8 | -1.374110 | -0.711162 | -1.589764 |
| 1 | -0.190142 | 0.661253 | -2.352406 |
| 30 | -3.191376 | -0.467768 | 0.009626 |
| 17 | -4.728508 | -1.062344 | -1.547899 |
| 6 | 1.122658 | -3.122630 | 0.071942 |
| 8 | 2.147654 | -3.026941 | 0.871860 |
| 1 | 2.585438 | -2.132536 | 0.769903 |
| 6 | 0.325061 | -4.369945 | 0.199749 |
| 1 | 0.880904 | -5.151492 | 0.719090 |
| 1 | -0.577627 | -4.111934 | 0.771371 |
| 1 | 0.003399 | -4.706010 | -0.788518 |
| 1 | -0.895724 | -1.501948 | -1.240546 |
| 17 | -1.919145 | -1.796377 | 1.341942 |
| 8 | -4.467842 | 0.570778 | 1.285108 |
| 6 | -5.678153 | 0.277830 | 1.175159 |
| 6 | -6.215144 | -0.953596 | 1.842182 |
| 1 | -7.085635 | -0.746410 | 2.473090 |
| 1 | -6.505601 | -1.686097 | 1.079041 |
| 1 | -5.415941 | -1.380320 | 2.451608 |
| 7 | -6.509939 | 1.049774 | 0.455016 |
| 6 | -7.833388 | 0.606627 | 0.057460 |
| 1 | -8.454642 | 1.482484 | -0.153169 |
| 1 | -7.771631 | -0.011965 | -0.849594 |

| | | | |
|---|---|---|---|
| 1 | -8.317493 | 0.032115 | 0.848880 |
| 6 | -5.947901 | 2.120547 | -0.353796 |
| 1 | -5.776575 | 1.759704 | -1.377848 |
| 1 | -6.645110 | 2.964503 | -0.372352 |
| 1 | -4.994790 | 2.433924 | 0.073860 |

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**$(6a'\text{-}9')_{5s}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -2579.7421744
Zero-point correction= 0.443556
Thermal correction to Energy= 0.480791
Thermal correction to Enthalpy= 0.481735
Thermal correction to Gibbs Free Energy= 0.373192
Sum of electronic and zero-point Energies= -2579.298619
Sum of electronic and thermal Energies= -2579.261383
Sum of electronic and thermal Enthalpies= -2579.260439
Sum of electronic and thermal Free Energies= -2579.368983

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.226382 | 3.792713 | -1.243126 |
| 6 | -3.178308 | 2.764952 | -0.328875 |
| 6 | -1.939745 | 2.144608 | -0.036314 |
| 6 | -0.763312 | 2.708486 | -0.615767 |
| 6 | -0.849798 | 3.701609 | -1.614688 |
| 6 | -2.072855 | 4.244496 | -1.923464 |
| 1 | -4.187090 | 4.254153 | -1.465289 |
| 1 | -4.087295 | 2.381376 | 0.130004 |
| 1 | 0.067853 | 4.056797 | -2.080346 |
| 1 | -2.156494 | 5.031337 | -2.667801 |
| 6 | 0.496292 | 2.225773 | -0.130101 |
| 8 | 1.554301 | 2.014639 | -0.723031 |
| 7 | 0.420811 | 1.957841 | 1.303174 |
| 46 | -1.502442 | 1.033946 | 1.565619 |
| 8 | 1.554556 | 1.263910 | 1.748277 |
| 8 | -0.297699 | -0.502822 | 2.807589 |
| 8 | -3.227046 | -0.281924 | 1.090430 |
| 6 | -3.081520 | -0.466306 | -0.179798 |
| 7 | -2.209078 | 0.323526 | -0.778456 |
| 8 | -1.921520 | 0.198924 | -2.115371 |
| 1 | -1.000137 | -0.134278 | -2.097284 |
| 6 | -3.868652 | -1.544186 | -0.822418 |
| 6 | -4.095104 | -1.618422 | -2.202206 |
| 6 | -4.442998 | -2.510572 | 0.013682 |

| | | | |
|---|---|---|---|
| 6 | -4.871468 | -2.644866 | -2.725471 |
| 1 | -3.664770 | -0.872393 | -2.859228 |
| 6 | -5.205861 | -3.540487 | -0.516407 |
| 1 | -4.293534 | -2.438020 | 1.087144 |
| 6 | -5.421818 | -3.610698 | -1.889483 |
| 1 | -5.046228 | -2.689177 | -3.797855 |
| 1 | -5.638197 | -4.287126 | 0.145406 |
| 1 | -6.023117 | -4.415457 | -2.306759 |
| 6 | -0.425073 | -1.702164 | 2.520130 |
| 8 | -1.545711 | -2.211311 | 2.078087 |
| 1 | -2.217315 | -1.503237 | 1.884223 |
| 1 | 0.376696 | 2.843391 | 1.813306 |
| 30 | 2.476587 | 0.169849 | -0.104981 |
| 17 | 3.815358 | -0.852197 | 1.470817 |
| 17 | 0.713840 | -1.159748 | -0.779471 |
| 8 | 3.928568 | 0.463035 | -1.525677 |
| 6 | 5.043458 | -0.091720 | -1.384813 |
| 6 | 6.221619 | 0.736165 | -0.970397 |
| 1 | 7.124601 | 0.531176 | -1.552470 |
| 1 | 5.948345 | 1.786602 | -1.078290 |
| 1 | 6.432367 | 0.538932 | 0.088629 |
| 7 | 5.203050 | -1.407248 | -1.592176 |
| 6 | 4.042209 | -2.232213 | -1.895821 |
| 1 | 3.280379 | -1.639283 | -2.403431 |
| 1 | 4.354714 | -3.057903 | -2.542585 |
| 1 | 3.609927 | -2.637804 | -0.970263 |
| 6 | 6.360965 | -2.143404 | -1.117505 |
| 1 | 6.167371 | -2.526370 | -0.105469 |
| 1 | 6.551897 | -2.987335 | -1.787939 |
| 1 | 7.254016 | -1.518276 | -1.092851 |
| 1 | 1.183771 | 0.527589 | 2.294091 |
| 6 | 0.699958 | -2.665765 | 2.634137 |
| 1 | 1.292429 | -2.580704 | 1.711733 |
| 1 | 1.353170 | -2.389586 | 3.464332 |
| 1 | 0.338271 | -3.690811 | 2.729032 |

---

**$(6a_1'\text{-}9)_{3s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2579.7375323
Zero-point correction= 0.441629
Thermal correction to Energy= 0.480364
Thermal correction to Enthalpy= 0.481308
Thermal correction to Gibbs Free Energy= 0.365455
Sum of electronic and zero-point Energies= -2579.295903

Sum of electronic and thermal Energies= -2579.257169
Sum of electronic and thermal Enthalpies= -2579.256224
Sum of electronic and thermal Free Energies= -2579.372078

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -2.366108 | -1.777379 | 0.034732 |
| 6 | -0.234234 | -0.917664 | 1.998917 |
| 6 | -1.602483 | -0.887723 | 1.659875 |
| 6 | 0.130181 | -0.908080 | 3.348188 |
| 6 | -2.573219 | -0.817529 | 2.669044 |
| 6 | -0.832386 | -0.897071 | 4.345919 |
| 1 | 1.190214 | -0.910755 | 3.592235 |
| 6 | -2.183331 | -0.857569 | 4.001747 |
| 1 | -3.618863 | -0.700132 | 2.393739 |
| 1 | -0.532797 | -0.897652 | 5.390254 |
| 1 | -2.943680 | -0.825706 | 4.778875 |
| 8 | -4.093677 | 0.399584 | 0.230138 |
| 6 | -3.032365 | 1.051918 | 0.158601 |
| 7 | -1.868548 | 0.339205 | 0.164566 |
| 8 | -0.667812 | 0.999199 | 0.096503 |
| 1 | -0.342268 | 1.005926 | -0.831333 |
| 6 | -3.081826 | 2.533134 | 0.024234 |
| 6 | -4.312146 | 3.047716 | -0.408762 |
| 6 | -2.043387 | 3.421587 | 0.331815 |
| 6 | -4.497170 | 4.413809 | -0.552802 |
| 1 | -5.117108 | 2.350882 | -0.623578 |
| 6 | -2.241018 | 4.790884 | 0.199908 |
| 1 | -1.086553 | 3.049029 | 0.675584 |
| 6 | -3.458958 | 5.289878 | -0.248732 |
| 1 | -5.453568 | 4.796732 | -0.900846 |
| 1 | -1.428686 | 5.470392 | 0.444831 |
| 1 | -3.599928 | 6.362726 | -0.360138 |
| 6 | 0.852722 | -0.880791 | 1.000794 |
| 8 | 1.888912 | -0.218812 | 1.180547 |
| 8 | -3.503002 | -2.839375 | -1.547641 |
| 6 | -4.537941 | -2.375303 | -2.024101 |
| 6 | -5.295494 | -3.077021 | -3.103854 |
| 1 | -6.334558 | -3.221545 | -2.793821 |
| 1 | -5.312666 | -2.449450 | -4.000442 |
| 1 | -4.828891 | -4.035792 | -3.329701 |
| 8 | -5.090932 | -1.242263 | -1.668383 |
| 1 | -4.606747 | -0.762477 | -0.939874 |
| 7 | 0.727373 | -1.692605 | -0.078961 |
| 8 | 1.504723 | -1.383648 | -1.173128 |

| | | | |
|---|---|---|---|
| 1 | 2.345493 | -1.867798 | -1.084755 |
| 1 | -0.197208 | -2.052863 | -0.341971 |
| 30 | 2.910762 | 0.709956 | -0.372611 |
| 17 | 4.656234 | 1.765343 | 0.642436 |
| 17 | 1.577661 | 1.794705 | -1.846957 |
| 8 | 4.079274 | -0.917755 | -1.137028 |
| 6 | 5.313790 | -0.690328 | -1.178301 |
| 7 | 6.127142 | -1.134014 | -0.211351 |
| 6 | 7.497598 | -0.670764 | -0.076483 |
| 1 | 7.525233 | 0.260201 | 0.507321 |
| 1 | 8.083183 | -1.435557 | 0.442518 |
| 1 | 7.955379 | -0.495054 | -1.050854 |
| 6 | 5.547455 | -1.690994 | 1.002447 |
| 1 | 6.228218 | -2.442468 | 1.413743 |
| 1 | 5.388457 | -0.888001 | 1.735792 |
| 1 | 4.585695 | -2.150958 | 0.775845 |
| 6 | 5.880168 | 0.101544 | -2.316756 |
| 1 | 5.073795 | 0.296993 | -3.026468 |
| 1 | 6.255434 | 1.060343 | -1.939304 |
| 1 | 6.696911 | -0.418395 | -2.828175 |

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**9a'$_s$**

---

Number of imaginary frequencies : 0
Electronic energy = -2579.8049095
Zero-point correction= 0.444940
Thermal correction to Energy= 0.483508
Thermal correction to Enthalpy= 0.484453
Thermal correction to Gibbs Free Energy= 0.369303
Sum of electronic and zero-point Energies= -2579.359970
Sum of electronic and thermal Energies= -2579.321401
Sum of electronic and thermal Enthalpies= -2579.320457
Sum of electronic and thermal Free Energies= -2579.435606

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 3.378283 | -1.494471 | -0.189866 |
| 6 | 0.471936 | -1.642308 | -0.814742 |
| 6 | 1.577607 | -0.811990 | -1.202113 |
| 6 | 0.336597 | -2.907152 | -1.367980 |
| 6 | 2.521432 | -1.327240 | -2.141597 |
| 6 | 1.288923 | -3.420119 | -2.255556 |
| 1 | -0.523826 | -3.503460 | -1.075316 |
| 6 | 2.378455 | -2.652196 | -2.620509 |
| 1 | 3.164902 | -0.626631 | -2.673401 |

| | | | |
|---|---|---|---|
| 1 | 1.165944 | -4.421837 | -2.657920 |
| 1 | 3.105106 | -3.032114 | -3.334642 |
| 8 | 2.166286 | 0.965137 | 0.922498 |
| 6 | 1.829213 | 1.454801 | -0.176177 |
| 7 | 1.435919 | 0.627077 | -1.172123 |
| 8 | 0.990928 | 1.139224 | -2.374288 |
| 1 | 0.010354 | 1.189536 | -2.281915 |
| 6 | 1.811283 | 2.928146 | -0.354172 |
| 6 | 1.568135 | 3.677324 | 0.802553 |
| 6 | 2.100419 | 3.588652 | -1.553235 |
| 6 | 1.582041 | 5.063559 | 0.757728 |
| 1 | 1.365766 | 3.153575 | 1.732741 |
| 6 | 2.139405 | 4.976432 | -1.585413 |
| 1 | 2.296867 | 3.017137 | -2.453402 |
| 6 | 1.870403 | 5.715437 | -0.437333 |
| 1 | 1.372408 | 5.636300 | 1.657694 |
| 1 | 2.375528 | 5.484243 | -2.517318 |
| 1 | 1.888475 | 6.802253 | -0.474280 |
| 6 | -0.554329 | -1.250431 | 0.172844 |
| 8 | -1.755401 | -1.619628 | 0.057385 |
| 8 | 4.671129 | -1.667725 | 1.591887 |
| 6 | 4.924000 | -0.792189 | 2.412054 |
| 6 | 5.962815 | -0.966084 | 3.472482 |
| 1 | 5.506561 | -0.842030 | 4.459314 |
| 1 | 6.421899 | -1.951281 | 3.390260 |
| 1 | 6.723625 | -0.186060 | 3.370726 |
| 8 | 4.333571 | 0.380080 | 2.469193 |
| 1 | 3.626531 | 0.485501 | 1.784323 |
| 7 | -0.157741 | -0.527748 | 1.210936 |
| 8 | -1.016449 | -0.161009 | 2.207964 |
| 1 | -1.862441 | 0.114750 | 1.785836 |
| 1 | 0.797556 | -0.171397 | 1.330637 |
| 30 | -3.139711 | -0.356812 | -0.704621 |
| 17 | -5.066918 | -1.373016 | -1.202768 |
| 17 | -2.016958 | 1.394368 | -1.603804 |
| 8 | -3.547760 | 0.441807 | 1.228712 |
| 6 | -4.561384 | -0.093962 | 1.753795 |
| 6 | -4.406137 | -1.356242 | 2.543830 |
| 1 | -4.888950 | -1.309299 | 3.524545 |
| 1 | -4.848362 | -2.184928 | 1.976020 |
| 1 | -3.339700 | -1.555342 | 2.667217 |
| 7 | -5.770686 | 0.444559 | 1.577899 |
| 6 | -5.929677 | 1.580728 | 0.678303 |
| 1 | -6.274918 | 1.226486 | -0.302074 |
| 1 | -6.667507 | 2.270692 | 1.099645 |

| | | | |
|---|---|---|---|
| 1 | -4.972950 | 2.089902 | 0.556514 |
| 6 | -7.001097 | -0.255540 | 1.903043 |
| 1 | -6.864770 | -0.936177 | 2.743919 |
| 1 | -7.767465 | 0.476998 | 2.173911 |
| 1 | -7.345565 | -0.827852 | 1.030542 |

## Involvement of Pd-Zn Heterobimetallic Species in Various Catalytic Steps

---

**$2b_N$**

---

Number of imaginary frequencies : 0
Electronic energy = -2045.2628608
Zero-point correction= 0.241866
Thermal correction to Energy= 0.267515
Thermal correction to Enthalpy= 0.268459
Thermal correction to Gibbs Free Energy= 0.183848
Sum of electronic and zero-point Energies= -2045.020994
Sum of electronic and thermal Energies= -2044.995346
Sum of electronic and thermal Enthalpies= -2044.994402
Sum of electronic and thermal Free Energies= -2045.079012

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -2.043829 | 0.082298 | 0.413079 |
| 6 | 2.511985 | 1.369061 | -0.252252 |
| 6 | 2.903755 | 2.514428 | 0.449506 |
| 6 | 3.359767 | 0.255237 | -0.298549 |
| 6 | 4.132171 | 2.551657 | 1.090241 |
| 6 | 4.586079 | 0.297455 | 0.351427 |
| 1 | 3.076516 | -0.664493 | -0.812481 |
| 6 | 4.973552 | 1.442266 | 1.041173 |
| 1 | 4.435138 | 3.443898 | 1.631981 |
| 1 | 5.237188 | -0.571836 | 0.320745 |
| 1 | 5.936359 | 1.469411 | 1.546089 |
| 6 | 1.194314 | 1.418391 | -0.915245 |
| 8 | 0.407342 | 2.335970 | -0.826648 |
| 8 | -2.151610 | 2.100327 | 0.952267 |
| 6 | -2.378743 | 2.405866 | -0.256096 |
| 8 | -2.487528 | 1.431007 | -1.091321 |
| 7 | 0.811792 | 0.249814 | -1.656192 |
| 1 | 1.581253 | -0.133326 | -2.210335 |
| 8 | -0.206183 | 0.490746 | -2.587880 |
| 1 | -0.928700 | 0.926993 | -2.088886 |
| 8 | -1.543995 | -0.812788 | 2.161074 |

| | | | |
|---|---|---|---|
| 6 | -0.363834 | -1.255236 | 2.314536 |
| 8 | 0.516891 | -1.340440 | 1.417878 |
| 30 | 0.322583 | -1.645061 | -0.542674 |
| 17 | 1.848906 | -2.912915 | -1.542264 |
| 17 | -2.000634 | -1.985113 | -0.745039 |
| 1 | 2.227041 | 3.364277 | 0.475146 |
| 6 | -0.002646 | -1.704484 | 3.698891 |
| 1 | -0.813847 | -1.521706 | 4.404058 |
| 1 | 0.237450 | -2.771708 | 3.670648 |
| 1 | 0.902314 | -1.177359 | 4.014606 |
| 6 | -2.490377 | 3.809139 | -0.709051 |
| 1 | -3.237492 | 3.894027 | -1.501985 |
| 1 | -2.736436 | 4.460291 | 0.132261 |
| 1 | -1.516824 | 4.104168 | -1.116207 |

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**$2b_O$**

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Number of imaginary frequencies : 0
Electronic energy = -2045.270003
Zero-point correction= 0.241566
Thermal correction to Energy= 0.267223
Thermal correction to Enthalpy= 0.268167
Thermal correction to Gibbs Free Energy= 0.184306
Sum of electronic and zero-point Energies= -2045.028437
Sum of electronic and thermal Energies= -2045.002780
Sum of electronic and thermal Enthalpies= -2045.001836
Sum of electronic and thermal Free Energies= -2045.085697

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.567312 | 0.996024 | -1.000626 |
| 6 | 1.296284 | -1.390936 | 1.239091 |
| 6 | 2.608813 | -1.852177 | 1.084757 |
| 6 | 1.015025 | -0.388625 | 2.172225 |
| 6 | 3.632731 | -1.287377 | 1.833277 |
| 6 | 2.045433 | 0.174836 | 2.913383 |
| 1 | -0.009974 | -0.046199 | 2.293775 |
| 6 | 3.353355 | -0.267503 | 2.740324 |
| 1 | 4.649962 | -1.655188 | 1.720384 |
| 1 | 1.826646 | 0.961683 | 3.630182 |
| 1 | 4.157227 | 0.172992 | 3.324934 |
| 6 | 0.183589 | -1.939730 | 0.445455 |
| 8 | -1.017797 | -1.888274 | 0.814475 |
| 8 | 2.576626 | 1.448061 | -0.568715 |
| 6 | 2.946210 | 0.433289 | -1.230190 |

| | | | |
|---|---|---|---|
| 8 | 2.032291 | -0.295914 | -1.759470 |
| 7 | 0.493588 | -2.552293 | -0.703371 |
| 1 | 1.276238 | -2.228411 | -1.268707 |
| 8 | -0.503815 | -3.089045 | -1.472408 |
| 1 | -1.316275 | -2.925013 | -0.955953 |
| 8 | -0.399221 | 2.515416 | -0.082315 |
| 6 | -1.256388 | 2.345867 | 0.839941 |
| 8 | -1.723294 | 1.246369 | 1.235831 |
| 30 | -2.345931 | -0.396015 | 0.279386 |
| 17 | -4.414626 | -1.113712 | 0.392343 |
| 17 | -1.452326 | 0.160226 | -1.883712 |
| 1 | 2.825190 | -2.673564 | 0.404259 |
| 6 | -1.735808 | 3.596678 | 1.517662 |
| 1 | -1.160019 | 4.469359 | 1.208322 |
| 1 | -2.791794 | 3.742211 | 1.268180 |
| 1 | -1.676983 | 3.459020 | 2.600933 |
| 6 | 4.383875 | 0.114229 | -1.421451 |
| 1 | 4.749630 | 0.643525 | -2.308123 |
| 1 | 4.960070 | 0.452528 | -0.556610 |
| 1 | 4.517674 | -0.958469 | -1.583525 |

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**2b**

---

Number of imaginary frequencies : 0
Electronic energy =-2332.939979
Zero-point correction= 0.373696
Thermal correction to Energy= 0.408380
Thermal correction to Enthalpy= 0.409324
Thermal correction to Gibbs Free Energy= 0.305995
Sum of electronic and zero-point Energies= -2332.566283
Sum of electronic and thermal Energies= -2332.531599
Sum of electronic and thermal Enthalpies= -2332.530655
Sum of electronic and thermal Free Energies= -2332.633984

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.623997 | -1.191352 | -0.312154 |
| 8 | 0.444620 | -2.853281 | -0.240737 |
| 6 | -0.824483 | -2.787651 | -0.138226 |
| 8 | -1.529677 | -1.762016 | -0.068796 |
| 6 | -1.509799 | -4.131391 | -0.131725 |
| 1 | -1.979451 | -4.283808 | -1.109164 |
| 1 | -0.801496 | -4.939399 | 0.054989 |
| 1 | -2.299203 | -4.130349 | 0.624632 |
| 30 | -0.905702 | 0.240056 | -0.074859 |

| | | | |
|---|---|---|---|
| 8 | -0.259314 | 2.247311 | -0.274879 |
| 6 | 0.908320 | 2.625327 | -0.111259 |
| 7 | 1.240371 | 3.682084 | 0.638128 |
| 8 | -0.646962 | 0.089373 | 1.891216 |
| 8 | 0.770726 | 1.713265 | 2.535214 |
| 6 | 0.149208 | 0.650885 | 2.724346 |
| 6 | 0.364351 | -0.113190 | 4.005669 |
| 1 | -0.563520 | -0.582074 | 4.344110 |
| 1 | 1.079385 | -0.917635 | 3.786656 |
| 1 | 0.781383 | 0.532697 | 4.781304 |
| 17 | 0.325627 | -0.424537 | -2.185020 |
| 6 | 2.058416 | 1.913593 | -0.742214 |
| 6 | 2.403257 | 2.126979 | -2.058927 |
| 6 | 2.694909 | 0.899518 | 0.015184 |
| 6 | 3.386436 | 1.328927 | -2.667619 |
| 1 | 1.893826 | 2.899512 | -2.630790 |
| 6 | 3.665779 | 0.092494 | -0.609639 |
| 6 | 3.993095 | 0.310999 | -1.963967 |
| 1 | 3.652130 | 1.508393 | -3.706114 |
| 1 | 4.242897 | -0.607833 | -0.011079 |
| 1 | 4.749326 | -0.310406 | -2.435530 |
| 1 | 2.213943 | 3.822027 | 0.887968 |
| 8 | 0.339650 | 4.167921 | 1.539083 |
| 1 | 0.200189 | 3.374666 | 2.114110 |
| 1 | 2.521907 | 0.854670 | 1.092520 |
| 17 | 2.672189 | -1.973338 | 1.621070 |
| 8 | -2.815930 | 0.782251 | -0.558004 |
| 6 | -3.874644 | 0.346666 | -0.065694 |
| 6 | -3.906866 | -0.303646 | 1.287217 |
| 1 | -4.644261 | 0.174381 | 1.940234 |
| 1 | -4.160656 | -1.365224 | 1.194950 |
| 1 | -2.917630 | -0.233751 | 1.746604 |
| 7 | -5.028798 | 0.471039 | -0.753336 |
| 6 | -5.047357 | 1.131147 | -2.047561 |
| 1 | -5.706703 | 2.007366 | -2.012055 |
| 1 | -4.038078 | 1.446753 | -2.307714 |
| 1 | -5.423221 | 0.441241 | -2.812701 |
| 6 | -6.324038 | 0.036769 | -0.271503 |
| 1 | -6.847761 | -0.492863 | -1.076034 |
| 1 | -6.233815 | -0.644409 | 0.574296 |
| 1 | -6.940249 | 0.895426 | 0.027984 |

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**(2b-3b)$_{a\text{-}a}$‡**

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Number of imaginary frequencies: 1

Electronic energy=-2045.2324076
Zero-point correction= 0.233574
Thermal correction to Energy= 0.259338
Thermal correction to Enthalpy= 0.260282
Thermal correction to Gibbs Free Energy= 0.175969
Sum of electronic and zero-point Energies= -2044.998833
Sum of electronic and thermal Energies= -2044.973070
Sum of electronic and thermal Enthalpies= -2044.972126
Sum of electronic and thermal Free Energies= -2045.056438

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| 46 | 0.308824 | -1.431578 | 0.049543 |
| 8 | -1.528978 | -2.422921 | 0.259859 |
| 6 | -2.578344 | -1.885337 | -0.182608 |
| 8 | -2.688544 | -0.689713 | -0.587277 |
| 6 | -3.816085 | -2.733416 | -0.254112 |
| 1 | -4.121342 | -2.820812 | -1.301600 |
| 1 | -3.643636 | -3.725099 | 0.165668 |
| 1 | -4.630800 | -2.229951 | 0.274482 |
| 30 | -1.645674 | 0.921460 | -0.187882 |
| 8 | 0.115044 | 1.149486 | -1.280568 |
| 6 | 1.106000 | 1.681551 | -0.738290 |
| 7 | 1.133849 | 2.993832 | -0.476370 |
| 8 | -0.908963 | 0.879884 | 1.692824 |
| 8 | 0.336670 | -0.959658 | 2.050108 |
| 6 | -0.291588 | 0.073333 | 2.431191 |
| 6 | -0.288451 | 0.342875 | 3.910141 |
| 1 | -1.306523 | 0.209860 | 4.289661 |
| 1 | 0.388693 | -0.328607 | 4.439230 |
| 1 | -0.014397 | 1.386376 | 4.087590 |
| 17 | 0.750475 | -2.023854 | -2.299431 |
| 6 | 2.286588 | 0.882031 | -0.318132 |
| 6 | 3.545546 | 1.468381 | -0.160586 |
| 6 | 2.148404 | -0.512398 | -0.144411 |
| 6 | 4.642718 | 0.703638 | 0.217507 |
| 1 | 3.693602 | 2.526478 | -0.369698 |
| 6 | 3.265195 | -1.268127 | 0.222079 |
| 6 | 4.504546 | -0.665999 | 0.415709 |
| 1 | 5.613800 | 1.177432 | 0.335729 |
| 1 | 3.159744 | -2.345035 | 0.347181 |
| 1 | 5.363640 | -1.267085 | 0.703159 |
| 1 | 1.890933 | 3.443922 | 0.019338 |
| 8 | 0.265318 | 3.869655 | -1.052602 |
| 1 | -0.644516 | 3.647141 | -0.732957 |

| | | | |
|---|---|---|---|
| 1 | 1.594607 | -1.176395 | -1.442195 |
| 17 | -2.632121 | 2.942718 | -0.357817 |

---

**(2b-3b)$_{a\text{-}a\text{-}s}$‡**

---

Number of imaginary frequencies : 1
Electronic energy =-2332.8966128
Zero-point correction= 0.366789
Thermal correction to Energy= 0.401305
Thermal correction to Enthalpy= 0.402250
Thermal correction to Gibbs Free Energy= 0.298444
Sum of electronic and zero-point Energies= -2332.529824
Sum of electronic and thermal Energies= -2332.495307
Sum of electronic and thermal Enthalpies= -2332.494363
Sum of electronic and thermal Free Energies= -2332.598168

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.219497 | -1.340161 | 0.021692 |
| 8 | -0.173504 | -2.923219 | -0.147303 |
| 6 | -1.304019 | -2.704839 | -0.654175 |
| 8 | -1.826323 | -1.566116 | -0.853684 |
| 6 | -2.097857 | -3.908665 | -1.080614 |
| 1 | -1.891249 | -4.087634 | -2.141561 |
| 1 | -1.793625 | -4.793688 | -0.518951 |
| 1 | -3.169769 | -3.725229 | -0.971280 |
| 30 | -1.006715 | 0.079047 | -0.053907 |
| 8 | 0.096355 | 1.684285 | -0.597392 |
| 6 | 1.262036 | 2.097058 | -0.658585 |
| 7 | 1.530451 | 3.401909 | -0.437069 |
| 8 | -0.967519 | -0.233234 | 1.930290 |
| 8 | 0.981086 | -1.355317 | 2.080885 |
| 6 | -0.037170 | -0.798473 | 2.578753 |
| 6 | -0.120085 | -0.783681 | 4.075707 |
| 1 | -1.160244 | -0.758129 | 4.407235 |
| 1 | 0.409091 | -1.636723 | 4.504249 |
| 1 | 0.377389 | 0.135241 | 4.408196 |
| 17 | 1.408746 | -1.365577 | -2.302740 |
| 8 | -2.736913 | 1.143976 | -0.291506 |
| 6 | -3.898373 | 0.759021 | -0.050641 |
| 7 | -4.934961 | 1.313322 | -0.707713 |
| 6 | -4.165097 | -0.308296 | 0.971257 |
| 1 | -4.364837 | -1.263677 | 0.471866 |
| 1 | -3.271014 | -0.426027 | 1.588642 |
| 1 | -5.013023 | -0.064741 | 1.617230 |

| | | | |
|---|---|---|---|
| 6 | -4.710433 | 2.383985 | -1.665272 |
| 1 | -4.983477 | 2.051865 | -2.674162 |
| 1 | -5.330247 | 3.249026 | -1.400570 |
| 1 | -3.659416 | 2.669368 | -1.651005 |
| 6 | -6.320159 | 0.921014 | -0.539793 |
| 1 | -6.879164 | 1.675410 | 0.029736 |
| 1 | -6.785415 | 0.825555 | -1.527668 |
| 1 | -6.407794 | -0.042091 | -0.036963 |
| 6 | 2.489493 | 1.285606 | -0.864814 |
| 6 | 3.497444 | 1.724514 | -1.708895 |
| 6 | 2.674941 | 0.180851 | 0.006296 |
| 6 | 4.712550 | 1.037042 | -1.738076 |
| 1 | 3.333228 | 2.580173 | -2.361562 |
| 6 | 3.933229 | -0.447439 | -0.012411 |
| 6 | 4.939452 | -0.031983 | -0.879361 |
| 1 | 5.491220 | 1.355161 | -2.427164 |
| 1 | 4.111619 | -1.283693 | 0.662160 |
| 1 | 5.897010 | -0.546603 | -0.892931 |
| 1 | 2.244023 | 0.668440 | 1.216553 |
| 17 | 1.850769 | 1.738729 | 2.361675 |
| 1 | 2.471289 | 3.654291 | -0.152086 |
| 8 | 0.553933 | 4.187023 | 0.109109 |
| 1 | 0.346166 | 3.756023 | 0.961553 |

---

**(2b-3b)$_{c\text{-}c}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2045.2310715
Zero-point correction= 0.235200
Thermal correction to Energy= 0.260848
Thermal correction to Enthalpy= 0.261792
Thermal correction to Gibbs Free Energy= 0.177637
Sum of electronic and zero-point Energies= -2044.995872
Sum of electronic and thermal Energies= -2044.970223
Sum of electronic and thermal Enthalpies= -2044.969279
Sum of electronic and thermal Free Energies= -2045.053435

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.648933 | 2.582734 | -0.481722 |
| 6 | 2.792091 | 3.634736 | -0.182611 |
| 6 | 1.499380 | 3.391846 | 0.283256 |
| 6 | 1.031741 | 2.089488 | 0.416992 |
| 6 | 1.919521 | 1.007529 | 0.186966 |
| 6 | 3.218935 | 1.278141 | -0.264999 |

| | | | |
|---|---|---|---|
| 1 | 4.652575 | 2.780304 | -0.848796 |
| 1 | 3.130537 | 4.661179 | -0.300727 |
| 1 | 0.879942 | 4.245063 | 0.553122 |
| 1 | 3.902632 | 0.443625 | -0.414904 |
| 6 | -0.381720 | 1.779767 | 0.799109 |
| 7 | -1.254245 | 2.787966 | 0.674666 |
| 1 | -1.018759 | 3.678461 | 0.258459 |
| 8 | -0.747770 | 0.641541 | 1.151044 |
| 8 | -2.559884 | 2.665959 | 1.033846 |
| 1 | -2.953982 | 1.991629 | 0.420947 |
| 46 | 1.101392 | -0.784873 | -0.720641 |
| 30 | -1.663885 | -0.663453 | -0.281211 |
| 17 | -0.512520 | -2.599844 | -1.079094 |
| 17 | -0.340317 | 0.560760 | -2.064547 |
| 8 | -3.408091 | 0.529174 | -0.341840 |
| 6 | -3.919116 | -0.277490 | 0.516999 |
| 8 | -3.289875 | -1.314523 | 0.844950 |
| 6 | -5.232789 | 0.064382 | 1.140602 |
| 1 | -5.935857 | 0.408337 | 0.377789 |
| 1 | -5.639273 | -0.786563 | 1.688245 |
| 1 | -5.073747 | 0.895028 | 1.838813 |
| 8 | 2.323675 | -2.060791 | 0.297126 |
| 6 | 2.548528 | -1.821801 | 1.530734 |
| 8 | 2.238647 | -0.765492 | 2.124099 |
| 1 | 1.887630 | 0.129671 | 1.082989 |
| 6 | 3.227665 | -2.931045 | 2.285155 |
| 1 | 2.480641 | -3.700070 | 2.506400 |
| 1 | 4.000433 | -3.391440 | 1.665645 |
| 1 | 3.645023 | -2.555477 | 3.220368 |

---

**(2b-3b)$_{a\text{-}c\text{-}10}^{\ddagger}$**

---

Number of imaginary frequencies: 1
Electronic energy =-2392.061865
Zero-point correction= 0.383080
Thermal correction to Energy= 0.417654
Thermal correction to Enthalpy= 0.418598
Thermal correction to Gibbs Free Energy= 0.315357
Sum of electronic and zero-point Energies= -2391.678785
Sum of electronic and thermal Energies= -2391.644211
Sum of electronic and thermal Enthalpies= -2391.643267
Sum of electronic and thermal Free Energies= -2391.746508

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.302995 | 1.025949 | 0.605045 |
| 6 | 0.063736 | -1.792842 | 1.167512 |
| 6 | -0.649975 | -0.627703 | 1.580217 |
| 6 | 0.511623 | -2.725257 | 2.087348 |
| 6 | -0.849083 | -0.442983 | 2.962744 |
| 6 | 0.254118 | -2.522759 | 3.444437 |
| 1 | 1.087417 | -3.584290 | 1.751622 |
| 6 | -0.416941 | -1.384557 | 3.887185 |
| 1 | -1.374394 | 0.450379 | 3.301445 |
| 1 | 0.607721 | -3.253821 | 4.167697 |
| 1 | -0.587137 | -1.233180 | 4.949901 |
| 6 | 0.516929 | -1.908537 | -0.253054 |
| 8 | 1.710817 | -2.189386 | -0.516394 |
| 8 | -1.562054 | 1.766963 | 0.049340 |
| 6 | -2.033889 | 2.714236 | 0.717335 |
| 8 | -3.300328 | 2.791529 | 0.929232 |
| 7 | -0.366417 | -1.595678 | -1.191926 |
| 1 | -1.351790 | -1.378745 | -0.983357 |
| 8 | 0.016446 | -1.492942 | -2.498288 |
| 1 | 0.657284 | -0.751897 | -2.509747 |
| 8 | 1.322824 | 2.394407 | -0.646792 |
| 6 | 1.913551 | 1.833072 | -1.607603 |
| 8 | 1.958049 | 0.568513 | -1.785941 |
| 30 | 3.052566 | -0.664621 | -0.565282 |
| 17 | 5.173633 | -0.910342 | -1.045853 |
| 17 | 2.391278 | 0.356019 | 1.523664 |
| 1 | -1.727262 | -0.455971 | 0.873218 |
| 8 | -2.704566 | -0.867620 | 0.043848 |
| 6 | -3.836534 | -0.371363 | -0.310198 |
| 8 | -4.355470 | 0.662395 | 0.138061 |
| 6 | -4.553019 | -1.128881 | -1.434315 |
| 1 | -3.745508 | 1.906081 | 0.609363 |
| 6 | 2.629551 | 2.700482 | -2.596951 |
| 1 | 2.446683 | 3.759720 | -2.412648 |
| 1 | 3.702545 | 2.489407 | -2.519277 |
| 1 | 2.324571 | 2.426625 | -3.610907 |
| 6 | -1.194142 | 3.787782 | 1.323157 |
| 1 | -1.795422 | 4.675866 | 1.526743 |
| 1 | -0.788401 | 3.421331 | 2.274823 |
| 1 | -0.349230 | 4.022408 | 0.670502 |
| 6 | -6.053314 | -0.863366 | -1.370783 |
| 1 | -6.269289 | 0.207152 | -1.428617 |
| 1 | -6.555385 | -1.369965 | -2.204602 |
| 1 | -6.483454 | -1.240362 | -0.435158 |
| 6 | -4.285867 | -2.629601 | -1.367667 |

| | | | |
|---|---|---|---|
| 1 | -4.822827 | -3.135458 | -2.179869 |
| 1 | -3.221493 | -2.865334 | -1.472920 |
| 1 | -4.632433 | -3.055150 | -0.418161 |
| 6 | -3.985924 | -0.557358 | -2.741246 |
| 1 | -4.480716 | -1.031714 | -3.598131 |
| 1 | -4.157551 | 0.524167 | -2.802834 |
| 1 | -2.907928 | -0.742082 | -2.835252 |

---

**(2b-3b)$_{a\text{-}c\text{-}6}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2045.241475
Zero-point correction= 0.235863
Thermal correction to Energy= 0.261075
Thermal correction to Enthalpy= 0.262019
Thermal correction to Gibbs Free Energy= 0.179790
Sum of electronic and zero-point Energies= -2045.005612
Sum of electronic and thermal Energies= -2044.980400
Sum of electronic and thermal Enthalpies= -2044.979456
Sum of electronic and thermal Free Energies= -2045.061685

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.820330 | -0.488464 | -0.908762 |
| 6 | -0.960863 | 1.879162 | 0.814218 |
| 6 | -1.814616 | 1.270876 | -0.142224 |
| 6 | -0.744486 | 3.248876 | 0.816683 |
| 6 | -2.433514 | 2.098591 | -1.092620 |
| 6 | -1.396148 | 4.043513 | -0.125017 |
| 1 | -0.049684 | 3.684115 | 1.531058 |
| 6 | -2.234821 | 3.473895 | -1.080171 |
| 1 | -3.078104 | 1.649448 | -1.846029 |
| 1 | -1.229586 | 5.117913 | -0.124854 |
| 1 | -2.719528 | 4.104003 | -1.821349 |
| 6 | -0.113685 | 1.011947 | 1.680599 |
| 8 | 1.124162 | 1.182926 | 1.743501 |
| 8 | -2.236257 | -1.904969 | -0.408109 |
| 6 | -3.156930 | -1.667140 | 0.418585 |
| 6 | -4.078357 | -2.793506 | 0.781016 |
| 1 | -4.021058 | -2.969579 | 1.859381 |
| 1 | -5.107502 | -2.498811 | 0.556335 |
| 1 | -3.816785 | -3.701876 | 0.238092 |
| 8 | -3.354773 | -0.539124 | 0.967910 |
| 7 | -0.721018 | -0.002926 | 2.291921 |
| 1 | -1.721985 | -0.178096 | 2.216432 |

| | | | |
|---|---|---|---|
| 8 | -0.000578 | -0.991297 | 2.897661 |
| 1 | 0.565032 | -1.361838 | 2.183130 |
| 8 | 0.425742 | -2.127933 | -1.366704 |
| 6 | 1.326767 | -2.287189 | -0.505771 |
| 8 | 1.480672 | -1.528163 | 0.515289 |
| 6 | 2.302166 | -3.407369 | -0.689612 |
| 1 | 2.335444 | -4.013669 | 0.220300 |
| 1 | 2.051337 | -4.023343 | -1.553749 |
| 1 | 3.298734 | -2.967199 | -0.815730 |
| 30 | 2.262853 | 0.351328 | 0.262933 |
| 17 | 4.445076 | 0.498647 | 0.177206 |
| 17 | 0.924144 | 0.961062 | -1.657061 |
| 1 | -2.571147 | 0.332405 | 0.335611 |

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**(2b-3b)**$_{a\text{-}c\text{-}6\text{-}s}^{\ddagger}$

---

Number of imaginary frequencies : 1
Electronic energy =-2332.9118925
Zero-point correction= 0.368939
Thermal correction to Energy= 0.402868
Thermal correction to Enthalpy= 0.403813
Thermal correction to Gibbs Free Energy= 0.302571
Sum of electronic and zero-point Energies= -2332.542954
Sum of electronic and thermal Energies= -2332.509024
Sum of electronic and thermal Enthalpies= -2332.508080
Sum of electronic and thermal Free Energies= -2332.609321

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.991127 | -0.531447 | -0.732077 |
| 6 | -1.513268 | 2.033913 | 0.637369 |
| 6 | -2.626290 | 1.385851 | 0.046190 |
| 6 | -1.265634 | 3.380859 | 0.420294 |
| 6 | -3.471560 | 2.149835 | -0.773120 |
| 6 | -2.140421 | 4.115754 | -0.375981 |
| 1 | -0.376702 | 3.840668 | 0.845154 |
| 6 | -3.238710 | 3.504590 | -0.976836 |
| 1 | -4.320341 | 1.665612 | -1.253183 |
| 1 | -1.949832 | 5.172529 | -0.547721 |
| 1 | -3.900313 | 4.085102 | -1.614898 |
| 6 | -0.473784 | 1.207162 | 1.310902 |
| 8 | 0.731945 | 1.343249 | 1.020595 |
| 8 | -3.382917 | -1.747811 | 0.229760 |
| 6 | -3.969788 | -1.351623 | 1.268407 |
| 8 | -3.858430 | -0.179852 | 1.753116 |

| | | | |
|---|---|---|---|
| 7 | -0.910496 | 0.267302 | 2.153214 |
| 1 | -1.897518 | 0.128057 | 2.366090 |
| 8 | -0.063002 | -0.684406 | 2.645043 |
| 1 | 0.195791 | -1.225629 | 1.864875 |
| 8 | -1.054613 | -2.299017 | -1.364704 |
| 6 | 0.075397 | -2.472259 | -0.845564 |
| 8 | 0.579062 | -1.730122 | 0.064813 |
| 17 | -0.359945 | 0.637947 | -1.970730 |
| 1 | -3.242558 | 0.547495 | 0.828795 |
| 17 | 3.232658 | 0.199166 | -1.880333 |
| 8 | 2.945233 | -0.530220 | 1.249077 |
| 6 | 4.174868 | -0.471258 | 1.058046 |
| 6 | 4.949411 | -1.731080 | 0.804095 |
| 1 | 4.288657 | -2.574538 | 1.009400 |
| 1 | 5.241737 | -1.764250 | -0.252777 |
| 1 | 5.851197 | -1.814108 | 1.418528 |
| 7 | 4.831472 | 0.704912 | 1.074784 |
| 6 | 6.164320 | 0.868043 | 0.526052 |
| 1 | 6.105785 | 1.105229 | -0.546211 |
| 1 | 6.669844 | 1.689807 | 1.043855 |
| 1 | 6.764163 | -0.033844 | 0.655235 |
| 6 | 4.066796 | 1.934483 | 1.202990 |
| 1 | 4.662380 | 2.669790 | 1.753993 |
| 1 | 3.827131 | 2.337933 | 0.207979 |
| 1 | 3.137641 | 1.734373 | 1.738831 |
| 30 | 1.605711 | -0.001052 | -0.319510 |
| 6 | -4.857833 | -2.319006 | 1.993772 |
| 1 | -4.457058 | -2.484260 | 2.998752 |
| 1 | -5.851499 | -1.877445 | 2.111452 |
| 1 | -4.921472 | -3.266965 | 1.458810 |
| 6 | 0.911334 | -3.610884 | -1.349381 |
| 1 | 0.340530 | -4.271491 | -2.003199 |
| 1 | 1.750128 | -3.179097 | -1.910360 |
| 1 | 1.332640 | -4.164118 | -0.505499 |

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**(2b-3b)$_{a\text{-}c\text{-}8}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2392.0524331
Zero-point correction= 0.383175
Thermal correction to Energy= 0.418321
Thermal correction to Enthalpy= 0.419265
Thermal correction to Gibbs Free Energy= 0.313021
Sum of electronic and zero-point Energies= -2391.669258
Sum of electronic and thermal Energies= -2391.634112

Sum of electronic and thermal Enthalpies= -2391.633168
Sum of electronic and thermal Free Energies= -2391.739412

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.267931 | 0.557436 | -1.105329 |
| 6 | -0.054260 | -2.162558 | -0.013479 |
| 6 | 0.703494 | -1.334445 | -0.891309 |
| 6 | -0.338768 | -3.474591 | -0.347040 |
| 6 | 1.148878 | -1.878150 | -2.108213 |
| 6 | 0.131209 | -3.987557 | -1.559191 |
| 1 | -0.942621 | -4.085280 | 0.319962 |
| 6 | 0.870455 | -3.199672 | -2.437772 |
| 1 | 1.734748 | -1.245480 | -2.772552 |
| 1 | -0.098573 | -5.016918 | -1.824326 |
| 1 | 1.218221 | -3.616077 | -3.379425 |
| 6 | -0.681602 | -1.563897 | 1.203090 |
| 8 | -1.901627 | -1.723711 | 1.440731 |
| 8 | 1.413775 | 1.774426 | -1.554575 |
| 6 | 2.058132 | 2.581015 | -0.877986 |
| 6 | 2.681714 | 3.783731 | -1.496440 |
| 1 | 2.236845 | 3.983895 | -2.470993 |
| 1 | 2.571103 | 4.643737 | -0.830791 |
| 1 | 3.754079 | 3.596058 | -1.617235 |
| 8 | 2.278224 | 2.454663 | 0.403867 |
| 7 | 0.090536 | -0.786620 | 1.955327 |
| 1 | 1.091095 | -0.638371 | 1.779742 |
| 8 | -0.451298 | -0.047465 | 2.968150 |
| 1 | -1.033963 | 0.598995 | 2.514639 |
| 8 | -1.381513 | 2.345532 | -0.806565 |
| 6 | -2.057031 | 2.306438 | 0.255300 |
| 8 | -2.079716 | 1.306631 | 1.054510 |
| 6 | -2.907459 | 3.489296 | 0.601175 |
| 1 | -2.694465 | 3.805732 | 1.626379 |
| 1 | -2.758135 | 4.313898 | -0.096622 |
| 1 | -3.955723 | 3.167301 | 0.579915 |
| 30 | -3.179196 | -0.375141 | 0.623072 |
| 17 | -5.324210 | -0.248935 | 1.032274 |
| 17 | -2.297115 | -0.596630 | -1.605512 |
| 1 | 1.559206 | -0.627901 | -0.267978 |
| 8 | 2.432933 | -0.149095 | 0.674581 |
| 6 | 3.667680 | -0.328889 | 0.210932 |
| 1 | 2.128666 | 1.501829 | 0.666096 |
| 6 | 4.745456 | -0.402352 | 1.291663 |
| 6 | 6.120427 | -0.399394 | 0.636889 |

| | | | |
|---|---|---|---|
| 1 | 6.900839 | -0.481936 | 1.403780 |
| 1 | 6.225511 | -1.233945 | -0.063509 |
| 1 | 6.287913 | 0.525105 | 0.072561 |
| 6 | 4.615097 | 0.784002 | 2.247649 |
| 1 | 4.711240 | 1.739849 | 1.716920 |
| 1 | 3.652000 | 0.779233 | 2.770309 |
| 1 | 5.409178 | 0.739040 | 3.003517 |
| 6 | 4.539232 | -1.709839 | 2.063256 |
| 1 | 3.559795 | -1.737080 | 2.554951 |
| 1 | 4.617039 | -2.578225 | 1.397101 |
| 1 | 5.310347 | -1.809731 | 2.837623 |
| 8 | 3.900374 | -0.442158 | -0.978260 |

---

**(2b-3b)$_{a\text{-}c}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2045.2191503
Zero-point correction= 0.235170
Thermal correction to Energy= 0.260844
Thermal correction to Enthalpy= 0.261789
Thermal correction to Gibbs Free Energy= 0.178711
Sum of electronic and zero-point Energies= -2044.983980
Sum of electronic and thermal Energies= -2044.958306
Sum of electronic and thermal Enthalpies= -2044.957362
Sum of electronic and thermal Free Energies= -2045.040440

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.732939 | -1.119202 | 0.125523 |
| 8 | -2.712293 | -1.051013 | -0.563505 |
| 6 | -3.145918 | -0.003431 | -1.115418 |
| 8 | -2.508009 | 1.078241 | -1.310221 |
| 6 | -4.571995 | -0.031213 | -1.586610 |
| 1 | -5.129279 | 0.754608 | -1.067859 |
| 1 | -4.597617 | 0.200741 | -2.655365 |
| 1 | -5.031149 | -1.002025 | -1.398841 |
| 30 | -0.628801 | 1.249484 | -0.750434 |
| 8 | 1.348109 | 1.648010 | -1.041176 |
| 6 | 2.335854 | 0.927449 | -0.751174 |
| 7 | 3.541796 | 1.483224 | -0.907388 |
| 8 | -0.720050 | 2.279628 | 0.939538 |
| 8 | 0.877011 | 1.244056 | 2.148146 |
| 6 | -0.076102 | 2.066575 | 2.007096 |
| 6 | -0.485294 | 2.830646 | 3.229196 |
| 1 | -1.035806 | 3.735175 | 2.965285 |

| | | | |
|---|---|---|---|
| 1 | -1.142622 | 2.173620 | 3.811242 |
| 1 | 0.384686 | 3.061215 | 3.848159 |
| 17 | -0.068685 | -0.962181 | -2.168820 |
| 6 | 2.336776 | -0.460469 | -0.226402 |
| 6 | 3.374055 | -1.306231 | -0.595692 |
| 6 | 1.355077 | -0.871037 | 0.721800 |
| 6 | 3.457570 | -2.590957 | -0.050882 |
| 1 | 4.100025 | -0.995767 | -1.345048 |
| 6 | 1.522158 | -2.140348 | 1.302818 |
| 6 | 2.548251 | -3.003683 | 0.907929 |
| 1 | 4.248891 | -3.259870 | -0.380331 |
| 1 | 0.821925 | -2.450599 | 2.076361 |
| 1 | 2.627917 | -3.994509 | 1.347828 |
| 1 | 4.390115 | 1.137394 | -0.482969 |
| 8 | 3.646153 | 2.779635 | -1.332613 |
| 1 | 2.713088 | 3.068702 | -1.365938 |
| 1 | 0.941675 | 0.185075 | 1.427779 |
| 17 | -1.511032 | -1.116043 | 2.317824 |

---

**(2b-3b)$_{a\text{-}c\text{-}s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2332.9074077
Zero-point correction= 0.368135
Thermal correction to Energy= 0.402458
Thermal correction to Enthalpy= 0.403402
Thermal correction to Gibbs Free Energy= 0.301370
Sum of electronic and zero-point Energies= -2332.539273
Sum of electronic and thermal Energies= -2332.504950
Sum of electronic and thermal Enthalpies= -2332.504006
Sum of electronic and thermal Free Energies= -2332.606038

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.266517 | -1.290832 | -0.461984 |
| 8 | -0.009952 | -2.826455 | -1.009915 |
| 6 | -1.247533 | -2.662851 | -0.810146 |
| 8 | -1.807937 | -1.634646 | -0.344126 |
| 6 | -2.129212 | -3.826652 | -1.180107 |
| 1 | -2.801606 | -3.519499 | -1.987478 |
| 1 | -1.538273 | -4.685993 | -1.499026 |
| 1 | -2.747580 | -4.096724 | -0.318710 |
| 30 | -0.895219 | 0.190668 | -0.015324 |
| 8 | 0.082139 | 2.067581 | 0.079256 |
| 6 | 1.254507 | 2.460772 | -0.063608 |

| | | | |
|---|---|---|---|
| 7 | 1.486777 | 3.770805 | 0.167275 |
| 8 | -0.654263 | -0.021019 | 1.985892 |
| 8 | 1.512005 | 0.463793 | 2.392201 |
| 6 | 0.352021 | 0.098709 | 2.740135 |
| 6 | 0.178797 | -0.254315 | 4.190665 |
| 1 | -0.869619 | -0.208298 | 4.492182 |
| 1 | 0.538035 | -1.282705 | 4.314689 |
| 1 | 0.797842 | 0.389443 | 4.819937 |
| 17 | 0.293412 | 0.004735 | -2.254047 |
| 6 | 2.450503 | 1.670699 | -0.442164 |
| 6 | 3.461270 | 2.302437 | -1.160386 |
| 6 | 2.617476 | 0.344758 | 0.038865 |
| 6 | 4.661886 | 1.638375 | -1.413476 |
| 1 | 3.306692 | 3.304377 | -1.556223 |
| 6 | 3.866336 | -0.262142 | -0.171749 |
| 6 | 4.874929 | 0.367831 | -0.901141 |
| 1 | 5.433164 | 2.130171 | -2.001463 |
| 1 | 4.035698 | -1.252845 | 0.245715 |
| 1 | 5.821534 | -0.139198 | -1.071718 |
| 1 | 2.385422 | 4.113622 | 0.477663 |
| 8 | 0.445538 | 4.535030 | 0.636466 |
| 1 | -0.269927 | 3.871981 | 0.723205 |
| 1 | 1.958052 | 0.217453 | 1.165921 |
| 17 | 1.997776 | -2.621592 | 1.308285 |
| 8 | -2.703793 | 1.137932 | -0.196129 |
| 6 | -3.802347 | 0.687723 | 0.189583 |
| 6 | -3.901330 | -0.225285 | 1.376888 |
| 1 | -4.679645 | 0.097128 | 2.075185 |
| 1 | -4.121295 | -1.245694 | 1.044686 |
| 1 | -2.937704 | -0.247010 | 1.892863 |
| 7 | -4.930426 | 1.033585 | -0.462200 |
| 6 | -4.879401 | 1.952912 | -1.586560 |
| 1 | -5.465480 | 2.852735 | -1.361498 |
| 1 | -3.844036 | 2.229786 | -1.779948 |
| 1 | -5.301028 | 1.474795 | -2.478510 |
| 6 | -6.259066 | 0.591842 | -0.087094 |
| 1 | -6.823993 | 0.354670 | -0.995455 |
| 1 | -6.225061 | -0.307801 | 0.527370 |
| 1 | -6.801944 | 1.377040 | 0.456635 |

---

**(2b-3b)$_{a\text{-}c\text{-}6\text{-}N}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2280.9306861
Zero-point correction= 0.404781

Thermal correction to Energy= 0.437646
Thermal correction to Enthalpy= 0.438590
Thermal correction to Gibbs Free Energy= 0.340307
Sum of electronic and zero-point Energies= -2280.525905
Sum of electronic and thermal Energies= -2280.493040
Sum of electronic and thermal Enthalpies= -2280.492096
Sum of electronic and thermal Free Energies= -2280.590379

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.553932 | -0.026360 | -0.970843 |
| 6 | 0.519723 | -2.600412 | 0.417062 |
| 6 | 1.270767 | -2.065064 | -0.655605 |
| 6 | -0.053284 | -3.863334 | 0.332711 |
| 6 | 1.415704 | -2.845544 | -1.810787 |
| 6 | 0.124145 | -4.620789 | -0.824836 |
| 1 | -0.621649 | -4.279728 | 1.163571 |
| 6 | 0.852378 | -4.114188 | -1.896665 |
| 1 | 1.988603 | -2.445506 | -2.645298 |
| 1 | -0.316388 | -5.612494 | -0.888149 |
| 1 | 0.974319 | -4.708389 | -2.798377 |
| 6 | 0.283172 | -1.710139 | 1.578439 |
| 8 | 1.100571 | -1.007620 | 2.135618 |
| 8 | 2.161179 | 1.008375 | -0.261686 |
| 6 | 3.251986 | 0.438297 | 0.060143 |
| 6 | 4.305109 | 1.343757 | 0.706524 |
| 8 | 3.486434 | -0.786524 | -0.048403 |
| 7 | -1.086489 | -1.564710 | 1.923744 |
| 8 | -1.281066 | -0.805640 | 3.079399 |
| 1 | -0.404221 | -0.383040 | 3.199198 |
| 8 | -0.314715 | 1.850056 | -1.168933 |
| 6 | -1.176833 | 2.169734 | -0.307260 |
| 8 | -1.554455 | 1.426815 | 0.652550 |
| 6 | -1.875214 | 3.513204 | -0.479514 |
| 30 | -2.333916 | -0.366960 | 0.454339 |
| 17 | -4.348167 | -1.032412 | 1.041728 |
| 17 | -1.524322 | -0.993954 | -1.704198 |
| 1 | 2.284145 | -1.376518 | -0.381096 |
| 6 | -2.067597 | 4.182873 | 0.878950 |
| 1 | -2.616977 | 5.123120 | 0.746307 |
| 1 | -2.632514 | 3.543265 | 1.563102 |
| 1 | -1.103972 | 4.420341 | 1.346097 |
| 6 | -1.104642 | 4.429120 | -1.421841 |
| 1 | -1.640773 | 5.380418 | -1.527243 |
| 1 | -0.101270 | 4.642722 | -1.035406 |

| | | | |
|---|---|---|---|
| 1 | -0.992220 | 3.982833 | -2.414775 |
| 6 | -3.241502 | 3.159636 | -1.087446 |
| 1 | -3.122030 | 2.631075 | -2.042478 |
| 1 | -3.827501 | 2.527072 | -0.409023 |
| 1 | -3.810304 | 4.078500 | -1.275686 |
| 6 | 4.242209 | 2.754506 | 0.131578 |
| 1 | 4.469613 | 2.758041 | -0.941254 |
| 1 | 3.252359 | 3.199815 | 0.267661 |
| 1 | 4.983975 | 3.386813 | 0.635343 |
| 6 | 3.942010 | 1.364903 | 2.197384 |
| 1 | 3.930279 | 0.351221 | 2.616033 |
| 1 | 4.683971 | 1.959629 | 2.744965 |
| 1 | 2.953910 | 1.812714 | 2.354696 |
| 6 | 5.697451 | 0.753651 | 0.516392 |
| 1 | 6.435628 | 1.399454 | 1.008108 |
| 1 | 5.770115 | -0.249707 | 0.946206 |
| 1 | 5.960901 | 0.686794 | -0.545834 |
| 1 | -1.620695 | -2.430854 | 2.018005 |

---

**3b**

---

Number of imaginary frequencies : 0
Electronic energy =-2332.9579214
Zero-point correction= 0.375338
Thermal correction to Energy= 0.409196
Thermal correction to Enthalpy= 0.410140
Thermal correction to Gibbs Free Energy= 0.310091
Sum of electronic and zero-point Energies= -2332.582584
Sum of electronic and thermal Energies= -2332.548726
Sum of electronic and thermal Enthalpies= -2332.547782
Sum of electronic and thermal Free Energies= -2332.647830

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.977556 | -1.418833 | 0.487974 |
| 8 | -0.757831 | -2.248340 | 1.525912 |
| 6 | -1.923008 | -1.821443 | 1.391786 |
| 8 | -2.271421 | -0.789292 | 0.728348 |
| 6 | -3.039461 | -2.597515 | 2.043867 |
| 1 | -3.570150 | -3.163601 | 1.268979 |
| 1 | -2.647584 | -3.298056 | 2.782951 |
| 1 | -3.757658 | -1.914149 | 2.506810 |
| 30 | -0.896068 | 0.254629 | -0.323955 |
| 8 | 0.647611 | 1.470691 | -1.051345 |
| 6 | 1.895162 | 1.528476 | -0.968084 |

| | | | |
|---|---|---|---|
| 7 | 2.422385 | 2.766472 | -0.874551 |
| 8 | -0.906558 | 1.762348 | 1.249787 |
| 8 | 1.125211 | 2.216476 | 2.101628 |
| 6 | -0.087545 | 2.541651 | 1.731311 |
| 6 | -0.377953 | 3.993036 | 1.938009 |
| 1 | -1.406964 | 4.221728 | 1.657964 |
| 1 | -0.196099 | 4.266212 | 2.981282 |
| 1 | 0.320235 | 4.572869 | 1.323475 |
| 17 | -0.120988 | -1.710761 | -1.655962 |
| 6 | 2.863236 | 0.421812 | -1.031006 |
| 6 | 4.083956 | 0.658393 | -1.692795 |
| 6 | 2.621320 | -0.831589 | -0.451083 |
| 6 | 5.055478 | -0.323592 | -1.761997 |
| 1 | 4.242383 | 1.612144 | -2.193782 |
| 6 | 3.617723 | -1.805401 | -0.511696 |
| 6 | 4.821907 | -1.558428 | -1.160143 |
| 1 | 5.986184 | -0.133275 | -2.290021 |
| 1 | 3.451916 | -2.771578 | -0.038041 |
| 1 | 5.580338 | -2.337376 | -1.201048 |
| 1 | 3.325260 | 2.956359 | -0.464161 |
| 8 | 1.552698 | 3.828695 | -0.754177 |
| 1 | 0.698599 | 3.401296 | -0.974264 |
| 1 | 1.283931 | 1.230107 | 2.122031 |
| 17 | 1.953098 | -0.683385 | 2.504253 |
| 8 | -2.379731 | 1.176382 | -1.408348 |
| 6 | -3.548600 | 0.984824 | -0.999911 |
| 6 | -4.122557 | 1.865450 | 0.070862 |
| 1 | -5.033219 | 2.377862 | -0.257469 |
| 1 | -4.360338 | 1.267184 | 0.957711 |
| 1 | -3.363115 | 2.598794 | 0.345871 |
| 7 | -4.305046 | -0.002404 | -1.503210 |
| 6 | -3.697878 | -0.985163 | -2.389717 |
| 1 | -4.427177 | -1.286555 | -3.148151 |
| 1 | -2.821594 | -0.550525 | -2.870780 |
| 1 | -3.378588 | -1.866774 | -1.816869 |
| 6 | -5.559116 | -0.402339 | -0.893257 |
| 1 | -5.380190 | -1.066013 | -0.034563 |
| 1 | -6.138404 | 0.461213 | -0.561033 |
| 1 | -6.156347 | -0.943117 | -1.633020 |

---

**4b**

---

Number of imaginary frequencies : 0
Electronic energy =-2521.1122134
Zero-point correction= 0.374456

Thermal correction to Energy= 0.409894
Thermal correction to Enthalpy= 0.410838
Thermal correction to Gibbs Free Energy= 0.304895
Sum of electronic and zero-point Energies= -2520.737758
Sum of electronic and thermal Energies= -2520.702320
Sum of electronic and thermal Enthalpies= -2520.701376
Sum of electronic and thermal Free Energies= -2520.807319

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.088619 | 0.625831 | -0.421828 |
| 6 | -0.898363 | -2.221088 | 0.106755 |
| 6 | -0.995509 | -1.122778 | -0.755226 |
| 6 | -1.704054 | -3.353729 | -0.082390 |
| 6 | -1.866157 | -1.197926 | -1.841569 |
| 6 | -2.578862 | -3.406211 | -1.156561 |
| 1 | -1.609989 | -4.195934 | 0.601204 |
| 6 | -2.651459 | -2.329862 | -2.039147 |
| 1 | -1.947022 | -0.357130 | -2.529290 |
| 1 | -3.192811 | -4.288816 | -1.315084 |
| 1 | -3.332470 | -2.366709 | -2.886858 |
| 6 | 0.049162 | -2.185196 | 1.234143 |
| 8 | 1.274923 | -1.921146 | 1.149040 |
| 7 | -0.451642 | -2.465881 | 2.437865 |
| 1 | -1.431079 | -2.269717 | 2.631595 |
| 8 | 0.349048 | -2.299458 | 3.541553 |
| 1 | 1.171735 | -1.926907 | 3.165926 |
| 30 | 2.358079 | -1.117101 | -0.347520 |
| 17 | 1.422513 | 0.050234 | -2.186349 |
| 8 | 0.799832 | 2.596822 | -0.209241 |
| 6 | 0.168672 | 3.569356 | 0.305774 |
| 8 | -0.952210 | 3.501973 | 0.874421 |
| 17 | 4.228025 | -2.235222 | -0.924185 |
| 8 | 3.107684 | 0.486526 | 0.703867 |
| 6 | 3.975461 | 1.241201 | 0.249432 |
| 8 | 4.947052 | 0.841567 | -0.533597 |
| 1 | 4.893543 | -0.133371 | -0.698316 |
| 7 | -1.244562 | 0.995985 | 1.369194 |
| 1 | -1.260188 | 2.082570 | 1.214176 |
| 6 | -2.468769 | 0.303762 | 1.483505 |
| 8 | -2.600590 | -0.517625 | 2.384904 |
| 6 | -3.497074 | 0.586510 | 0.469172 |
| 6 | -3.458158 | 1.713996 | -0.359756 |
| 6 | -4.522584 | -0.352874 | 0.330936 |
| 6 | -4.438118 | 1.882073 | -1.328570 |

| | | | |
|---|---|---|---|
| 1 | -2.678056 | 2.466809 | -0.244927 |
| 6 | -5.490642 | -0.183231 | -0.648057 |
| 1 | -4.529785 | -1.220616 | 0.985953 |
| 6 | -5.446276 | 0.932450 | -1.479948 |
| 1 | -4.415642 | 2.760464 | -1.968274 |
| 1 | -6.279966 | -0.921529 | -0.764757 |
| 1 | -6.205272 | 1.067107 | -2.247248 |
| 8 | -0.394529 | 0.742277 | 2.451117 |
| 1 | -0.946238 | 0.199912 | 3.051591 |
| 6 | 3.952599 | 2.696908 | 0.528527 |
| 1 | 4.873427 | 3.191348 | 0.218562 |
| 1 | 3.088065 | 3.088339 | -0.025043 |
| 1 | 3.747621 | 2.859594 | 1.589768 |
| 6 | 0.848980 | 4.916017 | 0.251747 |
| 1 | 0.112373 | 5.717896 | 0.335752 |
| 1 | 1.535799 | 4.998640 | 1.102732 |
| 1 | 1.431593 | 5.023193 | -0.667245 |

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**$(4b\text{-}7a)_6^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2521.1121864
Zero-point correction= 0.372950
Thermal correction to Energy= 0.407553
Thermal correction to Enthalpy= 0.408497
Thermal correction to Gibbs Free Energy= 0.305407
Sum of electronic and zero-point Energies= -2520.739236
Sum of electronic and thermal Energies= -2520.704634
Sum of electronic and thermal Enthalpies= -2520.703690
Sum of electronic and thermal Free Energies= -2520.806780

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.085784 | 0.624846 | -0.429551 |
| 6 | -0.907267 | -2.214542 | 0.115417 |
| 6 | -0.997330 | -1.121904 | -0.754553 |
| 6 | -1.715632 | -3.345924 | -0.070126 |
| 6 | -1.863790 | -1.201014 | -1.843867 |
| 6 | -2.586044 | -3.402711 | -1.147598 |
| 1 | -1.626764 | -4.183978 | 0.619215 |
| 6 | -2.651603 | -2.331903 | -2.037398 |
| 1 | -1.940001 | -0.364108 | -2.536750 |
| 1 | -3.202053 | -4.284427 | -1.303001 |
| 1 | -3.329230 | -2.372039 | -2.887654 |
| 6 | 0.036142 | -2.175530 | 1.245976 |

| | | | |
|---|---|---|---|
| 8 | 1.261903 | -1.910200 | 1.164224 |
| 7 | -0.467907 | -2.454410 | 2.448859 |
| 1 | -1.446756 | -2.252464 | 2.639921 |
| 8 | 0.330850 | -2.285975 | 3.553703 |
| 1 | 1.154486 | -1.914744 | 3.178891 |
| 30 | 2.348373 | -1.121372 | -0.337505 |
| 17 | 1.427298 | 0.038996 | -2.190132 |
| 8 | 0.801685 | 2.603314 | -0.218811 |
| 6 | 0.179954 | 3.565023 | 0.320099 |
| 8 | -0.932860 | 3.484089 | 0.910401 |
| 17 | 4.212356 | -2.256994 | -0.901001 |
| 8 | 3.109873 | 0.491831 | 0.692247 |
| 6 | 3.982064 | 1.234301 | 0.226713 |
| 8 | 4.952210 | 0.817686 | -0.549040 |
| 1 | 4.892614 | -0.159207 | -0.700216 |
| 7 | -1.237534 | 1.007685 | 1.354925 |
| 1 | -1.235098 | 2.119104 | 1.194231 |
| 6 | -2.460092 | 0.321817 | 1.479916 |
| 8 | -2.599231 | -0.486549 | 2.393364 |
| 6 | -3.489122 | 0.595242 | 0.462070 |
| 6 | -3.451920 | 1.716358 | -0.375190 |
| 6 | -4.513886 | -0.345435 | 0.330031 |
| 6 | -4.431292 | 1.876891 | -1.345917 |
| 1 | -2.673145 | 2.470663 | -0.264792 |
| 6 | -5.481850 | -0.183955 | -0.650706 |
| 1 | -4.521128 | -1.208228 | 0.991500 |
| 6 | -5.438501 | 0.925285 | -1.491029 |
| 1 | -4.409408 | 2.750869 | -1.991721 |
| 1 | -6.270391 | -0.923944 | -0.762173 |
| 1 | -6.197328 | 1.053712 | -2.259558 |
| 8 | -0.382537 | 0.754666 | 2.434604 |
| 1 | -0.935810 | 0.222394 | 3.042692 |
| 6 | 3.966527 | 2.694756 | 0.481811 |
| 1 | 4.894597 | 3.177298 | 0.174628 |
| 1 | 3.112541 | 3.084278 | -0.089006 |
| 1 | 3.749817 | 2.876371 | 1.537624 |
| 6 | 0.847061 | 4.917101 | 0.275693 |
| 1 | 0.105377 | 5.711742 | 0.380645 |
| 1 | 1.544492 | 4.993209 | 1.118539 |
| 1 | 1.416365 | 5.040765 | -0.649390 |

---

**(4b-7a)$_8^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2521.0905499

Zero-point correction= 0.368469
Thermal correction to Energy= 0.404979
Thermal correction to Enthalpy= 0.405923
Thermal correction to Gibbs Free Energy= 0.294951
Sum of electronic and zero-point Energies= -2520.722081
Sum of electronic and thermal Energies= -2520.685571
Sum of electronic and thermal Enthalpies= -2520.684627
Sum of electronic and thermal Free Energies= -2520.795599

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.055626 | 1.060584 | 0.342793 |
| 6 | 0.092541 | -1.906148 | 0.483961 |
| 6 | 0.046030 | -0.729483 | 1.249640 |
| 6 | 0.343087 | -3.147405 | 1.077145 |
| 6 | 0.229629 | -0.822585 | 2.627074 |
| 6 | 0.539908 | -3.219030 | 2.450077 |
| 1 | 0.337355 | -4.047953 | 0.465090 |
| 6 | 0.476359 | -2.060095 | 3.220095 |
| 1 | 0.178547 | 0.075194 | 3.240530 |
| 1 | 0.717312 | -4.181019 | 2.923643 |
| 1 | 0.614329 | -2.120177 | 4.297454 |
| 6 | -0.244447 | -1.812617 | -0.945965 |
| 8 | -1.260771 | -1.203080 | -1.364981 |
| 7 | 0.551420 | -2.425851 | -1.825324 |
| 1 | 1.544261 | -2.520052 | -1.635397 |
| 8 | 0.278255 | -2.290063 | -3.165232 |
| 1 | -0.378790 | -1.568370 | -3.191978 |
| 30 | -2.450404 | -0.352917 | 0.115617 |
| 17 | -2.045889 | 1.640289 | 1.323878 |
| 8 | 1.769933 | 0.276550 | -0.572110 |
| 6 | 2.929227 | 0.581624 | -0.155140 |
| 7 | 3.133337 | 1.672121 | 0.560014 |
| 6 | 4.017854 | -0.370980 | -0.493846 |
| 6 | 3.781131 | -1.726921 | -0.245871 |
| 6 | 5.212268 | 0.027422 | -1.092815 |
| 6 | 4.734723 | -2.676730 | -0.591620 |
| 1 | 2.858760 | -2.019630 | 0.259016 |
| 6 | 6.152762 | -0.929355 | -1.458409 |
| 1 | 5.398005 | 1.081903 | -1.276761 |
| 6 | 5.917810 | -2.277942 | -1.208343 |
| 1 | 4.557479 | -3.728134 | -0.377000 |
| 1 | 7.077222 | -0.618417 | -1.938867 |
| 1 | 6.660798 | -3.020278 | -1.490114 |
| 8 | 0.112225 | 2.953218 | -0.645678 |

| | | | |
|---|---|---|---|
| 6 | 0.801873 | 3.896034 | -0.170869 |
| 8 | 1.784207 | 3.767390 | 0.613845 |
| 8 | 4.453753 | 1.961959 | 0.893808 |
| 1 | 4.439986 | 2.056078 | 1.855353 |
| 17 | -3.579225 | -2.000578 | 1.208829 |
| 8 | -3.868534 | 0.300195 | -1.251370 |
| 6 | -5.065148 | 0.042543 | -1.398312 |
| 8 | -5.724310 | -0.847282 | -0.702828 |
| 1 | -5.134496 | -1.293829 | -0.039218 |
| 1 | 2.410033 | 2.599107 | 0.602329 |
| 6 | 0.393365 | 5.291998 | -0.560691 |
| 1 | -0.477312 | 5.578211 | 0.039527 |
| 1 | 1.200408 | 6.003583 | -0.376147 |
| 1 | 0.086587 | 5.315308 | -1.609396 |
| 6 | -5.905236 | 0.752193 | -2.404310 |
| 1 | -6.627263 | 1.385175 | -1.878080 |
| 1 | -5.279275 | 1.369467 | -3.048418 |
| 1 | -6.477440 | 0.029254 | -2.991854 |

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**7a**

---

Number of imaginary frequencies : 0
Electronic energy =-2521.1221644
Zero-point correction= 0.375793
Thermal correction to Energy= 0.410775
Thermal correction to Enthalpy= 0.411719
Thermal correction to Gibbs Free Energy= 0.308333
Sum of electronic and zero-point Energies= -2520.746371
Sum of electronic and thermal Energies= -2520.711390
Sum of electronic and thermal Enthalpies= -2520.710445
Sum of electronic and thermal Free Energies= -2520.813831

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.067151 | 0.623519 | -0.497091 |
| 6 | -1.076536 | -2.091666 | 0.214700 |
| 6 | -1.094280 | -1.063016 | -0.733336 |
| 6 | -1.938192 | -3.190479 | 0.090857 |
| 6 | -1.941836 | -1.170822 | -1.833383 |
| 6 | -2.789389 | -3.279841 | -1.000079 |
| 1 | -1.909435 | -3.975543 | 0.844394 |
| 6 | -2.781269 | -2.273636 | -1.963959 |
| 1 | -1.965700 | -0.381583 | -2.582468 |
| 1 | -3.451196 | -4.135426 | -1.104892 |
| 1 | -3.444495 | -2.339329 | -2.823825 |

| | | | |
|---|---|---|---|
| 6 | -0.137458 | -2.035028 | 1.350003 |
| 8 | 1.111573 | -1.920012 | 1.244738 |
| 7 | -0.669259 | -2.125736 | 2.567665 |
| 1 | -1.603891 | -1.733703 | 2.725743 |
| 8 | 0.158745 | -1.953231 | 3.650837 |
| 1 | 1.003787 | -1.671533 | 3.247652 |
| 30 | 2.211524 | -1.273576 | -0.307692 |
| 17 | 1.429618 | -0.123807 | -2.230627 |
| 8 | 1.049456 | 2.593444 | -0.349293 |
| 6 | 0.621907 | 3.625713 | 0.166169 |
| 8 | -0.485451 | 3.707497 | 0.860769 |
| 17 | 4.009489 | -2.552360 | -0.796604 |
| 8 | 3.085494 | 0.342406 | 0.655080 |
| 6 | 4.070413 | 0.952681 | 0.229988 |
| 8 | 5.004317 | 0.416700 | -0.514235 |
| 1 | 4.830530 | -0.547471 | -0.671389 |
| 7 | -1.191447 | 1.116810 | 1.211326 |
| 1 | -0.874747 | 2.791194 | 0.989464 |
| 6 | -2.406960 | 0.548925 | 1.478135 |
| 8 | -2.619483 | -0.058451 | 2.543774 |
| 6 | -3.459173 | 0.713345 | 0.448102 |
| 6 | -3.424072 | 1.722779 | -0.518497 |
| 6 | -4.516789 | -0.197038 | 0.457379 |
| 6 | -4.421485 | 1.796996 | -1.481605 |
| 1 | -2.618597 | 2.454484 | -0.513992 |
| 6 | -5.509387 | -0.125436 | -0.511239 |
| 1 | -4.534157 | -0.959795 | 1.231866 |
| 6 | -5.459209 | 0.867333 | -1.485715 |
| 1 | -4.393283 | 2.586651 | -2.228561 |
| 1 | -6.325372 | -0.844176 | -0.505947 |
| 1 | -6.237351 | 0.926815 | -2.243299 |
| 8 | -0.305691 | 0.952330 | 2.297354 |
| 1 | -0.866453 | 0.524887 | 2.979765 |
| 6 | 4.266537 | 2.401496 | 0.501909 |
| 1 | 5.321883 | 2.677374 | 0.476052 |
| 1 | 3.734228 | 2.942551 | -0.289608 |
| 1 | 3.804071 | 2.659796 | 1.456608 |
| 6 | 1.360671 | 4.921709 | 0.063649 |
| 1 | 0.669017 | 5.766205 | 0.091423 |
| 1 | 2.031790 | 5.010448 | 0.925701 |
| 1 | 1.960089 | 4.941300 | -0.848434 |

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**(7a-9)$_3^{‡}$**

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Number of imaginary frequencies : 1

Electronic energy =-2521.074288
Zero-point correction= 0.373789
Thermal correction to Energy= 0.409380
Thermal correction to Enthalpy= 0.410324
Thermal correction to Gibbs Free Energy= 0.304020
Sum of electronic and zero-point Energies= -2520.700499
Sum of electronic and thermal Energies= -2520.664908
Sum of electronic and thermal Enthalpies= -2520.663964
Sum of electronic and thermal Free Energies= -2520.770268

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.578125 | -0.258017 | -0.871648 |
| 6 | 0.660581 | 2.467861 | -0.333544 |
| 6 | 0.763180 | 1.253733 | -1.047775 |
| 6 | 1.080375 | 3.656348 | -0.959850 |
| 6 | 1.329789 | 1.258850 | -2.338306 |
| 6 | 1.605730 | 3.657855 | -2.238381 |
| 1 | 0.934532 | 4.599776 | -0.436728 |
| 6 | 1.730483 | 2.445904 | -2.923433 |
| 1 | 1.459997 | 0.313970 | -2.861947 |
| 1 | 1.903837 | 4.591692 | -2.706087 |
| 1 | 2.145773 | 2.426961 | -3.928618 |
| 8 | 1.852129 | -1.755933 | -1.480093 |
| 6 | 2.251084 | -1.014391 | -0.568180 |
| 7 | 1.344380 | -0.149913 | 0.000401 |
| 8 | 1.682906 | 0.395816 | 1.224205 |
| 1 | 1.154328 | -0.130984 | 1.867599 |
| 6 | 3.668748 | -1.002366 | -0.152660 |
| 6 | 4.388143 | -2.194838 | -0.263612 |
| 6 | 4.323876 | 0.174661 | 0.223072 |
| 6 | 5.743232 | -2.220818 | 0.033877 |
| 1 | 3.866376 | -3.092986 | -0.584619 |
| 6 | 5.685107 | 0.148924 | 0.493256 |
| 1 | 3.765029 | 1.105117 | 0.290091 |
| 6 | 6.392188 | -1.048159 | 0.411061 |
| 1 | 6.296854 | -3.153807 | -0.035486 |
| 1 | 6.198563 | 1.065711 | 0.772617 |
| 1 | 7.455767 | -1.065275 | 0.637760 |
| 6 | 0.114103 | 2.562408 | 1.029127 |
| 8 | -0.870130 | 1.951618 | 1.512583 |
| 30 | -1.814667 | 0.146343 | 1.406303 |
| 17 | -4.023983 | 0.241660 | 1.325764 |
| 17 | -0.540880 | -1.241122 | 2.698396 |
| 8 | -2.454730 | 0.505818 | -1.779325 |

| | | | |
|---|---|---|---|
| 8 | -1.695629 | -2.307634 | -0.601122 |
| 6 | -3.574441 | 0.033095 | -1.969495 |
| 6 | -1.116361 | -3.280013 | -0.102778 |
| 6 | -1.804339 | -4.243124 | 0.796999 |
| 1 | -2.871205 | -4.278433 | 0.571210 |
| 1 | -1.350043 | -5.234171 | 0.745990 |
| 1 | -1.683353 | -3.856134 | 1.817742 |
| 6 | -4.716984 | 0.872593 | -2.425121 |
| 1 | -5.283146 | 1.155865 | -1.529549 |
| 1 | -4.351701 | 1.776702 | -2.913255 |
| 1 | -5.382030 | 0.306371 | -3.080898 |
| 8 | -3.896317 | -1.225109 | -1.778488 |
| 1 | -3.160325 | -1.707870 | -1.337905 |
| 8 | 0.153864 | -3.521009 | -0.283812 |
| 1 | 0.597257 | -2.828832 | -0.844687 |
| 7 | 0.696152 | 3.477123 | 1.820744 |
| 1 | 1.649091 | 3.785709 | 1.693841 |
| 8 | 0.265468 | 3.617017 | 3.116837 |
| 1 | -0.440313 | 2.943674 | 3.179079 |

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**(7a-9)$_7^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2521.0791663
Zero-point correction= 0.374629
Thermal correction to Energy= 0.409571
Thermal correction to Enthalpy= 0.410515
Thermal correction to Gibbs Free Energy= 0.306747
Sum of electronic and zero-point Energies= -2520.704537
Sum of electronic and thermal Energies= -2520.669596
Sum of electronic and thermal Enthalpies= -2520.668651
Sum of electronic and thermal Free Energies= -2520.772420

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.667480 | 0.878062 | -1.165480 |
| 6 | 1.717663 | -1.887141 | -0.841079 |
| 6 | 0.677827 | -1.115623 | -1.426502 |
| 6 | 2.350187 | -2.884996 | -1.605172 |
| 6 | 0.238672 | -1.460573 | -2.726109 |
| 6 | 1.953497 | -3.163745 | -2.896493 |
| 1 | 3.206073 | -3.411555 | -1.183925 |
| 6 | 0.882636 | -2.445502 | -3.447377 |
| 1 | -0.602094 | -0.924364 | -3.162104 |
| 1 | 2.465592 | -3.924678 | -3.477920 |

| | | | |
|---|---|---|---|
| 1 | 0.549783 | -2.662618 | -4.460422 |
| 8 | -1.530569 | 0.721233 | -1.203981 |
| 6 | -1.885860 | -0.355204 | -0.663353 |
| 7 | -0.876600 | -1.178159 | -0.240600 |
| 8 | -1.240905 | -2.497926 | -0.023357 |
| 1 | -1.025258 | -2.670435 | 0.919535 |
| 6 | -3.318779 | -0.611316 | -0.425489 |
| 6 | -4.087754 | 0.496583 | -0.043590 |
| 6 | -3.929775 | -1.858837 | -0.590774 |
| 6 | -5.446094 | 0.352094 | 0.193304 |
| 1 | -3.603923 | 1.461239 | 0.091325 |
| 6 | -5.297578 | -1.985041 | -0.380688 |
| 1 | -3.338826 | -2.715171 | -0.893841 |
| 6 | -6.054036 | -0.888219 | 0.018376 |
| 1 | -6.032104 | 1.210440 | 0.511285 |
| 1 | -5.773294 | -2.952001 | -0.524409 |
| 1 | -7.121391 | -0.999892 | 0.194388 |
| 6 | 2.106904 | -1.633622 | 0.541329 |
| 8 | 1.900989 | -0.543252 | 1.136844 |
| 30 | -0.036871 | -0.185456 | 1.623083 |
| 17 | -0.812798 | 1.843539 | 2.078902 |
| 17 | -0.290207 | -2.090243 | 2.922141 |
| 8 | 2.929121 | 1.037606 | -1.090900 |
| 8 | 0.583027 | 3.186644 | -0.713320 |
| 6 | 3.456278 | 1.529664 | -0.096171 |
| 6 | -0.435307 | 3.834315 | -0.465240 |
| 6 | -0.408655 | 5.136898 | 0.254639 |
| 1 | 0.573569 | 5.602818 | 0.165601 |
| 1 | -1.194402 | 5.802026 | -0.109732 |
| 1 | -0.607072 | 4.926190 | 1.312502 |
| 6 | 4.737348 | 1.013097 | 0.466434 |
| 1 | 5.332857 | 1.815235 | 0.907292 |
| 1 | 4.479218 | 0.303639 | 1.263135 |
| 1 | 5.296991 | 0.485050 | -0.307015 |
| 8 | 2.947357 | 2.529059 | 0.595189 |
| 1 | 2.102032 | 2.833412 | 0.191031 |
| 8 | -1.643098 | 3.444884 | -0.798014 |
| 1 | -1.642038 | 2.506241 | -1.095558 |
| 7 | 2.664730 | -2.650935 | 1.224492 |
| 1 | 2.622326 | -3.608384 | 0.900651 |
| 8 | 2.967130 | -2.502199 | 2.546713 |
| 1 | 2.100718 | -2.352128 | 2.983112 |

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**(7a-9)$_{c\text{-}3\text{-}AcOH}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2521.0631241
Zero-point correction= 0.372473
Thermal correction to Energy= 0.408536
Thermal correction to Enthalpy= 0.409480
Thermal correction to Gibbs Free Energy= 0.300728
Sum of electronic and zero-point Energies= -2520.690651
Sum of electronic and thermal Energies= -2520.654588
Sum of electronic and thermal Enthalpies= -2520.653644
Sum of electronic and thermal Free Energies= -2520.762396

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.243733 | 0.364043 | 1.134368 |
| 8 | -0.249362 | 2.780207 | 1.082023 |
| 6 | 0.712974 | 3.415173 | 1.477078 |
| 8 | 1.841727 | 2.872717 | 1.922509 |
| 30 | -2.598433 | -0.294323 | -0.384177 |
| 8 | -1.431764 | -1.774100 | -1.067884 |
| 6 | -0.508956 | -2.545782 | -0.727424 |
| 7 | -0.156188 | -3.501499 | -1.612806 |
| 6 | 0.159842 | -2.623064 | 0.582810 |
| 6 | 0.240543 | -3.900038 | 1.157591 |
| 6 | 0.596937 | -1.487869 | 1.334127 |
| 6 | 0.705472 | -4.106699 | 2.446590 |
| 1 | -0.131325 | -4.743363 | 0.578635 |
| 6 | 1.029439 | -1.721658 | 2.668727 |
| 6 | 1.064402 | -2.997143 | 3.207938 |
| 1 | 0.738307 | -5.107530 | 2.866280 |
| 1 | 1.261113 | -0.870489 | 3.306564 |
| 1 | 1.365395 | -3.121102 | 4.246343 |
| 1 | 0.813665 | -3.791293 | -1.635455 |
| 8 | -0.706403 | -3.448553 | -2.872553 |
| 1 | -1.107318 | -2.559099 | -2.909235 |
| 7 | 1.668413 | -0.310232 | 0.587927 |
| 6 | 0.767737 | 4.909259 | 1.498189 |
| 1 | -0.218283 | 5.322809 | 1.282606 |
| 1 | 1.120815 | 5.261182 | 2.471421 |
| 1 | 1.486945 | 5.257390 | 0.749097 |
| 17 | -2.626580 | 0.250651 | 1.862362 |
| 8 | -1.717846 | 1.320674 | -1.381184 |
| 6 | -2.243612 | 2.379780 | -1.735310 |
| 6 | -1.432675 | 3.612559 | -1.934188 |
| 1 | -1.104385 | 3.943268 | -0.941847 |
| 1 | -0.536560 | 3.362926 | -2.507839 |

| | | | |
|---|---|---|---|
| 1 | -2.004750 | 4.400396 | -2.425349 |
| 8 | -3.524661 | 2.529967 | -1.949827 |
| 1 | -4.005980 | 1.669458 | -1.820075 |
| 6 | 2.101369 | -0.498619 | -0.719935 |
| 8 | 1.364326 | -1.064907 | -1.515939 |
| 6 | 3.455340 | -0.027154 | -1.129948 |
| 6 | 4.030346 | 1.176793 | -0.712530 |
| 6 | 4.111722 | -0.804453 | -2.088581 |
| 6 | 5.253252 | 1.579695 | -1.234619 |
| 1 | 3.516716 | 1.808922 | 0.006164 |
| 6 | 5.345276 | -0.411479 | -2.588819 |
| 1 | 3.633152 | -1.716050 | -2.437429 |
| 6 | 5.918132 | 0.782796 | -2.161937 |
| 1 | 5.689487 | 2.522595 | -0.913728 |
| 1 | 5.855605 | -1.031735 | -3.321563 |
| 1 | 6.880148 | 1.098467 | -2.559090 |
| 8 | 2.639637 | 0.145295 | 1.485631 |
| 1 | 2.874701 | -0.639018 | 2.018798 |
| 1 | 1.816593 | 1.893040 | 1.880628 |
| 17 | -4.604913 | -0.337587 | -1.455136 |

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**(7a-9)$_{c\text{-}3\text{-}OAc}$‡**

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Number of imaginary frequencies : 1
Electronic energy =-2060.2521607
Zero-point correction= 0.358810
Thermal correction to Energy= 0.392985
Thermal correction to Enthalpy= 0.393929
Thermal correction to Gibbs Free Energy= 0.288042
Sum of electronic and zero-point Energies= -2059.893350
Sum of electronic and thermal Energies= -2059.859176
Sum of electronic and thermal Enthalpies= -2059.858232
Sum of electronic and thermal Free Energies= -2059.964118

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.512771 | -0.296882 | -1.274649 |
| 8 | -0.617022 | -2.647778 | -1.455343 |
| 6 | 0.375391 | -3.325211 | -1.646660 |
| 8 | 1.571146 | -2.827882 | -1.968114 |
| 30 | -2.448034 | -0.141361 | 0.584665 |
| 8 | -1.612909 | 1.548409 | 1.284426 |
| 6 | -0.736021 | 2.373537 | 0.976460 |
| 7 | -0.306346 | 3.233995 | 1.930187 |
| 6 | -0.151638 | 2.609950 | -0.361522 |

| | | | |
|---|---|---|---|
| 6 | -0.143666 | 3.938738 | -0.809133 |
| 6 | 0.292203 | 1.578939 | -1.239097 |
| 6 | 0.264414 | 4.288510 | -2.086973 |
| 1 | -0.523291 | 4.705941 | -0.136552 |
| 6 | 0.694997 | 1.955988 | -2.544247 |
| 6 | 0.659556 | 3.277751 | -2.959489 |
| 1 | 0.240385 | 5.325854 | -2.406762 |
| 1 | 0.977255 | 1.181746 | -3.255366 |
| 1 | 0.938198 | 3.516613 | -3.983815 |
| 1 | 0.643856 | 3.578135 | 1.853446 |
| 8 | -0.690122 | 3.000557 | 3.226318 |
| 1 | -0.648447 | 2.032314 | 3.327106 |
| 7 | 1.404608 | 0.307887 | -0.650051 |
| 6 | 0.398480 | -4.814910 | -1.550031 |
| 1 | -0.601136 | -5.185357 | -1.324162 |
| 1 | 0.761285 | -5.243160 | -2.489184 |
| 1 | 1.096480 | -5.119079 | -0.763794 |
| 17 | -2.996752 | -0.128358 | -1.659674 |
| 8 | -1.765194 | -1.731837 | 1.752994 |
| 6 | -2.890552 | -1.699643 | 2.332769 |
| 6 | -3.216440 | -2.690112 | 3.408364 |
| 1 | -3.702763 | -2.184019 | 4.246341 |
| 1 | -3.932268 | -3.416892 | 3.010141 |
| 1 | -2.319993 | -3.215526 | 3.741325 |
| 8 | -3.764009 | -0.839197 | 1.995986 |
| 6 | 1.863471 | 0.359945 | 0.660478 |
| 8 | 1.147820 | 0.841080 | 1.530182 |
| 6 | 3.229890 | -0.140615 | 0.985569 |
| 6 | 3.777797 | -1.315220 | 0.461531 |
| 6 | 3.928291 | 0.564413 | 1.969722 |
| 6 | 5.016878 | -1.758825 | 0.906055 |
| 1 | 3.228357 | -1.894959 | -0.274920 |
| 6 | 5.178071 | 0.132406 | 2.391330 |
| 1 | 3.472348 | 1.451997 | 2.401468 |
| 6 | 5.724011 | -1.031971 | 1.859187 |
| 1 | 5.431858 | -2.680730 | 0.505763 |
| 1 | 5.721005 | 0.696722 | 3.145587 |
| 1 | 6.697957 | -1.379859 | 2.195834 |
| 8 | 2.355891 | -0.048873 | -1.609950 |
| 1 | 2.668434 | 0.790401 | -1.994462 |
| 1 | 1.540335 | -1.851703 | -2.028482 |

---

**(7a-9)$_{a\text{-}c\text{-}3\text{-}s\text{-}AcOH}^{‡}$**

---

Number of imaginary frequencies : 1

Electronic energy =-2347.9402662
Zero-point correction= 0.493861
Thermal correction to Energy= 0.534936
Thermal correction to Enthalpy= 0.535881
Thermal correction to Gibbs Free Energy= 0.420577
Sum of electronic and zero-point Energies= -2347.446405
Sum of electronic and thermal Energies= -2347.405330
Sum of electronic and thermal Enthalpies= -2347.404386
Sum of electronic and thermal Free Energies= -2347.519689

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.428379 | 0.539846 | -1.477140 |
| 8 | -0.509221 | -1.359787 | -2.320860 |
| 6 | -1.617391 | -1.804709 | -1.967308 |
| 8 | -2.306442 | -1.404912 | -0.969167 |
| 30 | -1.591921 | 0.095458 | 0.199248 |
| 8 | -0.411319 | 1.161904 | 1.567576 |
| 6 | 0.622959 | 1.842522 | 1.663459 |
| 7 | 1.140788 | 2.090164 | 2.889269 |
| 8 | -3.405679 | 0.088309 | 1.266266 |
| 6 | -4.268558 | -0.697593 | 0.807421 |
| 7 | -5.129536 | -0.306565 | -0.145334 |
| 6 | -4.357464 | -2.102355 | 1.327157 |
| 1 | -3.853448 | -2.764509 | 0.612368 |
| 1 | -3.825500 | -2.156452 | 2.277564 |
| 1 | -5.384891 | -2.446832 | 1.473411 |
| 6 | -5.018487 | 1.031200 | -0.710517 |
| 1 | -6.021287 | 1.385580 | -0.971009 |
| 1 | -4.565708 | 1.701487 | 0.020213 |
| 1 | -4.382906 | 1.024167 | -1.605978 |
| 6 | -5.857323 | -1.251291 | -0.971287 |
| 1 | -6.776905 | -0.780947 | -1.333264 |
| 1 | -5.242287 | -1.540538 | -1.835617 |
| 1 | -6.129544 | -2.151074 | -0.418678 |
| 6 | 1.365555 | 2.525173 | 0.576281 |
| 6 | 1.668414 | 3.878717 | 0.788908 |
| 6 | 1.661682 | 1.942027 | -0.692272 |
| 6 | 2.243879 | 4.675349 | -0.188103 |
| 1 | 1.383226 | 4.324669 | 1.740363 |
| 6 | 2.240684 | 2.776853 | -1.682170 |
| 6 | 2.504437 | 4.112123 | -1.437083 |
| 1 | 2.448576 | 5.724010 | 0.006812 |
| 1 | 2.420381 | 2.362521 | -2.672050 |
| 1 | 2.909042 | 4.726395 | -2.239399 |

| | | | |
|---|---|---|---|
| 1 | 2.099783 | 2.395369 | 2.989702 |
| 8 | 0.568172 | 1.577162 | 4.021531 |
| 1 | 0.693024 | 0.610029 | 3.955305 |
| 7 | 2.449479 | 0.349225 | -0.808138 |
| 6 | -2.240983 | -2.901280 | -2.800942 |
| 1 | -1.468311 | -3.492690 | -3.296794 |
| 1 | -2.883840 | -3.543031 | -2.190996 |
| 1 | -2.860409 | -2.439184 | -3.578551 |
| 17 | -1.750448 | 1.836895 | -1.473019 |
| 8 | -0.779158 | -1.518528 | 1.544559 |
| 6 | -0.552494 | -1.301970 | 2.727017 |
| 6 | -1.617929 | -1.172465 | 3.765660 |
| 1 | -2.079213 | -2.153438 | 3.925481 |
| 1 | -1.227006 | -0.806743 | 4.716914 |
| 1 | -2.385750 | -0.495028 | 3.375845 |
| 8 | 0.675596 | -1.171605 | 3.208073 |
| 1 | 1.318443 | -1.079169 | 2.445620 |
| 6 | 2.708073 | -0.485691 | 0.240210 |
| 8 | 2.206452 | -0.248313 | 1.350333 |
| 6 | 3.576487 | -1.672754 | 0.034567 |
| 6 | 3.485954 | -2.461660 | -1.116288 |
| 6 | 4.406333 | -2.067219 | 1.085803 |
| 6 | 4.238697 | -3.624182 | -1.214110 |
| 1 | 2.809533 | -2.169474 | -1.915920 |
| 6 | 5.175265 | -3.218092 | 0.972840 |
| 1 | 4.440433 | -1.458246 | 1.986547 |
| 6 | 5.090914 | -3.997164 | -0.177689 |
| 1 | 4.158680 | -4.244176 | -2.103624 |
| 1 | 5.834075 | -3.513225 | 1.786034 |
| 1 | 5.685290 | -4.904099 | -0.263281 |
| 8 | 3.311510 | 0.236867 | -1.895707 |
| 1 | 3.919662 | 0.988955 | -1.795435 |

---

**$(7a\text{-}9)_5^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2521.0636816
Zero-point correction= 0.374449
Thermal correction to Energy= 0.409768
Thermal correction to Enthalpy= 0.410712
Thermal correction to Gibbs Free Energy= 0.306224
Sum of electronic and zero-point Energies= -2520.689232
Sum of electronic and thermal Energies= -2520.653914
Sum of electronic and thermal Enthalpies= -2520.652970
Sum of electronic and thermal Free Energies= -2520.757458

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.900248 | 0.022441 | -1.008900 |
| 6 | 0.216893 | 2.426389 | 0.479408 |
| 6 | -0.145453 | 1.885207 | -0.778623 |
| 6 | -0.051348 | 3.768104 | 0.770842 |
| 6 | -0.677273 | 2.757742 | -1.746980 |
| 6 | -0.664042 | 4.591939 | -0.161223 |
| 1 | 0.224282 | 4.150343 | 1.752387 |
| 6 | -0.963135 | 4.075864 | -1.423860 |
| 1 | -0.894567 | 2.376385 | -2.743209 |
| 1 | -0.888578 | 5.626171 | 0.082613 |
| 1 | -1.418764 | 4.716430 | -2.176595 |
| 6 | 1.960247 | -0.030682 | -1.069427 |
| 6 | 3.332327 | -0.475329 | -0.756350 |
| 6 | 3.450404 | -1.502256 | 0.191217 |
| 6 | 4.479506 | 0.061353 | -1.348957 |
| 6 | 4.706321 | -1.971247 | 0.551069 |
| 1 | 2.547567 | -1.915470 | 0.641350 |
| 6 | 5.729985 | -0.426927 | -0.995205 |
| 1 | 4.386038 | 0.851212 | -2.086654 |
| 6 | 5.845760 | -1.435834 | -0.042361 |
| 1 | 4.794594 | -2.760090 | 1.293738 |
| 1 | 6.620775 | -0.016503 | -1.464449 |
| 1 | 6.829163 | -1.807070 | 0.236929 |
| 6 | 1.042944 | 1.643460 | 1.414598 |
| 8 | 0.791050 | 0.524860 | 1.922143 |
| 30 | -0.859043 | -0.658873 | 1.644634 |
| 17 | -2.740806 | 0.314327 | 2.329824 |
| 17 | -0.168975 | -2.777709 | 1.792248 |
| 8 | -2.969878 | 0.811347 | -1.047886 |
| 8 | -1.775581 | -2.159975 | -1.207953 |
| 6 | -4.005926 | 0.262554 | -0.668507 |
| 6 | -1.176243 | -3.240884 | -1.268472 |
| 6 | -1.873120 | -4.546074 | -1.110259 |
| 1 | -2.920264 | -4.464150 | -1.405859 |
| 1 | -1.364217 | -5.332182 | -1.671422 |
| 1 | -1.827550 | -4.803134 | -0.044801 |
| 6 | -5.210505 | 1.046915 | -0.281051 |
| 1 | -5.174438 | 1.159779 | 0.809146 |
| 1 | -5.177601 | 2.037001 | -0.737071 |
| 1 | -6.128787 | 0.516275 | -0.541371 |
| 8 | -4.165686 | -1.034523 | -0.553704 |
| 1 | -3.334500 | -1.519725 | -0.771265 |

| | | | |
|---|---|---|---|
| 8 | 0.108607 | -3.344465 | -1.465316 |
| 1 | 0.559287 | -2.467075 | -1.358519 |
| 7 | 2.221940 | 2.207563 | 1.709908 |
| 1 | 2.665032 | 2.818248 | 1.031375 |
| 8 | 3.120783 | 1.514749 | 2.482473 |
| 1 | 2.720026 | 0.626602 | 2.554612 |
| 7 | 1.589209 | 1.185438 | -1.436204 |
| 8 | 1.019240 | -0.886349 | -0.910251 |
| 8 | 2.562260 | 2.183989 | -1.331775 |
| 1 | 2.243017 | 2.848518 | -1.958716 |

---

**(7a-9)$_{c\text{-}7\text{-}s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2579.7540417
Zero-point correction= 0.443640
Thermal correction to Energy= 0.481540
Thermal correction to Enthalpy= 0.482484
Thermal correction to Gibbs Free Energy= 0.374192
Sum of electronic and zero-point Energies= -2579.310401
Sum of electronic and thermal Energies= -2579.272502
Sum of electronic and thermal Enthalpies= -2579.271557
Sum of electronic and thermal Free Energies= -2579.379850

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.701675 | -0.685914 | 1.093589 |
| 30 | -0.056975 | 1.279098 | -0.005493 |
| 8 | 1.266876 | 1.571926 | -1.839945 |
| 6 | 2.435999 | 1.166595 | -1.717117 |
| 7 | 3.470383 | 2.017358 | -1.595972 |
| 8 | -1.301174 | 2.360639 | -1.254167 |
| 6 | -2.389895 | 2.802480 | -0.820011 |
| 7 | -3.542683 | 2.159255 | -1.051425 |
| 6 | -2.411477 | 4.079826 | -0.033099 |
| 1 | -2.739938 | 3.880886 | 0.993682 |
| 1 | -1.393829 | 4.473706 | -0.003811 |
| 1 | -3.074319 | 4.831848 | -0.473955 |
| 6 | -3.530256 | 0.822932 | -1.628629 |
| 1 | -3.715764 | 0.080772 | -0.838848 |
| 1 | -4.314355 | 0.744447 | -2.390027 |
| 1 | -2.558252 | 0.613834 | -2.079490 |
| 6 | -4.785177 | 2.526267 | -0.398723 |
| 1 | -5.623495 | 2.207192 | -1.025923 |
| 1 | -4.866737 | 2.028682 | 0.578389 |

| | | | |
|---|---|---|---|
| 1 | -4.861334 | 3.605352 | -0.256368 |
| 6 | 2.795427 | -0.264558 | -1.659206 |
| 6 | 3.855832 | -0.770823 | -2.416872 |
| 6 | 2.089233 | -1.134189 | -0.800590 |
| 6 | 4.176984 | -2.121856 | -2.382611 |
| 1 | 4.410550 | -0.090432 | -3.061941 |
| 6 | 2.367244 | -2.509974 | -0.822176 |
| 6 | 3.428003 | -2.985776 | -1.585793 |
| 1 | 4.990325 | -2.503522 | -2.993487 |
| 1 | 1.756560 | -3.190330 | -0.232164 |
| 1 | 3.658029 | -4.049036 | -1.570022 |
| 1 | 4.350227 | 1.688937 | -1.213136 |
| 8 | 3.233848 | 3.350986 | -1.432241 |
| 1 | 2.711296 | 3.393758 | -0.600792 |
| 7 | 0.035738 | -0.754743 | -1.051872 |
| 6 | -0.678035 | -1.673390 | -0.354248 |
| 8 | -0.329915 | -0.567686 | -2.383047 |
| 1 | 0.066654 | 0.310569 | -2.564242 |
| 8 | -0.196353 | -2.044271 | 0.745051 |
| 6 | -2.003324 | -2.184394 | -0.773250 |
| 6 | -2.343518 | -2.487479 | -2.094816 |
| 6 | -2.943845 | -2.376124 | 0.247325 |
| 6 | -3.614406 | -2.973152 | -2.385808 |
| 1 | -1.615646 | -2.349861 | -2.886476 |
| 6 | -4.217105 | -2.836442 | -0.055787 |
| 1 | -2.671078 | -2.128569 | 1.270395 |
| 6 | -4.553765 | -3.138840 | -1.373473 |
| 1 | -3.870445 | -3.221311 | -3.413193 |
| 1 | -4.947582 | -2.965214 | 0.739209 |
| 1 | -5.549127 | -3.508661 | -1.609739 |
| 17 | 1.816175 | 2.109270 | 1.181930 |
| 17 | -1.724816 | 0.918718 | 1.580841 |
| 8 | 1.268930 | -0.511404 | 3.322377 |
| 6 | 0.246976 | -0.853436 | 3.904403 |
| 8 | -0.646064 | -1.696842 | 3.425650 |
| 1 | -0.473206 | -1.883372 | 2.473492 |
| 6 | -0.124421 | -0.321810 | 5.248087 |
| 1 | -0.586320 | -1.096610 | 5.864627 |
| 1 | 0.748978 | 0.107745 | 5.739584 |
| 1 | -0.868190 | 0.467470 | 5.086668 |

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**(7a-9)$_{c\text{-}3\text{-}s\text{-}AcOH}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2579.7382754

Zero-point correction= 0.442694
Thermal correction to Energy= 0.481015
Thermal correction to Enthalpy= 0.481959
Thermal correction to Gibbs Free Energy= 0.370533
Sum of electronic and zero-point Energies= -2579.295581
Sum of electronic and thermal Energies= -2579.257261
Sum of electronic and thermal Enthalpies= -2579.256316
Sum of electronic and thermal Free Energies= -2579.367743

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.176824 | 0.336665 | -1.357333 |
| 30 | -1.870553 | 0.243728 | 0.282308 |
| 8 | -0.872654 | 1.208842 | 1.706204 |
| 6 | -0.058435 | 2.152118 | 1.632148 |
| 7 | 0.495502 | 2.627422 | 2.771359 |
| 6 | 0.342937 | 2.874573 | 0.413235 |
| 6 | 0.275924 | 4.275727 | 0.435487 |
| 6 | 0.780785 | 2.200489 | -0.762882 |
| 6 | 0.596555 | 5.036639 | -0.676094 |
| 1 | -0.084898 | 4.760992 | 1.341629 |
| 6 | 1.117996 | 3.002483 | -1.881584 |
| 6 | 1.002056 | 4.379905 | -1.841173 |
| 1 | 0.510806 | 6.118808 | -0.646699 |
| 1 | 1.432230 | 2.511323 | -2.800827 |
| 1 | 1.228333 | 4.954575 | -2.737447 |
| 1 | 1.389810 | 3.095937 | 2.676877 |
| 8 | 0.401305 | 1.855097 | 3.900267 |
| 1 | 0.762040 | 0.992115 | 3.622834 |
| 7 | 2.057919 | 0.909245 | -0.575074 |
| 17 | -2.316416 | 0.617632 | -1.948239 |
| 8 | -3.809144 | 0.571344 | 1.009223 |
| 6 | -4.777975 | -0.170623 | 0.838429 |
| 8 | -4.676842 | -1.453121 | 0.582463 |
| 6 | 2.476691 | 0.310556 | 0.591610 |
| 8 | 1.885011 | 0.506547 | 1.657196 |
| 6 | 3.645319 | -0.610036 | 0.530044 |
| 6 | 3.744701 | -1.587230 | -0.465938 |
| 6 | 4.568346 | -0.578104 | 1.576275 |
| 6 | 4.782961 | -2.509606 | -0.414436 |
| 1 | 2.989565 | -1.642281 | -1.250607 |
| 6 | 5.620118 | -1.484888 | 1.604443 |
| 1 | 4.448072 | 0.164519 | 2.362373 |
| 6 | 5.727066 | -2.451187 | 0.607525 |
| 1 | 4.855632 | -3.277848 | -1.180603 |

| | | | |
|---|---|---|---|
| 1 | 6.351481 | -1.444966 | 2.408414 |
| 1 | 6.545499 | -3.167533 | 0.632690 |
| 8 | 2.960347 | 0.880703 | -1.634048 |
| 1 | 3.337034 | 1.776102 | -1.650689 |
| 6 | -6.178482 | 0.332437 | 0.878207 |
| 1 | -6.225423 | 1.253110 | 1.460930 |
| 1 | -6.485940 | 0.557549 | -0.149307 |
| 1 | -6.857546 | -0.424589 | 1.275492 |
| 1 | -3.722211 | -1.726061 | 0.600155 |
| 17 | 0.287017 | -2.111783 | -1.922055 |
| 8 | -2.022059 | -1.730240 | 0.825743 |
| 6 | -1.112829 | -2.618194 | 0.831266 |
| 6 | 0.173669 | -2.364690 | 1.544178 |
| 1 | 1.022245 | -2.549320 | 0.876437 |
| 1 | 0.206940 | -1.322981 | 1.874344 |
| 1 | 0.263169 | -3.017114 | 2.421250 |
| 7 | -1.346474 | -3.790067 | 0.253991 |
| 6 | -2.488903 | -3.889898 | -0.650239 |
| 1 | -2.517351 | -3.009291 | -1.303265 |
| 1 | -2.359002 | -4.775289 | -1.274788 |
| 1 | -3.428984 | -3.986924 | -0.095474 |
| 6 | -0.306944 | -4.800827 | 0.125411 |
| 1 | 0.327635 | -4.819085 | 1.013152 |
| 1 | -0.776776 | -5.782269 | 0.022238 |
| 1 | 0.304414 | -4.574780 | -0.759848 |

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**(7a-9)$_{c\text{-}5\text{-}AcOH}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2521.0689448
Zero-point correction= 0.373063
Thermal correction to Energy= 0.408936
Thermal correction to Enthalpy= 0.409880
Thermal correction to Gibbs Free Energy= 0.300226
Sum of electronic and zero-point Energies= -2520.695882
Sum of electronic and thermal Energies= -2520.660009
Sum of electronic and thermal Enthalpies= -2520.659064
Sum of electronic and thermal Free Energies= -2520.768719

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.158607 | -0.376700 | 1.222053 |
| 6 | 0.108486 | 2.503227 | 0.265977 |
| 6 | -0.633765 | 1.558708 | 1.020987 |
| 6 | 0.221660 | 3.834674 | 0.714443 |

| | | | |
|---|---|---|---|
| 6 | -1.307568 | 2.026858 | 2.173052 |
| 6 | -0.374889 | 4.247822 | 1.885515 |
| 1 | 0.844178 | 4.524823 | 0.142598 |
| 6 | -1.158296 | 3.328572 | 2.603275 |
| 1 | -1.944765 | 1.337352 | 2.724824 |
| 1 | -0.246607 | 5.264653 | 2.245138 |
| 1 | -1.661227 | 3.645378 | 3.514964 |
| 6 | 0.663105 | 2.141468 | -1.027989 |
| 8 | 1.321120 | 1.125647 | -1.324267 |
| 8 | 0.369287 | -2.591090 | 1.497457 |
| 6 | -0.051726 | -3.522317 | 0.817139 |
| 6 | 0.655592 | -4.834130 | 0.741218 |
| 1 | -0.053507 | -5.659897 | 0.648789 |
| 1 | 1.283022 | -4.815945 | -0.157979 |
| 1 | 1.300481 | -4.959891 | 1.611764 |
| 8 | -1.132349 | -3.468097 | 0.069363 |
| 7 | 0.482223 | 3.041287 | -2.057531 |
| 1 | 0.723040 | 2.667095 | -2.971220 |
| 8 | -0.730331 | 3.725062 | -2.119087 |
| 1 | -0.542151 | 4.617011 | -1.795642 |
| 17 | 2.140625 | 0.139096 | 2.061270 |
| 8 | -2.089527 | -1.008345 | 0.537416 |
| 6 | -2.705683 | -0.106566 | -0.143727 |
| 7 | -2.071201 | 1.031511 | -0.330520 |
| 8 | -2.831966 | 2.114485 | -0.746509 |
| 1 | -2.188827 | 2.683629 | -1.205838 |
| 6 | -4.054188 | -0.449615 | -0.653054 |
| 6 | -4.632818 | 0.179244 | -1.760560 |
| 6 | -4.742157 | -1.494141 | -0.024561 |
| 6 | -5.876175 | -0.230325 | -2.222921 |
| 1 | -4.104490 | 0.987460 | -2.252671 |
| 6 | -5.990925 | -1.891181 | -0.482674 |
| 1 | -4.282006 | -1.986945 | 0.827808 |
| 6 | -6.560577 | -1.260092 | -1.584128 |
| 1 | -6.314583 | 0.259180 | -3.089468 |
| 1 | -6.518650 | -2.698506 | 0.019548 |
| 1 | -7.537144 | -1.573003 | -1.946975 |
| 30 | 2.228584 | -0.310728 | -0.204098 |
| 17 | 2.286197 | -2.277839 | -1.357950 |
| 8 | 4.160346 | 0.397738 | -0.654348 |
| 6 | 5.135701 | -0.075986 | -1.237840 |
| 8 | 5.151018 | -1.242414 | -1.831756 |
| 1 | 4.267613 | -1.688812 | -1.749698 |
| 6 | 6.437132 | 0.647249 | -1.323521 |
| 1 | 6.341596 | 1.645664 | -0.897121 |

| | | | |
|---|---|---|---|
| 1 | 7.197702 | 0.081392 | -0.776136 |
| 1 | 6.764457 | 0.700421 | -2.365727 |
| 1 | -1.561115 | -2.576698 | 0.151535 |

---

**(7a-9)$_{a\text{-}a\text{-}5\text{-}s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1887.13375
Zero-point correction= 0.477540
Thermal correction to Energy= 0.517640
Thermal correction to Enthalpy= 0.518584
Thermal correction to Gibbs Free Energy= 0.402784
Sum of electronic and zero-point Energies= -1886.656210
Sum of electronic and thermal Energies= -1886.616110
Sum of electronic and thermal Enthalpies= -1886.615166
Sum of electronic and thermal Free Energies= -1886.730966

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 1.147304 | -0.141705 | -1.414618 |
| 30 | -0.156736 | -1.426374 | 0.436027 |
| 8 | 0.273335 | 0.251850 | 1.567866 |
| 6 | 1.476872 | 0.478396 | 1.887127 |
| 7 | 1.844857 | 0.100943 | 3.135279 |
| 8 | -1.486141 | -2.007273 | 1.928839 |
| 6 | -2.650799 | -2.294913 | 1.565878 |
| 7 | -3.493488 | -1.355070 | 1.111300 |
| 6 | -3.106636 | -3.720980 | 1.629787 |
| 1 | -2.369885 | -4.285707 | 2.202275 |
| 1 | -4.094866 | -3.839192 | 2.083874 |
| 1 | -3.141688 | -4.126991 | 0.610877 |
| 6 | -3.005286 | 0.006985 | 0.924555 |
| 1 | -2.529719 | 0.118546 | -0.062344 |
| 1 | -3.847644 | 0.702837 | 0.989695 |
| 1 | -2.274291 | 0.255831 | 1.696809 |
| 6 | -4.674331 | -1.692106 | 0.337749 |
| 1 | -5.404284 | -0.882095 | 0.423924 |
| 1 | -4.404922 | -1.815672 | -0.721699 |
| 1 | -5.141743 | -2.611028 | 0.694424 |
| 6 | 2.460240 | 1.102486 | 1.027383 |
| 6 | 3.649658 | 1.631775 | 1.577958 |
| 6 | 2.222176 | 1.202620 | -0.373459 |
| 6 | 4.626745 | 2.190127 | 0.787116 |
| 1 | 3.777258 | 1.634023 | 2.660405 |
| 6 | 3.252904 | 1.776050 | -1.166109 |

| | | | |
|---|---|---|---|
| 6 | 4.422681 | 2.236523 | -0.605062 |
| 1 | 5.530003 | 2.601196 | 1.228903 |
| 1 | 3.090269 | 1.866853 | -2.239337 |
| 1 | 5.190665 | 2.661262 | -1.249663 |
| 1 | 2.794851 | -0.175146 | 3.338969 |
| 8 | 0.945735 | -0.634661 | 3.879937 |
| 1 | 0.166454 | -0.691741 | 3.289732 |
| 6 | -0.508323 | 2.114808 | -0.789605 |
| 6 | -1.746046 | 2.857049 | -0.448762 |
| 6 | -1.877211 | 3.570858 | 0.744871 |
| 6 | -2.837659 | 2.756853 | -1.317419 |
| 6 | -3.088349 | 4.179439 | 1.058414 |
| 1 | -1.031833 | 3.636633 | 1.423175 |
| 6 | -4.036983 | 3.384832 | -1.009956 |
| 1 | -2.727220 | 2.174542 | -2.229304 |
| 6 | -4.165677 | 4.095565 | 0.181682 |
| 1 | -3.188948 | 4.725593 | 1.993684 |
| 1 | -4.876582 | 3.316719 | -1.698386 |
| 1 | -5.106897 | 4.583016 | 0.426824 |
| 8 | -0.039795 | -1.623355 | -2.620536 |
| 6 | -1.086218 | -2.120654 | -2.167422 |
| 8 | -1.432011 | -2.140846 | -0.932529 |
| 6 | -2.068695 | -2.740153 | -3.129048 |
| 1 | -1.575117 | -3.014996 | -4.062946 |
| 1 | -2.557842 | -3.609476 | -2.680068 |
| 1 | -2.844059 | -1.998848 | -3.355692 |
| 8 | 2.687257 | -1.586474 | -1.066116 |
| 6 | 2.518558 | -2.428224 | -0.149725 |
| 8 | 1.515664 | -2.510231 | 0.631056 |
| 6 | 3.601861 | -3.452448 | 0.060027 |
| 1 | 3.194924 | -4.447083 | -0.148275 |
| 1 | 4.457153 | -3.260777 | -0.589190 |
| 1 | 3.911962 | -3.447695 | 1.109218 |
| 8 | -0.657713 | 0.962738 | -1.337057 |
| 7 | 0.711891 | 2.540447 | -0.581699 |
| 8 | 0.876338 | 3.714618 | 0.147234 |
| 1 | 1.749044 | 4.014549 | -0.143881 |

---

**(7a-9)$_{a\text{-}a\text{-}7\text{-}s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1887.1411759
Zero-point correction= 0.481670
Thermal correction to Energy= 0.519811
Thermal correction to Enthalpy= 0.520756

Thermal correction to Gibbs Free Energy= 0.413524
Sum of electronic and zero-point Energies= -1886.659505
Sum of electronic and thermal Energies= -1886.621364
Sum of electronic and thermal Enthalpies= -1886.620420
Sum of electronic and thermal Free Energies= -1886.727652

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.342520 | 0.264953 | 1.499915 |
| 8 | -0.576239 | -1.557811 | 2.706783 |
| 6 | 0.452710 | -2.048123 | 2.214143 |
| 8 | 0.886956 | -1.860119 | 1.018240 |
| 6 | 1.313973 | -2.958648 | 3.058095 |
| 1 | 0.884244 | -3.095190 | 4.051781 |
| 1 | 1.422214 | -3.929065 | 2.561048 |
| 1 | 2.318205 | -2.529475 | 3.148865 |
| 30 | -0.254596 | -1.082131 | -0.458923 |
| 8 | -1.219086 | -0.070081 | -2.126901 |
| 6 | -2.295665 | 0.484579 | -1.798221 |
| 7 | -3.462269 | -0.069255 | -2.177784 |
| 8 | -1.942452 | -2.261188 | -0.490274 |
| 8 | -3.092527 | -0.975654 | 0.965726 |
| 6 | -2.957603 | -1.986104 | 0.244040 |
| 6 | -4.111552 | -2.951447 | 0.146943 |
| 1 | -3.750242 | -3.976745 | 0.265144 |
| 1 | -4.873086 | -2.728317 | 0.895527 |
| 1 | -4.549269 | -2.875848 | -0.856023 |
| 8 | 1.287307 | -1.413547 | -1.775956 |
| 6 | 2.360031 | -1.992199 | -1.498333 |
| 7 | 3.530640 | -1.363552 | -1.695402 |
| 6 | 2.366015 | -3.405831 | -0.988886 |
| 1 | 2.847074 | -3.472277 | -0.008532 |
| 1 | 1.332480 | -3.736433 | -0.880019 |
| 1 | 2.886152 | -4.071647 | -1.686995 |
| 6 | 3.564678 | -0.003263 | -2.214941 |
| 1 | 4.324251 | 0.565857 | -1.665599 |
| 1 | 3.826428 | -0.011808 | -3.280855 |
| 1 | 2.596928 | 0.483504 | -2.079691 |
| 6 | 4.833765 | -1.942370 | -1.439820 |
| 1 | 5.443814 | -1.908180 | -2.351490 |
| 1 | 5.348009 | -1.363500 | -0.660997 |
| 1 | 4.761832 | -2.979313 | -1.113261 |
| 6 | -2.377736 | 1.691038 | -0.971582 |
| 6 | -3.268917 | 2.716070 | -1.319728 |
| 6 | -1.565318 | 1.811708 | 0.191669 |

| | | | |
|---|---|---|---|
| 6 | -3.335326 | 3.887062 | -0.586224 |
| 1 | -3.883619 | 2.590641 | -2.210845 |
| 6 | -1.604309 | 3.041631 | 0.888591 |
| 6 | -2.487055 | 4.039395 | 0.516970 |
| 1 | -4.013552 | 4.683593 | -0.878455 |
| 1 | -0.948457 | 3.179754 | 1.745655 |
| 1 | -2.515203 | 4.960121 | 1.097209 |
| 1 | -4.313627 | 0.129646 | -1.664701 |
| 8 | -3.455366 | -1.277849 | -2.826436 |
| 1 | -2.803688 | -1.813812 | -2.324059 |
| 7 | 0.253555 | 1.307178 | -0.308372 |
| 6 | 1.109391 | 1.435146 | 0.733519 |
| 8 | 0.675026 | 1.821588 | -1.531624 |
| 1 | 0.211300 | 1.219780 | -2.148705 |
| 8 | 0.663579 | 1.177168 | 1.873368 |
| 6 | 2.544237 | 1.750179 | 0.556481 |
| 6 | 3.004394 | 2.819543 | -0.214362 |
| 6 | 3.454984 | 0.928677 | 1.228770 |
| 6 | 4.369800 | 3.068413 | -0.301353 |
| 1 | 2.292715 | 3.449495 | -0.739545 |
| 6 | 4.819287 | 1.165245 | 1.112904 |
| 1 | 3.070983 | 0.107113 | 1.830666 |
| 6 | 5.278262 | 2.240090 | 0.352793 |
| 1 | 4.726307 | 3.912639 | -0.886816 |
| 1 | 5.526823 | 0.523659 | 1.634280 |
| 1 | 6.345478 | 2.436520 | 0.276689 |

---

**(7a-9)$_{a\text{-}a\text{-}3\text{-}s\text{-}N^{\ddagger}}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1887.1408835
Zero-point correction= 0.481256
Thermal correction to Energy= 0.519810
Thermal correction to Enthalpy= 0.520754
Thermal correction to Gibbs Free Energy= 0.410764
Sum of electronic and zero-point Energies= -1886.659628
Sum of electronic and thermal Energies= -1886.621073
Sum of electronic and thermal Enthalpies= -1886.620129
Sum of electronic and thermal Free Energies= -1886.730119

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.902360 | 1.519980 | -1.065192 |
| 8 | -1.897291 | 0.301208 | -2.758702 |
| 6 | -1.770521 | -0.935730 | -2.767478 |

| | | | |
|---|---|---|---|
| 8 | -1.333779 | -1.653443 | -1.796722 |
| 30 | -1.266249 | -0.797261 | 0.041086 |
| 8 | -0.664406 | -0.078034 | 1.933201 |
| 6 | 0.340037 | 0.616486 | 2.150344 |
| 7 | 1.300234 | 0.178518 | 2.987385 |
| 6 | 0.592249 | 1.967035 | 1.587802 |
| 6 | 0.729581 | 2.990595 | 2.527243 |
| 6 | 0.532440 | 2.298256 | 0.188141 |
| 6 | 0.800715 | 4.333234 | 2.174016 |
| 1 | 0.721777 | 2.718950 | 3.582675 |
| 6 | 0.648467 | 3.679108 | -0.146638 |
| 6 | 0.734636 | 4.663636 | 0.823734 |
| 1 | 0.885652 | 5.100819 | 2.937048 |
| 1 | 0.612383 | 3.955753 | -1.198691 |
| 1 | 0.756206 | 5.706187 | 0.513028 |
| 1 | 2.104212 | 0.740385 | 3.233491 |
| 8 | 1.106350 | -0.917604 | 3.782453 |
| 1 | 1.082105 | -1.686829 | 3.165539 |
| 7 | 1.329210 | 1.396858 | -0.898573 |
| 6 | -2.168889 | -1.703465 | -4.005519 |
| 1 | -2.358027 | -1.026413 | -4.840147 |
| 1 | -1.388419 | -2.423494 | -4.269164 |
| 1 | -3.078521 | -2.276071 | -3.794011 |
| 6 | 1.753405 | 0.110964 | -0.630493 |
| 8 | 0.943846 | -0.692230 | -0.145913 |
| 6 | 3.164593 | -0.322748 | -0.797762 |
| 6 | 4.028476 | 0.056741 | -1.831782 |
| 6 | 3.608352 | -1.246735 | 0.163236 |
| 6 | 5.314418 | -0.468620 | -1.888671 |
| 1 | 3.686940 | 0.739302 | -2.601111 |
| 6 | 4.901672 | -1.745021 | 0.111089 |
| 1 | 2.923153 | -1.572612 | 0.945625 |
| 6 | 5.758462 | -1.357556 | -0.915962 |
| 1 | 5.972068 | -0.181161 | -2.705448 |
| 1 | 5.239226 | -2.445859 | 0.870800 |
| 1 | 6.768987 | -1.756932 | -0.963435 |
| 8 | 2.214501 | 2.157252 | -1.646698 |
| 1 | 2.584514 | 2.809740 | -1.022191 |
| 8 | -2.885881 | 1.630707 | 0.025062 |
| 6 | -3.582454 | 0.667551 | 0.406668 |
| 8 | -3.206499 | -0.554137 | 0.464663 |
| 6 | -5.004414 | 0.934144 | 0.834177 |
| 1 | -5.209108 | 2.005462 | 0.864254 |
| 1 | -5.685953 | 0.453419 | 0.124463 |
| 1 | -5.189045 | 0.484337 | 1.814299 |

| | | | |
|---|---|---|---|
| 8 | 0.991118 | -2.943894 | 1.942756 |
| 6 | 0.245794 | -3.207402 | 1.007118 |
| 7 | -1.130571 | -2.967131 | 1.077053 |
| 6 | -2.026002 | -3.758869 | 0.215886 |
| 1 | -2.080039 | -4.799736 | 0.565391 |
| 1 | -3.022179 | -3.311214 | 0.270469 |
| 1 | -1.705858 | -3.713219 | -0.825118 |
| 6 | -1.698633 | -2.785007 | 2.422968 |
| 1 | -2.672780 | -2.300167 | 2.312891 |
| 1 | -1.819719 | -3.759937 | 2.914441 |
| 1 | -1.062055 | -2.136597 | 3.019807 |
| 6 | 0.774781 | -3.764113 | -0.281140 |
| 1 | 0.465107 | -4.808809 | -0.405121 |
| 1 | 0.402277 | -3.193249 | -1.139014 |
| 1 | 1.864353 | -3.714523 | -0.248251 |

---

**(7a-9)*a-c-3-AcOH*‡**

---

Number of imaginary frequencies : 1
Electronic energy =-2060.2722242
Zero-point correction= 0.359867
Thermal correction to Energy= 0.393381
Thermal correction to Enthalpy= 0.394325
Thermal correction to Gibbs Free Energy= 0.290748
Sum of electronic and zero-point Energies= -2059.912357
Sum of electronic and thermal Energies= -2059.878843
Sum of electronic and thermal Enthalpies= -2059.877899
Sum of electronic and thermal Free Energies= -2059.981476

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.013650 | 0.038208 | -1.450017 |
| 30 | -2.174055 | 0.063789 | 0.084468 |
| 8 | -0.993920 | 0.769041 | 1.536056 |
| 6 | 0.003999 | 1.512150 | 1.601901 |
| 7 | 0.522461 | 1.784140 | 2.826030 |
| 6 | 0.662397 | 2.232793 | 0.493460 |
| 6 | 0.865475 | 3.609199 | 0.673650 |
| 6 | 1.031499 | 1.623308 | -0.744153 |
| 6 | 1.387202 | 4.412720 | -0.327051 |
| 1 | 0.551547 | 4.055157 | 1.616209 |
| 6 | 1.546472 | 2.469393 | -1.758703 |
| 6 | 1.700536 | 3.829830 | -1.555086 |
| 1 | 1.511397 | 5.479706 | -0.167555 |
| 1 | 1.763036 | 2.041986 | -2.735339 |

| | | | |
|---|---|---|---|
| 1 | 2.060316 | 4.447880 | -2.375445 |
| 1 | 1.512196 | 2.001650 | 2.857436 |
| 8 | 0.108304 | 1.008144 | 3.879710 |
| 1 | 0.190725 | 0.093565 | 3.554128 |
| 7 | 1.983523 | 0.103192 | -0.710764 |
| 17 | -2.311149 | 1.125294 | -1.953128 |
| 8 | -0.905686 | -2.074360 | -1.815434 |
| 6 | -1.782353 | -2.556456 | -1.096726 |
| 6 | -2.266459 | -3.964071 | -1.317559 |
| 1 | -1.737498 | -4.427280 | -2.151327 |
| 1 | -2.114276 | -4.552246 | -0.406783 |
| 1 | -3.342585 | -3.957029 | -1.522240 |
| 8 | -2.354221 | -1.931646 | -0.108265 |
| 6 | 2.386673 | -0.448139 | 0.487791 |
| 8 | 1.658153 | -0.350789 | 1.474983 |
| 6 | 3.713474 | -1.125458 | 0.597287 |
| 6 | 4.285955 | -1.914587 | -0.405427 |
| 6 | 4.349829 | -1.031654 | 1.839272 |
| 6 | 5.485362 | -2.575365 | -0.169278 |
| 1 | 3.788619 | -2.017958 | -1.363847 |
| 6 | 5.560103 | -1.672792 | 2.062993 |
| 1 | 3.872984 | -0.452261 | 2.625833 |
| 6 | 6.130747 | -2.446674 | 1.056736 |
| 1 | 5.918041 | -3.196249 | -0.950118 |
| 1 | 6.053763 | -1.577461 | 3.027282 |
| 1 | 7.075259 | -2.957208 | 1.231350 |
| 8 | 2.913682 | 0.100458 | -1.740000 |
| 1 | 3.352405 | 0.968951 | -1.686748 |
| 8 | -3.958605 | 0.178605 | 1.124945 |
| 6 | -4.785077 | -0.699242 | 1.397220 |
| 6 | -6.039166 | -0.386509 | 2.140399 |
| 1 | -6.894477 | -0.849368 | 1.640949 |
| 1 | -5.974795 | -0.822773 | 3.142693 |
| 1 | -6.172750 | 0.692256 | 2.219546 |
| 8 | -4.649945 | -1.959484 | 1.090460 |
| 1 | -3.778844 | -2.114317 | 0.607026 |

## Pd-Zn Heterobimetallic Complexes when Acetate as Ligand

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**Pd-Zn-1**

---

Number of imaginary frequencies : 0
Electronic energy =-1569.4183989
Zero-point correction= 0.106385
Thermal correction to Energy= 0.123106

Thermal correction to Enthalpy= 0.124050
Thermal correction to Gibbs Free Energy= 0.056462
Sum of electronic and zero-point Energies= -1569.312014
Sum of electronic and thermal Energies= -1569.295293
Sum of electronic and thermal Enthalpies= -1569.294348
Sum of electronic and thermal Free Energies= -1569.361937

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -1.493741 | 0.001224 | -0.064980 |
| 17 | 0.184176 | 1.687584 | -0.188519 |
| 17 | 0.190693 | -1.677443 | -0.195171 |
| 30 | 1.808352 | 0.008263 | -0.080685 |
| 8 | -3.244788 | 1.080220 | 0.101212 |
| 8 | -3.235810 | -1.090612 | 0.096595 |
| 8 | 3.391144 | 0.001082 | 1.212895 |
| 8 | 3.633726 | 0.004663 | -0.973438 |
| 6 | -3.907473 | -0.008042 | 0.164341 |
| 6 | 4.146772 | -0.002191 | 0.192386 |
| 6 | 5.632037 | -0.023924 | 0.343449 |
| 1 | 6.066708 | 0.805334 | -0.221695 |
| 1 | 5.920304 | 0.038105 | 1.393176 |
| 1 | 6.020139 | -0.948406 | -0.095192 |
| 6 | -5.378634 | -0.014530 | 0.331638 |
| 1 | -5.617320 | 0.038916 | 1.399202 |
| 1 | -5.814532 | 0.858330 | -0.160359 |
| 1 | -5.796911 | -0.939587 | -0.071776 |

---

**Pd-Zn-2**

---

Number of imaginary frequencies : 0
Electronic energy =-2144.7948332
Zero-point correction= 0.373175
Thermal correction to Energy= 0.406488
Thermal correction to Enthalpy= 0.407432
Thermal correction to Gibbs Free Energy= 0.306228
Sum of electronic and zero-point Energies= -2144.421658
Sum of electronic and thermal Energies= -2144.388345
Sum of electronic and thermal Enthalpies= -2144.387401
Sum of electronic and thermal Free Energies= -2144.488605

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 1.639609 | -1.317830 | -0.035053 |
| 8 | 0.285223 | -2.794719 | -0.584198 |

| | | | |
|---|---|---|---|
| 6 | -0.861363 | -2.490095 | -1.000745 |
| 8 | -1.393561 | -1.340171 | -0.962858 |
| 6 | -1.666960 | -3.599682 | -1.617527 |
| 1 | -1.546145 | -3.539679 | -2.704549 |
| 1 | -1.307048 | -4.574036 | -1.283373 |
| 1 | -2.729162 | -3.475315 | -1.390757 |
| 30 | -0.567932 | 0.249868 | -0.061042 |
| 8 | 0.205603 | 1.828785 | -0.980513 |
| 6 | 1.289390 | 2.462730 | -0.959880 |
| 6 | 2.148645 | 2.468113 | -2.180279 |
| 1 | 1.529439 | 2.176050 | -3.029568 |
| 1 | 2.626921 | 3.431115 | -2.376100 |
| 1 | 2.913488 | 1.687750 | -2.053361 |
| 7 | 1.652298 | 3.146608 | 0.132267 |
| 6 | 0.829522 | 3.046348 | 1.327066 |
| 1 | 1.066252 | 2.121605 | 1.872107 |
| 1 | 1.036839 | 3.908641 | 1.967464 |
| 1 | -0.229974 | 3.043585 | 1.058980 |
| 6 | 2.980213 | 3.689369 | 0.350801 |
| 1 | 2.912981 | 4.746352 | 0.635074 |
| 1 | 3.469005 | 3.127115 | 1.156410 |
| 1 | 3.600954 | 3.594845 | -0.538939 |
| 8 | -0.421824 | -0.011830 | 1.938051 |
| 8 | 1.161544 | -1.615756 | 1.974392 |
| 6 | 0.298816 | -0.884918 | 2.517821 |
| 6 | 0.093281 | -1.049860 | 3.998807 |
| 1 | -0.969962 | -1.203355 | 4.208770 |
| 1 | 0.681504 | -1.881935 | 4.387197 |
| 1 | 0.392478 | -0.123995 | 4.500673 |
| 17 | 2.102631 | -1.004197 | -2.279150 |
| 8 | -2.441826 | 1.173710 | 0.000767 |
| 6 | -3.528424 | 0.628503 | 0.268115 |
| 7 | -4.662758 | 1.057065 | -0.323564 |
| 6 | -3.609087 | -0.501083 | 1.256123 |
| 1 | -3.732528 | -1.455439 | 0.730631 |
| 1 | -2.670577 | -0.530735 | 1.815944 |
| 1 | -4.437791 | -0.380703 | 1.959658 |
| 6 | -4.629875 | 2.174791 | -1.251374 |
| 1 | -4.946073 | 1.845913 | -2.248628 |
| 1 | -5.313911 | 2.960982 | -0.908726 |
| 1 | -3.616139 | 2.569109 | -1.307011 |
| 6 | -5.974804 | 0.481789 | -0.104213 |
| 1 | -6.596633 | 1.135918 | 0.521950 |
| 1 | -6.476749 | 0.358871 | -1.070956 |
| 1 | -5.911884 | -0.501136 | 0.363044 |

| | | | |
|---|---|---|---|
| 17 | 3.165984 | 0.308947 | 0.620526 |

---

**Pd-Zn-3**

---

Number of imaginary frequencies : 0
Electronic energy =-2144.7468444
Zero-point correction= 0.373546
Thermal correction to Energy= 0.405588
Thermal correction to Enthalpy= 0.406532
Thermal correction to Gibbs Free Energy= 0.309517
Sum of electronic and zero-point Energies= -2144.373298
Sum of electronic and thermal Energies= -2144.341256
Sum of electronic and thermal Enthalpies= -2144.340312
Sum of electronic and thermal Free Energies= -2144.437328

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.706118 | 0.025320 | -0.688521 |
| 8 | 0.228842 | -1.466481 | -1.729638 |
| 6 | 1.479498 | -1.715557 | -1.577908 |
| 8 | 2.250468 | -1.166828 | -0.778262 |
| 6 | 2.008100 | -2.815033 | -2.460024 |
| 1 | 2.178399 | -3.701663 | -1.839272 |
| 1 | 1.315668 | -3.063433 | -3.265731 |
| 1 | 2.978004 | -2.514339 | -2.864121 |
| 30 | 2.546074 | -0.026059 | 0.928234 |
| 8 | 1.746180 | 1.671756 | 0.035030 |
| 8 | 0.511111 | 1.269129 | -1.782391 |
| 6 | 1.561775 | 1.712149 | -1.200089 |
| 6 | 2.616568 | 2.300411 | -2.088042 |
| 1 | 3.474483 | 1.616392 | -2.058227 |
| 1 | 2.276305 | 2.421199 | -3.117468 |
| 1 | 2.959375 | 3.250771 | -1.670542 |
| 17 | 0.976455 | -0.707250 | 2.427135 |
| 17 | 4.732176 | 0.260309 | 1.146583 |
| 7 | -1.679247 | 1.799776 | 0.206441 |
| 7 | -2.012721 | -1.685181 | -0.036987 |
| 6 | -1.388976 | 3.009526 | -0.613604 |
| 1 | -1.994215 | 3.847222 | -0.239474 |
| 1 | -0.335386 | 3.260201 | -0.498804 |
| 1 | -1.598190 | 2.833523 | -1.669416 |
| 6 | -1.127815 | 2.011784 | 1.569271 |
| 1 | -1.342863 | 1.153056 | 2.203408 |
| 1 | -0.046488 | 2.121633 | 1.478315 |
| 1 | -1.580889 | 2.906616 | 2.013008 |

| | | | |
|---|---|---|---|
| 6 | -1.145942 | -2.781063 | 0.480921 |
| 1 | -0.525919 | -3.138042 | -0.341099 |
| 1 | -0.494929 | -2.416755 | 1.280776 |
| 1 | -1.776614 | -3.607331 | 0.836554 |
| 6 | -2.645404 | -2.107437 | -1.311176 |
| 1 | -1.853274 | -2.310293 | -2.032734 |
| 1 | -3.247127 | -3.009590 | -1.142080 |
| 1 | -3.305099 | -1.320860 | -1.679368 |
| 6 | -3.034858 | -1.319823 | 0.939131 |
| 6 | -3.131179 | 1.624034 | 0.244255 |
| 6 | -3.818484 | 1.506596 | -1.083117 |
| 1 | -3.149793 | 1.188059 | -1.888773 |
| 1 | -4.636141 | 0.791764 | -0.961142 |
| 1 | -4.253079 | 2.476538 | -1.352396 |
| 6 | -2.618412 | -1.247756 | 2.372417 |
| 1 | -1.569735 | -0.969654 | 2.519500 |
| 1 | -3.287554 | -0.545449 | 2.873885 |
| 1 | -2.760951 | -2.235566 | 2.828838 |
| 8 | -3.705833 | 1.603450 | 1.299657 |
| 8 | -4.162889 | -1.122040 | 0.560571 |

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**Pd-Zn-4**

---

Number of imaginary frequencies : 0
Electronic energy =-2144.7849537
Zero-point correction= 0.374122
Thermal correction to Energy= 0.406770
Thermal correction to Enthalpy= 0.407714
Thermal correction to Gibbs Free Energy= 0.309325
Sum of electronic and zero-point Energies= -2144.410831
Sum of electronic and thermal Energies= -2144.378184
Sum of electronic and thermal Enthalpies= -2144.377240
Sum of electronic and thermal Free Energies= -2144.475628

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.713691 | 0.843208 | -0.522486 |
| 8 | -2.307127 | 1.084516 | 1.449701 |
| 6 | -1.600594 | 0.616812 | 2.382234 |
| 8 | -0.601595 | -0.147564 | 2.255976 |
| 6 | -1.977080 | 1.011136 | 3.783588 |
| 1 | -1.116550 | 1.491997 | 4.260366 |
| 1 | -2.835438 | 1.683727 | 3.791809 |
| 1 | -2.198120 | 0.109265 | 4.362303 |
| 30 | 0.019839 | -1.259544 | 0.727873 |

| | | | |
|---|---|---|---|
| 17 | 1.449962 | -2.932588 | 1.324402 |
| 8 | 1.479902 | -0.115914 | -0.253082 |
| 6 | 2.298803 | -0.832466 | -0.882120 |
| 6 | 1.856216 | -1.556187 | -2.114955 |
| 1 | 0.887561 | -1.146185 | -2.418142 |
| 1 | 2.563852 | -1.467264 | -2.944638 |
| 1 | 1.737603 | -2.621562 | -1.875387 |
| 7 | 3.563469 | -0.961722 | -0.448536 |
| 6 | 3.917227 | -0.449837 | 0.868092 |
| 1 | 4.965078 | -0.131085 | 0.859851 |
| 1 | 3.275117 | 0.395344 | 1.116900 |
| 1 | 3.767828 | -1.235082 | 1.621576 |
| 6 | 4.448609 | -2.003634 | -0.942766 |
| 1 | 5.486445 | -1.691621 | -0.791771 |
| 1 | 4.271376 | -2.937474 | -0.390801 |
| 1 | 4.299909 | -2.185160 | -2.007511 |
| 8 | -1.463589 | -2.182492 | -0.252127 |
| 8 | -3.047193 | -0.654111 | -0.738347 |
| 6 | -2.618646 | -1.841917 | -0.610272 |
| 6 | -3.602266 | -2.929935 | -0.931774 |
| 1 | -3.591139 | -3.675954 | -0.132847 |
| 1 | -4.606417 | -2.529825 | -1.076013 |
| 1 | -3.273617 | -3.427488 | -1.849822 |
| 17 | -1.164209 | 0.554691 | -2.764358 |
| 8 | -0.381275 | 2.400258 | -0.062452 |
| 6 | 0.771557 | 2.641516 | -0.482698 |
| 7 | 1.756682 | 2.799596 | 0.419756 |
| 6 | 1.083076 | 2.818727 | -1.933645 |
| 1 | 1.704492 | 3.702102 | -2.111761 |
| 1 | 1.615651 | 1.937883 | -2.314107 |
| 1 | 0.147303 | 2.893348 | -2.487788 |
| 6 | 1.448030 | 2.518573 | 1.818840 |
| 1 | 1.309772 | 1.439862 | 1.987431 |
| 1 | 2.262253 | 2.892821 | 2.443640 |
| 1 | 0.518540 | 3.021097 | 2.098501 |
| 6 | 3.138038 | 2.984380 | 0.010753 |
| 1 | 3.275606 | 3.912966 | -0.554638 |
| 1 | 3.764969 | 3.042319 | 0.903176 |
| 1 | 3.492895 | 2.143324 | -0.600476 |

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**Pd-Zn-5**

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Number of imaginary frequencies : 0
Electronic energy =-1857.1087826
Zero-point correction= 0.241483

Thermal correction to Energy= 0.265492
Thermal correction to Enthalpy= 0.266436
Thermal correction to Gibbs Free Energy= 0.186539
Sum of electronic and zero-point Energies= -1856.867299
Sum of electronic and thermal Energies= -1856.843291
Sum of electronic and thermal Enthalpies= -1856.842347
Sum of electronic and thermal Free Energies= -1856.922244

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.590601 | -1.204687 | -0.512483 |
| 8 | -2.409087 | -1.643061 | 0.483762 |
| 6 | -3.009774 | -0.861614 | -0.315363 |
| 6 | -4.490903 | -0.721384 | -0.277487 |
| 1 | -4.821423 | 0.092514 | -0.926447 |
| 1 | -4.942789 | -1.657979 | -0.620125 |
| 1 | -4.827329 | -0.558307 | 0.751411 |
| 8 | -2.308296 | -0.216504 | -1.166904 |
| 8 | 0.716409 | -2.467798 | 0.372320 |
| 6 | 1.783839 | -2.137922 | 0.981209 |
| 8 | 2.272964 | -0.987907 | 1.086171 |
| 6 | 2.521660 | -3.270867 | 1.636934 |
| 1 | 2.743684 | -2.999786 | 2.672754 |
| 1 | 1.951251 | -4.199250 | 1.596800 |
| 1 | 3.479518 | -3.402276 | 1.123626 |
| 30 | 1.940058 | 0.689366 | 0.073904 |
| 17 | 3.412140 | 2.300436 | -0.247720 |
| 17 | 1.069329 | -0.343334 | -1.947739 |
| 8 | 0.233990 | 1.359109 | 0.979121 |
| 6 | -0.704766 | 2.015268 | 0.474419 |
| 6 | -0.532166 | 2.735136 | -0.825926 |
| 1 | -0.872195 | 2.076181 | -1.637291 |
| 1 | -1.092441 | 3.671579 | -0.879403 |
| 1 | 0.531046 | 2.947658 | -0.977006 |
| 7 | -1.900129 | 2.049457 | 1.084862 |
| 6 | -3.056921 | 2.689236 | 0.477355 |
| 1 | -3.162909 | 2.387993 | -0.570557 |
| 1 | -3.951827 | 2.367962 | 1.016808 |
| 1 | -3.002975 | 3.783031 | 0.537966 |
| 6 | -2.102005 | 1.346035 | 2.343724 |
| 1 | -2.575512 | 2.016615 | 3.068729 |
| 1 | -2.738712 | 0.463170 | 2.197408 |
| 1 | -1.137171 | 1.014570 | 2.726222 |

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**Pd-Zn-6**

---

Number of imaginary frequencies : 0
Electronic energy =-2144.7885957
Zero-point correction= 0.372240
Thermal correction to Energy= 0.405923
Thermal correction to Enthalpy= 0.406868
Thermal correction to Gibbs Free Energy= 0.304560
Sum of electronic and zero-point Energies= -2144.416356
Sum of electronic and thermal Energies= -2144.382672
Sum of electronic and thermal Enthalpies= -2144.381728
Sum of electronic and thermal Free Energies= -2144.484035

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.898729 | -0.596223 | -0.334624 |
| 8 | -0.316608 | -2.336163 | 0.586132 |
| 6 | 0.744030 | -2.472756 | 1.273195 |
| 8 | 1.672246 | -1.641911 | 1.400842 |
| 6 | 0.882172 | -3.784032 | 1.999817 |
| 1 | 1.148514 | -3.588079 | 3.042192 |
| 1 | -0.031651 | -4.377042 | 1.944132 |
| 1 | 1.711697 | -4.340162 | 1.551539 |
| 30 | 2.327455 | -0.203214 | 0.164107 |
| 17 | 0.943282 | -0.588935 | -1.794240 |
| 8 | 1.167840 | 1.278732 | 1.025612 |
| 6 | 0.770034 | 2.361450 | 0.542310 |
| 6 | 1.401868 | 2.947028 | -0.682378 |
| 1 | 0.789998 | 2.677564 | -1.554464 |
| 1 | 1.489520 | 4.035491 | -0.635996 |
| 1 | 2.400150 | 2.516826 | -0.802505 |
| 7 | -0.255835 | 2.990267 | 1.143272 |
| 6 | -1.009769 | 4.078963 | 0.554736 |
| 1 | -1.979766 | 3.705940 | 0.197191 |
| 1 | -1.175463 | 4.865570 | 1.300311 |
| 1 | -0.488657 | 4.511668 | -0.299001 |
| 6 | -0.899419 | 2.309233 | 2.258873 |
| 1 | -0.149059 | 1.945703 | 2.963276 |
| 1 | -1.559450 | 3.020391 | 2.764800 |
| 1 | -1.483372 | 1.446703 | 1.904508 |
| 17 | -1.832245 | 1.266212 | -1.414616 |
| 8 | 4.002775 | 1.021465 | -0.091841 |
| 6 | 4.670954 | -0.002072 | -0.449125 |
| 6 | 6.117634 | 0.157398 | -0.811157 |
| 1 | 6.459576 | -0.684439 | -1.415819 |
| 1 | 6.276211 | 1.102636 | -1.335827 |

| | | | |
|---|---|---|---|
| 1 | 6.709156 | 0.187629 | 0.110292 |
| 8 | 4.129488 | -1.139234 | -0.472190 |
| 8 | -2.543794 | -0.534277 | 1.028219 |
| 6 | -3.682873 | -0.252616 | 0.583660 |
| 6 | -4.416068 | 0.893237 | 1.212586 |
| 1 | -5.496562 | 0.747241 | 1.284352 |
| 1 | -4.002413 | 1.044142 | 2.211780 |
| 1 | -4.210339 | 1.796053 | 0.621188 |
| 7 | -4.259730 | -0.958601 | -0.400036 |
| 6 | -5.355771 | -0.453598 | -1.207287 |
| 1 | -4.971104 | -0.141168 | -2.187511 |
| 1 | -6.106236 | -1.238231 | -1.353829 |
| 1 | -5.834354 | 0.407140 | -0.740589 |
| 6 | -3.556626 | -2.095653 | -0.974277 |
| 1 | -4.299264 | -2.789628 | -1.380483 |
| 1 | -2.885358 | -1.772298 | -1.784373 |
| 1 | -2.965140 | -2.600690 | -0.207716 |

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**Pd-Zn-7**

---

Number of imaginary frequencies : 0
Electronic energy =-2144.7804376
Zero-point correction= 0.373789
Thermal correction to Energy= 0.406553
Thermal correction to Enthalpy= 0.407497
Thermal correction to Gibbs Free Energy= 0.309245
Sum of electronic and zero-point Energies= -2144.406649
Sum of electronic and thermal Energies= -2144.373884
Sum of electronic and thermal Enthalpies= -2144.372940
Sum of electronic and thermal Free Energies= -2144.471193

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.387014 | -0.599832 | -0.401786 |
| 8 | -2.975827 | 0.504107 | -1.553013 |
| 6 | -2.170869 | 1.410744 | -1.354211 |
| 6 | -2.535940 | 2.853645 | -1.637439 |
| 1 | -2.728171 | 3.371970 | -0.689015 |
| 1 | -1.714622 | 3.372845 | -2.141285 |
| 1 | -3.438564 | 2.894610 | -2.250455 |
| 8 | -0.973112 | 1.285693 | -0.868111 |
| 8 | 0.167966 | -2.510622 | 0.110769 |
| 6 | 1.267142 | -2.811956 | 0.669511 |
| 8 | 2.228737 | -2.039058 | 0.905101 |
| 6 | 1.423216 | -4.247494 | 1.088364 |

| | | | |
|---|---|---|---|
| 1 | 1.738706 | -4.281125 | 2.134971 |
| 1 | 0.500366 | -4.812063 | 0.949732 |
| 1 | 2.225371 | -4.698403 | 0.495633 |
| 30 | 2.750368 | -0.307571 | 0.077504 |
| 17 | 4.874678 | 0.266417 | -0.182401 |
| 17 | 1.406777 | -0.384345 | -1.929387 |
| 8 | 1.667908 | 1.060604 | 1.131308 |
| 6 | 1.368388 | 2.220903 | 0.766244 |
| 6 | 2.112706 | 2.900230 | -0.338524 |
| 1 | 1.553583 | 2.739599 | -1.270809 |
| 1 | 2.227493 | 3.976041 | -0.186689 |
| 1 | 3.102310 | 2.444101 | -0.446252 |
| 7 | 0.346821 | 2.865079 | 1.349690 |
| 6 | -0.120480 | 4.151027 | 0.860160 |
| 1 | -0.381384 | 4.106409 | -0.204401 |
| 1 | -1.018263 | 4.426571 | 1.418944 |
| 1 | 0.623999 | 4.940128 | 1.013752 |
| 6 | -0.521953 | 2.156327 | 2.276380 |
| 1 | -0.767266 | 2.806929 | 3.122106 |
| 1 | -1.440976 | 1.846732 | 1.758913 |
| 1 | -0.015527 | 1.260632 | 2.635415 |
| 8 | -2.028445 | -0.714580 | 0.923004 |
| 6 | -3.070697 | -1.223686 | 0.438269 |
| 6 | -3.027672 | -2.406118 | -0.476362 |
| 1 | -3.220706 | -2.062941 | -1.498941 |
| 1 | -2.033889 | -2.856120 | -0.431208 |
| 1 | -3.775033 | -3.158042 | -0.205461 |
| 7 | -4.265345 | -0.718134 | 0.798299 |
| 6 | -4.270041 | 0.536408 | 1.531731 |
| 1 | -4.039880 | 1.371459 | 0.852386 |
| 1 | -5.260218 | 0.689507 | 1.969337 |
| 1 | -3.526043 | 0.509157 | 2.328705 |
| 6 | -5.461462 | -0.981071 | 0.013932 |
| 1 | -6.344294 | -0.773959 | 0.625399 |
| 1 | -5.472532 | -0.337726 | -0.877010 |
| 1 | -5.509761 | -2.023673 | -0.303058 |

## 3. Nucleophilic Addition Elimination

3.2. Concerted pathway

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**$(9\text{-}P)_4^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-950.3461629

Zero-point correction= 0.241372
Thermal correction to Energy= 0.257919
Thermal correction to Enthalpy= 0.258863
Thermal correction to Gibbs Free Energy= 0.196148
Sum of electronic and zero-point Energies= -950.104791
Sum of electronic and thermal Energies= -950.088244
Sum of electronic and thermal Enthalpies= -950.087300
Sum of electronic and thermal Free Energies= -950.150015

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -2.368067 | 1.977660 | 0.225510 |
| 6 | -1.880258 | 0.665208 | 0.280545 |
| 6 | -0.571439 | 0.359058 | -0.157541 |
| 6 | 0.172034 | 1.383038 | -0.778115 |
| 6 | -0.345107 | 2.662920 | -0.854914 |
| 6 | -1.606943 | 2.983837 | -0.340679 |
| 1 | -3.364058 | 2.177431 | 0.617563 |
| 1 | 1.152539 | 1.173529 | -1.191706 |
| 1 | 0.250075 | 3.434896 | -1.337506 |
| 1 | -1.990051 | 3.997944 | -0.404761 |
| 6 | -2.755561 | -0.382607 | 0.831244 |
| 8 | -3.351296 | -0.446197 | 1.866580 |
| 7 | -3.336472 | -1.280104 | -0.346580 |
| 1 | -4.123881 | -1.817470 | 0.023052 |
| 8 | -3.819736 | -0.570912 | -1.446140 |
| 1 | -3.158648 | 0.135333 | -1.573154 |
| 7 | -0.161145 | -0.941285 | 0.063320 |
| 6 | 1.098437 | -1.525229 | -0.153448 |
| 8 | 1.198378 | -2.707158 | -0.406974 |
| 6 | 2.298519 | -0.659723 | 0.020928 |
| 6 | 3.381493 | -0.861453 | -0.836014 |
| 6 | 2.409303 | 0.248106 | 1.076735 |
| 6 | 4.548101 | -0.125751 | -0.670173 |
| 1 | 3.289686 | -1.604987 | -1.624516 |
| 6 | 3.584630 | 0.967073 | 1.253685 |
| 1 | 1.573934 | 0.380411 | 1.761399 |
| 6 | 4.649500 | 0.789906 | 0.373919 |
| 1 | 5.384176 | -0.273378 | -1.349611 |
| 1 | 3.672584 | 1.665824 | 2.082156 |
| 1 | 5.566071 | 1.359641 | 0.509386 |
| 8 | -1.153734 | -1.790653 | 0.407293 |
| 1 | -2.445855 | -1.852356 | -0.525640 |

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**$(9\text{-P})_6^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1297.1979727
Zero-point correction= 0.389598
Thermal correction to Energy= 0.414741
Thermal correction to Enthalpy= 0.415685
Thermal correction to Gibbs Free Energy= 0.334430
Sum of electronic and zero-point Energies= -1296.808374
Sum of electronic and thermal Energies= -1296.783232
Sum of electronic and thermal Enthalpies= -1296.782288
Sum of electronic and thermal Free Energies= -1296.863543

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.050282 | 3.634805 | -0.533216 |
| 6 | -0.578243 | 2.333777 | -0.412998 |
| 6 | -1.443656 | 1.235933 | -0.489186 |
| 6 | -2.806764 | 1.449156 | -0.701889 |
| 6 | -3.269438 | 2.756375 | -0.808285 |
| 6 | -2.409321 | 3.850129 | -0.726005 |
| 1 | -0.343266 | 4.460645 | -0.489358 |
| 1 | -3.495583 | 0.616958 | -0.806017 |
| 1 | -4.330502 | 2.919404 | -0.982061 |
| 1 | -2.795810 | 4.859921 | -0.830812 |
| 6 | 0.856488 | 2.044488 | -0.193214 |
| 8 | 1.846536 | 2.488852 | -0.678084 |
| 7 | 1.062594 | 1.684319 | 1.458956 |
| 1 | 0.271433 | 2.046687 | 1.994678 |
| 7 | -0.759368 | 0.012267 | -0.395385 |
| 6 | -1.192870 | -1.305190 | -0.497086 |
| 8 | -0.443751 | -2.179853 | -0.891294 |
| 6 | -2.564028 | -1.595942 | 0.001069 |
| 6 | -3.037370 | -1.071473 | 1.205668 |
| 6 | -3.348578 | -2.496659 | -0.719599 |
| 6 | -4.298293 | -1.423717 | 1.669574 |
| 1 | -2.411105 | -0.391102 | 1.779868 |
| 6 | -4.618197 | -2.830460 | -0.264929 |
| 1 | -2.945658 | -2.925197 | -1.634349 |
| 6 | -5.093908 | -2.293288 | 0.928447 |
| 1 | -4.661306 | -1.022339 | 2.612670 |
| 1 | -5.235527 | -3.518154 | -0.837656 |
| 1 | -6.084603 | -2.561647 | 1.287817 |
| 8 | 0.573350 | 0.206071 | -0.690303 |
| 8 | 2.194102 | 2.291777 | 1.963336 |
| 1 | 1.159389 | 0.654883 | 1.574222 |

| | | | |
|---|---|---|---|
| 1 | 2.929674 | 1.666553 | 1.717804 |
| 8 | 1.982053 | -0.829204 | 0.951764 |
| 1 | 1.340316 | -0.594070 | 0.116810 |
| 6 | 3.263424 | -0.600797 | 0.669508 |
| 6 | 3.887958 | -1.515238 | -0.368394 |
| 8 | 3.874578 | 0.310555 | 1.211778 |
| 6 | 3.228557 | -1.175929 | -1.715460 |
| 1 | 3.733951 | -1.739729 | -2.509207 |
| 1 | 2.164252 | -1.439671 | -1.732455 |
| 1 | 3.319653 | -0.105784 | -1.945052 |
| 6 | 5.387729 | -1.261457 | -0.443677 |
| 1 | 5.835416 | -1.918394 | -1.199421 |
| 1 | 5.600612 | -0.222168 | -0.714479 |
| 1 | 5.873765 | -1.460385 | 0.518372 |
| 6 | 3.605302 | -2.977011 | -0.016423 |
| 1 | 4.044583 | -3.247497 | 0.951956 |
| 1 | 2.530040 | -3.179164 | 0.020516 |
| 1 | 4.051688 | -3.626444 | -0.779850 |

---

**$(9\text{-P})_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1297.2137176
Zero-point correction= 0.388123
Thermal correction to Energy= 0.412708
Thermal correction to Enthalpy= 0.413652
Thermal correction to Gibbs Free Energy= 0.335020
Sum of electronic and zero-point Energies= -1296.825595
Sum of electronic and thermal Energies= -1296.801010
Sum of electronic and thermal Enthalpies= -1296.800065
Sum of electronic and thermal Free Energies= -1296.878698

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.034925 | 0.581974 | -0.722301 |
| 6 | -2.880334 | 0.110494 | -0.100780 |
| 6 | -1.800516 | 0.960839 | 0.178848 |
| 6 | -1.899245 | 2.309570 | -0.188116 |
| 6 | -3.041784 | 2.757945 | -0.834274 |
| 6 | -4.116700 | 1.911099 | -1.107004 |
| 1 | -4.862211 | -0.105932 | -0.888174 |
| 1 | -1.101585 | 3.006127 | 0.046621 |
| 1 | -3.102216 | 3.808226 | -1.109894 |
| 1 | -5.009998 | 2.291209 | -1.593689 |
| 6 | -2.779290 | -1.307355 | 0.278738 |

| | | | |
|---|---|---|---|
| 8 | -3.543327 | -2.003150 | 0.897054 |
| 7 | -1.905397 | -2.100574 | -0.734778 |
| 1 | -2.398601 | -2.056561 | -1.636317 |
| 7 | -0.759677 | 0.369861 | 0.887420 |
| 6 | 0.368286 | 0.978544 | 1.465564 |
| 8 | 0.792000 | 0.636213 | 2.547880 |
| 6 | 1.094313 | 1.947834 | 0.599545 |
| 6 | 1.213647 | 1.750232 | -0.780239 |
| 6 | 1.796530 | 2.983857 | 1.217886 |
| 6 | 2.016377 | 2.599299 | -1.532364 |
| 1 | 0.712400 | 0.905091 | -1.250741 |
| 6 | 2.580269 | 3.842589 | 0.458251 |
| 1 | 1.724364 | 3.091577 | 2.297574 |
| 6 | 2.691295 | 3.650385 | -0.916787 |
| 1 | 2.123511 | 2.433525 | -2.601921 |
| 1 | 3.116832 | 4.656128 | 0.940544 |
| 1 | 3.316160 | 4.314962 | -1.509173 |
| 8 | -1.129642 | -0.846919 | 1.428131 |
| 8 | -1.824903 | -3.425951 | -0.339038 |
| 1 | -0.842135 | -1.747792 | -0.875270 |
| 1 | -2.553287 | -3.487884 | 0.321744 |
| 8 | 0.537981 | -1.553457 | -1.151997 |
| 6 | 1.302681 | -1.865380 | -0.202708 |
| 8 | 0.908966 | -2.037962 | 0.997862 |
| 1 | -0.131749 | -1.541606 | 1.236928 |
| 6 | 2.794799 | -2.036727 | -0.445006 |
| 6 | 3.532331 | -1.007140 | 0.418829 |
| 1 | 4.615601 | -1.151788 | 0.318496 |
| 1 | 3.300605 | 0.017546 | 0.098157 |
| 1 | 3.258493 | -1.102567 | 1.474796 |
| 6 | 3.136515 | -1.824437 | -1.913884 |
| 1 | 2.870264 | -0.813087 | -2.244244 |
| 1 | 4.214945 | -1.959286 | -2.064827 |
| 1 | 2.605722 | -2.535129 | -2.557000 |
| 6 | 3.189361 | -3.450193 | -0.008314 |
| 1 | 2.956267 | -3.614021 | 1.048463 |
| 1 | 2.664552 | -4.211250 | -0.599455 |
| 1 | 4.267316 | -3.593258 | -0.155556 |

### 3.2.1. Lewis Acid Participation in Nucleophilic Addition Elimination

---

**(9a'-P)$_4$‡**

---

Number of imaginary frequencies : 1
Electronic energy =-1936.2791232
Zero-point correction= 0.243227
Thermal correction to Energy= 0.264729
Thermal correction to Enthalpy= 0.265673
Thermal correction to Gibbs Free Energy= 0.190114
Sum of electronic and zero-point Energies= -1936.035896
Sum of electronic and thermal Energies= -1936.014394
Sum of electronic and thermal Enthalpies= -1936.013450
Sum of electronic and thermal Free Energies= -1936.089010

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 0.108866 | 2.928098 | 0.387063 |
| 6 | -0.165112 | 1.607245 | 0.056386 |
| 6 | -1.454374 | 1.193471 | -0.260684 |
| 6 | -2.512115 | 2.096807 | -0.223557 |
| 6 | -2.235617 | 3.413053 | 0.133869 |
| 6 | -0.940866 | 3.836488 | 0.432897 |
| 1 | 1.134063 | 3.227976 | 0.593337 |
| 1 | -3.523359 | 1.795190 | -0.476809 |
| 1 | -3.053497 | 4.128728 | 0.162348 |
| 1 | -0.752090 | 4.875918 | 0.685372 |
| 6 | 0.857461 | 0.537886 | -0.043177 |
| 8 | 1.924524 | 0.662384 | -0.660241 |
| 7 | 0.919725 | -0.367868 | 1.238825 |
| 1 | 0.434987 | 0.059038 | 2.031311 |
| 7 | -1.514705 | -0.189503 | -0.630156 |
| 6 | -2.317205 | -1.031308 | 0.221107 |
| 8 | -1.791121 | -1.782461 | 1.014008 |
| 6 | -3.768868 | -0.919876 | 0.007823 |
| 6 | -4.616840 | -1.302176 | 1.051608 |
| 6 | -4.303093 | -0.511820 | -1.219369 |
| 6 | -5.991641 | -1.242743 | 0.880289 |
| 1 | -4.177582 | -1.641784 | 1.986421 |
| 6 | -5.681013 | -0.465197 | -1.388255 |
| 1 | -3.632077 | -0.254974 | -2.036032 |
| 6 | -6.522474 | -0.822912 | -0.338145 |
| 1 | -6.653336 | -1.528512 | 1.693699 |
| 1 | -6.099671 | -0.158546 | -2.343209 |
| 1 | -7.600798 | -0.783403 | -0.472652 |
| 8 | -0.195467 | -0.671167 | -0.660269 |
| 1 | 0.183034 | -1.082920 | 0.506754 |
| 30 | 3.637282 | -0.358253 | -0.299204 |
| 17 | 5.402577 | 0.903736 | -0.069293 |

| | | | |
|---|---|---|---|
| 17 | 3.217356 | -2.578461 | -0.399988 |
| 8 | 2.207398 | -0.682949 | 1.654799 |
| 1 | 2.342541 | -1.625764 | 1.389170 |

---

**$(9a'\text{-}P)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2283.1090165
Zero-point correction= 0.390501
Thermal correction to Energy= 0.421285
Thermal correction to Enthalpy= 0.422229
Thermal correction to Gibbs Free Energy= 0.326228
Sum of electronic and zero-point Energies= -2282.718516
Sum of electronic and thermal Energies= -2282.687732
Sum of electronic and thermal Enthalpies= -2282.686787
Sum of electronic and thermal Free Energies= -2282.782789

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.442413 | -3.315186 | -0.013478 |
| 6 | 0.693120 | -1.961231 | -0.154790 |
| 6 | 1.992895 | -1.465640 | -0.202594 |
| 6 | 3.088546 | -2.313903 | -0.110607 |
| 6 | 2.829709 | -3.675304 | 0.047097 |
| 6 | 1.531449 | -4.176938 | 0.098671 |
| 1 | -0.585558 | -3.676959 | 0.005427 |
| 1 | 4.106996 | -1.944870 | -0.172977 |
| 1 | 3.672067 | -4.359401 | 0.114661 |
| 1 | 1.367338 | -5.244988 | 0.210580 |
| 6 | -0.317631 | -0.861245 | -0.306602 |
| 8 | -1.339895 | -0.970872 | -1.044911 |
| 7 | -0.654489 | -0.209106 | 1.065725 |
| 1 | -0.667638 | 1.348323 | 0.750694 |
| 7 | 1.942702 | -0.054906 | -0.372189 |
| 6 | 2.897364 | 0.876647 | -0.805290 |
| 8 | 2.571361 | 1.807417 | -1.509485 |
| 6 | 4.265917 | 0.701851 | -0.260388 |
| 6 | 4.506129 | 0.292377 | 1.053533 |
| 6 | 5.331952 | 1.067421 | -1.084470 |
| 6 | 5.809755 | 0.223787 | 1.528446 |
| 1 | 3.671492 | 0.040245 | 1.704747 |
| 6 | 6.634142 | 0.979828 | -0.611635 |
| 1 | 5.118871 | 1.420281 | -2.090523 |
| 6 | 6.873025 | 0.557457 | 0.693637 |
| 1 | 5.997230 | -0.083973 | 2.554025 |

| | | | |
|---|---|---|---|
| 1 | 7.465080 | 1.249766 | -1.258187 |
| 1 | 7.892781 | 0.497233 | 1.066175 |
| 8 | 0.659706 | 0.222270 | -0.907370 |
| 8 | -1.909603 | -0.627850 | 1.536249 |
| 1 | -1.882037 | -1.592350 | 1.744710 |
| 1 | 0.277248 | 1.433043 | -0.552749 |
| 30 | -3.167235 | -1.363527 | -0.359387 |
| 17 | -4.873218 | -0.168741 | -1.046145 |
| 17 | -3.072819 | -3.318740 | 0.811427 |
| 8 | -0.258860 | 2.113018 | 0.162720 |
| 1 | 0.041894 | -0.476722 | 1.765083 |
| 6 | -0.967267 | 3.270225 | -0.240274 |
| 6 | -2.138699 | 3.582367 | 0.660000 |
| 8 | -0.583008 | 3.847042 | -1.205629 |
| 6 | -1.703117 | 3.602420 | 2.128124 |
| 1 | -0.906824 | 4.334725 | 2.305993 |
| 1 | -2.563959 | 3.882586 | 2.745778 |
| 1 | -1.359567 | 2.622082 | 2.481003 |
| 6 | -2.690739 | 4.943762 | 0.252289 |
| 1 | -3.557231 | 5.187993 | 0.876822 |
| 1 | -1.939534 | 5.731765 | 0.375232 |
| 1 | -3.007758 | 4.942911 | -0.795179 |
| 6 | -3.198502 | 2.495134 | 0.437674 |
| 1 | -3.479818 | 2.397866 | -0.616792 |
| 1 | -2.875220 | 1.509184 | 0.794277 |
| 1 | -4.104004 | 2.751162 | 0.999607 |

---

**(9a-P)$_{10}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2283.1442693
Zero-point correction= 0.392528
Thermal correction to Energy= 0.422587
Thermal correction to Enthalpy= 0.423532
Thermal correction to Gibbs Free Energy= 0.330698
Sum of electronic and zero-point Energies= -2282.751741
Sum of electronic and thermal Energies= -2282.721682
Sum of electronic and thermal Enthalpies= -2282.720738
Sum of electronic and thermal Free Energies= -2282.813571

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.924096 | -3.347786 | -0.509628 |
| 6 | 0.451877 | -2.150618 | 0.020454 |
| 6 | -0.905146 | -1.944567 | 0.290456 |

| | | | |
|---|---|---|---|
| 6 | -1.811203 | -2.974961 | 0.032920 |
| 6 | -1.334156 | -4.161723 | -0.511151 |
| 6 | 0.018197 | -4.360662 | -0.788911 |
| 1 | 1.990855 | -3.461830 | -0.697762 |
| 1 | -2.865229 | -2.865432 | 0.264467 |
| 1 | -2.044176 | -4.961535 | -0.706807 |
| 1 | 0.361258 | -5.303296 | -1.204412 |
| 6 | 1.368779 | -1.040262 | 0.313537 |
| 8 | 2.408552 | -1.073329 | 0.949237 |
| 7 | 1.368456 | -0.015518 | -0.856899 |
| 1 | 1.906955 | -0.476314 | -1.621042 |
| 7 | -1.176009 | -0.698496 | 0.869365 |
| 6 | -2.347309 | -0.176873 | 1.439351 |
| 8 | -2.297159 | 0.597320 | 2.369885 |
| 6 | -3.608760 | -0.525850 | 0.738091 |
| 6 | -3.701211 | -0.462207 | -0.655756 |
| 6 | -4.739526 | -0.803832 | 1.507083 |
| 6 | -4.922617 | -0.702959 | -1.273335 |
| 1 | -2.821825 | -0.202473 | -1.244748 |
| 6 | -5.950675 | -1.069866 | 0.881419 |
| 1 | -4.652074 | -0.808338 | 2.590991 |
| 6 | -6.041718 | -1.019870 | -0.507597 |
| 1 | -5.001886 | -0.640886 | -2.355884 |
| 1 | -6.828550 | -1.306503 | 1.477287 |
| 1 | -6.993466 | -1.217823 | -0.995108 |
| 8 | 0.002069 | -0.111497 | 1.326232 |
| 8 | 2.154114 | 1.094581 | -0.533137 |
| 1 | 0.388800 | 0.353372 | -1.170735 |
| 1 | 1.527059 | 1.706603 | -0.051274 |
| 8 | -0.824203 | 1.269233 | -1.436052 |
| 6 | -0.857326 | 2.169231 | -0.573500 |
| 8 | -0.088281 | 2.143893 | 0.478273 |
| 1 | -0.061742 | 0.991108 | 0.994307 |
| 6 | -1.782412 | 3.362797 | -0.705799 |
| 6 | -2.635568 | 3.469257 | 0.561870 |
| 1 | -3.281280 | 4.353014 | 0.489009 |
| 1 | -3.280399 | 2.590633 | 0.689712 |
| 1 | -2.014399 | 3.560223 | 1.457986 |
| 6 | -2.673379 | 3.218407 | -1.932645 |
| 1 | -3.310565 | 2.328099 | -1.860798 |
| 1 | -3.324561 | 4.096725 | -2.017972 |
| 1 | -2.082615 | 3.135043 | -2.851178 |
| 6 | -0.899424 | 4.610469 | -0.835352 |
| 1 | -0.247888 | 4.726197 | 0.036815 |
| 1 | -0.275398 | 4.568496 | -1.737066 |

| | | | |
|---|---|---|---|
| 1 | -1.536739 | 5.499857 | -0.910184 |
| 30 | 4.060021 | 0.034383 | 0.185925 |
| 17 | 4.133747 | -1.087189 | -1.774433 |
| 17 | 5.227680 | 1.287855 | 1.514129 |

### 3.3. Nucleophilic Addition Elimination via Stepwise Pathway

---

**$(9\text{-}11)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1297.1823976
Zero-point correction= 0.386400
Thermal correction to Energy= 0.411403
Thermal correction to Enthalpy= 0.412348
Thermal correction to Gibbs Free Energy= 0.331646
Sum of electronic and zero-point Energies= -1296.795998
Sum of electronic and thermal Energies= -1296.770994
Sum of electronic and thermal Enthalpies= -1296.770050
Sum of electronic and thermal Free Energies= -1296.850752

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.941810 | 3.363891 | 0.594748 |
| 6 | -1.162021 | 2.316221 | 0.127165 |
| 6 | -1.747982 | 1.129736 | -0.312855 |
| 6 | -3.130295 | 0.985021 | -0.307956 |
| 6 | -3.906688 | 2.041379 | 0.163328 |
| 6 | -3.326397 | 3.224569 | 0.608458 |
| 1 | -1.457247 | 4.274994 | 0.937172 |
| 1 | -3.602974 | 0.072771 | -0.655425 |
| 1 | -4.988576 | 1.933736 | 0.168950 |
| 1 | -3.951870 | 4.040037 | 0.961642 |
| 6 | 0.326686 | 2.329117 | 0.100138 |
| 8 | 0.949938 | 2.061191 | 1.169909 |
| 7 | 1.010320 | 3.171531 | -0.847361 |
| 1 | 0.449394 | 3.266479 | -1.692006 |
| 7 | -0.779109 | 0.171300 | -0.758012 |
| 6 | -0.590083 | -1.077073 | -0.149338 |
| 8 | 0.516526 | -1.460216 | 0.181769 |
| 6 | -1.789005 | -1.942412 | -0.047399 |
| 6 | -1.946142 | -2.718117 | 1.102241 |
| 6 | -2.670369 | -2.095288 | -1.119998 |
| 6 | -3.010256 | -3.604344 | 1.197352 |
| 1 | -1.225554 | -2.613164 | 1.909738 |

| | | | |
|---|---|---|---|
| 6 | -3.722647 | -2.998762 | -1.028782 |
| 1 | -2.511363 | -1.516838 | -2.028477 |
| 6 | -3.898635 | -3.744215 | 0.133583 |
| 1 | -3.143678 | -4.195389 | 2.099864 |
| 1 | -4.401862 | -3.126895 | -1.867925 |
| 1 | -4.725411 | -4.446811 | 0.206766 |
| 8 | 0.403904 | 0.863220 | -1.008789 |
| 8 | 1.011499 | 4.469637 | -0.265953 |
| 1 | 1.905043 | 4.543472 | 0.091769 |
| 1 | 1.937179 | 1.381741 | 0.815750 |
| 8 | 2.465722 | 0.613186 | 0.105856 |
| 6 | 3.100486 | -0.431418 | 0.711321 |
| 8 | 3.242331 | -0.456036 | 1.905286 |
| 6 | 3.728188 | -1.435661 | -0.244559 |
| 6 | 3.157579 | -1.382449 | -1.657481 |
| 1 | 3.692411 | -2.103551 | -2.288227 |
| 1 | 2.094788 | -1.647432 | -1.669950 |
| 1 | 3.274962 | -0.390064 | -2.108092 |
| 6 | 3.565124 | -2.833785 | 0.345725 |
| 1 | 4.097102 | -3.563817 | -0.277278 |
| 1 | 3.971521 | -2.876850 | 1.361059 |
| 1 | 2.506967 | -3.114978 | 0.386941 |
| 6 | 5.216791 | -1.057923 | -0.283530 |
| 1 | 5.358378 | -0.046957 | -0.686942 |
| 1 | 5.654290 | -1.095534 | 0.720246 |
| 1 | 5.759535 | -1.760438 | -0.928354 |
| 1 | 1.453969 | 0.446918 | -0.517188 |

---

**$(9\text{-}11)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1297.2028713
Zero-point correction= 0.385951
Thermal correction to Energy= 0.411441
Thermal correction to Enthalpy= 0.412385
Thermal correction to Gibbs Free Energy= 0.329272
Sum of electronic and zero-point Energies= -1296.816921
Sum of electronic and thermal Energies= -1296.791431
Sum of electronic and thermal Enthalpies= -1296.790487
Sum of electronic and thermal Free Energies= -1296.873600

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.151191 | 3.557734 | -0.341886 |
| 6 | 0.717160 | 2.244810 | -0.290871 |

| | | | |
|---|---|---|---|
| 6 | 1.620396 | 1.184744 | -0.414718 |
| 6 | 2.972707 | 1.433699 | -0.619818 |
| 6 | 3.400367 | 2.759761 | -0.660981 |
| 6 | 2.507589 | 3.817833 | -0.522054 |
| 1 | 0.422275 | 4.358662 | -0.242378 |
| 1 | 3.682588 | 0.625142 | -0.761759 |
| 1 | 4.456065 | 2.962456 | -0.825217 |
| 1 | 2.865805 | 4.842797 | -0.566491 |
| 6 | -0.694814 | 1.829004 | -0.052069 |
| 8 | -1.662496 | 2.299345 | -0.685612 |
| 7 | -0.998135 | 1.361877 | 1.299042 |
| 1 | -0.188229 | 0.884393 | 1.694830 |
| 7 | 0.958395 | -0.071506 | -0.355815 |
| 6 | 1.422571 | -1.363701 | -0.593922 |
| 8 | 0.716155 | -2.197499 | -1.123305 |
| 6 | 2.775601 | -1.675818 | -0.060068 |
| 6 | 3.571313 | -2.558365 | -0.791797 |
| 6 | 3.225627 | -1.190173 | 1.169858 |
| 6 | 4.827275 | -2.916929 | -0.319628 |
| 1 | 3.185669 | -2.953598 | -1.728664 |
| 6 | 4.474153 | -1.566000 | 1.648836 |
| 1 | 2.593756 | -0.522378 | 1.752390 |
| 6 | 5.279500 | -2.419859 | 0.899904 |
| 1 | 5.452481 | -3.591116 | -0.899875 |
| 1 | 4.819890 | -1.193731 | 2.610112 |
| 1 | 6.259961 | -2.706634 | 1.273065 |
| 8 | -0.355003 | 0.156062 | -0.753408 |
| 8 | -1.090646 | 2.558776 | 2.067868 |
| 1 | -2.044222 | 2.688247 | 2.140786 |
| 1 | -2.697586 | 1.435489 | -0.487580 |
| 8 | -3.542274 | 0.761858 | -0.337546 |
| 6 | -3.367027 | -0.483060 | -0.098888 |
| 8 | -2.266777 | -1.085957 | -0.065800 |
| 6 | -4.631541 | -1.304970 | 0.079978 |
| 6 | -5.743392 | -0.471474 | 0.710141 |
| 1 | -6.649503 | -1.082834 | 0.799944 |
| 1 | -5.466145 | -0.131439 | 1.715316 |
| 1 | -5.978316 | 0.410107 | 0.106597 |
| 6 | -4.349303 | -2.541441 | 0.927128 |
| 1 | -5.264973 | -3.138671 | 1.015121 |
| 1 | -3.568940 | -3.163998 | 0.480380 |
| 1 | -4.025160 | -2.266824 | 1.937913 |
| 6 | -5.040672 | -1.730476 | -1.338599 |
| 1 | -5.253305 | -0.857755 | -1.967097 |
| 1 | -4.249832 | -2.321322 | -1.815705 |

| | | | |
|---|---|---|---|
| 1 | -5.946656 | -2.346605 | -1.287863 |
| 1 | -1.231330 | -0.535577 | -0.347272 |

---

**$(9\text{-}11)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1644.0528578
Zero-point correction= 0.538246
Thermal correction to Energy= 0.572144
Thermal correction to Enthalpy= 0.573088
Thermal correction to Gibbs Free Energy= 0.474679
Sum of electronic and zero-point Energies= -1643.514612
Sum of electronic and thermal Energies= -1643.480714
Sum of electronic and thermal Enthalpies= -1643.479770
Sum of electronic and thermal Free Energies= -1643.578179

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.634457 | 3.390795 | 1.799130 |
| 6 | -1.009755 | 2.405244 | 1.034218 |
| 6 | -1.743484 | 1.346385 | 0.473716 |
| 6 | -3.116691 | 1.272260 | 0.750925 |
| 6 | -3.720719 | 2.256717 | 1.517310 |
| 6 | -2.997298 | 3.329483 | 2.037613 |
| 1 | -1.029696 | 4.194966 | 2.214856 |
| 1 | -3.708173 | 0.439848 | 0.386970 |
| 1 | -4.785334 | 2.173426 | 1.722886 |
| 1 | -3.487772 | 4.091122 | 2.636350 |
| 6 | 0.455206 | 2.485218 | 0.874567 |
| 8 | 1.222359 | 2.127231 | 1.865294 |
| 7 | 0.949057 | 3.316959 | -0.031051 |
| 1 | 0.391783 | 3.653656 | -0.806687 |
| 7 | -0.997498 | 0.440585 | -0.284663 |
| 6 | -1.383845 | -0.742845 | -0.906751 |
| 8 | -0.596948 | -1.666039 | -1.028113 |
| 6 | -2.762372 | -0.823923 | -1.454603 |
| 6 | -3.471377 | -2.009554 | -1.257322 |
| 6 | -3.318052 | 0.203418 | -2.219394 |
| 6 | -4.748163 | -2.149460 | -1.786618 |
| 1 | -3.006164 | -2.809396 | -0.683771 |
| 6 | -4.585091 | 0.050803 | -2.767458 |
| 1 | -2.751147 | 1.117817 | -2.383622 |
| 6 | -5.304617 | -1.120215 | -2.541669 |
| 1 | -5.307404 | -3.066577 | -1.618422 |
| 1 | -5.013955 | 0.845641 | -3.372831 |

| | | | |
|---|---|---|---|
| 1 | -6.300323 | -1.234856 | -2.963892 |
| 8 | 0.344733 | 0.584881 | -0.087756 |
| 8 | 2.265379 | 3.665941 | 0.012053 |
| 1 | 2.750331 | 3.054909 | -0.633507 |
| 1 | 2.154792 | 2.239277 | 1.580849 |
| 8 | 3.210291 | 0.818136 | 0.271505 |
| 6 | 3.449068 | 0.867965 | -1.030541 |
| 8 | 3.403123 | 1.957739 | -1.592436 |
| 6 | 3.771020 | -0.415428 | -1.774365 |
| 6 | 4.555293 | -1.394023 | -0.896799 |
| 1 | 4.876867 | -2.238643 | -1.517803 |
| 1 | 5.456070 | -0.927561 | -0.478330 |
| 1 | 3.953684 | -1.821535 | -0.084147 |
| 6 | 4.584300 | -0.059008 | -3.016712 |
| 1 | 4.796477 | -0.973362 | -3.583072 |
| 1 | 4.039662 | 0.635391 | -3.663353 |
| 1 | 5.540308 | 0.407485 | -2.749867 |
| 6 | 2.434214 | -1.042843 | -2.195481 |
| 1 | 1.821744 | -1.335185 | -1.338030 |
| 1 | 1.847216 | -0.345845 | -2.806776 |
| 1 | 2.638596 | -1.940920 | -2.790953 |
| 1 | 0.863760 | -0.325592 | 0.689936 |
| 8 | 1.631934 | -0.959268 | 1.197068 |
| 6 | 1.449848 | -2.257567 | 1.404325 |
| 8 | 2.284345 | -3.077540 | 1.078004 |
| 6 | 0.217135 | -2.675372 | 2.215945 |
| 6 | 0.772503 | -3.104438 | 3.581525 |
| 1 | -0.040382 | -3.484815 | 4.213679 |
| 1 | 1.524766 | -3.891058 | 3.463294 |
| 1 | 1.238267 | -2.256811 | 4.101378 |
| 6 | -0.442172 | -3.868945 | 1.528918 |
| 1 | -0.807212 | -3.587403 | 0.532785 |
| 1 | 0.275262 | -4.686489 | 1.407406 |
| 1 | -1.289294 | -4.227629 | 2.128917 |
| 6 | -0.800712 | -1.559893 | 2.430468 |
| 1 | -0.328049 | -0.627159 | 2.763983 |
| 1 | -1.370699 | -1.350007 | 1.518061 |
| 1 | -1.524053 | -1.867629 | 3.196364 |
| 1 | 2.898755 | -0.075172 | 0.596733 |

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**$(9\text{-}11)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1644.0578985
Zero-point correction= 0.540305

Thermal correction to Energy= 0.574419
Thermal correction to Enthalpy= 0.575363
Thermal correction to Gibbs Free Energy= 0.475237
Sum of electronic and zero-point Energies= -1643.517594
Sum of electronic and thermal Energies= -1643.483480
Sum of electronic and thermal Enthalpies= -1643.482536
Sum of electronic and thermal Free Energies= -1643.582661

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.658537 | 3.199834 | 1.848628 |
| 6 | -1.182055 | 2.280534 | 0.916946 |
| 6 | -2.053899 | 1.557801 | 0.091090 |
| 6 | -3.427595 | 1.828689 | 0.174168 |
| 6 | -3.888730 | 2.734830 | 1.116456 |
| 6 | -3.021298 | 3.417417 | 1.970042 |
| 1 | -0.944117 | 3.742980 | 2.464600 |
| 1 | -4.128863 | 1.343404 | -0.494707 |
| 1 | -4.958157 | 2.925182 | 1.171446 |
| 1 | -3.404922 | 4.127151 | 2.697194 |
| 6 | 0.274622 | 2.106632 | 0.745613 |
| 8 | 0.933453 | 1.333996 | 1.570716 |
| 7 | 0.910770 | 3.148731 | 0.182985 |
| 1 | 0.443272 | 3.652353 | -0.561771 |
| 7 | -1.423345 | 0.708603 | -0.808581 |
| 6 | -1.890701 | -0.325728 | -1.614021 |
| 8 | -1.150182 | -0.870865 | -2.408598 |
| 6 | -3.313235 | -0.746655 | -1.457935 |
| 6 | -3.796133 | -1.255103 | -0.249727 |
| 6 | -4.130974 | -0.727531 | -2.587733 |
| 6 | -5.107551 | -1.710017 | -0.174861 |
| 1 | -3.135802 | -1.290852 | 0.614820 |
| 6 | -5.448121 | -1.162537 | -2.499288 |
| 1 | -3.724159 | -0.367688 | -3.530673 |
| 6 | -5.937422 | -1.652322 | -1.291416 |
| 1 | -5.484783 | -2.111875 | 0.762873 |
| 1 | -6.090391 | -1.130579 | -3.376408 |
| 1 | -6.966071 | -1.999733 | -1.223267 |
| 8 | -0.054916 | 0.851314 | -0.783998 |
| 8 | 2.275953 | 3.264074 | 0.206055 |
| 1 | 2.654355 | 2.494857 | -0.273481 |
| 1 | 1.848508 | 1.188096 | 1.241748 |
| 8 | 3.116010 | 0.783443 | -0.072085 |
| 6 | 3.738924 | -0.123583 | -0.627181 |
| 8 | 3.303060 | -1.353988 | -0.670519 |

| | | | |
|---|---|---|---|
| 6 | 5.102377 | 0.081459 | -1.258078 |
| 6 | 5.364018 | 1.569955 | -1.454936 |
| 1 | 6.361570 | 1.715476 | -1.885753 |
| 1 | 4.633838 | 2.015539 | -2.142125 |
| 1 | 5.317670 | 2.116747 | -0.506572 |
| 6 | 5.191221 | -0.657887 | -2.592971 |
| 1 | 6.189343 | -0.513650 | -3.024340 |
| 1 | 5.019288 | -1.730969 | -2.468689 |
| 1 | 4.455579 | -0.276553 | -3.311168 |
| 6 | 6.122341 | -0.503067 | -0.270335 |
| 1 | 6.067997 | 0.003476 | 0.701345 |
| 1 | 5.953164 | -1.574101 | -0.114737 |
| 1 | 7.135082 | -0.366356 | -0.668519 |
| 1 | 0.384345 | -0.277546 | -0.333674 |
| 8 | 0.835839 | -1.205534 | 0.138151 |
| 6 | 0.080823 | -1.680523 | 1.113371 |
| 8 | -1.039444 | -1.261402 | 1.340576 |
| 6 | 0.757882 | -2.757660 | 1.956441 |
| 6 | -0.241008 | -3.318640 | 2.959702 |
| 1 | 0.246370 | -4.072195 | 3.591276 |
| 1 | -0.642687 | -2.527715 | 3.601058 |
| 1 | -1.088157 | -3.790735 | 2.449629 |
| 6 | 1.918046 | -2.089249 | 2.702568 |
| 1 | 2.672541 | -1.696184 | 2.010080 |
| 1 | 1.556127 | -1.259520 | 3.323556 |
| 1 | 2.410162 | -2.817032 | 3.360317 |
| 6 | 1.284571 | -3.885176 | 1.067030 |
| 1 | 0.472871 | -4.351181 | 0.495498 |
| 1 | 2.041859 | -3.539909 | 0.355450 |
| 1 | 1.743428 | -4.661932 | 1.692417 |
| 1 | 2.365193 | -1.387437 | -0.302094 |

---

**$(9\text{-}11)_{12}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1644.0599205
Zero-point correction= 0.538703
Thermal correction to Energy= 0.572373
Thermal correction to Enthalpy= 0.573318
Thermal correction to Gibbs Free Energy= 0.474870
Sum of electronic and zero-point Energies= -1643.521218
Sum of electronic and thermal Energies= -1643.487547
Sum of electronic and thermal Enthalpies= -1643.486603
Sum of electronic and thermal Free Energies= -1643.585050

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.321211 | 2.514955 | 2.484109 |
| 6 | 0.933891 | 1.371113 | 1.788462 |
| 6 | 1.807343 | 0.730812 | 0.894543 |
| 6 | 3.083529 | 1.280002 | 0.703089 |
| 6 | 3.454159 | 2.417563 | 1.403345 |
| 6 | 2.588470 | 3.044110 | 2.299794 |
| 1 | 0.608980 | 2.985928 | 3.159404 |
| 1 | 3.772510 | 0.842453 | -0.010535 |
| 1 | 4.443496 | 2.834581 | 1.229653 |
| 1 | 2.895018 | 3.939241 | 2.832777 |
| 6 | -0.449909 | 0.875061 | 1.950473 |
| 8 | -1.423297 | 1.570034 | 1.431883 |
| 7 | -0.668029 | 0.061819 | 2.980411 |
| 1 | 0.088697 | -0.526192 | 3.310584 |
| 7 | 1.265817 | -0.371583 | 0.229167 |
| 6 | 1.800542 | -1.120632 | -0.820633 |
| 8 | 1.082195 | -1.569457 | -1.693676 |
| 6 | 3.256976 | -1.421391 | -0.775415 |
| 6 | 3.957055 | -1.446338 | -1.982250 |
| 6 | 3.905589 | -1.772220 | 0.410782 |
| 6 | 5.307008 | -1.772918 | -1.997400 |
| 1 | 3.423500 | -1.207860 | -2.899341 |
| 6 | 5.250565 | -2.119081 | 0.390194 |
| 1 | 3.348875 | -1.775146 | 1.345898 |
| 6 | 5.954603 | -2.108503 | -0.811226 |
| 1 | 5.854312 | -1.775208 | -2.936895 |
| 1 | 5.751993 | -2.401026 | 1.312998 |
| 1 | 7.009588 | -2.372308 | -0.823868 |
| 8 | -0.095986 | -0.433864 | 0.351350 |
| 8 | -1.917032 | -0.311547 | 3.384493 |
| 1 | -2.361100 | -0.706764 | 2.591644 |
| 1 | -2.265057 | 1.045432 | 1.378412 |
| 8 | -3.094774 | -0.440744 | 1.064082 |
| 6 | -3.506509 | -1.171598 | 0.152003 |
| 8 | -4.185910 | -0.723188 | -0.859196 |
| 6 | -3.232619 | -2.662097 | 0.120260 |
| 6 | -2.499230 | -3.092173 | 1.384125 |
| 1 | -2.284259 | -4.166306 | 1.335669 |
| 1 | -1.542381 | -2.560646 | 1.472635 |
| 1 | -3.097369 | -2.913483 | 2.287259 |
| 6 | -2.336543 | -2.923054 | -1.100004 |
| 1 | -2.127863 | -3.998544 | -1.164052 |

| | | | |
|---|---|---|---|
| 1 | -2.828738 | -2.604860 | -2.024154 |
| 1 | -1.381046 | -2.388956 | -1.023323 |
| 6 | -4.552340 | -3.422412 | -0.023675 |
| 1 | -5.214455 | -3.246565 | 0.833604 |
| 1 | -5.083289 | -3.128708 | -0.934515 |
| 1 | -4.347830 | -4.498819 | -0.075874 |
| 1 | -0.765095 | 0.042625 | -0.715522 |
| 8 | -1.585182 | 0.280215 | -1.392567 |
| 6 | -2.087794 | 1.472312 | -1.497041 |
| 8 | -3.303774 | 1.665687 | -1.367289 |
| 1 | -3.996990 | 0.266561 | -0.996149 |
| 6 | -1.196117 | 2.632832 | -1.933742 |
| 6 | -1.587738 | 3.899261 | -1.177308 |
| 1 | -1.000003 | 4.750664 | -1.544188 |
| 1 | -2.650214 | 4.122067 | -1.313045 |
| 1 | -1.394858 | 3.789196 | -0.102329 |
| 6 | -1.488591 | 2.807839 | -3.431005 |
| 1 | -1.220845 | 1.902986 | -3.991208 |
| 1 | -2.551007 | 3.016467 | -3.597289 |
| 1 | -0.899919 | 3.644069 | -3.829434 |
| 6 | 0.285717 | 2.340239 | -1.740109 |
| 1 | 0.544248 | 2.291526 | -0.675780 |
| 1 | 0.579879 | 1.397896 | -2.218400 |
| 1 | 0.881173 | 3.148867 | -2.182544 |

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**$(11\text{-}P)_4^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-950.3382273
Zero-point correction= 0.238802
Thermal correction to Energy= 0.255368
Thermal correction to Enthalpy= 0.256312
Thermal correction to Gibbs Free Energy= 0.193824
Sum of electronic and zero-point Energies= -950.099425
Sum of electronic and thermal Energies= -950.082860
Sum of electronic and thermal Enthalpies= -950.081915
Sum of electronic and thermal Free Energies= -950.144403

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.761387 | 1.649521 | -0.553472 |
| 6 | -2.004062 | 0.498912 | -0.434989 |
| 6 | -0.614393 | 0.522613 | -0.459144 |
| 6 | 0.073163 | 1.721848 | -0.618656 |
| 6 | -0.693668 | 2.881140 | -0.732799 |

| | | | |
|---|---|---|---|
| 6 | -2.088489 | 2.861645 | -0.699705 |
| 1 | -3.848170 | 1.582895 | -0.559341 |
| 1 | 1.156650 | 1.767842 | -0.663413 |
| 1 | -0.179462 | 3.830281 | -0.865270 |
| 1 | -2.644450 | 3.789327 | -0.804582 |
| 6 | -2.425608 | -0.907097 | -0.232177 |
| 8 | -3.566314 | -1.415106 | -0.568390 |
| 7 | -2.708724 | -1.136815 | 1.404365 |
| 1 | -2.182661 | -1.963207 | 1.697951 |
| 7 | -0.172403 | -0.807429 | -0.316997 |
| 6 | 1.069672 | -1.395620 | -0.574822 |
| 8 | 1.174480 | -2.490211 | -1.079480 |
| 6 | 2.229634 | -0.598010 | -0.093672 |
| 6 | 3.407228 | -0.642323 | -0.841066 |
| 6 | 2.195034 | 0.104557 | 1.113861 |
| 6 | 4.530015 | 0.050904 | -0.408383 |
| 1 | 3.421812 | -1.227568 | -1.757576 |
| 6 | 3.325948 | 0.782543 | 1.552021 |
| 1 | 1.284462 | 0.110008 | 1.710729 |
| 6 | 4.488777 | 0.765254 | 0.786557 |
| 1 | 5.442055 | 0.029671 | -0.999757 |
| 1 | 3.301982 | 1.322281 | 2.495545 |
| 1 | 5.370284 | 1.303389 | 1.127445 |
| 8 | -1.267266 | -1.659340 | -0.561879 |
| 1 | -3.716165 | -1.411046 | 0.762908 |
| 8 | -2.443870 | -0.178005 | 2.385589 |
| 1 | -2.805881 | 0.641812 | 2.015737 |

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**$(11\text{-}P)_6^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1297.2054838
Zero-point correction= 0.391239
Thermal correction to Energy= 0.416152
Thermal correction to Enthalpy= 0.417096
Thermal correction to Gibbs Free Energy= 0.334662
Sum of electronic and zero-point Energies= -1296.814245
Sum of electronic and thermal Energies= -1296.789332
Sum of electronic and thermal Enthalpies= -1296.788387
Sum of electronic and thermal Free Energies= -1296.870822

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.425441 | 3.115802 | -0.700100 |
| 6 | 0.490964 | 1.763632 | -0.419724 |

| | | | |
|---|---|---|---|
| 6 | 1.697573 | 1.085920 | -0.299528 |
| 6 | 2.904865 | 1.756344 | -0.471764 |
| 6 | 2.836997 | 3.119468 | -0.753696 |
| 6 | 1.624310 | 3.801622 | -0.864365 |
| 1 | -0.542665 | 3.602162 | -0.789842 |
| 1 | 3.862295 | 1.250497 | -0.404192 |
| 1 | 3.767757 | 3.662575 | -0.899622 |
| 1 | 1.620347 | 4.864794 | -1.086896 |
| 6 | -0.604971 | 0.791009 | -0.210256 |
| 8 | -1.676957 | 0.882421 | -0.956871 |
| 7 | -1.063359 | 0.859720 | 1.335440 |
| 1 | -0.247674 | 0.794634 | 1.949034 |
| 7 | 1.415360 | -0.269144 | 0.010599 |
| 6 | 2.164989 | -1.413909 | -0.358961 |
| 8 | 1.645138 | -2.370354 | -0.879286 |
| 6 | 3.596496 | -1.366298 | 0.031310 |
| 6 | 4.499646 | -2.077322 | -0.762274 |
| 6 | 4.042453 | -0.725472 | 1.190181 |
| 6 | 5.844702 | -2.112429 | -0.421617 |
| 1 | 4.126058 | -2.597046 | -1.641110 |
| 6 | 5.387363 | -0.774304 | 1.535528 |
| 1 | 3.332922 | -0.198768 | 1.824887 |
| 6 | 6.288995 | -1.460044 | 0.725760 |
| 1 | 6.548292 | -2.655130 | -1.047663 |
| 1 | 5.731985 | -0.283970 | 2.442492 |
| 1 | 7.341850 | -1.493231 | 0.995594 |
| 8 | 0.031328 | -0.474585 | -0.235096 |
| 8 | -1.757112 | 2.012654 | 1.649157 |
| 1 | -2.689767 | 1.710654 | 1.428085 |
| 1 | -2.541718 | 0.555891 | -0.441195 |
| 1 | -1.716739 | 0.062896 | 1.465383 |
| 8 | -5.249546 | -0.156628 | 1.809879 |
| 6 | -4.565012 | -0.264364 | 0.810357 |
| 8 | -3.422367 | 0.371641 | 0.651567 |
| 6 | -4.959383 | -1.163054 | -0.369792 |
| 6 | -6.246572 | -1.905319 | -0.036792 |
| 1 | -6.541349 | -2.548678 | -0.876296 |
| 1 | -6.121487 | -2.528613 | 0.855345 |
| 1 | -7.060672 | -1.202991 | 0.171081 |
| 6 | -3.837177 | -2.168793 | -0.639645 |
| 1 | -4.115231 | -2.826607 | -1.473480 |
| 1 | -2.893247 | -1.678119 | -0.905905 |
| 1 | -3.656409 | -2.803808 | 0.237398 |
| 6 | -5.177155 | -0.289819 | -1.608663 |
| 1 | -5.959487 | 0.458875 | -1.430778 |

| | | | |
|---|---|---|---|
| 1 | -4.264178 | 0.236220 | -1.910853 |
| 1 | -5.495923 | -0.913492 | -2.454294 |

---

**$(11\text{-}P)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1297.223901
Zero-point correction= 0.391321
Thermal correction to Energy= 0.416073
Thermal correction to Enthalpy= 0.417017
Thermal correction to Gibbs Free Energy= 0.335256
Sum of electronic and zero-point Energies= -1296.832580
Sum of electronic and thermal Energies= -1296.807828
Sum of electronic and thermal Enthalpies= -1296.806884
Sum of electronic and thermal Free Energies= -1296.888645

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.639082 | 3.246695 | -0.406554 |
| 6 | 0.630502 | 1.866264 | -0.353133 |
| 6 | 1.797233 | 1.120541 | -0.248580 |
| 6 | 3.037178 | 1.749951 | -0.194804 |
| 6 | 3.043665 | 3.142875 | -0.245789 |
| 6 | 1.870969 | 3.891389 | -0.346803 |
| 1 | -0.298331 | 3.788870 | -0.498341 |
| 1 | 3.965512 | 1.192550 | -0.130915 |
| 1 | 4.001928 | 3.656158 | -0.214228 |
| 1 | 1.923460 | 4.975643 | -0.387457 |
| 6 | -0.512704 | 0.921373 | -0.418401 |
| 8 | -1.484573 | 1.232829 | -1.246928 |
| 7 | -1.113789 | 0.726965 | 1.016984 |
| 1 | -0.389907 | 0.418025 | 1.670871 |
| 7 | 1.439646 | -0.250821 | -0.213611 |
| 6 | 2.195442 | -1.361571 | -0.647762 |
| 8 | 1.724421 | -2.215890 | -1.359155 |
| 6 | 3.566883 | -1.430832 | -0.079493 |
| 6 | 4.556457 | -2.036673 | -0.856328 |
| 6 | 3.865753 | -1.000598 | 1.215846 |
| 6 | 5.844151 | -2.173229 | -0.356217 |
| 1 | 4.294735 | -2.395153 | -1.848858 |
| 6 | 5.151642 | -1.152951 | 1.719009 |
| 1 | 3.086514 | -0.554595 | 1.830376 |
| 6 | 6.142611 | -1.731173 | 0.930329 |
| 1 | 6.616799 | -2.632604 | -0.967514 |
| 1 | 5.379764 | -0.826963 | 2.730719 |

| | | | |
|---|---|---|---|
| 1 | 7.149723 | -1.846375 | 1.324115 |
| 8 | 0.090016 | -0.343945 | -0.645714 |
| 8 | -1.671427 | 1.902761 | 1.503044 |
| 1 | -2.630260 | 1.689808 | 1.440008 |
| 1 | -2.262288 | 0.550761 | -1.228006 |
| 1 | -1.984494 | 0.059054 | 0.984544 |
| 8 | -3.458220 | -0.334010 | -1.098687 |
| 6 | -4.020127 | -0.413810 | 0.015864 |
| 8 | -3.490439 | -0.044954 | 1.120228 |
| 6 | -5.411845 | -1.040322 | 0.109475 |
| 6 | -6.030213 | -1.207783 | -1.271691 |
| 1 | -7.019003 | -1.677286 | -1.184757 |
| 1 | -6.152996 | -0.239923 | -1.771608 |
| 1 | -5.401143 | -1.831621 | -1.914364 |
| 6 | -6.305590 | -0.165293 | 0.987316 |
| 1 | -7.294011 | -0.630162 | 1.097383 |
| 1 | -5.868158 | -0.032644 | 1.981797 |
| 1 | -6.451630 | 0.827158 | 0.541510 |
| 6 | -5.234506 | -2.411630 | 0.770267 |
| 1 | -4.593915 | -3.061260 | 0.160234 |
| 1 | -4.781798 | -2.311371 | 1.763079 |
| 1 | -6.209225 | -2.904745 | 0.880195 |

## Effect of Solvent Coordination on Lewis Acid in Nucleophilic Addition Elimination

---

**$(11a'\text{-}P)_{4s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2223.9635989
Zero-point correction= 0.376245
Thermal correction to Energy= 0.406487
Thermal correction to Enthalpy= 0.407431
Thermal correction to Gibbs Free Energy= 0.312533
Sum of electronic and zero-point Energies= -2223.587354
Sum of electronic and thermal Energies= -2223.557112
Sum of electronic and thermal Enthalpies= -2223.556168
Sum of electronic and thermal Free Energies= -2223.651066

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.134620 | -3.122154 | -1.228431 |
| 6 | 1.132010 | -1.837031 | -0.695147 |
| 6 | 2.266730 | -1.023053 | -0.757109 |
| 6 | 3.436472 | -1.521842 | -1.329856 |
| 6 | 3.437241 | -2.816827 | -1.836928 |

| | | | |
|---|---|---|---|
| 6 | 2.297915 | -3.618179 | -1.800706 |
| 1 | 0.223539 | -3.715514 | -1.187946 |
| 1 | 4.329845 | -0.909475 | -1.396488 |
| 1 | 4.349555 | -3.198930 | -2.288927 |
| 1 | 2.316331 | -4.617811 | -2.225169 |
| 6 | -0.068567 | -1.278953 | -0.036042 |
| 8 | -1.199433 | -1.307500 | -0.501015 |
| 7 | 0.064401 | -1.146310 | 1.492802 |
| 1 | 0.861225 | -1.690636 | 1.832460 |
| 7 | 2.072955 | 0.291198 | -0.233650 |
| 6 | 2.893581 | 0.677019 | 0.874240 |
| 8 | 2.418247 | 0.805299 | 1.983812 |
| 6 | 4.309460 | 0.957197 | 0.557836 |
| 6 | 5.249240 | 0.825403 | 1.583627 |
| 6 | 4.708424 | 1.423020 | -0.698447 |
| 6 | 6.584005 | 1.117127 | 1.343023 |
| 1 | 4.910487 | 0.492650 | 2.561755 |
| 6 | 6.044367 | 1.725925 | -0.931730 |
| 1 | 3.961338 | 1.557197 | -1.477953 |
| 6 | 6.981825 | 1.565339 | 0.085311 |
| 1 | 7.317627 | 1.000851 | 2.136704 |
| 1 | 6.354482 | 2.096590 | -1.905544 |
| 1 | 8.027366 | 1.799789 | -0.100856 |
| 8 | 0.727901 | 0.479919 | 0.048825 |
| 1 | 0.411294 | -0.019867 | 1.289414 |
| 30 | -3.044152 | -0.673768 | 0.228124 |
| 17 | -4.509865 | -2.266692 | 0.658195 |
| 17 | -2.457820 | 1.051464 | 1.700442 |
| 8 | -1.044718 | -1.537103 | 2.215140 |
| 1 | -1.506133 | -0.690249 | 2.431228 |
| 8 | -3.504084 | 0.492020 | -1.384423 |
| 6 | -3.756481 | 1.698186 | -1.155111 |
| 6 | -5.107786 | 2.088849 | -0.632903 |
| 1 | -5.011978 | 2.487558 | 0.384353 |
| 1 | -5.597721 | 2.843600 | -1.256763 |
| 1 | -5.727842 | 1.190448 | -0.600571 |
| 7 | -2.826966 | 2.641252 | -1.357786 |
| 6 | -1.465437 | 2.245979 | -1.692935 |
| 1 | -1.471090 | 1.240521 | -2.114339 |
| 1 | -1.057447 | 2.952858 | -2.423183 |
| 1 | -0.834214 | 2.238622 | -0.794544 |
| 6 | -2.979302 | 4.013777 | -0.915279 |
| 1 | -2.551777 | 4.141864 | 0.089174 |
| 1 | -2.448075 | 4.675081 | -1.607566 |
| 1 | -4.027543 | 4.314003 | -0.894532 |

---

**(11a'-P)$_{6s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2570.7966448
Zero-point correction= 0.522870
Thermal correction to Energy= 0.561938
Thermal correction to Enthalpy= 0.562883
Thermal correction to Gibbs Free Energy= 0.450039
Sum of electronic and zero-point Energies= -2570.273774
Sum of electronic and thermal Energies= -2570.234706
Sum of electronic and thermal Enthalpies= -2570.233762
Sum of electronic and thermal Free Energies= -2570.346606

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.442630 | -3.533039 | -0.554953 |
| 6 | -1.465662 | -2.180954 | -0.248914 |
| 6 | -2.640284 | -1.535321 | 0.133243 |
| 6 | -3.831112 | -2.253100 | 0.219239 |
| 6 | -3.805000 | -3.607484 | -0.104814 |
| 6 | -2.631378 | -4.252320 | -0.490073 |
| 1 | -0.497668 | -4.005549 | -0.821807 |
| 1 | -4.755080 | -1.787272 | 0.545419 |
| 1 | -4.729868 | -4.174886 | -0.034248 |
| 1 | -2.641538 | -5.313725 | -0.720532 |
| 6 | -0.256300 | -1.313280 | -0.293382 |
| 8 | 0.822523 | -1.617254 | 0.219260 |
| 7 | -0.154761 | -0.561190 | -1.637755 |
| 1 | -0.137847 | 0.742533 | -1.365736 |
| 7 | -2.395877 | -0.173766 | 0.424936 |
| 6 | -3.188142 | 0.789268 | 1.060834 |
| 8 | -2.691257 | 1.632171 | 1.775880 |
| 6 | -4.634331 | 0.763540 | 0.720359 |
| 6 | -5.091546 | 0.558524 | -0.583345 |
| 6 | -5.542941 | 1.042126 | 1.742247 |
| 6 | -6.453197 | 0.604250 | -0.854685 |
| 1 | -4.376774 | 0.371091 | -1.382268 |
| 6 | -6.904755 | 1.066143 | 1.471470 |
| 1 | -5.162788 | 1.236236 | 2.742317 |
| 6 | -7.360100 | 0.845303 | 0.174148 |
| 1 | -6.808889 | 0.454668 | -1.871070 |
| 1 | -7.613601 | 1.264723 | 2.271369 |
| 1 | -8.426164 | 0.870906 | -0.038723 |
| 8 | -1.028320 | -0.032921 | 0.688699 |

| | | | |
|---|---|---|---|
| 8 | 1.043188 | -0.795287 | -2.304071 |
| 1 | 1.233608 | -1.764317 | -2.333014 |
| 1 | -0.658582 | 1.050011 | 0.170397 |
| 30 | 2.810473 | -1.325906 | -0.315870 |
| 17 | 3.430985 | 0.844161 | -0.646008 |
| 17 | 2.941153 | -3.108953 | -1.728509 |
| 8 | -0.302560 | 1.706163 | -0.715337 |
| 1 | -0.935800 | -0.838635 | -2.239323 |
| 6 | 0.634377 | 2.686576 | -0.455712 |
| 6 | 1.046574 | 3.467322 | -1.686990 |
| 8 | 0.941958 | 2.924813 | 0.680257 |
| 8 | 3.533442 | -1.524695 | 1.586670 |
| 6 | 3.967986 | -0.490836 | 2.153934 |
| 6 | 5.447859 | -0.255250 | 2.194670 |
| 1 | 5.805318 | 0.122590 | 3.156471 |
| 1 | 5.941088 | -1.201468 | 1.966730 |
| 1 | 5.708585 | 0.465605 | 1.409372 |
| 7 | 3.138956 | 0.397207 | 2.715210 |
| 6 | 3.523278 | 1.750288 | 3.077368 |
| 1 | 3.076199 | 2.449964 | 2.357802 |
| 1 | 3.148114 | 1.987992 | 4.079512 |
| 1 | 4.604959 | 1.880840 | 3.064435 |
| 6 | 1.698049 | 0.191880 | 2.662984 |
| 1 | 1.261777 | 0.523906 | 3.611089 |
| 1 | 1.260892 | 0.793751 | 1.854661 |
| 1 | 1.475712 | -0.861909 | 2.498097 |
| 6 | -0.086803 | 4.476677 | -1.930480 |
| 1 | 0.158150 | 5.088700 | -2.807178 |
| 1 | -1.041773 | 3.972330 | -2.119404 |
| 1 | -0.211556 | 5.144762 | -1.069901 |
| 6 | 1.209908 | 2.567700 | -2.911473 |
| 1 | 1.559843 | 3.174604 | -3.755236 |
| 1 | 1.945249 | 1.773499 | -2.732849 |
| 1 | 0.258159 | 2.112892 | -3.215381 |
| 6 | 2.345545 | 4.208545 | -1.391843 |
| 1 | 2.608018 | 4.842571 | -2.247343 |
| 1 | 2.241959 | 4.842511 | -0.505322 |
| 1 | 3.163360 | 3.500663 | -1.216040 |

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**(11a'-P)$_{8s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2570.8275209
Zero-point correction= 0.526096
Thermal correction to Energy= 0.564668

Thermal correction to Enthalpy= 0.565612
Thermal correction to Gibbs Free Energy= 0.454434
Sum of electronic and zero-point Energies= -2570.301425
Sum of electronic and thermal Energies= -2570.262853
Sum of electronic and thermal Enthalpies= -2570.261908
Sum of electronic and thermal Free Energies= -2570.373087

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -0.005269 | -3.260343 | -0.966033 |
| 6 | -0.427768 | -2.096346 | -0.330906 |
| 6 | -1.720859 | -1.965411 | 0.187748 |
| 6 | -2.604501 | -3.041887 | 0.080036 |
| 6 | -2.180341 | -4.194168 | -0.570671 |
| 6 | -0.895463 | -4.316681 | -1.098423 |
| 1 | 1.011924 | -3.313883 | -1.351665 |
| 1 | -3.600099 | -2.992844 | 0.507613 |
| 1 | -2.874141 | -5.027736 | -0.649869 |
| 1 | -0.589421 | -5.233124 | -1.594015 |
| 6 | 0.482705 | -0.947477 | -0.195654 |
| 8 | 1.615340 | -0.946673 | 0.250395 |
| 7 | 0.218629 | 0.095457 | -1.299520 |
| 1 | 0.636864 | -0.318268 | -2.165361 |
| 7 | -1.945279 | -0.748551 | 0.839374 |
| 6 | -3.046223 | -0.274226 | 1.558366 |
| 8 | -2.906542 | 0.507121 | 2.476711 |
| 6 | -4.383028 | -0.670623 | 1.041407 |
| 6 | -4.677748 | -0.616313 | -0.324268 |
| 6 | -5.386089 | -0.967865 | 1.965021 |
| 6 | -5.969568 | -0.889473 | -0.758739 |
| 1 | -3.901426 | -0.333387 | -1.034186 |
| 6 | -6.668988 | -1.263847 | 1.521849 |
| 1 | -5.143039 | -0.958884 | 3.025095 |
| 6 | -6.960085 | -1.225744 | 0.160448 |
| 1 | -6.204725 | -0.835687 | -1.818956 |
| 1 | -7.446968 | -1.512265 | 2.239522 |
| 1 | -7.967341 | -1.447465 | -0.184601 |
| 8 | -0.745628 | -0.098975 | 1.098513 |
| 8 | 0.997276 | 1.231857 | -1.101030 |
| 1 | -0.809494 | 0.398594 | -1.415573 |
| 1 | 0.476744 | 1.795273 | -0.474718 |
| 8 | -2.129647 | 1.293479 | -1.417964 |
| 6 | -2.048629 | 2.175667 | -0.543607 |
| 8 | -1.126692 | 2.161886 | 0.377185 |
| 1 | -0.935268 | 1.035035 | 0.802068 |

| | | | |
|---|---|---|---|
| 30 | 3.205197 | 0.111949 | -0.775582 |
| 17 | 2.705340 | -0.787256 | -2.828910 |
| 17 | 3.960735 | 2.081433 | 0.025740 |
| 6 | -3.024273 | 3.336626 | -0.492300 |
| 8 | 4.636949 | -1.111096 | 0.059936 |
| 6 | 5.541515 | -0.594982 | 0.755023 |
| 6 | 6.869572 | -0.292435 | 0.129881 |
| 1 | 6.948677 | 0.791089 | -0.026086 |
| 1 | 7.719276 | -0.620882 | 0.735566 |
| 1 | 6.902332 | -0.785436 | -0.842561 |
| 7 | 5.339137 | -0.303465 | 2.049661 |
| 6 | 6.205100 | 0.588868 | 2.799134 |
| 1 | 5.848382 | 1.623984 | 2.701495 |
| 1 | 6.189144 | 0.305238 | 3.856166 |
| 1 | 7.235863 | 0.536644 | 2.447731 |
| 6 | 4.008175 | -0.481014 | 2.612146 |
| 1 | 4.100306 | -0.690853 | 3.681963 |
| 1 | 3.414000 | 0.433148 | 2.470798 |
| 1 | 3.503402 | -1.310885 | 2.116657 |
| 6 | -2.223192 | 4.629138 | -0.686054 |
| 1 | -2.900752 | 5.489960 | -0.628344 |
| 1 | -1.457031 | 4.739640 | 0.087976 |
| 1 | -1.733392 | 4.653419 | -1.667771 |
| 6 | -3.688495 | 3.346085 | 0.888462 |
| 1 | -4.392852 | 4.185342 | 0.946176 |
| 1 | -4.246796 | 2.419367 | 1.075801 |
| 1 | -2.945834 | 3.449912 | 1.685190 |
| 6 | -4.077069 | 3.198870 | -1.583680 |
| 1 | -4.758838 | 4.057480 | -1.548101 |
| 1 | -3.621079 | 3.158674 | -2.578826 |
| 1 | -4.670332 | 2.285938 | -1.449555 |

---

**$(11a'\text{-}9a')_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2570.7975395
Zero-point correction= 0.522692
Thermal correction to Energy= 0.561736
Thermal correction to Enthalpy= 0.562680
Thermal correction to Gibbs Free Energy= 0.450561
Sum of electronic and zero-point Energies= -2570.274848
Sum of electronic and thermal Energies= -2570.235804
Sum of electronic and thermal Enthalpies= -2570.234859
Sum of electronic and thermal Free Energies= -2570.346978
.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.130963 | -3.533108 | -0.675118 |
| 6 | 1.381920 | -2.182586 | -0.863743 |
| 6 | 2.660205 | -1.650549 | -0.704234 |
| 6 | 3.725723 | -2.479628 | -0.385232 |
| 6 | 3.472652 | -3.839333 | -0.205094 |
| 6 | 2.195204 | -4.368944 | -0.346242 |
| 1 | 0.109864 | -3.908762 | -0.755743 |
| 1 | 4.731348 | -2.090683 | -0.274169 |
| 1 | 4.303580 | -4.494694 | 0.044325 |
| 1 | 2.024167 | -5.431566 | -0.199360 |
| 6 | 0.329061 | -1.171923 | -1.134851 |
| 8 | -0.272785 | -0.618872 | -0.101870 |
| 7 | -0.424032 | -1.335973 | -2.289239 |
| 1 | -0.392178 | -2.259368 | -2.708208 |
| 7 | 2.684896 | -0.238941 | -0.937133 |
| 6 | 3.049824 | 0.721523 | 0.014203 |
| 8 | 2.381919 | 1.725313 | 0.184787 |
| 6 | 4.337608 | 0.500593 | 0.712884 |
| 6 | 4.387611 | 0.749604 | 2.085055 |
| 6 | 5.503852 | 0.179766 | 0.015046 |
| 6 | 5.591932 | 0.626101 | 2.764932 |
| 1 | 3.474940 | 1.033294 | 2.603709 |
| 6 | 6.711243 | 0.078256 | 0.696684 |
| 1 | 5.460387 | 0.030638 | -1.062601 |
| 6 | 6.752212 | 0.289990 | 2.071806 |
| 1 | 5.628158 | 0.799391 | 3.837336 |
| 1 | 7.622073 | -0.159965 | 0.152945 |
| 1 | 7.696122 | 0.202758 | 2.604699 |
| 8 | 1.521974 | 0.068288 | -1.641392 |
| 8 | -1.751721 | -0.948728 | -2.153787 |
| 1 | -1.800786 | -0.022579 | -2.436990 |
| 1 | -0.411887 | 0.553165 | -0.372042 |
| 8 | -0.170968 | 1.558363 | -0.986801 |
| 6 | -0.189886 | 2.717896 | -0.255089 |
| 8 | -0.703933 | 2.738985 | 0.830409 |
| 6 | 0.321124 | 3.946133 | -0.991047 |
| 6 | 1.226496 | 3.621534 | -2.173923 |
| 1 | 1.530677 | 4.555748 | -2.661479 |
| 1 | 2.134136 | 3.100437 | -1.851454 |
| 1 | 0.718033 | 3.005165 | -2.924616 |
| 6 | 1.046719 | 4.844146 | 0.007689 |
| 1 | 1.344100 | 5.778664 | -0.484012 |
| 1 | 0.400814 | 5.085724 | 0.857273 |

| | | | |
|---|---|---|---|
| 1 | 1.945492 | 4.349136 | 0.390777 |
| 6 | -0.947159 | 4.650762 | -1.497530 |
| 1 | -1.507521 | 4.010899 | -2.192768 |
| 1 | -1.604163 | 4.919340 | -0.661825 |
| 1 | -0.672576 | 5.569014 | -2.031096 |
| 1 | 0.854688 | 1.084064 | -1.300225 |
| 30 | -2.322764 | -1.271970 | 0.230969 |
| 17 | -2.515520 | -3.437985 | -0.380937 |
| 17 | -2.537509 | -0.580258 | 2.389131 |
| 8 | -3.487427 | 0.264109 | -0.598646 |
| 6 | -4.196173 | 0.957193 | 0.171517 |
| 6 | -3.824633 | 2.389540 | 0.383227 |
| 1 | -3.133261 | 2.446079 | 1.235055 |
| 1 | -3.269270 | 2.714193 | -0.499969 |
| 1 | -4.672216 | 3.058039 | 0.549603 |
| 7 | -5.268027 | 0.435938 | 0.785214 |
| 6 | -5.888694 | 1.034779 | 1.953100 |
| 1 | -5.661652 | 2.097846 | 2.027858 |
| 1 | -6.975594 | 0.910215 | 1.896835 |
| 1 | -5.515688 | 0.537298 | 2.858768 |
| 6 | -5.585620 | -0.972411 | 0.598263 |
| 1 | -5.095566 | -1.579978 | 1.372473 |
| 1 | -6.670047 | -1.100922 | 0.674588 |
| 1 | -5.251217 | -1.306235 | -0.385370 |

---

**(9a'-11a')$_{8's}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -2570.848441
Zero-point correction= 0.525080
Thermal correction to Energy= 0.563877
Thermal correction to Enthalpy= 0.564821
Thermal correction to Gibbs Free Energy= 0.453508
Sum of electronic and zero-point Energies= -2570.323361
Sum of electronic and thermal Energies= -2570.284564
Sum of electronic and thermal Enthalpies= -2570.283620
Sum of electronic and thermal Free Energies= -2570.394933

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.789519 | -2.179784 | 2.727720 |
| 6 | 1.573830 | -1.638943 | 1.469587 |
| 6 | 2.569794 | -0.922773 | 0.806895 |
| 6 | 3.810946 | -0.725457 | 1.410544 |
| 6 | 4.019622 | -1.277325 | 2.671074 |

| | | | |
|---|---|---|---|
| 6 | 3.028343 | -2.000037 | 3.332906 |
| 1 | 0.987243 | -2.728262 | 3.217011 |
| 1 | 4.591841 | -0.149411 | 0.925196 |
| 1 | 4.983021 | -1.124231 | 3.151848 |
| 1 | 3.220449 | -2.412315 | 4.319415 |
| 6 | 0.285084 | -1.743112 | 0.717948 |
| 8 | -0.806423 | -1.278753 | 1.232929 |
| 7 | 0.161027 | -2.960632 | 0.041737 |
| 1 | 0.965989 | -3.158620 | -0.548574 |
| 7 | 2.103209 | -0.461016 | -0.442594 |
| 6 | 2.647449 | 0.431960 | -1.363157 |
| 8 | 1.940655 | 1.192448 | -1.995699 |
| 6 | 4.117012 | 0.347395 | -1.566933 |
| 6 | 4.806506 | 1.533000 | -1.825970 |
| 6 | 4.794836 | -0.873625 | -1.601035 |
| 6 | 6.172714 | 1.502420 | -2.072157 |
| 1 | 4.252914 | 2.468847 | -1.832545 |
| 6 | 6.158215 | -0.902544 | -1.864810 |
| 1 | 4.249180 | -1.799144 | -1.428777 |
| 6 | 6.849108 | 0.285242 | -2.090075 |
| 1 | 6.710900 | 2.428382 | -2.259057 |
| 1 | 6.682692 | -1.854141 | -1.900682 |
| 1 | 7.917647 | 0.261083 | -2.290485 |
| 8 | 0.713332 | -0.527209 | -0.461659 |
| 8 | -0.978723 | -2.984613 | -0.768521 |
| 1 | -0.591522 | -0.091547 | 2.003763 |
| 1 | -1.596318 | -3.617215 | -0.348833 |
| 30 | -2.549613 | -1.232844 | 0.031863 |
| 17 | -3.825266 | -3.091642 | 0.290301 |
| 17 | -3.285827 | 0.861223 | 0.760468 |
| 8 | -2.185424 | -0.616479 | -1.890026 |
| 6 | -2.502454 | 0.521486 | -2.300294 |
| 7 | -3.781696 | 0.828336 | -2.578708 |
| 6 | -4.241833 | 2.198503 | -2.703102 |
| 1 | -5.121176 | 2.227126 | -3.354435 |
| 1 | -4.518967 | 2.593070 | -1.714239 |
| 1 | -3.474408 | 2.840674 | -3.137271 |
| 6 | -4.825630 | -0.147259 | -2.298528 |
| 1 | -5.212535 | -0.015027 | -1.278059 |
| 1 | -5.640288 | -0.008718 | -3.016370 |
| 1 | -4.426224 | -1.157921 | -2.395618 |
| 6 | -1.437399 | 1.555760 | -2.492780 |
| 1 | -1.519885 | 2.081561 | -3.448912 |
| 1 | -1.508855 | 2.293465 | -1.682298 |
| 1 | -0.459528 | 1.072621 | -2.422338 |

| | | | |
|---|---|---|---|
| 1 | 0.266154 | 0.656086 | 0.047031 |
| 8 | -0.518152 | 0.853614 | 2.455791 |
| 6 | -0.408436 | 1.802336 | 1.610905 |
| 8 | 0.005355 | 1.651817 | 0.420760 |
| 6 | -0.661890 | 3.205591 | 2.098404 |
| 6 | -1.663915 | 3.197759 | 3.249123 |
| 1 | -2.619443 | 2.767234 | 2.929043 |
| 1 | -1.296914 | 2.616288 | 4.100393 |
| 1 | -1.834634 | 4.228433 | 3.582131 |
| 6 | -1.175368 | 4.074451 | 0.952398 |
| 1 | -1.337607 | 5.093688 | 1.322459 |
| 1 | -0.460639 | 4.116948 | 0.123958 |
| 1 | -2.129684 | 3.686990 | 0.574627 |
| 6 | 0.701476 | 3.724719 | 2.584561 |
| 1 | 1.095584 | 3.102694 | 3.397319 |
| 1 | 1.433984 | 3.746253 | 1.768878 |
| 1 | 0.580069 | 4.745546 | 2.965487 |

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**$(9a'\text{-}11a')_{8s}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -2917.6275349
Zero-point correction= 0.673644
Thermal correction to Energy= 0.720749
Thermal correction to Enthalpy= 0.721694
Thermal correction to Gibbs Free Energy= 0.593302
Sum of electronic and zero-point Energies= -2916.953891
Sum of electronic and thermal Energies= -2916.906785
Sum of electronic and thermal Enthalpies= -2916.905841
Sum of electronic and thermal Free Energies= -2917.034233

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.248687 | -1.274118 | 3.145554 |
| 6 | 1.278564 | -0.862445 | 1.821288 |
| 6 | 2.201896 | -1.391329 | 0.922719 |
| 6 | 3.114206 | -2.356673 | 1.332497 |
| 6 | 3.062630 | -2.778624 | 2.658962 |
| 6 | 2.145361 | -2.253029 | 3.564809 |
| 1 | 0.538304 | -0.816112 | 3.831579 |
| 1 | 3.851736 | -2.767611 | 0.651217 |
| 1 | 3.771659 | -3.532838 | 2.990938 |
| 1 | 2.135898 | -2.597506 | 4.594733 |
| 6 | 0.373248 | 0.154923 | 1.209709 |
| 8 | 0.260915 | 1.273871 | 1.821722 |

| | | | |
|---|---|---|---|
| 7 | -0.838429 | -0.350367 | 0.573491 |
| 1 | -0.586571 | -1.028055 | -0.158706 |
| 7 | 2.055370 | -0.804180 | -0.352937 |
| 6 | 2.943898 | -0.693814 | -1.434161 |
| 8 | 3.059555 | 0.358268 | -2.025830 |
| 6 | 3.613667 | -1.956414 | -1.811515 |
| 6 | 4.923535 | -1.890721 | -2.290600 |
| 6 | 2.930565 | -3.176404 | -1.775545 |
| 6 | 5.567001 | -3.052906 | -2.692432 |
| 1 | 5.418625 | -0.923566 | -2.336482 |
| 6 | 3.575465 | -4.332059 | -2.197602 |
| 1 | 1.896650 | -3.213675 | -1.433113 |
| 6 | 4.893140 | -4.271623 | -2.644030 |
| 1 | 6.592571 | -3.010388 | -3.050356 |
| 1 | 3.045036 | -5.280508 | -2.182350 |
| 1 | 5.396895 | -5.180288 | -2.965778 |
| 8 | 1.219718 | 0.317600 | -0.235366 |
| 8 | -1.551818 | -1.099762 | 1.553946 |
| 1 | -0.283523 | 2.074744 | 1.177821 |
| 8 | -0.415864 | 2.949444 | 0.296812 |
| 6 | -1.555219 | 2.967646 | -0.368075 |
| 8 | -2.622608 | 2.699935 | 0.156057 |
| 6 | -1.433595 | 3.253036 | -1.864540 |
| 6 | -0.385379 | 4.320774 | -2.172098 |
| 1 | -0.396807 | 4.548496 | -3.245364 |
| 1 | -0.590010 | 5.253723 | -1.630925 |
| 1 | 0.631799 | 3.993089 | -1.928988 |
| 6 | -2.786243 | 3.691724 | -2.411615 |
| 1 | -2.712946 | 3.879652 | -3.490044 |
| 1 | -3.539188 | 2.915321 | -2.243115 |
| 1 | -3.138586 | 4.608915 | -1.924009 |
| 6 | -1.032370 | 1.918622 | -2.512330 |
| 1 | -0.041894 | 1.576966 | -2.183752 |
| 1 | -1.759946 | 1.131567 | -2.266693 |
| 1 | -1.000870 | 2.029551 | -3.603912 |
| 1 | 1.751277 | 1.340197 | -0.300721 |
| 8 | 1.989108 | 2.575681 | -0.228872 |
| 6 | 2.974530 | 2.770359 | 0.722761 |
| 8 | 3.713192 | 1.852148 | 0.945050 |
| 6 | 2.990708 | 4.134624 | 1.379738 |
| 6 | 1.921299 | 4.127564 | 2.483538 |
| 1 | 1.977413 | 5.075265 | 3.032717 |
| 1 | 0.907831 | 4.033537 | 2.077335 |
| 1 | 2.086150 | 3.307331 | 3.191414 |
| 6 | 2.687854 | 5.241230 | 0.368802 |

| | | | |
|---|---|---|---|
| 1 | 3.384002 | 5.219474 | -0.478017 |
| 1 | 1.665900 | 5.179283 | -0.023693 |
| 1 | 2.788568 | 6.214156 | 0.863969 |
| 6 | 4.369137 | 4.341938 | 1.999236 |
| 1 | 4.600016 | 3.551024 | 2.719292 |
| 1 | 5.153755 | 4.338413 | 1.234109 |
| 1 | 4.396507 | 5.307513 | 2.517329 |
| 1 | 1.065266 | 2.999344 | -0.080466 |
| 1 | -0.931971 | -1.760443 | 1.930519 |
| 30 | -2.855964 | -2.500826 | 0.392695 |
| 8 | -3.743588 | -1.062651 | -0.681993 |
| 6 | -4.335525 | -0.035027 | -0.265203 |
| 6 | -4.329451 | 0.343963 | 1.179704 |
| 1 | -5.247387 | 0.852430 | 1.482898 |
| 1 | -4.200575 | -0.550659 | 1.795021 |
| 1 | -3.486840 | 1.029215 | 1.347989 |
| 7 | -4.988001 | 0.749826 | -1.135753 |
| 6 | -5.622650 | 1.997533 | -0.727137 |
| 1 | -6.543554 | 1.815803 | -0.158871 |
| 1 | -4.923821 | 2.604882 | -0.143171 |
| 1 | -5.886459 | 2.556472 | -1.629009 |
| 6 | -5.084541 | 0.380216 | -2.538491 |
| 1 | -4.674021 | -0.619111 | -2.678916 |
| 1 | -6.135151 | 0.391439 | -2.850123 |
| 1 | -4.523810 | 1.086998 | -3.163810 |
| 17 | -4.108699 | -3.428708 | 1.967874 |
| 17 | -1.017593 | -3.312839 | -0.672512 |

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**(9a'-11a')$_{10s}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy = -2917.664351
Zero-point correction= 0.673618
Thermal correction to Energy= 0.722092
Thermal correction to Enthalpy= 0.723036
Thermal correction to Gibbs Free Energy= 0.589486
Sum of electronic and zero-point Energies= -2916.990733
Sum of electronic and thermal Energies= -2916.942259
Sum of electronic and thermal Enthalpies= -2916.941315
Sum of electronic and thermal Free Energies= -2917.074866

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.770820 | -3.343487 | 0.363990 |
| 6 | 1.258998 | -2.136392 | -0.144293 |

| | | | |
|---|---|---|---|
| 6 | 2.607667 | -1.978615 | -0.513463 |
| 6 | 3.445441 | -3.100675 | -0.406409 |
| 6 | 2.954187 | -4.285816 | 0.116134 |
| 6 | 1.624534 | -4.422333 | 0.515768 |
| 1 | -0.282783 | -3.411709 | 0.639001 |
| 1 | 4.474726 | -3.050919 | -0.741847 |
| 1 | 3.629614 | -5.135029 | 0.192280 |
| 1 | 1.257370 | -5.362054 | 0.917418 |
| 6 | 0.303531 | -1.027355 | -0.282933 |
| 8 | 0.130768 | -0.194440 | 0.696918 |
| 7 | -0.635257 | -1.184419 | -1.215580 |
| 1 | -0.486040 | -1.796263 | -2.007315 |
| 7 | 2.959252 | -0.756137 | -1.062983 |
| 6 | 4.194822 | -0.189311 | -1.385391 |
| 8 | 4.249721 | 0.805725 | -2.077938 |
| 6 | 5.422406 | -0.828842 | -0.833422 |
| 6 | 5.605465 | -1.012647 | 0.539258 |
| 6 | 6.443793 | -1.149723 | -1.727856 |
| 6 | 6.800670 | -1.552116 | 1.000944 |
| 1 | 4.815609 | -0.712152 | 1.224833 |
| 6 | 7.626847 | -1.709353 | -1.260398 |
| 1 | 6.296632 | -0.956039 | -2.788359 |
| 6 | 7.803778 | -1.913915 | 0.105480 |
| 1 | 6.950855 | -1.688678 | 2.069528 |
| 1 | 8.415845 | -1.975790 | -1.959960 |
| 1 | 8.732286 | -2.344552 | 0.474447 |
| 8 | 1.870793 | 0.033064 | -1.341121 |
| 8 | -1.760115 | -0.398177 | -1.292470 |
| 1 | -1.457970 | 0.562384 | -1.444293 |
| 1 | -0.364846 | 0.612090 | 0.431543 |
| 8 | -0.651474 | 1.812479 | -1.139509 |
| 6 | -0.669796 | 3.051924 | -1.143875 |
| 8 | 0.351314 | 3.738243 | -0.735772 |
| 6 | -1.860857 | 3.871653 | -1.594590 |
| 6 | -2.982855 | 2.956656 | -2.069705 |
| 1 | -3.829425 | 3.563204 | -2.412147 |
| 1 | -2.664008 | 2.324272 | -2.908024 |
| 1 | -3.340557 | 2.313867 | -1.254917 |
| 6 | -1.418844 | 4.806257 | -2.724596 |
| 1 | -2.269047 | 5.425179 | -3.036066 |
| 1 | -0.609338 | 5.468247 | -2.401945 |
| 1 | -1.074138 | 4.241930 | -3.599923 |
| 6 | -2.334766 | 4.693374 | -0.388606 |
| 1 | -2.619874 | 4.040959 | 0.446775 |
| 1 | -1.554113 | 5.379941 | -0.045622 |

| | | | |
|---|---|---|---|
| 1 | -3.213763 | 5.282875 | -0.677253 |
| 1 | 1.995407 | 0.980456 | -0.691081 |
| 8 | 2.006512 | 1.985790 | 0.077914 |
| 6 | 2.517680 | 1.714950 | 1.258176 |
| 8 | 3.127819 | 0.682854 | 1.492602 |
| 6 | 2.240046 | 2.760056 | 2.340740 |
| 6 | 2.964547 | 2.366710 | 3.622424 |
| 1 | 2.759728 | 3.103463 | 4.410101 |
| 1 | 2.641105 | 1.380732 | 3.971510 |
| 1 | 4.047824 | 2.320090 | 3.464677 |
| 6 | 0.728176 | 2.774647 | 2.597535 |
| 1 | 0.159229 | 3.103499 | 1.718494 |
| 1 | 0.368140 | 1.777384 | 2.883872 |
| 1 | 0.492919 | 3.463368 | 3.419221 |
| 6 | 2.715751 | 4.141559 | 1.888805 |
| 1 | 3.792844 | 4.139042 | 1.680944 |
| 1 | 2.199344 | 4.489561 | 0.988501 |
| 1 | 2.529289 | 4.874840 | 2.684405 |
| 1 | 1.079454 | 3.090711 | -0.399837 |
| 30 | -3.181228 | -0.630115 | 0.325407 |
| 17 | -2.851886 | 1.258250 | 1.471301 |
| 17 | -3.018952 | -2.808932 | 0.847633 |
| 8 | -4.866713 | -0.571563 | -0.824280 |
| 6 | -5.712311 | -1.490098 | -0.704613 |
| 6 | -5.974136 | -2.391245 | -1.871947 |
| 1 | -5.489042 | -3.359521 | -1.694708 |
| 1 | -7.038392 | -2.563658 | -2.055356 |
| 1 | -5.521048 | -1.936256 | -2.753523 |
| 7 | -6.374742 | -1.683533 | 0.444503 |
| 6 | -7.108549 | -2.897657 | 0.754951 |
| 1 | -6.497080 | -3.541110 | 1.402081 |
| 1 | -8.033448 | -2.642338 | 1.282775 |
| 1 | -7.365200 | -3.454063 | -0.146165 |
| 6 | -6.109027 | -0.825282 | 1.590378 |
| 1 | -7.037637 | -0.692129 | 2.153997 |
| 1 | -5.359986 | -1.282873 | 2.252424 |
| 1 | -5.751304 | 0.151358 | 1.258150 |

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**$(9a'\text{-}11a')_{12s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2917.6917439
Zero-point correction= 0.675291
Thermal correction to Energy= 0.722150
Thermal correction to Enthalpy= 0.723094

Thermal correction to Gibbs Free Energy= 0.597273
Sum of electronic and zero-point Energies= -2917.016453
Sum of electronic and thermal Energies= -2916.969594
Sum of electronic and thermal Enthalpies= -2916.968650
Sum of electronic and thermal Free Energies= -2917.094471

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.907352 | -3.465083 | 0.055721 |
| 6 | 1.038797 | -2.316537 | -0.703213 |
| 6 | 2.284003 | -1.810362 | -1.058139 |
| 6 | 3.450285 | -2.459071 | -0.664147 |
| 6 | 3.313143 | -3.632507 | 0.078013 |
| 6 | 2.064958 | -4.141728 | 0.432812 |
| 1 | -0.080650 | -3.800356 | 0.371307 |
| 1 | 4.435483 | -2.080131 | -0.916172 |
| 1 | 4.213707 | -4.158271 | 0.387399 |
| 1 | 1.998007 | -5.054636 | 1.018240 |
| 6 | -0.014805 | -1.320278 | -1.070751 |
| 8 | -0.453086 | -0.588765 | -0.036908 |
| 7 | -1.057501 | -1.908232 | -1.902778 |
| 1 | -1.496231 | -2.655286 | -1.354193 |
| 7 | 2.096292 | -0.606898 | -1.790787 |
| 6 | 2.738198 | 0.618934 | -1.626721 |
| 8 | 2.109981 | 1.664872 | -1.625308 |
| 6 | 4.215499 | 0.580960 | -1.558553 |
| 6 | 4.846506 | 1.470471 | -0.687194 |
| 6 | 4.974661 | -0.234436 | -2.400417 |
| 6 | 6.232557 | 1.506350 | -0.622440 |
| 1 | 4.227578 | 2.104569 | -0.056003 |
| 6 | 6.362783 | -0.181777 | -2.345175 |
| 1 | 4.472329 | -0.897909 | -3.102301 |
| 6 | 6.990231 | 0.680253 | -1.449855 |
| 1 | 6.725311 | 2.182749 | 0.071774 |
| 1 | 6.956197 | -0.809194 | -3.005660 |
| 1 | 8.076124 | 0.714985 | -1.402626 |
| 8 | 0.725174 | -0.454039 | -2.018011 |
| 8 | -2.126853 | -0.961709 | -1.974694 |
| 1 | -1.901170 | -0.396355 | -2.725852 |
| 1 | 0.264875 | -0.671328 | 1.167803 |
| 30 | -2.482548 | -0.353207 | 0.208461 |
| 17 | -3.256393 | -2.506665 | 0.621224 |
| 17 | -2.263328 | 1.196759 | 1.891017 |
| 8 | -4.217956 | 0.486898 | -0.717166 |
| 6 | -5.263933 | 0.039962 | -0.197052 |

| | | | |
|---|---|---|---|
| 6 | -5.702566 | 0.517479 | 1.157011 |
| 1 | -5.604916 | -0.297376 | 1.885908 |
| 1 | -5.036234 | 1.325165 | 1.467868 |
| 1 | -6.742353 | 0.860778 | 1.161019 |
| 7 | -6.008925 | -0.885206 | -0.830505 |
| 6 | -7.044105 | -1.649023 | -0.158436 |
| 1 | -7.578807 | -1.045489 | 0.576580 |
| 1 | -7.769236 | -1.997783 | -0.900736 |
| 1 | -6.604863 | -2.522222 | 0.345081 |
| 6 | -5.505516 | -1.486764 | -2.054823 |
| 1 | -4.967420 | -2.415365 | -1.819905 |
| 1 | -6.346803 | -1.702518 | -2.721957 |
| 1 | -4.812049 | -0.798850 | -2.536354 |
| 8 | -0.581181 | 1.961002 | -1.200352 |
| 6 | -0.381252 | 2.737140 | -0.186001 |
| 8 | 0.537693 | 2.577499 | 0.652403 |
| 1 | 1.169146 | 1.673416 | 0.749377 |
| 8 | 0.894223 | -0.827555 | 2.008910 |
| 6 | 1.948962 | -0.102010 | 1.974569 |
| 8 | 2.118846 | 0.853708 | 1.180486 |
| 6 | -1.217591 | 3.988374 | -0.143979 |
| 6 | 3.020350 | -0.423428 | 2.997629 |
| 1 | 0.150902 | 1.300258 | -1.321864 |
| 6 | -2.630120 | 3.720406 | -0.660836 |
| 1 | -3.138562 | 2.974270 | -0.039447 |
| 1 | -3.199330 | 4.657020 | -0.627889 |
| 1 | -2.624028 | 3.361042 | -1.695082 |
| 6 | -1.256352 | 4.574605 | 1.262301 |
| 1 | -0.250269 | 4.795237 | 1.633193 |
| 1 | -1.828877 | 5.509533 | 1.240607 |
| 1 | -1.738828 | 3.881250 | 1.958772 |
| 6 | -0.486337 | 4.959040 | -1.092435 |
| 1 | -1.036362 | 5.907051 | -1.117922 |
| 1 | 0.533394 | 5.162477 | -0.743729 |
| 1 | -0.434228 | 4.561422 | -2.112312 |
| 6 | 4.398759 | -0.299511 | 2.351848 |
| 1 | 4.577027 | 0.711542 | 1.972694 |
| 1 | 5.171754 | -0.533995 | 3.093789 |
| 1 | 4.507661 | -0.999693 | 1.511732 |
| 6 | 2.868440 | 0.623516 | 4.109587 |
| 1 | 1.880081 | 0.557130 | 4.580152 |
| 1 | 3.627819 | 0.449886 | 4.881970 |
| 1 | 2.998477 | 1.637813 | 3.715701 |
| 6 | 2.829450 | -1.824530 | 3.565875 |
| 1 | 2.862689 | -2.576590 | 2.768234 |

| | | | |
|---|---|---|---|
| 1 | 3.629451 | -2.040889 | 4.284560 |
| 1 | 1.866977 | -1.924374 | 4.076750 |

---

**$(11a'\text{-}P)_{4s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2223.9543319
Zero-point correction= 0.376080
Thermal correction to Energy= 0.406615
Thermal correction to Enthalpy= 0.407559
Thermal correction to Gibbs Free Energy= 0.311672
Sum of electronic and zero-point Energies= -2223.578252
Sum of electronic and thermal Energies= -2223.547717
Sum of electronic and thermal Enthalpies= -2223.546773
Sum of electronic and thermal Free Energies= -2223.642660

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.508334 | 3.206630 | -1.061956 |
| 6 | 1.449924 | 1.970039 | -0.444597 |
| 6 | 2.518502 | 1.082042 | -0.466195 |
| 6 | 3.702489 | 1.414977 | -1.119666 |
| 6 | 3.762047 | 2.665664 | -1.729403 |
| 6 | 2.689334 | 3.559020 | -1.708670 |
| 1 | 0.637077 | 3.860306 | -1.060717 |
| 1 | 4.545171 | 0.732548 | -1.166559 |
| 1 | 4.674628 | 2.943723 | -2.251245 |
| 1 | 2.774407 | 4.519158 | -2.209844 |
| 6 | 0.352088 | 1.328556 | 0.313484 |
| 8 | -0.942349 | 1.486649 | -0.070917 |
| 7 | 0.108530 | 2.013365 | 1.694017 |
| 1 | -0.178170 | 1.270615 | 2.357066 |
| 7 | 2.136170 | -0.079666 | 0.232443 |
| 6 | 2.564730 | -1.411802 | 0.027812 |
| 8 | 1.787165 | -2.328830 | -0.057371 |
| 6 | 4.041162 | -1.571731 | 0.015772 |
| 6 | 4.575643 | -2.570973 | -0.799517 |
| 6 | 4.878284 | -0.824306 | 0.848252 |
| 6 | 5.945986 | -2.792729 | -0.813994 |
| 1 | 3.899446 | -3.163218 | -1.411438 |
| 6 | 6.247761 | -1.060173 | 0.841392 |
| 1 | 4.451628 | -0.071990 | 1.508553 |
| 6 | 6.781606 | -2.035987 | 0.004193 |
| 1 | 6.364344 | -3.560769 | -1.459606 |
| 1 | 6.899147 | -0.486363 | 1.495901 |

| | | | |
|---|---|---|---|
| 1 | 7.854254 | -2.215308 | -0.003197 |
| 8 | 0.738941 | -0.006477 | 0.440945 |
| 1 | -0.908712 | 2.246410 | 1.006976 |
| 8 | 1.124834 | 2.736848 | 2.305236 |
| 1 | 1.205258 | 3.546751 | 1.782031 |
| 30 | -2.164652 | -0.163307 | 0.302716 |
| 17 | -1.917792 | -0.331462 | 2.566229 |
| 17 | -2.375100 | -1.736933 | -1.285893 |
| 8 | -3.938701 | 0.880026 | -0.027763 |
| 6 | -4.794012 | 0.307270 | -0.738299 |
| 6 | -5.018405 | 0.784417 | -2.141820 |
| 1 | -6.075949 | 0.887968 | -2.402032 |
| 1 | -4.517433 | 1.747142 | -2.250652 |
| 1 | -4.552324 | 0.072299 | -2.834557 |
| 7 | -5.511745 | -0.729677 | -0.274100 |
| 6 | -5.240468 | -1.251030 | 1.057508 |
| 1 | -6.182400 | -1.579850 | 1.508859 |
| 1 | -4.553816 | -2.107758 | 1.002822 |
| 1 | -4.788082 | -0.475398 | 1.677592 |
| 6 | -6.237695 | -1.638529 | -1.141570 |
| 1 | -7.116569 | -2.019769 | -0.611296 |
| 1 | -6.575327 | -1.142686 | -2.051996 |
| 1 | -5.591528 | -2.483889 | -1.417737 |

---

**$(11a'\text{-}P)_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2570.8307032
Zero-point correction= 0.529581
Thermal correction to Energy= 0.567235
Thermal correction to Enthalpy= 0.568179
Thermal correction to Gibbs Free Energy= 0.459853
Sum of electronic and zero-point Energies= -2570.301122
Sum of electronic and thermal Energies= -2570.263469
Sum of electronic and thermal Enthalpies= -2570.262524
Sum of electronic and thermal Free Energies= -2570.370850

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.595165 | -2.959683 | -0.397041 |
| 6 | -1.676435 | -1.824579 | 0.393187 |
| 6 | -2.895626 | -1.210064 | 0.664894 |
| 6 | -4.082241 | -1.719191 | 0.158640 |
| 6 | -3.997795 | -2.868967 | -0.625296 |
| 6 | -2.780525 | -3.487362 | -0.898975 |

| | | | |
|---|---|---|---|
| 1 | -0.637107 | -3.418828 | -0.622587 |
| 1 | -5.037794 | -1.242977 | 0.353350 |
| 1 | -4.913775 | -3.289135 | -1.033506 |
| 1 | -2.750779 | -4.375020 | -1.523653 |
| 6 | -0.626406 | -0.961046 | 0.993030 |
| 8 | 0.126589 | -0.274382 | 0.088069 |
| 7 | 0.330366 | -1.677081 | 1.946800 |
| 1 | -0.198599 | -1.986495 | 2.764456 |
| 7 | -2.678749 | -0.052256 | 1.475191 |
| 6 | -2.952286 | 1.248390 | 0.915201 |
| 8 | -2.080641 | 2.052926 | 0.707073 |
| 6 | -4.394498 | 1.497208 | 0.692901 |
| 6 | -4.751219 | 2.359915 | -0.346040 |
| 6 | -5.379355 | 0.960251 | 1.526909 |
| 6 | -6.088341 | 2.652108 | -0.574019 |
| 1 | -3.965792 | 2.783991 | -0.966675 |
| 6 | -6.716110 | 1.268751 | 1.304422 |
| 1 | -5.089657 | 0.318461 | 2.356423 |
| 6 | -7.070031 | 2.106018 | 0.250073 |
| 1 | -6.368098 | 3.308636 | -1.393882 |
| 1 | -7.482407 | 0.861749 | 1.959393 |
| 1 | -8.117139 | 2.340554 | 0.073181 |
| 8 | -1.327691 | -0.128023 | 1.887064 |
| 8 | 0.895899 | -2.811762 | 1.387482 |
| 1 | 1.593818 | -2.494023 | 0.747809 |
| 1 | 0.836464 | 0.266226 | 0.632353 |
| 1 | 1.099589 | -0.935169 | 2.187578 |
| 8 | 3.380950 | 1.394576 | 0.596698 |
| 6 | 3.061944 | 0.612972 | 1.490628 |
| 8 | 1.828634 | 0.325051 | 1.772519 |
| 30 | 1.069379 | -0.789066 | -1.805096 |
| 17 | 2.802521 | -1.966020 | -0.836384 |
| 17 | -0.351043 | -1.650941 | -3.265721 |
| 8 | 1.502976 | 1.139030 | -1.987251 |
| 6 | 2.551212 | 1.826723 | -1.963136 |
| 6 | 3.852157 | 1.257882 | -2.433064 |
| 1 | 4.397885 | 1.935579 | -3.095558 |
| 1 | 4.466755 | 1.046870 | -1.548729 |
| 1 | 3.663733 | 0.318649 | -2.958128 |
| 7 | 2.489924 | 3.093682 | -1.532608 |
| 6 | 1.289299 | 3.504351 | -0.815073 |
| 1 | 1.355316 | 3.168989 | 0.229574 |
| 1 | 1.207307 | 4.594199 | -0.850545 |
| 1 | 0.406916 | 3.055311 | -1.270159 |
| 6 | 3.691120 | 3.844885 | -1.208380 |

| | | | |
|---|---|---|---|
| 1 | 3.439612 | 4.908383 | -1.165865 |
| 1 | 4.085059 | 3.517934 | -0.237155 |
| 1 | 4.460882 | 3.715213 | -1.971850 |
| 6 | 4.145105 | -0.001649 | 2.386875 |
| 6 | 5.355620 | -0.367347 | 1.531165 |
| 1 | 6.162646 | -0.759197 | 2.164190 |
| 1 | 5.096749 | -1.131709 | 0.786579 |
| 1 | 5.726596 | 0.513052 | 0.996725 |
| 6 | 4.530928 | 1.087809 | 3.393757 |
| 1 | 3.668317 | 1.380769 | 4.006523 |
| 1 | 5.319814 | 0.724905 | 4.065769 |
| 1 | 4.900671 | 1.979246 | 2.874238 |
| 6 | 3.648338 | -1.231381 | 3.138607 |
| 1 | 3.302982 | -2.014511 | 2.450359 |
| 1 | 4.460936 | -1.659505 | 3.739311 |
| 1 | 2.829948 | -0.977511 | 3.824651 |

---

**(11a'-P)$_{8s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2570.8530847
Zero-point correction= 0.526168
Thermal correction to Energy= 0.564078
Thermal correction to Enthalpy= 0.565023
Thermal correction to Gibbs Free Energy= 0.457212
Sum of electronic and zero-point Energies= -2570.326916
Sum of electronic and thermal Energies= -2570.289006
Sum of electronic and thermal Enthalpies= -2570.288062
Sum of electronic and thermal Free Energies= -2570.395873

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.139160 | 0.955735 | -3.269824 |
| 6 | -0.670732 | -0.046604 | -2.433895 |
| 6 | -1.530732 | -0.979314 | -1.863879 |
| 6 | -2.891246 | -0.958287 | -2.129138 |
| 6 | -3.357801 | 0.042086 | -2.979160 |
| 6 | -2.503814 | 0.987131 | -3.544134 |
| 1 | -0.461816 | 1.704281 | -3.673804 |
| 1 | -3.573555 | -1.673576 | -1.681449 |
| 1 | -4.421509 | 0.084462 | -3.200024 |
| 1 | -2.904061 | 1.757998 | -4.196430 |
| 6 | 0.685397 | -0.280968 | -1.854570 |
| 8 | 1.132352 | 0.657441 | -1.005916 |
| 7 | 1.808171 | -0.491207 | -2.826508 |

| | | | |
|---|---|---|---|
| 1 | 1.508153 | -1.110633 | -3.580027 |
| 7 | -0.781617 | -1.848873 | -1.013763 |
| 6 | -1.015761 | -1.908875 | 0.389252 |
| 8 | -0.144437 | -1.684285 | 1.197964 |
| 6 | -2.374933 | -2.386080 | 0.738879 |
| 6 | -2.970113 | -3.439352 | 0.040601 |
| 6 | -3.024016 | -1.819794 | 1.837197 |
| 6 | -4.215464 | -3.916077 | 0.434088 |
| 1 | -2.446853 | -3.887820 | -0.801679 |
| 6 | -4.275040 | -2.287094 | 2.214903 |
| 1 | -2.545656 | -0.993846 | 2.358943 |
| 6 | -4.870042 | -3.335305 | 1.516147 |
| 1 | -4.674265 | -4.743200 | -0.102191 |
| 1 | -4.791548 | -1.831185 | 3.055919 |
| 1 | -5.847808 | -3.702738 | 1.819333 |
| 8 | 0.573667 | -1.593862 | -1.292531 |
| 8 | 2.116607 | 0.727653 | -3.453114 |
| 1 | 2.101153 | 1.364714 | -2.710424 |
| 1 | 2.069916 | 0.135823 | -0.157586 |
| 1 | 2.763133 | -0.962014 | -2.081974 |
| 8 | 2.786065 | -0.366701 | 0.477954 |
| 6 | 3.489045 | -1.271216 | -0.082577 |
| 8 | 3.539563 | -1.479588 | -1.326273 |
| 30 | -0.046682 | 2.148750 | -0.254163 |
| 17 | 0.312830 | 3.868691 | -1.646846 |
| 17 | -1.995797 | 1.360645 | 0.630710 |
| 8 | 1.147177 | 2.220213 | 1.443251 |
| 6 | 0.620223 | 1.940838 | 2.543172 |
| 6 | 0.908223 | 0.617754 | 3.181394 |
| 1 | 1.114778 | 0.690151 | 4.253306 |
| 1 | 0.053703 | -0.053922 | 3.026180 |
| 1 | 1.759833 | 0.174819 | 2.660748 |
| 7 | -0.202032 | 2.809202 | 3.159440 |
| 6 | -0.544772 | 4.060334 | 2.498376 |
| 1 | -1.477529 | 3.948894 | 1.927926 |
| 1 | -0.677679 | 4.838167 | 3.257246 |
| 1 | 0.256927 | 4.352135 | 1.817819 |
| 6 | -1.104769 | 2.409587 | 4.222774 |
| 1 | -2.049528 | 2.040660 | 3.797384 |
| 1 | -0.668966 | 1.628980 | 4.847708 |
| 1 | -1.318595 | 3.274868 | 4.858180 |
| 6 | 4.241404 | -2.196610 | 0.845743 |
| 6 | 4.870252 | -1.414703 | 1.997185 |
| 1 | 5.377023 | -2.113764 | 2.673288 |
| 1 | 5.615900 | -0.696954 | 1.634631 |

| | | | |
|---|---|---|---|
| 1 | 4.118853 | -0.865243 | 2.571641 |
| 6 | 3.157033 | -3.145002 | 1.384663 |
| 1 | 2.688681 | -3.707389 | 0.566960 |
| 1 | 3.612432 | -3.861561 | 2.079041 |
| 1 | 2.367733 | -2.589313 | 1.904060 |
| 6 | 5.306542 | -2.983847 | 0.093347 |
| 1 | 6.067666 | -2.320348 | -0.333593 |
| 1 | 5.804298 | -3.674071 | 0.784614 |
| 1 | 4.872131 | -3.566410 | -0.724672 |

## II. Pivalate as ligand

## III.

### Pathway A (LA=0)

---

**$(2a\text{-}3a)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1295.0200212
Zero-point correction= 0.402242
Thermal correction to Energy= 0.429589
Thermal correction to Enthalpy= 0.430533
Thermal correction to Gibbs Free Energy= 0.343873
Sum of electronic and zero-point Energies= -1294.617779
Sum of electronic and thermal Energies= -1294.590433
Sum of electronic and thermal Enthalpies= -1294.589488
Sum of electronic and thermal Free Energies= -1294.676148

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.879737 | 3.868312 | -1.970223 |
| 6 | -0.684344 | 4.310701 | -1.408871 |
| 6 | -0.161273 | 3.664567 | -0.299021 |
| 6 | -0.823920 | 2.559493 | 0.245354 |
| 6 | -2.027573 | 2.120059 | -0.316053 |
| 6 | -2.551694 | 2.780799 | -1.419287 |
| 1 | -2.292903 | 4.377016 | -2.838109 |
| 1 | -0.162214 | 5.162397 | -1.837305 |
| 1 | 0.764893 | 3.994568 | 0.164131 |
| 1 | -2.570729 | 1.284035 | 0.119292 |
| 1 | -3.492791 | 2.446462 | -1.848910 |
| 6 | -0.205300 | 1.938570 | 1.431838 |
| 8 | 0.602538 | 2.493761 | 2.153331 |
| 7 | -0.525165 | 0.570090 | 1.712695 |
| 1 | -1.578321 | 0.076252 | 1.574954 |
| 8 | -0.010514 | 0.186487 | 2.938431 |

| | | | |
|---|---|---|---|
| 46 | 0.473512 | -0.520317 | 0.260554 |
| 8 | -2.637602 | -0.668572 | 1.234778 |
| 8 | -1.251914 | -1.451691 | -0.350494 |
| 8 | 1.974213 | -1.429347 | -0.936526 |
| 8 | 2.424031 | 0.114235 | 0.538334 |
| 6 | -2.379140 | -1.384707 | 0.228339 |
| 6 | 2.839245 | -0.705567 | -0.355585 |
| 6 | -3.522194 | -2.158879 | -0.421557 |
| 6 | 4.312863 | -0.839593 | -0.643812 |
| 1 | 0.669695 | 0.874642 | 3.112646 |
| 6 | -2.999242 | -3.343995 | -1.225364 |
| 1 | -3.840069 | -3.868288 | -1.696560 |
| 1 | -2.304762 | -3.023011 | -2.007302 |
| 1 | -2.471365 | -4.057625 | -0.582011 |
| 6 | -4.512586 | -2.628516 | 0.639329 |
| 1 | -4.902551 | -1.788688 | 1.221369 |
| 1 | -5.353331 | -3.140532 | 0.154446 |
| 1 | -4.044311 | -3.334141 | 1.335861 |
| 6 | -4.202741 | -1.152225 | -1.359968 |
| 1 | -3.492267 | -0.761312 | -2.100074 |
| 1 | -5.022505 | -1.643679 | -1.898861 |
| 1 | -4.623987 | -0.310804 | -0.794803 |
| 6 | 4.863619 | -1.812783 | 0.408476 |
| 1 | 5.940221 | -1.952262 | 0.250832 |
| 1 | 4.710465 | -1.424562 | 1.422119 |
| 1 | 4.375516 | -2.791805 | 0.331844 |
| 6 | 4.996139 | 0.518344 | -0.503083 |
| 1 | 6.074169 | 0.404386 | -0.671099 |
| 1 | 4.612161 | 1.235498 | -1.238389 |
| 1 | 4.842769 | 0.941508 | 0.494606 |
| 6 | 4.522030 | -1.410437 | -2.042510 |
| 1 | 5.595602 | -1.536042 | -2.229479 |
| 1 | 4.032827 | -2.383161 | -2.154091 |
| 1 | 4.117454 | -0.740725 | -2.810331 |

---

**$(2a\text{-}3a)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1523.9863648
Zero-point correction= 0.463545
Thermal correction to Energy= 0.496143
Thermal correction to Enthalpy= 0.497087
Thermal correction to Gibbs Free Energy= 0.398574
Sum of electronic and zero-point Energies= -1523.522819
Sum of electronic and thermal Energies= -1523.490222

Sum of electronic and thermal Enthalpies= -1523.489277
Sum of electronic and thermal Free Energies= -1523.587791

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 4.991549 | -0.644957 | -0.952831 |
| 6 | 4.347308 | -0.960503 | -2.147930 |
| 6 | 3.060180 | -1.476306 | -2.123520 |
| 6 | 2.403774 | -1.661407 | -0.902702 |
| 6 | 3.052603 | -1.350716 | 0.295432 |
| 6 | 4.347461 | -0.846679 | 0.265169 |
| 1 | 6.003070 | -0.245605 | -0.970433 |
| 1 | 4.852224 | -0.806731 | -3.098175 |
| 1 | 2.542560 | -1.743667 | -3.041235 |
| 1 | 2.565839 | -1.515934 | 1.254090 |
| 1 | 4.855823 | -0.615818 | 1.198369 |
| 6 | 1.061645 | -2.267405 | -0.940536 |
| 8 | 0.668348 | -3.007726 | -1.823291 |
| 7 | 0.160407 | -1.961653 | 0.132033 |
| 1 | 0.440784 | -1.614021 | 1.247838 |
| 8 | -0.836345 | -2.919757 | 0.208430 |
| 46 | -0.797891 | -0.162106 | -0.334859 |
| 8 | 1.592594 | 1.161926 | 1.691801 |
| 8 | 0.907414 | 0.982149 | -0.452899 |
| 8 | -2.264264 | 1.307591 | -0.692444 |
| 8 | -2.784347 | -0.790085 | -0.433425 |
| 6 | 1.585045 | 1.509198 | 0.471362 |
| 6 | -3.167575 | 0.413128 | -0.630430 |
| 6 | 2.430127 | 2.718304 | 0.093568 |
| 6 | -4.621656 | 0.766103 | -0.811798 |
| 6 | -0.437005 | -0.826040 | 3.211222 |
| 8 | 0.588369 | -0.928580 | 2.339190 |
| 1 | 1.063618 | 0.201394 | 2.022730 |
| 8 | -0.598127 | 0.161751 | 3.884548 |
| 6 | -1.338686 | -2.026411 | 3.219619 |
| 1 | -0.760105 | -2.955139 | 3.249476 |
| 1 | -2.017262 | -1.972002 | 4.072067 |
| 1 | -1.921971 | -2.045021 | 2.289583 |
| 6 | -4.943858 | 1.993952 | 0.041132 |
| 1 | -4.310060 | 2.844042 | -0.229956 |
| 1 | -5.992238 | 2.278268 | -0.111347 |
| 1 | -4.800437 | 1.787167 | 1.108323 |
| 6 | -4.813023 | 1.101338 | -2.297052 |
| 1 | -4.570488 | 0.240162 | -2.931814 |
| 1 | -5.860196 | 1.372752 | -2.478730 |

| | | | |
|---|---|---|---|
| 1 | -4.179686 | 1.943465 | -2.596483 |
| 6 | -5.506830 | -0.410826 | -0.419185 |
| 1 | -5.282198 | -1.299153 | -1.018686 |
| 1 | -5.372885 | -0.676116 | 0.635518 |
| 1 | -6.559175 | -0.144135 | -0.575591 |
| 6 | 3.646290 | 2.828520 | 1.006990 |
| 1 | 4.222623 | 3.723656 | 0.742238 |
| 1 | 3.353543 | 2.898896 | 2.058442 |
| 1 | 4.302095 | 1.956391 | 0.893306 |
| 6 | 2.868883 | 2.630758 | -1.364799 |
| 1 | 3.487225 | 3.502340 | -1.612642 |
| 1 | 3.463010 | 1.724823 | -1.543294 |
| 1 | 2.011065 | 2.610663 | -2.043240 |
| 6 | 1.512728 | 3.932957 | 0.296110 |
| 1 | 0.618124 | 3.861728 | -0.334198 |
| 1 | 1.195488 | 4.016835 | 1.342175 |
| 1 | 2.053931 | 4.848191 | 0.025741 |
| 1 | -0.887085 | -3.265166 | -0.708964 |

---

**$(2a\text{-}3a)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1523.9955
Zero-point correction= 0.466746
Thermal correction to Energy= 0.498435
Thermal correction to Enthalpy= 0.499379
Thermal correction to Gibbs Free Energy= 0.404225
Sum of electronic and zero-point Energies= -1523.528754
Sum of electronic and thermal Energies= -1523.497065
Sum of electronic and thermal Enthalpies= -1523.496121
Sum of electronic and thermal Free Energies= -1523.591275

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.584366 | 3.358369 | -0.723733 |
| 6 | 3.600980 | 3.319542 | 0.668360 |
| 6 | 2.517331 | 2.795108 | 1.356635 |
| 6 | 1.413404 | 2.300336 | 0.657200 |
| 6 | 1.396277 | 2.349166 | -0.739745 |
| 6 | 2.480782 | 2.879247 | -1.424498 |
| 1 | 4.434145 | 3.768049 | -1.265365 |
| 1 | 4.461730 | 3.696448 | 1.215315 |
| 1 | 2.503798 | 2.750041 | 2.442493 |
| 1 | 0.542417 | 1.970524 | -1.295356 |
| 1 | 2.465878 | 2.917830 | -2.510791 |

| | | | |
|---|---|---|---|
| 6 | 0.313777 | 1.730763 | 1.456600 |
| 8 | 0.190859 | 1.900365 | 2.661269 |
| 7 | -0.656227 | 0.953169 | 0.755564 |
| 1 | -1.296683 | 1.666089 | -0.206285 |
| 8 | -1.733493 | 0.709292 | 1.611100 |
| 1 | -1.366753 | 0.925943 | 2.497199 |
| 46 | 0.259867 | -0.854226 | 0.228076 |
| 8 | -2.379233 | -0.451118 | -1.072911 |
| 8 | -1.545844 | -1.868833 | 0.388895 |
| 8 | 1.563513 | -2.436085 | -0.323810 |
| 8 | 2.292478 | -0.417493 | 0.054562 |
| 6 | -2.529109 | -1.390132 | -0.218239 |
| 6 | 2.541250 | -1.628053 | -0.271450 |
| 6 | -3.915144 | -1.934364 | 0.097669 |
| 6 | 3.955741 | -2.081945 | -0.533647 |
| 6 | 4.424737 | -2.798157 | 0.740121 |
| 1 | 5.453437 | -3.154521 | 0.604015 |
| 1 | 4.409270 | -2.119977 | 1.602061 |
| 1 | 3.786842 | -3.660249 | 0.965402 |
| 6 | 4.848309 | -0.878382 | -0.816332 |
| 1 | 5.875844 | -1.217876 | -0.996815 |
| 1 | 4.506692 | -0.326081 | -1.699767 |
| 1 | 4.854077 | -0.180847 | 0.027524 |
| 6 | 3.968661 | -3.056500 | -1.709864 |
| 1 | 3.630047 | -2.571140 | -2.633097 |
| 1 | 4.990896 | -3.419906 | -1.872948 |
| 1 | 3.319977 | -3.917309 | -1.520723 |
| 6 | -4.804441 | -1.891363 | -1.144015 |
| 1 | -5.782719 | -2.324015 | -0.901421 |
| 1 | -4.973364 | -0.871144 | -1.504330 |
| 1 | -4.372225 | -2.476230 | -1.964692 |
| 6 | -3.813568 | -3.365310 | 0.617702 |
| 1 | -3.385257 | -4.034572 | -0.137592 |
| 1 | -3.183437 | -3.420490 | 1.510030 |
| 1 | -4.815053 | -3.733269 | 0.872416 |
| 6 | -4.491741 | -1.028164 | 1.195038 |
| 1 | -4.548162 | 0.017933 | 0.871764 |
| 1 | -5.504419 | -1.367742 | 1.445958 |
| 1 | -3.872686 | -1.073456 | 2.097943 |
| 6 | -3.050854 | 2.510740 | -1.074555 |
| 8 | -3.760876 | 1.481801 | -1.189686 |
| 1 | -3.121205 | 0.400610 | -1.140055 |
| 8 | -1.815564 | 2.531823 | -0.755683 |
| 6 | -3.676166 | 3.846121 | -1.326408 |
| 1 | -4.656604 | 3.734788 | -1.790991 |

| | | | |
|---|---|---|---|
| 1 | -3.782948 | 4.370291 | -0.370834 |
| 1 | -3.016102 | 4.452331 | -1.952413 |

---

**$(3a\text{-}4a)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1294.9947405
Zero-point correction= 0.400766
Thermal correction to Energy= 0.428379
Thermal correction to Enthalpy= 0.429323
Thermal correction to Gibbs Free Energy= 0.341552
Sum of electronic and zero-point Energies= -1294.593975
Sum of electronic and thermal Energies= -1294.566362
Sum of electronic and thermal Enthalpies= -1294.565417
Sum of electronic and thermal Free Energies= -1294.653188

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.271591 | -1.663343 | -0.290278 |
| 6 | -2.977201 | -1.408189 | 0.155223 |
| 6 | -2.361477 | -0.155823 | -0.073878 |
| 6 | -3.054945 | 0.774094 | -0.869558 |
| 6 | -4.353343 | 0.526373 | -1.293881 |
| 6 | -4.968325 | -0.688197 | -0.989033 |
| 1 | -4.683184 | -2.655906 | -0.121155 |
| 1 | -1.692565 | 0.694341 | 0.724969 |
| 1 | -2.596329 | 1.737578 | -1.087111 |
| 1 | -4.892066 | 1.283853 | -1.858526 |
| 1 | -5.982837 | -0.882829 | -1.329263 |
| 6 | -2.171900 | -2.550603 | 0.632186 |
| 8 | -2.554728 | -3.718512 | 0.706282 |
| 7 | -0.874387 | -2.187768 | 0.892047 |
| 8 | -0.044165 | -3.261886 | 1.006651 |
| 1 | -0.608029 | -4.017546 | 0.724391 |
| 46 | -0.263277 | -0.522720 | -0.041422 |
| 8 | 0.293866 | 1.523955 | -0.451846 |
| 8 | -1.237531 | 1.939545 | 1.118090 |
| 8 | 1.800301 | -1.181784 | -0.201040 |
| 6 | -0.293679 | 2.304911 | 0.371373 |
| 6 | 0.100852 | 3.776628 | 0.366581 |
| 6 | 2.827448 | -0.530620 | -0.392107 |
| 8 | 2.848555 | 0.761479 | -0.625509 |
| 1 | 1.929989 | 1.138266 | -0.616393 |
| 6 | 4.193818 | -1.179179 | -0.301718 |
| 6 | 5.152183 | -0.583818 | -1.330986 |

| | | | |
|---|---|---|---|
| 1 | 5.287263 | 0.492229 | -1.185503 |
| 1 | 6.130573 | -1.069947 | -1.235358 |
| 1 | 4.794007 | -0.748770 | -2.354185 |
| 6 | 4.059223 | -2.685158 | -0.499232 |
| 1 | 5.040944 | -3.158252 | -0.377841 |
| 1 | 3.363980 | -3.122196 | 0.223993 |
| 1 | 3.688132 | -2.921298 | -1.503355 |
| 6 | 4.701258 | -0.883275 | 1.118194 |
| 1 | 4.020392 | -1.295732 | 1.872408 |
| 1 | 5.684933 | -1.348583 | 1.255391 |
| 1 | 4.805303 | 0.194363 | 1.289355 |
| 6 | -0.875581 | 4.447060 | -0.609957 |
| 1 | -0.656432 | 5.519931 | -0.676176 |
| 1 | -0.782691 | 4.017385 | -1.615699 |
| 1 | -1.911768 | 4.328635 | -0.270022 |
| 6 | 1.533146 | 3.961772 | -0.123391 |
| 1 | 1.793993 | 5.026830 | -0.104379 |
| 1 | 2.248877 | 3.430694 | 0.516997 |
| 1 | 1.660984 | 3.600764 | -1.149757 |
| 6 | -0.065632 | 4.374110 | 1.760296 |
| 1 | 0.614200 | 3.901808 | 2.479463 |
| 1 | 0.165322 | 5.446050 | 1.730674 |
| 1 | -1.087477 | 4.244989 | 2.128156 |

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**(3a-4a)$_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1523.9833118
Zero-point correction= 0.465032
Thermal correction to Energy= 0.497407
Thermal correction to Enthalpy= 0.498351
Thermal correction to Gibbs Free Energy= 0.401470
Sum of electronic and zero-point Energies= -1523.518280
Sum of electronic and thermal Energies= -1523.485905
Sum of electronic and thermal Enthalpies= -1523.484961
Sum of electronic and thermal Free Energies= -1523.581842

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.602948 | 4.007823 | -0.979983 |
| 6 | 2.970502 | 3.852200 | -1.159889 |
| 6 | 3.605188 | 2.655153 | -0.810662 |
| 6 | 2.868700 | 1.607475 | -0.280131 |
| 6 | 1.490487 | 1.753766 | -0.030631 |
| 6 | 0.870731 | 2.965260 | -0.420137 |

| | | | |
|---|---|---|---|
| 1 | 1.076706 | 4.906016 | -1.295155 |
| 1 | 3.553957 | 4.662069 | -1.592240 |
| 1 | 4.678266 | 2.550859 | -0.953196 |
| 1 | 3.370371 | 0.686430 | 0.017887 |
| 6 | -0.601678 | 3.041390 | -0.368534 |
| 8 | -1.299084 | 3.974236 | -0.763878 |
| 7 | -1.137867 | 1.875792 | 0.134525 |
| 8 | -2.494936 | 1.821987 | -0.054928 |
| 1 | -2.676434 | 2.614307 | -0.611539 |
| 46 | -0.001178 | 0.278114 | -0.336657 |
| 8 | -1.735892 | -0.934072 | -0.802581 |
| 1 | 1.270838 | 1.245559 | 1.183366 |
| 6 | -2.722625 | -1.101474 | -0.080142 |
| 8 | -2.704675 | -1.106620 | 1.225610 |
| 1 | -1.794674 | -1.004513 | 1.629253 |
| 8 | 1.294141 | 0.646871 | 2.345693 |
| 6 | 0.081363 | 0.285684 | 2.666241 |
| 8 | -0.345933 | -0.845394 | 2.397961 |
| 8 | 1.285187 | -1.399570 | -0.667268 |
| 6 | 2.148438 | -1.908624 | 0.054407 |
| 8 | 2.503124 | -1.480765 | 1.234129 |
| 1 | 1.957534 | -0.724822 | 1.613584 |
| 6 | -0.791243 | 1.300469 | 3.346044 |
| 6 | -4.090283 | -1.389367 | -0.670920 |
| 6 | 2.970312 | -3.086326 | -0.439779 |
| 1 | -1.806666 | 1.234915 | 2.940797 |
| 1 | -0.838251 | 1.072930 | 4.417035 |
| 1 | -0.399039 | 2.311719 | 3.216462 |
| 6 | 2.298563 | -3.724229 | -1.649242 |
| 1 | 1.307266 | -4.114902 | -1.393226 |
| 1 | 2.172007 | -3.004576 | -2.463839 |
| 1 | 2.913502 | -4.557312 | -2.009870 |
| 6 | 4.335376 | -2.510648 | -0.843743 |
| 1 | 4.844401 | -2.054962 | 0.013237 |
| 1 | 4.970427 | -3.315329 | -1.233721 |
| 1 | 4.226615 | -1.753792 | -1.631594 |
| 6 | 3.149080 | -4.115774 | 0.675491 |
| 1 | 3.751580 | -4.952803 | 0.302199 |
| 1 | 3.653772 | -3.684743 | 1.544930 |
| 1 | 2.183358 | -4.516749 | 1.005621 |
| 6 | -5.146824 | -0.551907 | 0.052284 |
| 1 | -4.921664 | 0.517634 | -0.028501 |
| 1 | -6.127485 | -0.734284 | -0.404310 |
| 1 | -5.205171 | -0.808330 | 1.114266 |
| 6 | -4.090655 | -1.065235 | -2.159227 |

| | | | |
|---|---|---|---|
| 1 | -3.344596 | -1.656143 | -2.699971 |
| 1 | -5.079533 | -1.282111 | -2.580889 |
| 1 | -3.866660 | -0.006226 | -2.332034 |
| 6 | -4.369290 | -2.881988 | -0.454892 |
| 1 | -4.363223 | -3.135858 | 0.610618 |
| 1 | -5.355322 | -3.131864 | -0.865483 |
| 1 | -3.622625 | -3.502173 | -0.966353 |

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**$(3a\text{-}4a)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1523.9916138
Zero-point correction= 0.463977
Thermal correction to Energy= 0.496696
Thermal correction to Enthalpy= 0.497640
Thermal correction to Gibbs Free Energy= 0.400172
Sum of electronic and zero-point Energies= -1523.527636
Sum of electronic and thermal Energies= -1523.494918
Sum of electronic and thermal Enthalpies= -1523.493974
Sum of electronic and thermal Free Energies= -1523.591442

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.776517 | 3.845784 | -1.035765 |
| 6 | 0.987174 | 2.868713 | -0.433688 |
| 6 | 1.547632 | 1.665618 | 0.066456 |
| 6 | 2.929566 | 1.459448 | -0.119729 |
| 6 | 3.720303 | 2.438155 | -0.697232 |
| 6 | 3.141147 | 3.629741 | -1.153415 |
| 1 | 1.297457 | 4.738454 | -1.431296 |
| 1 | 1.186617 | 1.336152 | 1.274843 |
| 1 | 3.390047 | 0.547480 | 0.260239 |
| 1 | 4.793314 | 2.288850 | -0.794273 |
| 1 | 3.769284 | 4.385546 | -1.619830 |
| 6 | -0.482159 | 2.997304 | -0.446338 |
| 8 | -1.129232 | 3.931326 | -0.915886 |
| 7 | -1.085320 | 1.865751 | 0.073668 |
| 8 | -2.427295 | 1.850721 | -0.206382 |
| 46 | 0.033804 | 0.247465 | -0.390503 |
| 8 | -1.722785 | -0.914149 | -0.939475 |
| 6 | -2.687716 | -1.090845 | -0.190681 |
| 8 | -2.629354 | -1.087362 | 1.115071 |
| 1 | -1.712412 | -0.925726 | 1.483245 |
| 8 | 0.813174 | 1.337501 | 2.559700 |
| 6 | -0.175110 | 0.574049 | 2.740305 |

| | | | |
|---|---|---|---|
| 8 | -0.263020 | -0.589454 | 2.232824 |
| 1 | 1.043334 | -1.274277 | 1.638835 |
| 8 | 1.348589 | -1.402493 | -0.777850 |
| 6 | 1.975813 | -2.025465 | 0.088471 |
| 8 | 1.827447 | -1.864845 | 1.370128 |
| 6 | -4.071111 | -1.386751 | -0.737940 |
| 6 | 3.070127 | -3.001708 | -0.306877 |
| 6 | -1.344223 | 1.085262 | 3.527971 |
| 1 | -1.837807 | 0.275601 | 4.071470 |
| 1 | -1.040450 | 1.885743 | 4.205295 |
| 1 | -2.062322 | 1.499754 | 2.806964 |
| 6 | 3.126533 | -4.180311 | 0.662390 |
| 1 | 3.931910 | -4.860093 | 0.358932 |
| 1 | 3.318216 | -3.852838 | 1.688307 |
| 1 | 2.187967 | -4.747268 | 0.656259 |
| 6 | 2.842738 | -3.494571 | -1.731546 |
| 1 | 1.895167 | -4.038793 | -1.817456 |
| 1 | 2.818006 | -2.665189 | -2.444518 |
| 1 | 3.654089 | -4.175540 | -2.015190 |
| 6 | 4.382114 | -2.206094 | -0.236213 |
| 1 | 4.362370 | -1.353106 | -0.927476 |
| 1 | 4.569849 | -1.836155 | 0.779295 |
| 1 | 5.218743 | -2.854667 | -0.523189 |
| 6 | -4.362822 | -2.868612 | -0.473328 |
| 1 | -3.638868 | -3.513240 | -0.987138 |
| 1 | -4.332313 | -3.093846 | 0.598165 |
| 1 | -5.362682 | -3.116211 | -0.850380 |
| 6 | -4.104912 | -1.101029 | -2.233471 |
| 1 | -5.107437 | -1.313078 | -2.624056 |
| 1 | -3.867889 | -0.050579 | -2.437486 |
| 1 | -3.381725 | -1.717058 | -2.777384 |
| 6 | -5.098187 | -0.515618 | -0.010598 |
| 1 | -4.856750 | 0.547998 | -0.118399 |
| 1 | -6.091098 | -0.690915 | -0.442755 |
| 1 | -5.138361 | -0.749107 | 1.057639 |
| 1 | -2.544752 | 2.630053 | -0.798882 |

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**$(5a\text{-}6a)_4^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1423.9640332
Zero-point correction= 0.386110
Thermal correction to Energy= 0.414127
Thermal correction to Enthalpy= 0.415072
Thermal correction to Gibbs Free Energy= 0.328143

Sum of electronic and zero-point Energies= -1423.577923
Sum of electronic and thermal Energies= -1423.549906
Sum of electronic and thermal Enthalpies= -1423.548962
Sum of electronic and thermal Free Energies= -1423.635890

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 4.880935 | 0.544101 | -0.237417 |
| 6 | 3.575859 | 0.047768 | -0.172147 |
| 6 | 2.476999 | 0.892638 | -0.401194 |
| 6 | 2.683399 | 2.234096 | -0.696975 |
| 6 | 3.989600 | 2.719925 | -0.757808 |
| 6 | 5.084539 | 1.883613 | -0.527563 |
| 1 | 5.708755 | -0.142605 | -0.069565 |
| 1 | 1.842628 | 2.905083 | -0.861398 |
| 1 | 4.156835 | 3.771815 | -0.982972 |
| 1 | 6.093103 | 2.285425 | -0.581243 |
| 6 | 3.324174 | -1.384509 | 0.018551 |
| 8 | 4.133789 | -2.280255 | 0.039955 |
| 7 | 1.894739 | -1.695256 | 0.047866 |
| 8 | 1.634682 | -2.600058 | -1.015768 |
| 1 | 2.124526 | -3.398093 | -0.755675 |
| 46 | 0.772759 | -0.002066 | 0.089473 |
| 7 | -0.070343 | -1.624747 | 1.594627 |
| 6 | -1.415497 | -1.377530 | 1.534433 |
| 8 | -1.978797 | -0.763686 | 2.454310 |
| 8 | 0.476226 | -1.129470 | 2.779330 |
| 1 | -0.297668 | -0.679111 | 3.189556 |
| 6 | -2.161790 | -1.799398 | 0.316633 |
| 6 | -3.499372 | -1.403777 | 0.234862 |
| 6 | -1.593587 | -2.520796 | -0.737940 |
| 6 | -4.253576 | -1.698088 | -0.894253 |
| 1 | -3.928110 | -0.868351 | 1.079525 |
| 6 | -2.349741 | -2.804592 | -1.869949 |
| 1 | -0.558514 | -2.850443 | -0.690115 |
| 6 | -3.676779 | -2.391012 | -1.954158 |
| 1 | -5.294511 | -1.385627 | -0.947052 |
| 1 | -1.898146 | -3.358265 | -2.689925 |
| 1 | -4.262511 | -2.617941 | -2.842128 |
| 1 | 1.051475 | -1.979300 | 0.934490 |
| 8 | -0.556990 | 1.665300 | 0.320345 |
| 6 | -1.589137 | 1.722116 | -0.352654 |
| 6 | -2.733665 | 2.628836 | 0.034195 |
| 8 | -1.759410 | 1.019960 | -1.455043 |
| 1 | -0.972107 | 0.452814 | -1.596998 |

| | | | |
|---|---|---|---|
| 6 | -2.938939 | 2.495066 | 1.545828 |
| 1 | -3.803365 | 3.098681 | 1.846234 |
| 1 | -3.114366 | 1.451902 | 1.838633 |
| 1 | -2.059948 | 2.844562 | 2.095853 |
| 6 | -4.012498 | 2.268120 | -0.714533 |
| 1 | -4.818119 | 2.936355 | -0.388782 |
| 1 | -3.893538 | 2.374337 | -1.797800 |
| 1 | -4.315117 | 1.234747 | -0.507534 |
| 6 | -2.301426 | 4.059516 | -0.314477 |
| 1 | -3.086676 | 4.757821 | -0.001625 |
| 1 | -1.374605 | 4.329094 | 0.204062 |
| 1 | -2.150661 | 4.181278 | -1.394382 |

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**$(5a\text{-}6a)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1423.9992548
Zero-point correction= 0.386019
Thermal correction to Energy= 0.414181
Thermal correction to Enthalpy= 0.415125
Thermal correction to Gibbs Free Energy= 0.326023
Sum of electronic and zero-point Energies= -1423.613236
Sum of electronic and thermal Energies= -1423.585074
Sum of electronic and thermal Enthalpies= -1423.584130
Sum of electronic and thermal Free Energies= -1423.673232

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 4.576867 | -1.529830 | -0.948612 |
| 6 | 3.323034 | -1.354492 | -0.356341 |
| 6 | 2.724991 | -0.087918 | -0.276188 |
| 6 | 3.393574 | 1.017180 | -0.794887 |
| 6 | 4.630629 | 0.833331 | -1.408633 |
| 6 | 5.222921 | -0.430847 | -1.490100 |
| 1 | 5.024835 | -2.521649 | -0.956168 |
| 1 | 2.945779 | 2.007132 | -0.733396 |
| 1 | 5.147484 | 1.692667 | -1.832741 |
| 1 | 6.194271 | -0.545106 | -1.964610 |
| 6 | 2.648908 | -2.429116 | 0.364983 |
| 8 | 3.132906 | -3.453174 | 0.807311 |
| 7 | 1.280103 | -2.097615 | 0.673989 |
| 8 | 0.890811 | -2.690489 | 1.887293 |
| 46 | 0.885686 | -0.092236 | 0.448772 |
| 8 | 0.611041 | 1.997728 | 0.127865 |
| 6 | -0.427694 | 2.650043 | 0.297080 |

| | | | |
|---|---|---|---|
| 6 | -0.429225 | 4.160282 | 0.152599 |
| 8 | -1.576919 | 2.139738 | 0.634683 |
| 1 | -1.556040 | 1.126758 | 0.714052 |
| 1 | 1.571518 | -3.380191 | 2.016702 |
| 8 | -1.286820 | -0.400845 | 0.715466 |
| 6 | -1.812658 | -1.378561 | 0.050030 |
| 7 | -1.055916 | -2.378084 | -0.331461 |
| 6 | -3.267102 | -1.283081 | -0.249797 |
| 6 | -3.773762 | -0.067570 | -0.713374 |
| 6 | -4.141950 | -2.346938 | -0.020324 |
| 6 | -5.132971 | 0.078838 | -0.961723 |
| 1 | -3.095582 | 0.764836 | -0.888362 |
| 6 | -5.503230 | -2.191080 | -0.246256 |
| 1 | -3.749090 | -3.292928 | 0.340081 |
| 6 | -6.000685 | -0.981640 | -0.723899 |
| 1 | -5.515647 | 1.025538 | -1.335967 |
| 1 | -6.180275 | -3.019705 | -0.052281 |
| 1 | -7.066285 | -0.866263 | -0.908978 |
| 1 | 0.374156 | -2.368101 | -0.009639 |
| 8 | -1.696888 | -3.310356 | -1.159214 |
| 1 | -1.323284 | -4.153153 | -0.874977 |
| 6 | 0.900192 | 4.634486 | -0.421011 |
| 1 | 1.739237 | 4.345271 | 0.221069 |
| 1 | 1.078114 | 4.213781 | -1.417680 |
| 1 | 0.891482 | 5.727500 | -0.507085 |
| 6 | -1.582681 | 4.585020 | -0.759175 |
| 1 | -2.549723 | 4.271897 | -0.354191 |
| 1 | -1.585040 | 5.677451 | -0.855035 |
| 1 | -1.474419 | 4.160443 | -1.764825 |
| 6 | -0.635996 | 4.745279 | 1.555825 |
| 1 | -0.641859 | 5.840205 | 1.494758 |
| 1 | -1.587136 | 4.416535 | 1.987014 |
| 1 | 0.174593 | 4.448704 | 2.232649 |

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**(5a-6a)$_8^‡$**

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Number of imaginary frequencies : 1
Electronic energy =-1652.9870088
Zero-point correction= 0.450705
Thermal correction to Energy= 0.484395
Thermal correction to Enthalpy= 0.485340
Thermal correction to Gibbs Free Energy= 0.382396
Sum of electronic and zero-point Energies= -1652.536303
Sum of electronic and thermal Energies= -1652.502613
Sum of electronic and thermal Enthalpies= -1652.501669

Sum of electronic and thermal Free Energies= -1652.604613

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.844354 | -0.884300 | -0.939072 |
| 6 | -3.448825 | -0.887769 | -0.888376 |
| 6 | -2.737514 | 0.145157 | -0.266834 |
| 6 | -3.427201 | 1.200007 | 0.316836 |
| 6 | -4.821079 | 1.182889 | 0.294951 |
| 6 | -5.529551 | 0.154022 | -0.330377 |
| 1 | -5.361807 | -1.691872 | -1.452531 |
| 1 | -2.891916 | 2.015720 | 0.796372 |
| 1 | -5.367908 | 1.991011 | 0.777477 |
| 1 | -6.616057 | 0.172900 | -0.340395 |
| 6 | -2.637337 | -1.907222 | -1.532392 |
| 8 | -2.891340 | -2.645926 | -2.457310 |
| 7 | -1.297492 | -1.924327 | -0.956300 |
| 8 | -0.392804 | -2.598432 | -1.773374 |
| 46 | -0.763960 | -0.006286 | -0.348679 |
| 8 | -0.514287 | 2.042033 | 0.247756 |
| 6 | 0.403926 | 2.810526 | -0.061183 |
| 8 | 1.501253 | 2.438304 | -0.662868 |
| 1 | 1.563991 | 1.435179 | -0.722599 |
| 8 | 1.459287 | -0.127948 | -0.461881 |
| 6 | 2.240529 | -0.988370 | 0.074444 |
| 7 | 1.728338 | -1.929089 | 0.829122 |
| 6 | 3.699367 | -0.873080 | -0.174190 |
| 6 | 4.267938 | 0.402369 | -0.224497 |
| 6 | 4.496444 | -1.992311 | -0.429083 |
| 6 | 5.618253 | 0.556738 | -0.508511 |
| 1 | 3.653127 | 1.277399 | -0.026366 |
| 6 | 5.841799 | -1.831365 | -0.734785 |
| 1 | 4.056959 | -2.983704 | -0.387536 |
| 6 | 6.406091 | -0.559979 | -0.769628 |
| 1 | 6.055400 | 1.551959 | -0.532975 |
| 1 | 6.453066 | -2.705319 | -0.946141 |
| 1 | 7.461851 | -0.439147 | -1.001157 |
| 1 | -1.266455 | -2.423210 | -0.014816 |
| 8 | 2.577391 | -2.820283 | 1.473658 |
| 1 | 1.969390 | -3.532854 | 1.724348 |
| 1 | 0.626386 | -2.197597 | 1.072591 |
| 8 | -0.501008 | -2.810364 | 1.388663 |
| 6 | -1.267473 | -2.245413 | 2.297479 |
| 8 | -2.479790 | -2.175217 | 2.193611 |
| 6 | 0.341237 | 4.289101 | 0.267375 |

| | | | |
|---|---|---|---|
| 1 | -0.973426 | -3.022217 | -2.439074 |
| 6 | -0.518039 | -1.619739 | 3.453374 |
| 1 | -1.191521 | -1.417588 | 4.288358 |
| 1 | 0.319509 | -2.246534 | 3.778135 |
| 1 | -0.093694 | -0.665805 | 3.109678 |
| 6 | 1.401996 | 4.559697 | 1.342465 |
| 1 | 2.406508 | 4.311788 | 0.983780 |
| 1 | 1.383950 | 5.622905 | 1.610196 |
| 1 | 1.202592 | 3.980389 | 2.252444 |
| 6 | 0.660355 | 5.100607 | -0.990966 |
| 1 | 0.622974 | 6.169253 | -0.747978 |
| 1 | 1.657156 | 4.869295 | -1.378129 |
| 1 | -0.071599 | 4.910849 | -1.785185 |
| 6 | -1.041022 | 4.654237 | 0.793430 |
| 1 | -1.818289 | 4.456438 | 0.046016 |
| 1 | -1.289930 | 4.089029 | 1.698161 |
| 1 | -1.066881 | 5.722629 | 1.037989 |

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**$(5a\text{-}6a)_{10}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1653.0078954
Zero-point correction= 0.451996
Thermal correction to Energy= 0.484492
Thermal correction to Enthalpy= 0.485436
Thermal correction to Gibbs Free Energy= 0.389424
Sum of electronic and zero-point Energies= -1652.555900
Sum of electronic and thermal Energies= -1652.523403
Sum of electronic and thermal Enthalpies= -1652.522459
Sum of electronic and thermal Free Energies= -1652.618471

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.767454 | -3.737624 | -0.234443 |
| 6 | -1.727567 | -2.811591 | -0.360364 |
| 6 | -1.976598 | -1.462263 | -0.648382 |
| 6 | -3.288851 | -1.034798 | -0.826034 |
| 6 | -4.325616 | -1.953288 | -0.668314 |
| 6 | -4.073256 | -3.295825 | -0.370712 |
| 1 | -2.532928 | -4.781627 | -0.036960 |
| 1 | -3.497362 | 0.003584 | -1.071969 |
| 1 | -5.354453 | -1.616348 | -0.781880 |
| 1 | -4.900164 | -3.992269 | -0.260176 |
| 6 | -0.323216 | -3.192724 | -0.294564 |
| 8 | 0.212926 | -4.254870 | -0.511724 |

| | | | |
|---|---|---|---|
| 7 | 0.500849 | -2.031218 | 0.030275 |
| 8 | 1.853346 | -2.277698 | -0.165865 |
| 46 | -0.370389 | -0.309529 | -0.802315 |
| 8 | -1.593879 | 1.407513 | -1.164899 |
| 6 | -1.299425 | 2.519841 | -0.698075 |
| 6 | -2.370956 | 3.509766 | -0.289702 |
| 8 | -0.080447 | 2.940555 | -0.535031 |
| 1 | 0.588869 | 2.218497 | -0.761455 |
| 1 | 1.879485 | -3.235299 | -0.372747 |
| 8 | 1.494268 | 0.910871 | -0.899610 |
| 6 | 2.247991 | 0.675053 | 0.133884 |
| 7 | 1.656758 | 0.632189 | 1.301280 |
| 6 | 3.694744 | 0.488872 | -0.090676 |
| 6 | 4.108987 | 0.089894 | -1.365778 |
| 6 | 4.651580 | 0.733644 | 0.900135 |
| 6 | 5.457550 | -0.086094 | -1.640221 |
| 1 | 3.353819 | -0.078382 | -2.128543 |
| 6 | 6.001170 | 0.569635 | 0.615174 |
| 1 | 4.335660 | 1.053633 | 1.887210 |
| 6 | 6.406081 | 0.153201 | -0.649091 |
| 1 | 5.771664 | -0.406863 | -2.630763 |
| 1 | 6.741658 | 0.766716 | 1.386778 |
| 1 | 7.463960 | 0.018685 | -0.864624 |
| 1 | 0.361744 | -1.787869 | 1.042514 |
| 8 | 2.345137 | 0.170686 | 2.413582 |
| 1 | 1.673598 | -0.425011 | 2.805826 |
| 6 | -3.729745 | 2.821509 | -0.276853 |
| 1 | -3.996120 | 2.436223 | -1.267620 |
| 1 | -3.736011 | 1.981487 | 0.430438 |
| 1 | -4.500063 | 3.537520 | 0.033155 |
| 6 | -2.039816 | 4.031319 | 1.112342 |
| 1 | -1.100057 | 4.591496 | 1.120015 |
| 1 | -2.844711 | 4.697248 | 1.446692 |
| 1 | -1.947225 | 3.202192 | 1.823919 |
| 6 | -2.362632 | 4.663200 | -1.298474 |
| 1 | -3.117442 | 5.404141 | -1.008341 |
| 1 | -1.386252 | 5.158652 | -1.325059 |
| 1 | -2.603374 | 4.312323 | -2.309580 |
| 1 | 0.448014 | 0.856178 | 1.582012 |
| 8 | -0.712027 | 0.920612 | 1.973173 |
| 6 | -1.019809 | -0.220369 | 2.477188 |
| 8 | -0.207173 | -1.160881 | 2.618322 |
| 6 | -2.462245 | -0.412997 | 2.850413 |
| 1 | -2.970583 | -0.886344 | 1.998248 |
| 1 | -2.548493 | -1.084925 | 3.707309 |

| | | | |
|---|---|---|---|
| 1 | -2.951312 | 0.543444 | 3.052926 |

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**$(6a_1\text{-}9)_3^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -1423.9740072
Zero-point correction= 0.388920
Thermal correction to Energy= 0.417518
Thermal correction to Enthalpy= 0.418462
Thermal correction to Gibbs Free Energy= 0.326203
Sum of electronic and zero-point Energies= -1423.585087
Sum of electronic and thermal Energies= -1423.556489
Sum of electronic and thermal Enthalpies= -1423.555545
Sum of electronic and thermal Free Energies= -1423.647804

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.563373 | -1.030378 | 0.202463 |
| 6 | 2.227598 | -2.075687 | 0.368464 |
| 6 | 1.316716 | -1.124217 | 0.872032 |
| 6 | 3.168004 | -2.611900 | 1.259943 |
| 6 | 1.389196 | -0.693178 | 2.201935 |
| 6 | 3.217489 | -2.219975 | 2.587272 |
| 1 | 3.854774 | -3.357182 | 0.866029 |
| 6 | 2.320528 | -1.262522 | 3.059862 |
| 1 | 0.726509 | 0.101062 | 2.539910 |
| 1 | 3.959147 | -2.652551 | 3.253385 |
| 1 | 2.357850 | -0.939308 | 4.097780 |
| 8 | -0.270421 | 1.667626 | 0.950701 |
| 6 | 0.693878 | 1.591916 | 0.160834 |
| 7 | 0.988610 | 0.381038 | -0.375196 |
| 8 | 2.008180 | 0.317088 | -1.302797 |
| 1 | 1.668299 | -0.298610 | -1.979091 |
| 6 | 1.482814 | 2.807942 | -0.163361 |
| 6 | 0.796946 | 4.026351 | -0.119955 |
| 6 | 2.858593 | 2.800786 | -0.412248 |
| 6 | 1.466972 | 5.217532 | -0.357958 |
| 1 | -0.265342 | 4.017935 | 0.109553 |
| 6 | 3.529523 | 3.998784 | -0.624838 |
| 1 | 3.402472 | 1.862425 | -0.429824 |
| 6 | 2.836126 | 5.204968 | -0.610065 |
| 1 | 0.923118 | 6.158931 | -0.337670 |
| 1 | 4.601608 | 3.988613 | -0.806054 |
| 1 | 3.364759 | 6.138662 | -0.789196 |
| 6 | 2.278567 | -2.635046 | -1.005153 |

| | | | |
|---|---|---|---|
| 8 | 3.193168 | -3.348302 | -1.402689 |
| 8 | -2.754619 | -0.942161 | -0.115241 |
| 6 | -3.405677 | 0.081996 | 0.094580 |
| 6 | -4.913278 | 0.132795 | -0.078770 |
| 8 | -2.888475 | 1.224635 | 0.475236 |
| 1 | -1.899966 | 1.205102 | 0.615138 |
| 7 | 1.261033 | -2.321791 | -1.897511 |
| 8 | 1.293180 | -3.073775 | -3.066261 |
| 1 | 2.112999 | -3.597838 | -2.938435 |
| 1 | 0.310652 | -2.301312 | -1.516341 |
| 6 | -5.545638 | 0.577296 | 1.243927 |
| 1 | -5.190884 | 1.567552 | 1.546099 |
| 1 | -6.635682 | 0.618850 | 1.129478 |
| 1 | -5.320590 | -0.131464 | 2.050393 |
| 6 | -5.236532 | 1.154420 | -1.175046 |
| 1 | -4.779885 | 0.870247 | -2.131111 |
| 1 | -6.322671 | 1.196556 | -1.321621 |
| 1 | -4.885386 | 2.155866 | -0.907224 |
| 6 | -5.437183 | -1.241211 | -0.474862 |
| 1 | -4.995000 | -1.582025 | -1.416949 |
| 1 | -5.209542 | -1.991366 | 0.290162 |
| 1 | -6.525564 | -1.194679 | -0.599907 |

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**$(6a\text{-}9)_5^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-1423.9734002
Zero-point correction= 0.390437
Thermal correction to Energy= 0.418276
Thermal correction to Enthalpy= 0.419220
Thermal correction to Gibbs Free Energy= 0.330709
Sum of electronic and zero-point Energies= -1423.582963
Sum of electronic and thermal Energies= -1423.555124
Sum of electronic and thermal Enthalpies= -1423.554180
Sum of electronic and thermal Free Energies= -1423.642691

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.778055 | -1.302556 | -1.825334 |
| 6 | -2.519740 | -0.774660 | -1.657177 |
| 6 | -1.730049 | -1.155012 | -0.532411 |
| 6 | -2.223799 | -2.244607 | 0.254644 |
| 6 | -3.547488 | -2.713520 | 0.107317 |
| 6 | -4.330578 | -2.234359 | -0.916574 |
| 1 | -4.372371 | -0.980760 | -2.679206 |

| | | | |
|---|---|---|---|
| 1 | -2.143961 | -0.011509 | -2.336853 |
| 1 | -3.897187 | -3.502462 | 0.772177 |
| 1 | -5.342051 | -2.603475 | -1.061233 |
| 6 | -1.267931 | -2.947405 | 1.067281 |
| 8 | -1.360711 | -3.541328 | 2.125777 |
| 7 | 0.050149 | -2.960674 | 0.388666 |
| 46 | 0.277838 | -1.012911 | -0.449912 |
| 8 | 1.037386 | -3.505946 | 1.202596 |
| 1 | 0.513376 | -3.847056 | 1.960900 |
| 8 | 2.527967 | -0.827159 | -0.296114 |
| 8 | 0.009613 | 1.136412 | -0.683914 |
| 6 | -1.032257 | 1.441015 | 0.007257 |
| 7 | -1.733589 | 0.429813 | 0.493719 |
| 8 | -2.974807 | 0.706407 | 1.044486 |
| 1 | -3.134410 | -0.067760 | 1.603722 |
| 6 | -1.341717 | 2.872184 | 0.212645 |
| 6 | -2.648748 | 3.366941 | 0.264061 |
| 6 | -0.266709 | 3.763842 | 0.310491 |
| 6 | -2.868936 | 4.730767 | 0.416520 |
| 1 | -3.487605 | 2.686397 | 0.173475 |
| 6 | -0.493588 | 5.120846 | 0.485405 |
| 1 | 0.749924 | 3.382316 | 0.256680 |
| 6 | -1.796946 | 5.608263 | 0.536604 |
| 1 | -3.888200 | 5.108679 | 0.443198 |
| 1 | 0.349074 | 5.802178 | 0.574386 |
| 1 | -1.975449 | 6.673360 | 0.665854 |
| 6 | 3.174123 | 0.214368 | -0.233127 |
| 6 | 4.681359 | 0.235204 | -0.058103 |
| 8 | 2.641291 | 1.415807 | -0.326484 |
| 1 | 1.658982 | 1.361728 | -0.470453 |
| 1 | -0.032727 | -3.559846 | -0.438042 |
| 6 | 5.199954 | -1.184771 | 0.126272 |
| 1 | 4.761096 | -1.658786 | 1.010894 |
| 1 | 4.958978 | -1.812157 | -0.738172 |
| 1 | 6.289694 | -1.163529 | 0.247755 |
| 6 | 5.292636 | 0.861520 | -1.316984 |
| 1 | 4.938773 | 1.887028 | -1.465094 |
| 1 | 6.385013 | 0.881219 | -1.219829 |
| 1 | 5.045092 | 0.276559 | -2.211455 |
| 6 | 5.030565 | 1.089204 | 1.164192 |
| 1 | 6.119533 | 1.107034 | 1.294591 |
| 1 | 4.679271 | 2.119298 | 1.048156 |
| 1 | 4.590238 | 0.674340 | 2.079187 |

**Lewis Acid Participation (LA=1)**

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**(2a'-3a')$_6^‡$**

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Number of imaginary frequencies : 1
Electronic energy =-2280.9444675
Zero-point correction= 0.405774
Thermal correction to Energy= 0.438946
Thermal correction to Enthalpy= 0.439890
Thermal correction to Gibbs Free Energy= 0.337460
Sum of electronic and zero-point Energies= -2280.538694
Sum of electronic and thermal Energies= -2280.505522
Sum of electronic and thermal Enthalpies= -2280.504577
Sum of electronic and thermal Free Energies= -2280.607007

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 0.014447 | 0.720922 | 5.155278 |
| 6 | 1.120303 | 0.416280 | 4.365190 |
| 6 | 0.949916 | -0.189869 | 3.129274 |
| 6 | -0.343525 | -0.497969 | 2.684705 |
| 6 | -1.452077 | -0.195148 | 3.484542 |
| 6 | -1.271153 | 0.414326 | 4.715880 |
| 1 | 0.156630 | 1.197922 | 6.122129 |
| 1 | 2.122078 | 0.649966 | 4.715074 |
| 1 | 1.826367 | -0.426061 | 2.529301 |
| 1 | -2.444582 | -0.443843 | 3.119556 |
| 1 | -2.132244 | 0.652582 | 5.334221 |
| 6 | -0.614952 | -1.136150 | 1.392557 |
| 8 | -1.723067 | -1.588226 | 1.100806 |
| 7 | 0.436626 | -1.159942 | 0.456795 |
| 8 | 0.204880 | -2.100577 | -0.569676 |
| 46 | 0.536382 | 0.814606 | -0.319544 |
| 1 | 1.555347 | -1.227547 | 0.706390 |
| 8 | 2.442420 | 0.418688 | -0.950901 |
| 8 | 0.203415 | 2.734398 | -1.026899 |
| 8 | -1.299923 | 1.646645 | 0.104433 |
| 6 | -0.990821 | 2.685046 | -0.578480 |
| 6 | -2.010138 | 3.732554 | -0.915199 |
| 6 | 3.237332 | -0.380059 | -0.352705 |
| 8 | 2.917614 | -1.138472 | 0.600067 |
| 6 | 4.654345 | -0.458873 | -0.913196 |
| 6 | -3.017771 | 3.869612 | 0.223300 |
| 1 | -3.517846 | 2.918604 | 0.431743 |
| 1 | -2.536208 | 4.215074 | 1.145955 |
| 1 | -3.780713 | 4.605610 | -0.057019 |

| | | | |
|---|---|---|---|
| 6 | -2.712695 | 3.212803 | -2.180523 |
| 1 | -3.477712 | 3.934135 | -2.492376 |
| 1 | -1.998481 | 3.086520 | -3.002766 |
| 1 | -3.193887 | 2.245506 | -1.996042 |
| 6 | -1.322357 | 5.063571 | -1.201914 |
| 1 | -0.592298 | 4.970314 | -2.011988 |
| 1 | -2.075376 | 5.803669 | -1.497957 |
| 1 | -0.800307 | 5.444335 | -0.316151 |
| 6 | 4.613542 | -1.578743 | -1.962904 |
| 1 | 5.609548 | -1.702125 | -2.405811 |
| 1 | 4.318682 | -2.533431 | -1.511491 |
| 1 | 3.910101 | -1.339394 | -2.769457 |
| 6 | 5.065187 | 0.854332 | -1.570582 |
| 1 | 6.081165 | 0.757762 | -1.972736 |
| 1 | 4.392215 | 1.123639 | -2.389741 |
| 1 | 5.063812 | 1.679757 | -0.848784 |
| 6 | 5.633738 | -0.827234 | 0.197179 |
| 1 | 5.670165 | -0.050793 | 0.970857 |
| 1 | 5.360058 | -1.772070 | 0.675455 |
| 1 | 6.640530 | -0.928371 | -0.226298 |
| 30 | -2.105269 | -2.322255 | -0.808084 |
| 1 | 0.189599 | -1.581805 | -1.404712 |
| 17 | -1.795426 | -0.707328 | -2.361019 |
| 17 | -3.039937 | -4.291300 | -0.768418 |

---

**$(2a'\text{-}3a')_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2509.9117114
Zero-point correction= 0.466877
Thermal correction to Energy= 0.505171
Thermal correction to Enthalpy= 0.506115
Thermal correction to Gibbs Free Energy= 0.394178
Sum of electronic and zero-point Energies= -2509.444834
Sum of electronic and thermal Energies= -2509.406541
Sum of electronic and thermal Enthalpies= -2509.405597
Sum of electronic and thermal Free Energies= -2509.517534

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.763727 | 2.393990 | -0.618935 |
| 6 | -3.860447 | 2.694764 | -1.637470 |
| 6 | -2.498687 | 2.575119 | -1.409616 |
| 6 | -2.037833 | 2.137339 | -0.161823 |
| 6 | -2.944825 | 1.838835 | 0.861135 |

| | | | |
|---|---|---|---|
| 6 | -4.307022 | 1.972184 | 0.627172 |
| 1 | -5.832242 | 2.492096 | -0.796511 |
| 1 | -4.220984 | 3.026093 | -2.607557 |
| 1 | -1.773885 | 2.809565 | -2.184527 |
| 1 | -2.600269 | 1.523446 | 1.843201 |
| 1 | -5.013676 | 1.748231 | 1.421962 |
| 6 | -0.585956 | 2.082904 | 0.032625 |
| 8 | 0.191427 | 2.797293 | -0.599437 |
| 7 | -0.081713 | 1.160019 | 0.976649 |
| 1 | -0.666223 | 0.640863 | 1.851114 |
| 8 | 1.244439 | 1.472172 | 1.340408 |
| 46 | 0.208364 | -0.740254 | -0.020101 |
| 8 | -2.841207 | -1.354827 | 1.116957 |
| 8 | -1.692450 | -0.876976 | -0.767514 |
| 8 | 1.036075 | -2.465521 | -0.790350 |
| 8 | 2.187481 | -1.073725 | 0.405895 |
| 6 | -2.711968 | -1.290188 | -0.140046 |
| 6 | 2.177241 | -2.124792 | -0.322929 |
| 6 | -3.864860 | -1.809894 | -0.988284 |
| 6 | 3.418783 | -2.900164 | -0.646028 |
| 30 | 2.283708 | 2.329429 | -0.493911 |
| 17 | 3.254471 | 3.829202 | 0.810505 |
| 6 | -0.547574 | -1.117809 | 3.353247 |
| 8 | -1.294054 | -0.272371 | 2.607453 |
| 1 | -2.053291 | -0.891127 | 1.845643 |
| 8 | -0.813424 | -2.290051 | 3.442564 |
| 6 | 0.632237 | -0.453492 | 4.003753 |
| 1 | 0.353699 | 0.513745 | 4.434790 |
| 1 | 1.044159 | -1.105218 | 4.775438 |
| 1 | 1.404394 | -0.275727 | 3.243629 |
| 6 | 3.593149 | -2.861745 | -2.169998 |
| 1 | 3.708728 | -1.831794 | -2.527996 |
| 1 | 4.493249 | -3.426501 | -2.441484 |
| 1 | 2.733531 | -3.311014 | -2.678043 |
| 6 | 4.624295 | -2.270113 | 0.041566 |
| 1 | 4.518070 | -2.276056 | 1.132073 |
| 1 | 5.524082 | -2.840804 | -0.217589 |
| 1 | 4.767859 | -1.233168 | -0.281551 |
| 6 | 3.214668 | -4.345290 | -0.178895 |
| 1 | 3.082414 | -4.401465 | 0.908274 |
| 1 | 2.339839 | -4.797817 | -0.657544 |
| 1 | 4.099006 | -4.937172 | -0.443636 |
| 6 | -5.200152 | -1.549166 | -0.297455 |
| 1 | -6.010497 | -1.968309 | -0.906468 |
| 1 | -5.237505 | -2.008736 | 0.694344 |

| | | | |
|---|---|---|---|
| 1 | -5.383711 | -0.472609 | -0.185081 |
| 6 | -3.850648 | -1.169400 | -2.372545 |
| 1 | -4.696959 | -1.548836 | -2.957867 |
| 1 | -3.943820 | -0.077840 | -2.302695 |
| 1 | -2.926463 | -1.393646 | -2.913165 |
| 6 | -3.624661 | -3.322478 | -1.107564 |
| 1 | -2.657896 | -3.532545 | -1.580811 |
| 1 | -3.643549 | -3.805356 | -0.123785 |
| 1 | -4.413461 | -3.767640 | -1.726423 |
| 1 | 1.233424 | 2.274130 | 1.900299 |
| 17 | 2.564917 | 0.909170 | -2.155673 |

---

**$(2a'\text{-}3a')_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2509.9214995
Zero-point correction= 0.468980
Thermal correction to Energy= 0.506298
Thermal correction to Enthalpy= 0.507242
Thermal correction to Gibbs Free Energy= 0.399872
Sum of electronic and zero-point Energies= -2509.452520
Sum of electronic and thermal Energies= -2509.415201
Sum of electronic and thermal Enthalpies= -2509.414257
Sum of electronic and thermal Free Energies= -2509.521627

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.348481 | 3.923676 | -0.511190 |
| 6 | -3.589781 | 2.852548 | -1.368239 |
| 6 | -2.558346 | 1.989181 | -1.697388 |
| 6 | -1.275245 | 2.193218 | -1.168103 |
| 6 | -1.035738 | 3.274514 | -0.309103 |
| 6 | -2.074762 | 4.134954 | 0.011711 |
| 1 | -4.158782 | 4.600100 | -0.248576 |
| 1 | -4.585482 | 2.685101 | -1.770102 |
| 1 | -2.734594 | 1.129021 | -2.338228 |
| 1 | -0.044398 | 3.462901 | 0.091557 |
| 1 | -1.890139 | 4.978144 | 0.672103 |
| 6 | -0.260683 | 1.198207 | -1.507461 |
| 8 | -0.399303 | 0.419271 | -2.470278 |
| 7 | 0.856590 | 1.048134 | -0.658123 |
| 1 | 1.456763 | 2.032505 | -0.108842 |
| 8 | 1.959119 | 0.509561 | -1.323281 |
| 1 | 1.669407 | -0.281311 | -1.825970 |
| 46 | -0.049715 | -0.315620 | 0.733715 |

| | | | |
|---|---|---|---|
| 8 | 2.660664 | 0.339341 | 1.512634 |
| 8 | 1.641268 | -1.462913 | 0.771652 |
| 8 | -1.342790 | -1.459587 | 1.919117 |
| 8 | -1.990710 | 0.375565 | 0.953837 |
| 6 | 2.702065 | -0.850284 | 1.076819 |
| 6 | -2.291722 | -0.651069 | 1.657819 |
| 6 | 4.019794 | -1.581574 | 0.873669 |
| 6 | -3.684020 | -0.858253 | 2.181932 |
| 6 | -4.670717 | -0.031761 | 1.361970 |
| 1 | -5.682634 | -0.177852 | 1.759353 |
| 1 | -4.431545 | 1.036803 | 1.407593 |
| 1 | -4.659335 | -0.338179 | 0.308657 |
| 6 | -3.674758 | -0.383237 | 3.642257 |
| 1 | -4.673609 | -0.517751 | 4.074991 |
| 1 | -2.959743 | -0.958930 | 4.241161 |
| 1 | -3.413409 | 0.679983 | 3.712183 |
| 6 | -4.030596 | -2.344895 | 2.115500 |
| 1 | -3.327597 | -2.944255 | 2.702794 |
| 1 | -5.039386 | -2.499179 | 2.517847 |
| 1 | -4.009161 | -2.706588 | 1.080709 |
| 6 | 5.029366 | -1.141510 | 1.931730 |
| 1 | 5.972054 | -1.680297 | 1.777763 |
| 1 | 5.242583 | -0.068649 | 1.874657 |
| 1 | 4.673437 | -1.366733 | 2.944133 |
| 6 | 3.806266 | -3.091830 | 0.931869 |
| 1 | 3.404001 | -3.401142 | 1.903682 |
| 1 | 3.111353 | -3.426526 | 0.155240 |
| 1 | 4.767612 | -3.598537 | 0.783100 |
| 6 | 4.521041 | -1.190103 | -0.524662 |
| 1 | 4.688326 | -0.109957 | -0.609922 |
| 1 | 5.473126 | -1.700717 | -0.715472 |
| 1 | 3.805547 | -1.497242 | -1.297001 |
| 6 | 3.335439 | 3.088172 | 0.365517 |
| 8 | 4.038141 | 2.139139 | 0.815853 |
| 1 | 3.427239 | 1.198055 | 1.165235 |
| 8 | 2.093254 | 3.035875 | 0.120070 |
| 6 | 4.015880 | 4.392865 | 0.101496 |
| 1 | 3.468838 | 5.196398 | 0.602812 |
| 1 | 5.052339 | 4.370104 | 0.439212 |
| 1 | 3.978968 | 4.602419 | -0.972215 |
| 30 | -0.745530 | -1.588231 | -1.970143 |
| 17 | 1.187317 | -2.547431 | -2.433462 |
| 17 | -2.882156 | -1.839400 | -1.552531 |

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**$(3a'\text{-}4a')_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1294.9947405
Zero-point correction= 0.400766
Thermal correction to Energy= 0.428379
Thermal correction to Enthalpy= 0.429323
Thermal correction to Gibbs Free Energy= 0.341552
Sum of electronic and zero-point Energies= -1294.593975
Sum of electronic and thermal Energies= -1294.566362
Sum of electronic and thermal Enthalpies= -1294.565417
Sum of electronic and thermal Free Energies= -1294.653188

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -4.271591 | -1.663343 | -0.290278 |
| 6 | -2.977201 | -1.408189 | 0.155223 |
| 6 | -2.361477 | -0.155823 | -0.073878 |
| 6 | -3.054945 | 0.774094 | -0.869558 |
| 6 | -4.353343 | 0.526373 | -1.293881 |
| 6 | -4.968325 | -0.688197 | -0.989033 |
| 1 | -4.683184 | -2.655906 | -0.121155 |
| 1 | -1.692565 | 0.694341 | 0.724969 |
| 1 | -2.596329 | 1.737578 | -1.087111 |
| 1 | -4.892066 | 1.283853 | -1.858526 |
| 1 | -5.982837 | -0.882829 | -1.329263 |
| 6 | -2.171900 | -2.550603 | 0.632186 |
| 8 | -2.554728 | -3.718512 | 0.706282 |
| 7 | -0.874387 | -2.187768 | 0.892047 |
| 8 | -0.044165 | -3.261886 | 1.006651 |
| 1 | -0.608029 | -4.017546 | 0.724391 |
| 46 | -0.263277 | -0.522720 | -0.041422 |
| 8 | 0.293866 | 1.523955 | -0.451846 |
| 8 | -1.237531 | 1.939545 | 1.118090 |
| 8 | 1.800301 | -1.181784 | -0.201040 |
| 6 | -0.293679 | 2.304911 | 0.371373 |
| 6 | 0.100852 | 3.776628 | 0.366581 |
| 6 | 2.827448 | -0.530620 | -0.392107 |
| 8 | 2.848555 | 0.761479 | -0.625509 |
| 1 | 1.929989 | 1.138266 | -0.616393 |
| 6 | 4.193818 | -1.179179 | -0.301718 |
| 6 | 5.152183 | -0.583818 | -1.330986 |
| 1 | 5.287263 | 0.492229 | -1.185503 |
| 1 | 6.130573 | -1.069947 | -1.235358 |
| 1 | 4.794007 | -0.748770 | -2.354185 |
| 6 | 4.059223 | -2.685158 | -0.499232 |

| | | | |
|---|---|---|---|
| 1 | 5.040944 | -3.158252 | -0.377841 |
| 1 | 3.363980 | -3.122196 | 0.223993 |
| 1 | 3.688132 | -2.921298 | -1.503355 |
| 6 | 4.701258 | -0.883275 | 1.118194 |
| 1 | 4.020392 | -1.295732 | 1.872408 |
| 1 | 5.684933 | -1.348583 | 1.255391 |
| 1 | 4.805303 | 0.194363 | 1.289355 |
| 6 | -0.875581 | 4.447060 | -0.609957 |
| 1 | -0.656432 | 5.519931 | -0.676176 |
| 1 | -0.782691 | 4.017385 | -1.615699 |
| 1 | -1.911768 | 4.328635 | -0.270022 |
| 6 | 1.533146 | 3.961772 | -0.123391 |
| 1 | 1.793993 | 5.026830 | -0.104379 |
| 1 | 2.248877 | 3.430694 | 0.516997 |
| 1 | 1.660984 | 3.600764 | -1.149757 |
| 6 | -0.065632 | 4.374110 | 1.760296 |
| 1 | 0.614200 | 3.901808 | 2.479463 |
| 1 | 0.165322 | 5.446050 | 1.730674 |
| 1 | -1.087477 | 4.244989 | 2.128156 |

---

**$(3a'\text{-}4a')_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1523.9833118
Zero-point correction= 0.465032
Thermal correction to Energy= 0.497407
Thermal correction to Enthalpy= 0.498351
Thermal correction to Gibbs Free Energy= 0.401470
Sum of electronic and zero-point Energies= -1523.518280
Sum of electronic and thermal Energies= -1523.485905
Sum of electronic and thermal Enthalpies= -1523.484961
Sum of electronic and thermal Free Energies= -1523.581842

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.602948 | 4.007823 | -0.979983 |
| 6 | 2.970502 | 3.852200 | -1.159889 |
| 6 | 3.605188 | 2.655153 | -0.810662 |
| 6 | 2.868700 | 1.607475 | -0.280131 |
| 6 | 1.490487 | 1.753766 | -0.030631 |
| 6 | 0.870731 | 2.965260 | -0.420137 |
| 1 | 1.076706 | 4.906016 | -1.295155 |
| 1 | 3.553957 | 4.662069 | -1.592240 |
| 1 | 4.678266 | 2.550859 | -0.953196 |
| 1 | 3.370371 | 0.686430 | 0.017887 |

| | | | |
|---|---|---|---|
| 6 | -0.601678 | 3.041390 | -0.368534 |
| 8 | -1.299084 | 3.974236 | -0.763878 |
| 7 | -1.137867 | 1.875792 | 0.134525 |
| 8 | -2.494936 | 1.821987 | -0.054928 |
| 1 | -2.676434 | 2.614307 | -0.611539 |
| 46 | -0.001178 | 0.278114 | -0.336657 |
| 8 | -1.735892 | -0.934072 | -0.802581 |
| 1 | 1.270838 | 1.245559 | 1.183366 |
| 6 | -2.722625 | -1.101474 | -0.080142 |
| 8 | -2.704675 | -1.106620 | 1.225610 |
| 1 | -1.794674 | -1.004513 | 1.629253 |
| 8 | 1.294141 | 0.646871 | 2.345693 |
| 6 | 0.081363 | 0.285684 | 2.666241 |
| 8 | -0.345933 | -0.845394 | 2.397961 |
| 8 | 1.285187 | -1.399570 | -0.667268 |
| 6 | 2.148438 | -1.908624 | 0.054407 |
| 8 | 2.503124 | -1.480765 | 1.234129 |
| 1 | 1.957534 | -0.724822 | 1.613584 |
| 6 | -0.791243 | 1.300469 | 3.346044 |
| 6 | -4.090283 | -1.389367 | -0.670920 |
| 6 | 2.970312 | -3.086326 | -0.439779 |
| 1 | -1.806666 | 1.234915 | 2.940797 |
| 1 | -0.838251 | 1.072930 | 4.417035 |
| 1 | -0.399039 | 2.311719 | 3.216462 |
| 6 | 2.298563 | -3.724229 | -1.649242 |
| 1 | 1.307266 | -4.114902 | -1.393226 |
| 1 | 2.172007 | -3.004576 | -2.463839 |
| 1 | 2.913502 | -4.557312 | -2.009870 |
| 6 | 4.335376 | -2.510648 | -0.843743 |
| 1 | 4.844401 | -2.054962 | 0.013237 |
| 1 | 4.970427 | -3.315329 | -1.233721 |
| 1 | 4.226615 | -1.753792 | -1.631594 |
| 6 | 3.149080 | -4.115774 | 0.675491 |
| 1 | 3.751580 | -4.952803 | 0.302199 |
| 1 | 3.653772 | -3.684743 | 1.544930 |
| 1 | 2.183358 | -4.516749 | 1.005621 |
| 6 | -5.146824 | -0.551907 | 0.052284 |
| 1 | -4.921664 | 0.517634 | -0.028501 |
| 1 | -6.127485 | -0.734284 | -0.404310 |
| 1 | -5.205171 | -0.808330 | 1.114266 |
| 6 | -4.090655 | -1.065235 | -2.159227 |
| 1 | -3.344596 | -1.656143 | -2.699971 |
| 1 | -5.079533 | -1.282111 | -2.580889 |
| 1 | -3.866660 | -0.006226 | -2.332034 |
| 6 | -4.369290 | -2.881988 | -0.454892 |

| | | | |
|---|---|---|---|
| 1 | -4.363223 | -3.135858 | 0.610618 |
| 1 | -5.355322 | -3.131864 | -0.865483 |
| 1 | -3.622625 | -3.502173 | -0.966353 |

---

**$(3a'\text{-}4a')_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2509.9317911
Zero-point correction= 0.468220
Thermal correction to Energy= 0.506882
Thermal correction to Enthalpy= 0.507826
Thermal correction to Gibbs Free Energy= 0.394374
Sum of electronic and zero-point Energies= -2509.463571
Sum of electronic and thermal Energies= -2509.424909
Sum of electronic and thermal Enthalpies= -2509.423965
Sum of electronic and thermal Free Energies= -2509.537417

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.248117 | -3.214105 | -2.149062 |
| 6 | 0.905145 | -2.227712 | -1.238915 |
| 6 | -0.423897 | -2.090377 | -0.757658 |
| 6 | -1.414299 | -2.937623 | -1.285027 |
| 6 | -1.073655 | -3.924818 | -2.200026 |
| 6 | 0.249787 | -4.061158 | -2.624905 |
| 1 | 2.277043 | -3.288885 | -2.492374 |
| 1 | -0.401947 | -2.177038 | 0.543190 |
| 1 | -2.437558 | -2.852255 | -0.923478 |
| 1 | -1.834971 | -4.600168 | -2.582308 |
| 1 | 0.503069 | -4.836060 | -3.344637 |
| 6 | 1.894586 | -1.232180 | -0.781037 |
| 8 | 3.122597 | -1.329546 | -0.998919 |
| 7 | 1.289355 | -0.222406 | -0.136078 |
| 8 | 2.100745 | 0.886570 | 0.064337 |
| 46 | -0.709925 | -0.078358 | -0.276483 |
| 8 | -0.663717 | 2.053992 | 0.055156 |
| 6 | -1.475686 | 2.907561 | -0.316534 |
| 8 | -2.656750 | 2.621490 | -0.805279 |
| 1 | -2.817327 | 1.639715 | -0.780951 |
| 8 | 0.049725 | -2.561691 | 1.758912 |
| 6 | -0.002894 | -1.763875 | 2.713158 |
| 8 | -0.958676 | -0.895031 | 2.865787 |
| 1 | -1.702415 | -1.034027 | 2.198544 |
| 8 | -2.784532 | -0.016715 | -0.482588 |
| 6 | -3.500210 | -0.663140 | 0.380170 |

| | | | |
|---|---|---|---|
| 8 | -3.029201 | -1.309642 | 1.324372 |
| 6 | -1.154246 | 4.385661 | -0.261710 |
| 6 | -5.004856 | -0.683938 | 0.112098 |
| 6 | 1.070654 | -1.736534 | 3.736745 |
| 1 | 0.759547 | -1.195180 | 4.630902 |
| 1 | 1.370543 | -2.758941 | 3.977857 |
| 1 | 1.952451 | -1.244699 | 3.296739 |
| 6 | -5.762464 | -0.860608 | 1.423721 |
| 1 | -6.837745 | -0.942331 | 1.222940 |
| 1 | -5.432986 | -1.760306 | 1.951194 |
| 1 | -5.607329 | -0.004498 | 2.091342 |
| 6 | -5.468220 | 0.584196 | -0.598708 |
| 1 | -5.251532 | 1.480776 | -0.003744 |
| 1 | -4.992363 | 0.698636 | -1.578934 |
| 1 | -6.553319 | 0.544073 | -0.753644 |
| 6 | -5.243042 | -1.900705 | -0.792243 |
| 1 | -4.687265 | -1.808520 | -1.734490 |
| 1 | -4.938533 | -2.827379 | -0.288629 |
| 1 | -6.310039 | -1.982321 | -1.034226 |
| 6 | -1.131487 | 4.902732 | -1.706749 |
| 1 | -0.366969 | 4.388312 | -2.301410 |
| 1 | -2.102062 | 4.773829 | -2.196691 |
| 1 | -0.887000 | 5.971437 | -1.699869 |
| 6 | 0.206484 | 4.597500 | 0.389941 |
| 1 | 0.446682 | 5.666853 | 0.390559 |
| 1 | 0.212394 | 4.246233 | 1.427787 |
| 1 | 0.997101 | 4.065165 | -0.149503 |
| 6 | -2.246580 | 5.108906 | 0.531258 |
| 1 | -2.296479 | 4.746931 | 1.565382 |
| 1 | -2.015447 | 6.180183 | 0.563603 |
| 1 | -3.231667 | 4.983534 | 0.070831 |
| 1 | 2.081883 | 1.047804 | 1.027356 |
| 30 | 4.253330 | 0.097053 | -0.058660 |
| 17 | 5.618878 | 1.252097 | -1.326040 |
| 17 | 4.066678 | -0.170056 | 2.186975 |

---

**$(5a'\text{-}6a')_4^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2409.8887571
Zero-point correction= 0.390640
Thermal correction to Energy= 0.424018
Thermal correction to Enthalpy= 0.424962
Thermal correction to Gibbs Free Energy= 0.322620
Sum of electronic and zero-point Energies= -2409.498117

Sum of electronic and thermal Energies= -2409.464739
Sum of electronic and thermal Enthalpies= -2409.463795
Sum of electronic and thermal Free Energies= -2409.566137

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 2.335627 | 3.658568 | 0.229754 |
| 6 | 1.618200 | 2.456044 | 0.151831 |
| 6 | 0.270213 | 2.453466 | -0.255597 |
| 6 | -0.356060 | 3.644869 | -0.590982 |
| 6 | 0.364651 | 4.834902 | -0.498133 |
| 6 | 1.700557 | 4.845962 | -0.087047 |
| 1 | 3.383411 | 3.631583 | 0.520771 |
| 1 | -1.399451 | 3.658798 | -0.897832 |
| 1 | -0.126323 | 5.774229 | -0.745279 |
| 1 | 2.241243 | 5.786345 | -0.027040 |
| 6 | 2.294906 | 1.178365 | 0.321222 |
| 8 | 3.515386 | 1.029618 | 0.280245 |
| 7 | 1.413009 | 0.055215 | 0.374267 |
| 8 | 1.970467 | -1.050284 | -0.298632 |
| 1 | 2.170602 | -1.714268 | 0.406789 |
| 46 | -0.559527 | 0.691713 | 0.120015 |
| 7 | -0.461556 | -0.929641 | 1.793437 |
| 6 | -1.712853 | -1.470784 | 1.612158 |
| 8 | -2.633352 | -1.180656 | 2.390691 |
| 8 | -0.467426 | -0.067792 | 2.891302 |
| 1 | -1.410032 | -0.099458 | 3.182701 |
| 6 | -1.947910 | -2.354789 | 0.437017 |
| 6 | -3.236925 | -2.874876 | 0.296047 |
| 6 | -0.987790 | -2.636633 | -0.540878 |
| 6 | -3.568330 | -3.650261 | -0.808382 |
| 1 | -3.966507 | -2.656278 | 1.073102 |
| 6 | -1.325141 | -3.404027 | -1.649711 |
| 1 | 0.025830 | -2.255665 | -0.449848 |
| 6 | -2.615561 | -3.909439 | -1.788508 |
| 1 | -4.574558 | -4.052522 | -0.904994 |
| 1 | -0.572039 | -3.613283 | -2.405601 |
| 1 | -2.874123 | -4.510526 | -2.657013 |
| 1 | 0.811531 | -0.443020 | 1.256106 |
| 8 | -2.616828 | 1.229091 | 0.120001 |
| 6 | -3.432889 | 0.675485 | -0.623669 |
| 6 | -4.919977 | 0.795266 | -0.391756 |
| 8 | -3.074291 | -0.011216 | -1.688295 |
| 1 | -2.098569 | -0.018746 | -1.756850 |
| 6 | -5.181682 | 0.745365 | 1.114492 |

| | | | |
|---|---|---|---|
| 1 | -6.261428 | 0.809276 | 1.291706 |
| 1 | -4.801555 | -0.183614 | 1.558285 |
| 1 | -4.694177 | 1.577952 | 1.630914 |
| 6 | -5.685495 | -0.314405 | -1.106948 |
| 1 | -6.753819 | -0.207657 | -0.887014 |
| 1 | -5.552873 | -0.269361 | -2.192649 |
| 1 | -5.360370 | -1.304957 | -0.766532 |
| 6 | -5.325743 | 2.165126 | -0.957070 |
| 1 | -6.399083 | 2.315534 | -0.792366 |
| 1 | -4.785141 | 2.976292 | -0.455599 |
| 1 | -5.136235 | 2.225864 | -2.035946 |
| 30 | 4.386738 | -0.803907 | -0.167526 |
| 17 | 4.052218 | -2.207112 | 1.546888 |
| 17 | 5.496676 | -0.712090 | -2.038663 |

---

**$(5a'\text{-}6a')_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2409.9432316
Zero-point correction= 0.391321
Thermal correction to Energy= 0.424492
Thermal correction to Enthalpy= 0.425436
Thermal correction to Gibbs Free Energy= 0.323367
Sum of electronic and zero-point Energies= -2409.551910
Sum of electronic and thermal Energies= -2409.518740
Sum of electronic and thermal Enthalpies= -2409.517796
Sum of electronic and thermal Free Energies= -2409.619865

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.991113 | -3.747128 | -1.501123 |
| 6 | -1.391685 | -2.635778 | -0.891510 |
| 6 | -0.026896 | -2.636016 | -0.548180 |
| 6 | 0.740963 | -3.764649 | -0.808592 |
| 6 | 0.143090 | -4.858706 | -1.430379 |
| 6 | -1.212716 | -4.855392 | -1.778167 |
| 1 | -3.054954 | -3.719759 | -1.726654 |
| 1 | 1.796222 | -3.782192 | -0.545146 |
| 1 | 0.745753 | -5.737299 | -1.653041 |
| 1 | -1.652303 | -5.727388 | -2.254393 |
| 6 | -2.169017 | -1.497012 | -0.460785 |
| 8 | -3.391008 | -1.435119 | -0.357503 |
| 7 | -1.335650 | -0.401014 | -0.044528 |
| 8 | -1.972951 | 0.300445 | 1.008413 |
| 46 | 0.644419 | -0.922015 | 0.168757 |

| | | | |
|---|---|---|---|
| 8 | 2.642777 | -1.621120 | 0.272784 |
| 6 | 3.649790 | -0.970711 | 0.593990 |
| 6 | 5.008425 | -1.637096 | 0.683363 |
| 8 | 3.646055 | 0.294445 | 0.893573 |
| 1 | 2.735646 | 0.727616 | 0.797884 |
| 1 | -1.623361 | 1.214089 | 0.868583 |
| 8 | 1.260621 | 1.157735 | 0.506070 |
| 6 | 0.705205 | 2.105653 | -0.185891 |
| 7 | -0.498994 | 1.907799 | -0.678082 |
| 6 | 1.473190 | 3.364620 | -0.347687 |
| 6 | 2.854479 | 3.289498 | -0.547392 |
| 6 | 0.864148 | 4.617795 | -0.233328 |
| 6 | 3.613980 | 4.447802 | -0.647211 |
| 1 | 3.334092 | 2.317685 | -0.639905 |
| 6 | 1.630892 | 5.772641 | -0.308273 |
| 1 | -0.209298 | 4.680293 | -0.089181 |
| 6 | 3.003930 | 5.691774 | -0.521420 |
| 1 | 4.685616 | 4.378354 | -0.817525 |
| 1 | 1.151765 | 6.743084 | -0.204226 |
| 1 | 3.598944 | 6.599569 | -0.588998 |
| 1 | -1.076706 | 0.475642 | -0.723165 |
| 8 | -0.976816 | 2.923839 | -1.498215 |
| 1 | -1.934422 | 2.739575 | -1.535692 |
| 30 | -4.175242 | 0.326760 | 0.485172 |
| 17 | -5.399481 | 0.036469 | 2.267295 |
| 17 | -3.985012 | 1.866439 | -1.142025 |
| 6 | 5.449031 | -1.590782 | 2.152143 |
| 1 | 5.526937 | -0.560925 | 2.514704 |
| 1 | 4.747576 | -2.135008 | 2.796094 |
| 1 | 6.432237 | -2.066435 | 2.248818 |
| 6 | 4.920432 | -3.081945 | 0.208814 |
| 1 | 4.595732 | -3.141993 | -0.836441 |
| 1 | 5.907999 | -3.551323 | 0.287304 |
| 1 | 4.216700 | -3.661069 | 0.816939 |
| 6 | 6.002502 | -0.854751 | -0.180435 |
| 1 | 6.988862 | -1.328684 | -0.112259 |
| 1 | 5.703480 | -0.854462 | -1.235780 |
| 1 | 6.095168 | 0.182915 | 0.154188 |

---

**$(5a'\text{-}6a')_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2638.9134776
Zero-point correction= 0.455720
Thermal correction to Energy= 0.494096

Thermal correction to Enthalpy= 0.495040
Thermal correction to Gibbs Free Energy= 0.381373
Sum of electronic and zero-point Energies= -2638.457758
Sum of electronic and thermal Energies= -2638.419382
Sum of electronic and thermal Enthalpies= -2638.418438
Sum of electronic and thermal Free Energies= -2638.532104

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 0.147432 | -4.427742 | -0.701851 |
| 6 | 0.023280 | -3.031451 | -0.642443 |
| 6 | -1.239472 | -2.403176 | -0.695378 |
| 6 | -2.377170 | -3.185678 | -0.842514 |
| 6 | -2.244729 | -4.571745 | -0.898855 |
| 6 | -0.994092 | -5.195519 | -0.824883 |
| 1 | 1.139565 | -4.870682 | -0.653144 |
| 1 | -3.359453 | -2.722343 | -0.893866 |
| 1 | -3.139220 | -5.184294 | -0.995256 |
| 1 | -0.924010 | -6.278609 | -0.868487 |
| 6 | 1.178845 | -2.180475 | -0.585431 |
| 8 | 2.363383 | -2.437997 | -0.745160 |
| 7 | 0.781112 | -0.786711 | -0.336508 |
| 8 | 1.704514 | 0.114179 | -0.902493 |
| 46 | -1.250478 | -0.437772 | -0.435945 |
| 8 | -3.364985 | -0.340300 | -0.456912 |
| 6 | -4.065115 | 0.589942 | -0.021424 |
| 6 | -5.576938 | 0.479086 | -0.003007 |
| 8 | -3.599947 | 1.716063 | 0.423879 |
| 1 | -2.590518 | 1.776693 | 0.355981 |
| 1 | 1.391931 | 0.291973 | -1.805435 |
| 8 | -1.075326 | 1.698369 | 0.041753 |
| 6 | -0.053435 | 2.260386 | 0.623076 |
| 7 | 0.471185 | 1.704329 | 1.682497 |
| 6 | 0.443194 | 3.508641 | -0.011581 |
| 6 | -0.493740 | 4.403150 | -0.534883 |
| 6 | 1.807076 | 3.757094 | -0.195384 |
| 6 | -0.077129 | 5.549736 | -1.197873 |
| 1 | -1.554092 | 4.191014 | -0.414967 |
| 6 | 2.219400 | 4.890395 | -0.885105 |
| 1 | 2.544500 | 3.057411 | 0.188970 |
| 6 | 1.281439 | 5.793464 | -1.376414 |
| 1 | -0.813635 | 6.249396 | -1.585916 |
| 1 | 3.281106 | 5.068972 | -1.036752 |
| 1 | 1.609883 | 6.685042 | -1.905637 |
| 1 | 0.827463 | -0.656143 | 0.709496 |

| | | | |
|---|---|---|---|
| 8 | 1.504815 | 2.415630 | 2.300885 |
| 1 | 2.287370 | 1.844075 | 2.183136 |
| 6 | -6.010894 | -0.929874 | -0.385521 |
| 1 | -5.660786 | -1.199681 | -1.387974 |
| 1 | -5.624149 | -1.672830 | 0.321900 |
| 1 | -7.105399 | -0.988576 | -0.376068 |
| 6 | -6.083684 | 0.826811 | 1.399993 |
| 1 | -5.802661 | 1.844021 | 1.688685 |
| 1 | -7.177414 | 0.751918 | 1.416129 |
| 1 | -5.688327 | 0.132773 | 2.151464 |
| 6 | -6.121391 | 1.493175 | -1.017279 |
| 1 | -7.216663 | 1.442602 | -1.024704 |
| 1 | -5.824892 | 2.514924 | -0.758778 |
| 1 | -5.767277 | 1.272559 | -2.031793 |
| 1 | 0.246713 | 0.408946 | 2.219914 |
| 8 | 0.190084 | -0.685561 | 2.264659 |
| 6 | 1.133802 | -1.404197 | 2.886088 |
| 8 | 1.502980 | -2.457017 | 2.409186 |
| 30 | 3.718464 | -0.767075 | -0.533279 |
| 17 | 4.832494 | -0.527062 | -2.401528 |
| 17 | 3.747149 | 0.066440 | 1.543294 |
| 6 | 1.638700 | -0.819228 | 4.170750 |
| 1 | 2.558817 | -1.320495 | 4.474349 |
| 1 | 1.815408 | 0.256210 | 4.052421 |
| 1 | 0.877382 | -0.941564 | 4.949343 |

---

**$(5a'\text{-}6a')_{10}^{\ddagger}$**

---

Number of imaginary frequencies: 1
Electronic energy =-2638.929832
Zero-point correction= 0.453971
Thermal correction to Energy= 0.492194
Thermal correction to Enthalpy= 0.493138
Thermal correction to Gibbs Free Energy= 0.381329
Sum of electronic and zero-point Energies= -2638.475861
Sum of electronic and thermal Energies= -2638.437638
Sum of electronic and thermal Enthalpies= -2638.436694
Sum of electronic and thermal Free Energies= -2638.548503

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.374553 | -4.277565 | -0.958076 |
| 6 | -0.304657 | -2.886275 | -0.804158 |
| 6 | -1.458181 | -2.080025 | -0.884463 |
| 6 | -2.686862 | -2.677186 | -1.134420 |

| | | | |
|---|---|---|---|
| 6 | -2.750132 | -4.063638 | -1.270922 |
| 6 | -1.606028 | -4.863650 | -1.185277 |
| 1 | 0.540686 | -4.862841 | -0.901510 |
| 1 | -3.585447 | -2.069447 | -1.210389 |
| 1 | -3.715882 | -4.533691 | -1.447520 |
| 1 | -1.687219 | -5.940709 | -1.301570 |
| 6 | 0.951169 | -2.207587 | -0.591040 |
| 8 | 2.094116 | -2.637037 | -0.692599 |
| 7 | 0.722954 | -0.834900 | -0.187456 |
| 8 | 1.843334 | -0.031456 | -0.466060 |
| 46 | -1.173307 | -0.136209 | -0.616759 |
| 8 | -3.229482 | 0.302985 | -0.830790 |
| 6 | -3.782085 | 1.286973 | -0.307993 |
| 6 | -5.292726 | 1.400955 | -0.269742 |
| 8 | -3.151647 | 2.294253 | 0.211801 |
| 1 | -2.149942 | 2.217559 | 0.119227 |
| 1 | 1.719296 | 0.324551 | -1.363531 |
| 8 | -0.616846 | 1.996674 | -0.267231 |
| 6 | 0.399927 | 2.170037 | 0.524569 |
| 7 | 0.379150 | 1.547943 | 1.675151 |
| 6 | 1.503259 | 3.022244 | 0.024640 |
| 6 | 1.164704 | 4.049195 | -0.863427 |
| 6 | 2.852621 | 2.780148 | 0.314670 |
| 6 | 2.151773 | 4.844758 | -1.428225 |
| 1 | 0.117159 | 4.211131 | -1.103720 |
| 6 | 3.836944 | 3.559808 | -0.279744 |
| 1 | 3.133066 | 1.974041 | 0.985946 |
| 6 | 3.490807 | 4.597013 | -1.140675 |
| 1 | 1.876888 | 5.650587 | -2.104429 |
| 1 | 4.882435 | 3.348121 | -0.070063 |
| 1 | 4.267516 | 5.207482 | -1.595359 |
| 1 | 0.597421 | -0.891519 | 0.926043 |
| 8 | 1.420818 | 1.737088 | 2.567039 |
| 1 | 1.847670 | 0.860473 | 2.641332 |
| 6 | -5.935047 | 0.099335 | -0.731649 |
| 1 | -5.628662 | -0.161863 | -1.750482 |
| 1 | -5.668406 | -0.733061 | -0.069666 |
| 1 | -7.025849 | 0.206929 | -0.717777 |
| 6 | -5.729802 | 1.727481 | 1.161346 |
| 1 | -5.310711 | 2.677835 | 1.504651 |
| 1 | -6.823460 | 1.798360 | 1.194367 |
| 1 | -5.419741 | 0.943657 | 1.862722 |
| 6 | -5.687488 | 2.547366 | -1.209689 |
| 1 | -6.777579 | 2.664639 | -1.197618 |
| 1 | -5.235042 | 3.493236 | -0.894942 |

| | | | |
|---|---|---|---|
| 1 | -5.382021 | 2.339688 | -2.242611 |
| 30 | 3.657267 | -1.240697 | -0.100145 |
| 17 | 4.929874 | -0.770778 | -1.822873 |
| 17 | 3.585559 | -0.906251 | 2.095315 |
| 1 | -0.574504 | 0.870218 | 2.070427 |
| 8 | -1.474190 | 0.113234 | 2.502942 |
| 6 | -0.983755 | -1.053677 | 2.666418 |
| 8 | 0.126667 | -1.423119 | 2.209990 |
| 6 | -1.809060 | -2.052222 | 3.424198 |
| 1 | -2.259799 | -2.745657 | 2.703776 |
| 1 | -1.165717 | -2.643213 | 4.080876 |
| 1 | -2.602264 | -1.563699 | 3.992914 |

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**$(6a_1'\text{-}9)_3^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2409.9139009
Zero-point correction= 0.393608
Thermal correction to Energy= 0.427352
Thermal correction to Enthalpy= 0.428297
Thermal correction to Gibbs Free Energy= 0.324172
Sum of electronic and zero-point Energies= -2409.520293
Sum of electronic and thermal Energies= -2409.486548
Sum of electronic and thermal Enthalpies= -2409.485604
Sum of electronic and thermal Free Energies= -2409.589729

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.332434 | -0.733405 | 0.869584 |
| 6 | 1.312822 | 0.161275 | 2.055656 |
| 6 | -0.038108 | 0.485022 | 1.815225 |
| 6 | 1.948852 | 0.678523 | 3.188862 |
| 6 | -0.715763 | 1.338821 | 2.697512 |
| 6 | 1.259745 | 1.479478 | 4.086012 |
| 1 | 2.994180 | 0.426046 | 3.352631 |
| 6 | -0.075382 | 1.800600 | 3.839723 |
| 1 | -1.728157 | 1.657976 | 2.457367 |
| 1 | 1.763627 | 1.866695 | 4.967047 |
| 1 | -0.617957 | 2.443504 | 4.528908 |
| 8 | -2.334338 | 1.791052 | 0.032755 |
| 6 | -1.138875 | 1.953482 | -0.257549 |
| 7 | -0.281812 | 0.899697 | -0.059695 |
| 8 | 1.020665 | 1.029256 | -0.488363 |
| 1 | 1.125749 | 0.541545 | -1.331043 |
| 6 | -0.653675 | 3.255817 | -0.766650 |

| | | | |
|---|---|---|---|
| 6 | -1.531759 | 4.004899 | -1.555168 |
| 6 | 0.575586 | 3.800765 | -0.382403 |
| 6 | -1.168156 | 5.270483 | -1.992034 |
| 1 | -2.497846 | 3.578606 | -1.813951 |
| 6 | 0.921816 | 5.078954 | -0.800291 |
| 1 | 1.251312 | 3.228736 | 0.247045 |
| 6 | 0.059285 | 5.808259 | -1.613730 |
| 1 | -1.845280 | 5.843457 | -2.620616 |
| 1 | 1.873336 | 5.505517 | -0.493254 |
| 1 | 0.342966 | 6.802765 | -1.950423 |
| 6 | 2.126419 | -0.675552 | 1.154931 |
| 8 | 3.310603 | -0.421575 | 0.888631 |
| 8 | -3.022565 | -1.950547 | 0.134267 |
| 6 | -3.999418 | -1.439428 | -0.416451 |
| 6 | -5.193071 | -2.258390 | -0.870693 |
| 8 | -4.125918 | -0.155763 | -0.652406 |
| 1 | -3.363964 | 0.396780 | -0.327967 |
| 7 | 1.545976 | -1.831183 | 0.716253 |
| 8 | 2.195375 | -2.479810 | -0.324148 |
| 1 | 2.642563 | -3.254235 | 0.063849 |
| 1 | 0.521111 | -1.895401 | 0.645180 |
| 30 | 3.974947 | -1.210092 | -0.925609 |
| 17 | 5.409133 | -2.865113 | -0.640285 |
| 17 | 3.075131 | -0.016574 | -2.575181 |
| 6 | -5.477403 | -1.962487 | -2.345970 |
| 1 | -6.337637 | -2.558527 | -2.673761 |
| 1 | -5.708000 | -0.905304 | -2.508731 |
| 1 | -4.623021 | -2.231115 | -2.979059 |
| 6 | -4.907436 | -3.742081 | -0.677474 |
| 1 | -4.701493 | -3.977305 | 0.371943 |
| 1 | -5.777621 | -4.326388 | -0.999075 |
| 1 | -4.041370 | -4.061854 | -1.267297 |
| 6 | -6.396374 | -1.839015 | -0.017032 |
| 1 | -7.274998 | -2.421787 | -0.318945 |
| 1 | -6.214922 | -2.032556 | 1.047523 |
| 1 | -6.625874 | -0.776161 | -0.143710 |

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**$(6a'\text{-}9)_5^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2409.8703732
Zero-point correction= 0.393135
Thermal correction to Energy= 0.426844
Thermal correction to Enthalpy= 0.427788
Thermal correction to Gibbs Free Energy= 0.324263

Sum of electronic and zero-point Energies= -2409.477238
Sum of electronic and thermal Energies= -2409.443529
Sum of electronic and thermal Enthalpies= -2409.442585
Sum of electronic and thermal Free Energies= -2409.546110

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.313314 | -3.521162 | -1.139428 |
| 6 | -2.192112 | -2.159525 | -1.213173 |
| 6 | -1.139480 | -1.503135 | -0.500088 |
| 6 | -0.081946 | -2.342563 | -0.004115 |
| 6 | -0.285373 | -3.743432 | 0.137803 |
| 6 | -1.396496 | -4.323334 | -0.405064 |
| 1 | -3.141363 | -4.004865 | -1.654945 |
| 1 | -2.937936 | -1.569961 | -1.744354 |
| 1 | 0.499231 | -4.331632 | 0.609487 |
| 1 | -1.548987 | -5.396837 | -0.340997 |
| 6 | 1.185854 | -1.777675 | 0.209691 |
| 8 | 2.154841 | -2.190593 | 0.869219 |
| 7 | 1.388667 | -0.575851 | -0.637807 |
| 46 | -0.466030 | 0.350232 | -0.955126 |
| 8 | 2.365085 | 0.234925 | 0.018024 |
| 8 | 0.410842 | 2.455282 | -1.017743 |
| 8 | -2.508937 | 1.011774 | -0.414874 |
| 6 | -2.896181 | 0.126293 | 0.381648 |
| 7 | -2.019503 | -0.725885 | 1.056628 |
| 8 | -0.975216 | 0.080564 | 1.623510 |
| 1 | -0.836644 | -0.340720 | 2.480612 |
| 6 | -4.323903 | -0.169792 | 0.521523 |
| 6 | -4.782451 | -1.092062 | 1.471271 |
| 6 | -5.236831 | 0.468577 | -0.330499 |
| 6 | -6.139231 | -1.368204 | 1.566221 |
| 1 | -4.060401 | -1.579957 | 2.119364 |
| 6 | -6.590563 | 0.196010 | -0.223464 |
| 1 | -4.858022 | 1.171427 | -1.068020 |
| 6 | -7.041265 | -0.723364 | 0.724093 |
| 1 | -6.497122 | -2.084857 | 2.300911 |
| 1 | -7.299604 | 0.691456 | -0.881751 |
| 1 | -8.104365 | -0.939079 | 0.803570 |
| 6 | 0.300132 | 3.181934 | -0.029280 |
| 6 | 0.745834 | 4.631179 | -0.019123 |
| 8 | -0.217964 | 2.792419 | 1.116065 |
| 1 | -0.513337 | 1.851981 | 1.110198 |
| 1 | 1.864610 | -0.925178 | -1.493620 |
| 30 | 3.986486 | -1.324859 | 0.394920 |

| | | | |
|---|---|---|---|
| 17 | 5.307689 | -0.721742 | 2.026482 |
| 1 | 2.494436 | 0.986766 | -0.582963 |
| 17 | 4.128675 | -1.646778 | -1.837689 |
| 6 | -0.497740 | 5.500865 | 0.206427 |
| 1 | -0.975940 | 5.276784 | 1.165252 |
| 1 | -0.202709 | 6.556989 | 0.205602 |
| 1 | -1.235519 | 5.356670 | -0.592277 |
| 6 | 1.393765 | 4.985611 | -1.351192 |
| 1 | 1.688278 | 6.041395 | -1.342482 |
| 1 | 2.291381 | 4.385319 | -1.536755 |
| 1 | 0.705289 | 4.824963 | -2.187191 |
| 6 | 1.739809 | 4.841611 | 1.127546 |
| 1 | 2.631669 | 4.214043 | 1.007766 |
| 1 | 2.067818 | 5.887839 | 1.131885 |
| 1 | 1.289465 | 4.617552 | 2.099303 |

## Effect of solvent in Monometallic Pathway (Pivalate as Ligand, LA=1, S=1)

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**(2a'-3a')$_{6s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2568.6286138
Zero-point correction= 0.538662
Thermal correction to Energy= 0.580266
Thermal correction to Enthalpy= 0.581210
Thermal correction to Gibbs Free Energy= 0.461257
Sum of electronic and zero-point Energies= -2568.089952
Sum of electronic and thermal Energies= -2568.048348
Sum of electronic and thermal Enthalpies= -2568.047404
Sum of electronic and thermal Free Energies= -2568.167357

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.864034 | 1.766458 | 4.825376 |
| 6 | 2.735607 | 1.187589 | 3.906698 |
| 6 | 2.245837 | 0.370661 | 2.897189 |
| 6 | 0.868488 | 0.128490 | 2.810125 |
| 6 | -0.002335 | 0.706568 | 3.740867 |
| 6 | 0.495041 | 1.524891 | 4.742913 |
| 1 | 2.254984 | 2.406951 | 5.612492 |
| 1 | 3.804525 | 1.369285 | 3.978890 |
| 1 | 2.945698 | -0.079603 | 2.196631 |
| 1 | -1.065313 | 0.497244 | 3.659232 |
| 1 | -0.184043 | 1.973623 | 5.463072 |

| | | | |
|---|---|---|---|
| 6 | 0.263888 | -0.729166 | 1.778232 |
| 8 | -0.902632 | -1.110131 | 1.853346 |
| 7 | 1.067597 | -1.054473 | 0.670656 |
| 8 | 0.555798 | -2.140442 | -0.051484 |
| 46 | 1.221790 | 0.689183 | -0.507326 |
| 1 | 2.221665 | -1.226983 | 0.712376 |
| 8 | 2.838872 | -0.160422 | -1.422482 |
| 8 | 1.064017 | 2.508768 | -1.497366 |
| 8 | -0.307447 | 1.967915 | 0.105220 |
| 6 | 0.027925 | 2.793090 | -0.812527 |
| 6 | 3.651690 | -0.937868 | -0.825893 |
| 8 | 3.498921 | -1.383032 | 0.343400 |
| 1 | 0.224851 | -1.772424 | -0.903895 |
| 17 | -1.593260 | -0.768259 | -1.624336 |
| 17 | -2.301121 | -4.264238 | 0.327242 |
| 30 | -1.970468 | -2.078808 | 0.320855 |
| 8 | -3.690762 | -1.099399 | 0.930039 |
| 6 | -4.083323 | -0.134412 | 0.237146 |
| 6 | -3.668869 | 1.245404 | 0.644265 |
| 1 | -2.708323 | 1.459521 | 0.150289 |
| 1 | -4.383556 | 2.037818 | 0.408083 |
| 1 | -3.482043 | 1.226570 | 1.720205 |
| 7 | -4.832815 | -0.332583 | -0.858674 |
| 6 | -5.094087 | -1.698919 | -1.294541 |
| 1 | -6.083958 | -1.739592 | -1.759936 |
| 1 | -4.336202 | -2.012686 | -2.026276 |
| 1 | -5.058558 | -2.375852 | -0.440372 |
| 6 | -5.049943 | 0.673697 | -1.880880 |
| 1 | -4.313054 | 0.549127 | -2.687112 |
| 1 | -6.055142 | 0.556233 | -2.299668 |
| 1 | -4.961861 | 1.683653 | -1.478919 |
| 6 | -0.813806 | 3.998316 | -1.133584 |
| 6 | 4.867185 | -1.401902 | -1.620972 |
| 6 | -1.521604 | 4.501791 | 0.121444 |
| 1 | -2.160766 | 5.353954 | -0.139701 |
| 1 | -2.148781 | 3.726100 | 0.573102 |
| 1 | -0.802610 | 4.836748 | 0.878257 |
| 6 | -1.843574 | 3.517089 | -2.167899 |
| 1 | -2.490686 | 4.355075 | -2.455185 |
| 1 | -1.348050 | 3.135164 | -3.067965 |
| 1 | -2.469835 | 2.713784 | -1.760240 |
| 6 | 0.056198 | 5.096600 | -1.739153 |
| 1 | -0.572092 | 5.956298 | -2.002204 |
| 1 | 0.819301 | 5.438233 | -1.030069 |
| 1 | 0.565202 | 4.750921 | -2.644013 |

| | | | |
|---|---|---|---|
| 6 | 6.108579 | -1.300409 | -0.735323 |
| 1 | 6.978939 | -1.679915 | -1.284792 |
| 1 | 6.316572 | -0.259638 | -0.457184 |
| 1 | 5.992811 | -1.886288 | 0.181356 |
| 6 | 5.055749 | -0.584660 | -2.892830 |
| 1 | 5.220281 | 0.475389 | -2.668220 |
| 1 | 5.931181 | -0.958171 | -3.438424 |
| 1 | 4.183179 | -0.654376 | -3.549692 |
| 6 | 4.599162 | -2.870438 | -1.974117 |
| 1 | 4.469698 | -3.475942 | -1.070924 |
| 1 | 3.697069 | -2.970034 | -2.590529 |
| 1 | 5.446414 | -3.269807 | -2.545199 |

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**$(2a'\text{-}3a')_{8s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2797.5910631
Zero-point correction= 0.600856
Thermal correction to Energy= 0.647296
Thermal correction to Enthalpy= 0.648240
Thermal correction to Gibbs Free Energy= 0.518268
Sum of electronic and zero-point Energies= -2796.990207
Sum of electronic and thermal Energies= -2796.943767
Sum of electronic and thermal Enthalpies= -2796.942823
Sum of electronic and thermal Free Energies= -2797.072795

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 1.472820 | -4.195460 | -2.219415 |
| 6 | 0.822336 | -3.271364 | -3.034777 |
| 6 | 0.200804 | -2.166898 | -2.470583 |
| 6 | 0.261748 | -1.963167 | -1.088225 |
| 6 | 0.917275 | -2.889240 | -0.271751 |
| 6 | 1.508566 | -4.010148 | -0.839683 |
| 1 | 1.948193 | -5.068394 | -2.660683 |
| 1 | 0.792206 | -3.418491 | -4.111087 |
| 1 | -0.330814 | -1.445905 | -3.086581 |
| 1 | 0.957009 | -2.754233 | 0.805952 |
| 1 | 1.994193 | -4.742213 | -0.199057 |
| 6 | -0.450333 | -0.796688 | -0.539711 |
| 8 | -1.470976 | -0.353690 | -1.055919 |
| 7 | 0.108465 | -0.181460 | 0.604984 |
| 1 | 0.658365 | -0.745479 | 1.480465 |
| 8 | -0.810138 | 0.668794 | 1.230020 |
| 46 | 1.731814 | 0.985103 | -0.061461 |

| | | | |
|---|---|---|---|
| 8 | 3.565274 | -1.520620 | 1.365227 |
| 8 | 3.034141 | -0.494698 | -0.579246 |
| 8 | 2.762153 | 2.797141 | -0.561728 |
| 8 | 0.720879 | 2.721543 | 0.167499 |
| 6 | 3.735152 | -1.269014 | 0.144867 |
| 6 | 1.708836 | 3.432684 | -0.265516 |
| 6 | 1.049430 | -1.861539 | 3.491309 |
| 8 | 1.465270 | -1.116852 | 2.435407 |
| 1 | 2.522740 | -1.286687 | 1.990428 |
| 8 | 1.810372 | -2.548042 | 4.120717 |
| 1 | -0.637825 | 1.593979 | 0.937418 |
| 6 | 1.532154 | 4.913385 | -0.426893 |
| 6 | 4.941098 | -1.901370 | -0.545917 |
| 30 | -2.965360 | 0.597093 | 0.167516 |
| 17 | -3.595528 | -1.060014 | 1.620681 |
| 17 | -2.796794 | 2.842736 | 0.296797 |
| 8 | -4.358316 | 0.168539 | -1.318126 |
| 6 | -5.401746 | -0.389437 | -0.914763 |
| 6 | -6.460459 | 0.414996 | -0.219551 |
| 1 | -6.179768 | 1.468454 | -0.286585 |
| 1 | -7.454854 | 0.274923 | -0.655536 |
| 1 | -6.500863 | 0.128618 | 0.838883 |
| 7 | -5.581845 | -1.710241 | -1.086263 |
| 6 | -4.461353 | -2.507000 | -1.563854 |
| 1 | -3.859090 | -2.848940 | -0.709002 |
| 1 | -4.844813 | -3.370808 | -2.115927 |
| 1 | -3.832790 | -1.896691 | -2.212904 |
| 6 | -6.614823 | -2.453621 | -0.389850 |
| 1 | -6.887073 | -3.333251 | -0.981910 |
| 1 | -6.247369 | -2.784589 | 0.592166 |
| 1 | -7.512230 | -1.850300 | -0.247521 |
| 6 | 6.137830 | -1.017336 | -0.169064 |
| 1 | 7.044752 | -1.405324 | -0.649328 |
| 1 | 5.987145 | 0.015006 | -0.508291 |
| 1 | 6.297309 | -1.009881 | 0.915098 |
| 6 | 4.760800 | -1.917006 | -2.059784 |
| 1 | 5.621610 | -2.412985 | -2.525111 |
| 1 | 3.852249 | -2.463790 | -2.342845 |
| 1 | 4.681370 | -0.904981 | -2.468162 |
| 6 | 5.158982 | -3.318030 | -0.022690 |
| 1 | 4.322450 | -3.971826 | -0.300304 |
| 1 | 6.072147 | -3.735517 | -0.464785 |
| 1 | 5.257562 | -3.331673 | 1.066352 |
| 6 | 2.855638 | 5.567333 | -0.803175 |
| 1 | 2.702107 | 6.645325 | -0.932193 |

| | | | |
|---|---|---|---|
| 1 | 3.612907 | 5.420133 | -0.024851 |
| 1 | 3.252551 | 5.162384 | -1.740280 |
| 6 | 0.988255 | 5.485074 | 0.886285 |
| 1 | 0.828986 | 6.563200 | 0.766586 |
| 1 | 0.032004 | 5.023670 | 1.154975 |
| 1 | 1.695184 | 5.337465 | 1.711595 |
| 6 | 0.490342 | 5.110961 | -1.538876 |
| 1 | 0.310217 | 6.184280 | -1.672720 |
| 1 | 0.846388 | 4.705470 | -2.493963 |
| 1 | -0.459092 | 4.627198 | -1.282312 |
| 6 | -0.421816 | -1.707167 | 3.731269 |
| 1 | -0.676276 | -0.652087 | 3.880581 |
| 1 | -1.001648 | -2.032056 | 2.855749 |
| 1 | -0.723148 | -2.292467 | 4.600511 |

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**$(2a'\text{-}3a')_{10s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2797.6088274
Zero-point correction= 0.602484
Thermal correction to Energy= 0.648438
Thermal correction to Enthalpy= 0.649382
Thermal correction to Gibbs Free Energy= 0.522216
Sum of electronic and zero-point Energies= -2797.006344
Sum of electronic and thermal Energies= -2796.960390
Sum of electronic and thermal Enthalpies= -2796.959445
Sum of electronic and thermal Free Energies= -2797.086611

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.947463 | 2.762463 | 4.428016 |
| 6 | 0.087477 | 1.851447 | 4.619982 |
| 6 | 0.300935 | 0.841403 | 3.693020 |
| 6 | -0.523700 | 0.733388 | 2.569527 |
| 6 | -1.564305 | 1.651983 | 2.379975 |
| 6 | -1.770489 | 2.661900 | 3.308841 |
| 1 | -1.113861 | 3.555022 | 5.154005 |
| 1 | 0.728581 | 1.928312 | 5.494393 |
| 1 | 1.099932 | 0.116360 | 3.824245 |
| 1 | -2.204648 | 1.593441 | 1.502043 |
| 1 | -2.575550 | 3.376289 | 3.157469 |
| 6 | -0.240768 | -0.364771 | 1.623601 |
| 8 | 0.665087 | -1.171849 | 1.837190 |
| 7 | -1.086178 | -0.441747 | 0.505235 |
| 1 | -2.359555 | -0.608626 | 0.975530 |

| | | | |
|---|---|---|---|
| 8 | -0.896695 | -1.690208 | -0.144081 |
| 1 | -0.547637 | -1.473447 | -1.033436 |
| 46 | -0.499090 | 1.124058 | -0.789849 |
| 8 | -3.462807 | 0.897119 | -0.730289 |
| 8 | -1.853261 | 0.340680 | -2.128707 |
| 8 | 0.402532 | 2.682486 | -1.837613 |
| 8 | 1.090278 | 2.101580 | 0.145380 |
| 6 | -3.060400 | 0.295027 | -1.777054 |
| 6 | 1.262213 | 2.806592 | -0.907767 |
| 6 | -4.435480 | -0.769689 | 1.629524 |
| 8 | -5.017932 | 0.007495 | 0.824357 |
| 1 | -4.306058 | 0.465903 | -0.029612 |
| 8 | -3.197473 | -1.055960 | 1.620217 |
| 30 | 1.398011 | -2.470186 | 0.357397 |
| 17 | 0.967613 | -4.642996 | 0.278055 |
| 17 | 1.762305 | -1.091372 | -1.535121 |
| 6 | 2.483702 | 3.669240 | -1.079494 |
| 6 | -4.006996 | -0.555165 | -2.610448 |
| 8 | 3.277888 | -2.175372 | 1.212076 |
| 6 | 3.995085 | -1.279764 | 0.717471 |
| 6 | 3.875656 | 0.112209 | 1.262636 |
| 1 | 4.787755 | 0.712379 | 1.213561 |
| 1 | 3.073384 | 0.627325 | 0.711500 |
| 1 | 3.550209 | 0.026369 | 2.302087 |
| 7 | 4.843164 | -1.560236 | -0.286436 |
| 6 | 4.819702 | -2.898148 | -0.864601 |
| 1 | 4.121813 | -2.928254 | -1.713261 |
| 1 | 5.826431 | -3.151578 | -1.212027 |
| 1 | 4.492180 | -3.619798 | -0.115514 |
| 6 | 5.477661 | -0.561058 | -1.122727 |
| 1 | 5.547809 | 0.403982 | -0.619655 |
| 1 | 6.490679 | -0.889331 | -1.380760 |
| 1 | 4.901342 | -0.430408 | -2.049937 |
| 6 | -5.250987 | -1.448722 | 2.679465 |
| 1 | -6.272669 | -1.068017 | 2.687165 |
| 1 | -5.257079 | -2.524624 | 2.476650 |
| 1 | -4.778489 | -1.312408 | 3.655980 |
| 6 | 3.015356 | 4.114039 | 0.279148 |
| 1 | 3.931955 | 4.699726 | 0.137602 |
| 1 | 2.288566 | 4.741924 | 0.807662 |
| 1 | 3.246610 | 3.256228 | 0.919893 |
| 6 | 3.514860 | 2.771691 | -1.781036 |
| 1 | 3.136631 | 2.413643 | -2.745749 |
| 1 | 4.438629 | 3.338344 | -1.952967 |
| 1 | 3.749892 | 1.894399 | -1.165473 |

| | | | |
|---|---|---|---|
| 6 | 2.156091 | 4.872146 | -1.958998 |
| 1 | 1.403022 | 5.516378 | -1.490068 |
| 1 | 3.063462 | 5.468163 | -2.115346 |
| 1 | 1.774577 | 4.559116 | -2.935618 |
| 6 | -3.426516 | -0.792642 | -4.000919 |
| 1 | -3.270717 | 0.152098 | -4.534051 |
| 1 | -2.464435 | -1.311125 | -3.952133 |
| 1 | -4.123096 | -1.406260 | -4.584553 |
| 6 | -5.374906 | 0.116411 | -2.718806 |
| 1 | -6.040735 | -0.517994 | -3.316159 |
| 1 | -5.845829 | 0.266731 | -1.741856 |
| 1 | -5.302235 | 1.090227 | -3.217653 |
| 6 | -4.127423 | -1.895772 | -1.867264 |
| 1 | -4.634875 | -1.778334 | -0.903181 |
| 1 | -4.719165 | -2.591588 | -2.474066 |
| 1 | -3.143294 | -2.346519 | -1.687831 |

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**(5a'-6a')$_{4s}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy = -2697.5882146
Zero-point correction= 0.522695
Thermal correction to Energy= 0.564880
Thermal correction to Enthalpy= 0.565824
Thermal correction to Gibbs Free Energy= 0.444250
Sum of electronic and zero-point Energies= -2697.065519
Sum of electronic and thermal Energies= -2697.023334
Sum of electronic and thermal Enthalpies= -2697.022390
Sum of electronic and thermal Free Energies= -2697.143964

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.399415 | 3.971070 | 0.180851 |
| 6 | -0.639712 | 2.611252 | -0.053662 |
| 6 | -1.886534 | 2.176149 | -0.539281 |
| 6 | -2.886989 | 3.101199 | -0.806129 |
| 6 | -2.641101 | 4.450902 | -0.558236 |
| 6 | -1.408243 | 4.886860 | -0.063726 |
| 1 | 0.582719 | 4.279576 | 0.533291 |
| 1 | -3.852406 | 2.771549 | -1.185299 |
| 1 | -3.426852 | 5.179500 | -0.749723 |
| 1 | -1.240855 | 5.945151 | 0.117554 |
| 6 | 0.426211 | 1.625642 | 0.050185 |
| 8 | 1.625151 | 1.870506 | 0.142994 |

| | | | |
|---|---|---|---|
| 7 | -0.043161 | 0.283995 | -0.117563 |
| 8 | 0.910327 | -0.421129 | -0.868317 |
| 1 | 0.969957 | -1.311962 | -0.461575 |
| 46 | -2.063479 | 0.207007 | -0.504370 |
| 7 | -1.458066 | -1.518375 | 0.961718 |
| 6 | -1.051888 | -2.826923 | 1.042633 |
| 8 | -1.275532 | -3.515619 | 2.037597 |
| 8 | -2.201955 | -1.188280 | 2.128540 |
| 1 | -2.089112 | -2.007092 | 2.674274 |
| 6 | -0.260402 | -3.273674 | -0.133071 |
| 6 | -0.732493 | -3.110134 | -1.439015 |
| 6 | 1.009801 | -3.815198 | 0.087256 |
| 6 | 0.071153 | -3.464343 | -2.516990 |
| 1 | -1.729980 | -2.703875 | -1.603567 |
| 6 | 1.821051 | -4.135528 | -0.994834 |
| 1 | 1.362410 | -3.931268 | 1.109006 |
| 6 | 1.352434 | -3.960162 | -2.294922 |
| 1 | -0.296785 | -3.336151 | -3.531871 |
| 1 | 2.826739 | -4.510386 | -0.824481 |
| 1 | 1.993437 | -4.203859 | -3.138357 |
| 1 | -0.416826 | -0.460545 | 0.731408 |
| 8 | -4.172925 | 0.243758 | -0.639508 |
| 6 | -4.974565 | -0.108096 | 0.239142 |
| 6 | -6.456369 | 0.169814 | 0.068603 |
| 8 | -4.662422 | -0.666508 | 1.368414 |
| 1 | -3.685198 | -0.828156 | 1.566416 |
| 30 | 2.991489 | 0.237924 | 0.265079 |
| 17 | 4.186430 | -0.644650 | -1.456196 |
| 17 | 2.208635 | -1.051411 | 1.973086 |
| 8 | 4.464073 | 1.524332 | 0.962032 |
| 6 | 5.614059 | 1.035462 | 0.891358 |
| 6 | 5.997618 | -0.121463 | 1.766635 |
| 1 | 6.175175 | -1.009694 | 1.147744 |
| 1 | 6.900584 | 0.080575 | 2.352107 |
| 1 | 5.165035 | -0.329624 | 2.442801 |
| 7 | 6.516130 | 1.527511 | 0.025932 |
| 6 | 7.765032 | 0.852024 | -0.270901 |
| 1 | 7.618877 | 0.098145 | -1.057821 |
| 1 | 8.494087 | 1.588702 | -0.622882 |
| 1 | 8.177921 | 0.365287 | 0.614044 |
| 6 | 6.087325 | 2.497358 | -0.969957 |
| 1 | 6.889275 | 3.223727 | -1.138225 |
| 1 | 5.850646 | 1.982878 | -1.911105 |
| 1 | 5.193039 | 3.007687 | -0.614054 |
| 6 | -7.291038 | -0.999678 | 0.588592 |

| | | | |
|---|---|---|---|
| 1 | -7.104462 | -1.191940 | 1.648845 |
| 1 | -8.354992 | -0.766696 | 0.461685 |
| 1 | -7.080491 | -1.920003 | 0.030855 |
| 6 | -6.779003 | 0.439892 | -1.396399 |
| 1 | -7.849650 | 0.652080 | -1.498801 |
| 1 | -6.218705 | 1.297181 | -1.783009 |
| 1 | -6.541195 | -0.426039 | -2.024635 |
| 6 | -6.737318 | 1.427212 | 0.905421 |
| 1 | -6.125640 | 2.272933 | 0.565012 |
| 1 | -7.792492 | 1.706007 | 0.798910 |
| 1 | -6.530779 | 1.253084 | 1.967043 |

---

**$(5a'\text{-}6a')_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2697.6223186
Zero-point correction= 0.523937
Thermal correction to Energy= 0.565822
Thermal correction to Enthalpy= 0.566766
Thermal correction to Gibbs Free Energy= 0.445504
Sum of electronic and zero-point Energies= -2697.098381
Sum of electronic and thermal Energies= -2697.056497
Sum of electronic and thermal Enthalpies= -2697.055553
Sum of electronic and thermal Free Energies= -2697.176814

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.111387 | -3.525954 | -1.833905 |
| 6 | -0.491134 | -2.479091 | -1.138400 |
| 6 | 0.839784 | -2.580337 | -0.694899 |
| 6 | 1.549208 | -3.752026 | -0.938101 |
| 6 | 0.932801 | -4.782605 | -1.643482 |
| 6 | -0.387931 | -4.675097 | -2.094746 |
| 1 | -2.149994 | -3.417181 | -2.139378 |
| 1 | 2.577115 | -3.849126 | -0.594097 |
| 1 | 1.492386 | -5.692972 | -1.851534 |
| 1 | -0.844363 | -5.498433 | -2.637486 |
| 6 | -1.225001 | -1.304966 | -0.716644 |
| 8 | -2.443994 | -1.172820 | -0.695211 |
| 7 | -0.357631 | -0.281904 | -0.196448 |
| 8 | -1.014618 | 0.387757 | 0.849019 |
| 46 | 1.566136 | -0.934553 | 0.119877 |
| 8 | 3.505530 | -1.763492 | 0.349609 |
| 6 | 4.523646 | -1.186381 | 0.761093 |
| 6 | 5.824386 | -1.946208 | 0.939625 |

| | | | |
|---|---|---|---|
| 8 | 4.582607 | 0.072069 | 1.079147 |
| 1 | 3.710269 | 0.569452 | 0.915643 |
| 1 | -0.715773 | 1.318485 | 0.731115 |
| 8 | 2.303149 | 1.087170 | 0.536898 |
| 6 | 1.866617 | 2.076747 | -0.186150 |
| 7 | 0.686909 | 1.978024 | -0.749941 |
| 6 | 2.754186 | 3.260930 | -0.310104 |
| 6 | 4.124583 | 3.054541 | -0.485160 |
| 6 | 2.265849 | 4.565402 | -0.197507 |
| 6 | 4.994259 | 4.134856 | -0.562795 |
| 1 | 4.509308 | 2.041248 | -0.575180 |
| 6 | 3.141316 | 5.641964 | -0.250578 |
| 1 | 1.200002 | 4.726568 | -0.072639 |
| 6 | 4.504154 | 5.430770 | -0.439871 |
| 1 | 6.057493 | 3.963779 | -0.714323 |
| 1 | 2.755027 | 6.653350 | -0.149311 |
| 1 | 5.184453 | 6.277824 | -0.491547 |
| 1 | -0.012225 | 0.587098 | -0.827189 |
| 8 | 0.341723 | 3.027867 | -1.593159 |
| 1 | -0.634909 | 2.995456 | -1.579455 |
| 30 | -3.357861 | 0.551268 | 0.137572 |
| 17 | -4.147043 | 0.424665 | 2.254803 |
| 17 | -2.713344 | 2.455447 | -0.957810 |
| 8 | -5.111117 | 0.009242 | -0.854478 |
| 6 | -6.157448 | 0.259986 | -0.217630 |
| 6 | -6.684483 | 1.663845 | -0.165992 |
| 1 | -6.608894 | 2.048227 | 0.858698 |
| 1 | -6.060914 | 2.279630 | -0.817606 |
| 1 | -7.729322 | 1.733214 | -0.486161 |
| 7 | -6.814289 | -0.712673 | 0.436972 |
| 6 | -7.854553 | -0.435282 | 1.409322 |
| 1 | -8.515945 | -1.304391 | 1.482223 |
| 1 | -7.408052 | -0.243691 | 2.395871 |
| 1 | -8.458447 | 0.425339 | 1.117468 |
| 6 | -6.197952 | -2.024401 | 0.559980 |
| 1 | -5.696969 | -2.106629 | 1.534264 |
| 1 | -6.968743 | -2.797845 | 0.474546 |
| 1 | -5.455141 | -2.149656 | -0.228200 |
| 6 | 6.186534 | -1.912571 | 2.429229 |
| 1 | 7.129613 | -2.450292 | 2.584137 |
| 1 | 6.310946 | -0.885979 | 2.788015 |
| 1 | 5.415934 | -2.402081 | 3.037164 |
| 6 | 5.660589 | -3.386880 | 0.472550 |
| 1 | 4.882385 | -3.906477 | 1.042630 |
| 1 | 5.390969 | -3.434953 | -0.588799 |

| | | | |
|---|---|---|---|
| 1 | 6.606086 | -3.924271 | 0.611140 |
| 6 | 6.916486 | -1.246400 | 0.124574 |
| 1 | 7.065297 | -0.214294 | 0.456567 |
| 1 | 7.862085 | -1.788053 | 0.246724 |
| 1 | 6.672242 | -1.235385 | -0.944817 |

---

**(5a'-6a')$_{10s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2926.6138981
Zero-point correction= 0.585295
Thermal correction to Energy= 0.632317
Thermal correction to Enthalpy= 0.633261
Thermal correction to Gibbs Free Energy= 0.501455
Sum of electronic and zero-point Energies= -2926.028603
Sum of electronic and thermal Energies= -2925.981581
Sum of electronic and thermal Enthalpies= -2925.980637
Sum of electronic and thermal Free Energies= -2926.112443

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.170565 | -4.195649 | -0.944052 |
| 6 | -0.210196 | -2.887428 | -0.618117 |
| 6 | -1.561263 | -2.495152 | -0.607679 |
| 6 | -2.537223 | -3.426485 | -0.947140 |
| 6 | -2.153875 | -4.728436 | -1.260027 |
| 6 | -0.809744 | -5.118172 | -1.259278 |
| 1 | 1.227872 | -4.452095 | -0.950461 |
| 1 | -3.587106 | -3.142287 | -0.950622 |
| 1 | -2.919658 | -5.461534 | -1.507655 |
| 1 | -0.541186 | -6.140595 | -1.511176 |
| 6 | 0.761938 | -1.851972 | -0.354810 |
| 8 | 1.975123 | -1.883728 | -0.530797 |
| 7 | 0.133027 | -0.662146 | 0.166048 |
| 8 | 0.907429 | 0.469940 | -0.124465 |
| 46 | -1.924107 | -0.636446 | -0.016399 |
| 8 | -4.011579 | -0.833004 | -0.329729 |
| 6 | -4.859893 | 0.076445 | -0.311700 |
| 8 | -4.619766 | 1.304796 | 0.017564 |
| 1 | -3.655377 | 1.446650 | 0.351658 |
| 1 | 0.778505 | 0.686357 | -1.066388 |
| 8 | -2.266552 | 1.324142 | 0.875078 |
| 6 | -1.270871 | 2.169257 | 0.950367 |
| 7 | -0.394628 | 1.966259 | 1.889219 |
| 6 | -1.204806 | 3.243085 | -0.068396 |

| | | | |
|---|---|---|---|
| 6 | -1.769955 | 2.982383 | -1.323327 |
| 6 | -0.633948 | 4.497863 | 0.171922 |
| 6 | -1.747702 | 3.943606 | -2.324294 |
| 1 | -2.223093 | 2.009195 | -1.508822 |
| 6 | -0.631813 | 5.463797 | -0.826438 |
| 1 | -0.194241 | 4.708054 | 1.140568 |
| 6 | -1.180131 | 5.189709 | -2.075498 |
| 1 | -2.177154 | 3.722369 | -3.298639 |
| 1 | -0.192320 | 6.438456 | -0.627946 |
| 1 | -1.164988 | 5.947292 | -2.855777 |
| 1 | 0.156656 | -0.794269 | 1.305214 |
| 8 | 0.705809 | 2.807044 | 1.910197 |
| 1 | 1.448507 | 2.210878 | 2.139640 |
| 1 | -0.373222 | 1.045863 | 2.930928 |
| 8 | -0.184667 | 0.444941 | 3.854420 |
| 6 | 0.147260 | -0.775334 | 3.668685 |
| 8 | 0.157962 | -1.363235 | 2.565036 |
| 6 | -6.301074 | -0.210822 | -0.693657 |
| 30 | 3.137171 | -0.128139 | 0.066098 |
| 17 | 3.423124 | 1.117995 | -1.845759 |
| 17 | 3.012612 | 0.496911 | 2.251410 |
| 8 | 4.870379 | -1.252190 | -0.063891 |
| 6 | 5.646723 | -1.003156 | -1.012403 |
| 6 | 5.598607 | -1.852472 | -2.246993 |
| 1 | 6.581383 | -2.225593 | -2.551634 |
| 1 | 4.933672 | -2.693285 | -2.042974 |
| 1 | 5.174340 | -1.265285 | -3.070813 |
| 7 | 6.517479 | 0.016940 | -0.944847 |
| 6 | 7.205105 | 0.541902 | -2.109932 |
| 1 | 6.602665 | 1.333643 | -2.577624 |
| 1 | 8.167345 | 0.962825 | -1.801256 |
| 1 | 7.396455 | -0.238112 | -2.848180 |
| 6 | 6.449679 | 0.924411 | 0.192443 |
| 1 | 7.444477 | 1.343153 | 0.372494 |
| 1 | 5.745249 | 1.741715 | -0.018643 |
| 1 | 6.111335 | 0.387403 | 1.079809 |
| 6 | 0.583819 | -1.522922 | 4.888114 |
| 1 | 1.667700 | -1.384432 | 4.980363 |
| 1 | 0.109233 | -1.122652 | 5.786198 |
| 1 | 0.385313 | -2.590428 | 4.775240 |
| 6 | -6.466559 | -1.674130 | -1.082994 |
| 1 | -6.184018 | -2.340348 | -0.260122 |
| 1 | -7.515195 | -1.868098 | -1.338014 |
| 1 | -5.850748 | -1.930008 | -1.952951 |
| 6 | -7.187124 | 0.117230 | 0.512850 |

| | | | |
|---|---|---|---|
| 1 | -7.096189 | 1.169117 | 0.800908 |
| 1 | -8.234845 | -0.083708 | 0.258453 |
| 1 | -6.926601 | -0.502752 | 1.379407 |
| 6 | -6.676061 | 0.693727 | -1.872364 |
| 1 | -6.046877 | 0.489884 | -2.747666 |
| 1 | -7.717928 | 0.502886 | -2.156884 |
| 1 | -6.576649 | 1.752263 | -1.613208 |

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**$(6a'\text{-}9)_{5s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2697.5913132
Zero-point correction= 0.526721
Thermal correction to Energy= 0.568784
Thermal correction to Enthalpy= 0.569729
Thermal correction to Gibbs Free Energy= 0.448761
Sum of electronic and zero-point Energies= -2697.064593
Sum of electronic and thermal Energies= -2697.022529
Sum of electronic and thermal Enthalpies= -2697.021585
Sum of electronic and thermal Free Energies= -2697.142553

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -2.039576 | -4.301511 | -1.875025 |
| 6 | -2.411139 | -2.982108 | -1.758195 |
| 6 | -1.424133 | -1.993743 | -1.523557 |
| 6 | -0.056685 | -2.401547 | -1.540577 |
| 6 | 0.289000 | -3.769881 | -1.573982 |
| 6 | -0.693128 | -4.713420 | -1.745953 |
| 1 | -2.808682 | -5.052404 | -2.047787 |
| 1 | -3.458621 | -2.689795 | -1.790159 |
| 1 | 1.340876 | -4.044471 | -1.518063 |
| 1 | -0.441320 | -5.768552 | -1.805285 |
| 6 | 0.934632 | -1.368264 | -1.518320 |
| 8 | 2.044523 | -1.354027 | -0.978861 |
| 7 | 0.482061 | -0.203699 | -2.263059 |
| 46 | -1.629762 | -0.036519 | -1.835923 |
| 8 | 1.300436 | 0.908315 | -2.039960 |
| 8 | -1.168172 | 2.208973 | -1.582101 |
| 8 | -3.469697 | -0.098389 | -0.556802 |
| 6 | -3.042212 | -0.769580 | 0.458918 |
| 7 | -1.870990 | -1.361913 | 0.304109 |
| 8 | -1.275057 | -2.053626 | 1.330720 |
| 1 | -0.507528 | -1.485111 | 1.544022 |
| 6 | -3.872004 | -0.794730 | 1.684353 |

| | | | |
|---|---|---|---|
| 6 | -3.757538 | -1.782381 | 2.670201 |
| 6 | -4.846178 | 0.201014 | 1.825280 |
| 6 | -4.599733 | -1.760342 | 3.774961 |
| 1 | -3.010323 | -2.561258 | 2.566148 |
| 6 | -5.674067 | 0.225619 | 2.937935 |
| 1 | -4.951950 | 0.950172 | 1.045520 |
| 6 | -5.552426 | -0.756542 | 3.916516 |
| 1 | -4.507834 | -2.534930 | 4.532767 |
| 1 | -6.420700 | 1.009586 | 3.039286 |
| 1 | -6.203062 | -0.741924 | 4.788150 |
| 6 | -1.577418 | 2.798583 | -0.572914 |
| 8 | -2.651085 | 2.424419 | 0.076734 |
| 1 | -3.021029 | 1.571768 | -0.277846 |
| 1 | 0.508806 | -0.414383 | -3.263816 |
| 30 | 2.506108 | 0.481940 | 0.047655 |
| 17 | 3.909188 | 2.125891 | -0.592865 |
| 6 | -0.935780 | 4.067399 | -0.052420 |
| 17 | 0.560675 | 0.707905 | 1.248712 |
| 8 | 3.752771 | -0.600014 | 1.306802 |
| 6 | 4.939848 | -0.897761 | 1.075176 |
| 6 | 5.419260 | -1.073672 | -0.335149 |
| 1 | 6.213229 | -1.815205 | -0.445728 |
| 1 | 4.562475 | -1.378253 | -0.941994 |
| 1 | 5.762798 | -0.103846 | -0.718549 |
| 7 | 5.807102 | -1.061770 | 2.093598 |
| 6 | 5.349919 | -0.943717 | 3.468210 |
| 1 | 4.267209 | -0.825991 | 3.479730 |
| 1 | 5.628922 | -1.843935 | 4.029087 |
| 1 | 5.812140 | -0.072630 | 3.948266 |
| 6 | 7.218709 | -1.348786 | 1.922781 |
| 1 | 7.775399 | -0.845153 | 2.719860 |
| 1 | 7.427298 | -2.425357 | 1.987925 |
| 1 | 7.593537 | -0.966656 | 0.971951 |
| 6 | -1.006574 | 4.126528 | 1.472728 |
| 1 | -0.518949 | 5.046986 | 1.816046 |
| 1 | -2.040905 | 4.129914 | 1.829760 |
| 1 | -0.485843 | 3.271399 | 1.919741 |
| 6 | 0.515342 | 4.152417 | -0.513586 |
| 1 | 1.124620 | 3.349610 | -0.079229 |
| 1 | 0.603017 | 4.112405 | -1.605528 |
| 1 | 0.946650 | 5.103032 | -0.179652 |
| 6 | -1.747744 | 5.220403 | -0.664519 |
| 1 | -2.798555 | 5.177355 | -0.355249 |
| 1 | -1.328895 | 6.174977 | -0.324109 |
| 1 | -1.702627 | 5.199254 | -1.760409 |

| | | | |
|---|---|---|---|
| 1 | 0.658763 | 1.623147 | -1.823441 |

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**$(6a_1'\text{-}9)_{3s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2697.5888006
Zero-point correction= 0.526183
Thermal correction to Energy= 0.568756
Thermal correction to Enthalpy= 0.569700
Thermal correction to Gibbs Free Energy= 0.445358
Sum of electronic and zero-point Energies= -2697.062618
Sum of electronic and thermal Energies= -2697.020045
Sum of electronic and thermal Enthalpies= -2697.019101
Sum of electronic and thermal Free Energies= -2697.143442

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -2.146739 | -1.023029 | 0.899240 |
| 6 | 0.311074 | 0.035678 | 2.300143 |
| 6 | -1.068254 | 0.202284 | 2.060750 |
| 6 | 0.836119 | 0.418652 | 3.537843 |
| 6 | -1.885268 | 0.778989 | 3.043377 |
| 6 | 0.016044 | 0.932344 | 4.530747 |
| 1 | 1.905455 | 0.300937 | 3.699032 |
| 6 | -1.344820 | 1.107133 | 4.280124 |
| 1 | -2.926826 | 0.992517 | 2.812705 |
| 1 | 0.437698 | 1.218095 | 5.490464 |
| 1 | -1.990353 | 1.532049 | 5.045542 |
| 8 | -3.507641 | 1.365156 | 0.427982 |
| 6 | -2.375434 | 1.761400 | 0.087391 |
| 7 | -1.337281 | 0.889976 | 0.253426 |
| 8 | -0.070990 | 1.270981 | -0.113276 |
| 1 | 0.139582 | 0.917135 | -1.006055 |
| 6 | -2.211260 | 3.116891 | -0.503690 |
| 6 | -3.379024 | 3.686207 | -1.029591 |
| 6 | -1.024870 | 3.861308 | -0.515656 |
| 6 | -3.360790 | 4.961039 | -1.573784 |
| 1 | -4.298152 | 3.108228 | -0.997156 |
| 6 | -1.018102 | 5.145368 | -1.047050 |
| 1 | -0.110967 | 3.441694 | -0.112237 |
| 6 | -2.177852 | 5.694845 | -1.582774 |
| 1 | -4.272504 | 5.385203 | -1.987815 |
| 1 | -0.092870 | 5.715988 | -1.046703 |
| 1 | -2.160348 | 6.696273 | -2.007081 |
| 6 | 1.258351 | -0.452419 | 1.278123 |

| | | | |
|---|---|---|---|
| 8 | 2.393408 | 0.039413 | 1.147116 |
| 8 | -3.606953 | -2.337266 | -0.128119 |
| 6 | -4.628593 | -1.897455 | -0.656202 |
| 6 | -5.614306 | -2.793295 | -1.384837 |
| 8 | -4.971731 | -0.631886 | -0.664647 |
| 1 | -4.329741 | -0.030696 | -0.195027 |
| 7 | 0.883571 | -1.537320 | 0.559778 |
| 8 | 1.533352 | -1.758886 | -0.633016 |
| 1 | 2.344933 | -2.261554 | -0.437681 |
| 1 | -0.103172 | -1.815837 | 0.526741 |
| 30 | 3.355601 | 0.297019 | -0.664710 |
| 17 | 5.331623 | 1.314646 | -0.172100 |
| 17 | 2.026566 | 1.023430 | -2.341608 |
| 8 | 4.161690 | -1.670745 | -0.895902 |
| 6 | 5.403093 | -1.682672 | -1.091340 |
| 7 | 6.252577 | -1.916764 | -0.083317 |
| 6 | 7.676521 | -1.647901 | -0.188411 |
| 1 | 7.878124 | -0.597011 | 0.062045 |
| 1 | 8.215766 | -2.293235 | 0.511438 |
| 1 | 8.047341 | -1.851238 | -1.193570 |
| 6 | 5.734509 | -1.949398 | 1.277530 |
| 1 | 6.374555 | -2.591854 | 1.889421 |
| 1 | 5.722269 | -0.930651 | 1.690008 |
| 1 | 4.716281 | -2.337999 | 1.277410 |
| 6 | 5.932859 | -1.406336 | -2.464776 |
| 1 | 5.084960 | -1.368410 | -3.151492 |
| 1 | 6.424951 | -0.425611 | -2.465071 |
| 1 | 6.648412 | -2.160278 | -2.807414 |
| 6 | -7.001422 | -2.621276 | -0.759317 |
| 1 | -7.351322 | -1.587193 | -0.835017 |
| 1 | -7.716749 | -3.268017 | -1.281782 |
| 1 | -7.000156 | -2.909675 | 0.299097 |
| 6 | -5.652436 | -2.357523 | -2.854518 |
| 1 | -4.666753 | -2.457558 | -3.325460 |
| 1 | -6.353353 | -2.997738 | -3.403929 |
| 1 | -5.980314 | -1.318172 | -2.956067 |
| 6 | -5.168528 | -4.246137 | -1.283125 |
| 1 | -4.174718 | -4.391156 | -1.719641 |
| 1 | -5.126670 | -4.579805 | -0.240508 |
| 1 | -5.879451 | -4.884680 | -1.820975 |

## Pd-Zn Heterobimetallic Pathway (Pivalate as Ligand)

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**(2b-3b)$_{p\text{-}c\text{-}6}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2280.9487979
Zero-point correction= 0.405311
Thermal correction to Energy= 0.437964
Thermal correction to Enthalpy= 0.438908
Thermal correction to Gibbs Free Energy= 0.342373
Sum of electronic and zero-point Energies= -2280.543486
Sum of electronic and thermal Energies= -2280.510834
Sum of electronic and thermal Enthalpies= -2280.509889
Sum of electronic and thermal Free Energies= -2280.606425

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.553034 | 0.136261 | -1.031228 |
| 6 | -0.637951 | 2.543515 | 0.642154 |
| 6 | -1.392827 | 2.050496 | -0.453303 |
| 6 | -0.223955 | 3.866415 | 0.693081 |
| 6 | -1.709706 | 2.943551 | -1.488636 |
| 6 | -0.580114 | 4.732562 | -0.338687 |
| 1 | 0.394306 | 4.207004 | 1.520335 |
| 6 | -1.317334 | 4.275692 | -1.428945 |
| 1 | -2.274387 | 2.581211 | -2.345698 |
| 1 | -0.259947 | 5.770864 | -0.300361 |
| 1 | -1.570153 | 4.957396 | -2.236903 |
| 6 | -0.079069 | 1.572348 | 1.623557 |
| 8 | 1.145503 | 1.558178 | 1.878927 |
| 8 | -2.168490 | -1.082899 | -0.630323 |
| 6 | -3.174898 | -0.681849 | 0.013649 |
| 6 | -4.201647 | -1.717818 | 0.459190 |
| 8 | -3.349889 | 0.521123 | 0.380697 |
| 7 | -0.915003 | 0.659810 | 2.115662 |
| 1 | -1.909032 | 0.643736 | 1.892016 |
| 8 | -0.448145 | -0.448607 | 2.764311 |
| 1 | 0.193733 | -0.856836 | 2.138217 |
| 8 | 0.498676 | -1.661275 | -1.294579 |
| 6 | 1.290744 | -1.904885 | -0.347766 |
| 8 | 1.404691 | -1.153493 | 0.683215 |
| 6 | 2.223329 | -3.098831 | -0.493231 |
| 30 | 2.406778 | 0.627362 | 0.567309 |
| 17 | 4.571510 | 0.605773 | 0.915534 |
| 17 | 1.470561 | 1.306553 | -1.549262 |
| 1 | -2.347992 | 1.240912 | -0.132994 |
| 6 | 2.675371 | -3.601936 | 0.873753 |
| 1 | 3.366407 | -4.443112 | 0.740028 |

| | | | |
|---|---|---|---|
| 1 | 3.192348 | -2.819502 | 1.438684 |
| 1 | 1.827093 | -3.955461 | 1.472796 |
| 6 | 1.558449 | -4.217254 | -1.288641 |
| 1 | 2.264777 | -5.047605 | -1.408889 |
| 1 | 0.669713 | -4.600404 | -0.772147 |
| 1 | 1.252227 | -3.875194 | -2.281561 |
| 6 | 3.433354 | -2.551438 | -1.270370 |
| 1 | 3.127602 | -2.150836 | -2.244530 |
| 1 | 3.950815 | -1.759924 | -0.710946 |
| 1 | 4.151956 | -3.362796 | -1.439789 |
| 6 | -3.983473 | -3.050091 | -0.245522 |
| 1 | -4.083556 | -2.948269 | -1.331785 |
| 1 | -2.988744 | -3.457317 | -0.039261 |
| 1 | -4.733135 | -3.771460 | 0.101648 |
| 6 | -3.978824 | -1.876001 | 1.969999 |
| 1 | -4.195774 | -0.942028 | 2.501325 |
| 1 | -4.645685 | -2.654609 | 2.359553 |
| 1 | -2.944915 | -2.171914 | 2.191976 |
| 6 | -5.610464 | -1.193220 | 0.188262 |
| 1 | -6.345354 | -1.913967 | 0.567101 |
| 1 | -5.782190 | -0.230818 | 0.679575 |
| 1 | -5.788775 | -1.067910 | -0.886682 |

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**(2b-3b)$_{p\text{-}c\text{-}8}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2509.9104461
Zero-point correction= 0.470268
Thermal correction to Energy= 0.508011
Thermal correction to Enthalpy= 0.508956
Thermal correction to Gibbs Free Energy= 0.401522
Sum of electronic and zero-point Energies= -2509.440178
Sum of electronic and thermal Energies= -2509.402435
Sum of electronic and thermal Enthalpies= -2509.401490
Sum of electronic and thermal Free Energies= -2509.508924

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.292242 | 0.050511 | -1.105323 |
| 6 | 1.533918 | -2.153810 | 0.311379 |
| 6 | 1.917835 | -1.275398 | -0.748366 |
| 6 | 1.777717 | -3.510585 | 0.247327 |
| 6 | 2.506408 | -1.850937 | -1.893068 |
| 6 | 2.414613 | -4.029991 | -0.883706 |
| 1 | 1.459221 | -4.162084 | 1.057363 |

| | | | |
|---|---|---|---|
| 6 | 2.767726 | -3.211969 | -1.954105 |
| 1 | 2.784839 | -1.202707 | -2.721753 |
| 1 | 2.617482 | -5.097017 | -0.934914 |
| 1 | 3.243230 | -3.642184 | -2.831238 |
| 6 | 0.702183 | -1.598026 | 1.415102 |
| 8 | -0.363611 | -2.162170 | 1.756915 |
| 8 | 1.398233 | 1.864498 | -0.888616 |
| 6 | 1.608039 | 2.799788 | -0.104285 |
| 6 | 0.705468 | 4.012116 | -0.005200 |
| 8 | 2.613551 | 2.795785 | 0.723613 |
| 7 | 1.076194 | -0.421437 | 1.909659 |
| 1 | 1.969097 | 0.024870 | 1.670031 |
| 8 | 0.249317 | 0.286308 | 2.735205 |
| 1 | -0.577235 | 0.408324 | 2.217499 |
| 8 | -1.503543 | 1.191289 | -1.162159 |
| 6 | -2.256404 | 0.973589 | -0.177347 |
| 8 | -1.924057 | 0.216226 | 0.801298 |
| 6 | -3.652930 | 1.579525 | -0.196684 |
| 17 | -1.022466 | -1.867294 | -1.576362 |
| 1 | 2.617366 | -0.353390 | -0.272935 |
| 6 | -4.182544 | 1.762136 | 1.221972 |
| 1 | -5.192784 | 2.186910 | 1.179113 |
| 1 | -4.233460 | 0.809051 | 1.757923 |
| 1 | -3.553369 | 2.449234 | 1.802446 |
| 6 | -3.663196 | 2.906501 | -0.949164 |
| 1 | -4.685940 | 3.301495 | -0.976712 |
| 1 | -3.027061 | 3.653231 | -0.455778 |
| 1 | -3.310904 | 2.788633 | -1.978685 |
| 6 | -4.516548 | 0.549937 | -0.945603 |
| 1 | -4.143211 | 0.387535 | -1.963949 |
| 1 | -4.544563 | -0.415278 | -0.421323 |
| 1 | -5.545903 | 0.923190 | -1.011852 |
| 6 | -0.027537 | 4.234745 | -1.324325 |
| 1 | 0.677680 | 4.456375 | -2.134317 |
| 1 | -0.618294 | 3.359455 | -1.611446 |
| 1 | -0.702906 | 5.093374 | -1.222717 |
| 6 | -0.297232 | 3.662136 | 1.108679 |
| 1 | 0.208614 | 3.494983 | 2.067098 |
| 1 | -1.008732 | 4.488487 | 1.232738 |
| 1 | -0.864246 | 2.758341 | 0.852787 |
| 6 | 1.492317 | 5.259876 | 0.388015 |
| 1 | 0.804250 | 6.110288 | 0.463555 |
| 1 | 1.995874 | 5.137142 | 1.351457 |
| 1 | 2.250467 | 5.506204 | -0.364666 |
| 17 | -3.934549 | -2.817017 | 1.035136 |

| | | | |
|---|---|---|---|
| 30 | -2.026117 | -1.816974 | 0.641286 |
| 1 | 3.095817 | 1.906422 | 0.650048 |
| 8 | 3.471887 | 0.397143 | 0.560235 |
| 6 | 4.615600 | -0.253944 | 0.736889 |
| 6 | 5.674285 | 0.566760 | 1.428904 |
| 1 | 6.567315 | -0.036981 | 1.598524 |
| 1 | 5.931828 | 1.436464 | 0.813998 |
| 1 | 5.296795 | 0.949454 | 2.383192 |
| 8 | 4.789057 | -1.399761 | 0.371698 |

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**(2b-3b)$_{p\text{-}c\text{-}10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2509.9152522
Zero-point correction= 0.467527
Thermal correction to Energy= 0.505688
Thermal correction to Enthalpy= 0.506632
Thermal correction to Gibbs Free Energy= 0.397461
Sum of electronic and zero-point Energies= -2509.447725
Sum of electronic and thermal Energies= -2509.409564
Sum of electronic and thermal Enthalpies= -2509.408620
Sum of electronic and thermal Free Energies= -2509.517791

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 0.450202 | 0.271038 | -0.343121 |
| 6 | 0.492804 | -2.624053 | -0.266123 |
| 6 | 1.459725 | -1.607574 | -0.523928 |
| 6 | 0.361357 | -3.712734 | -1.109756 |
| 6 | 2.257085 | -1.730140 | -1.677931 |
| 6 | 1.194794 | -3.816234 | -2.225726 |
| 1 | -0.406833 | -4.457612 | -0.916914 |
| 6 | 2.135631 | -2.830549 | -2.516937 |
| 1 | 2.988423 | -0.951129 | -1.894899 |
| 1 | 1.088978 | -4.670241 | -2.890509 |
| 1 | 2.759409 | -2.918921 | -3.402376 |
| 6 | -0.531697 | -2.411169 | 0.801510 |
| 8 | -1.745801 | -2.599754 | 0.545444 |
| 8 | 2.081609 | 1.213063 | 0.661958 |
| 6 | 2.932880 | 1.666400 | -0.143064 |
| 6 | 2.726126 | 2.954643 | -0.924984 |
| 8 | 4.047302 | 1.058457 | -0.362928 |
| 7 | -0.123937 | -1.914684 | 1.963541 |
| 1 | 0.863203 | -1.783348 | 2.217892 |
| 8 | -1.040632 | -1.518391 | 2.894367 |

| | | | |
|---|---|---|---|
| 1 | -1.499630 | -0.755030 | 2.480612 |
| 8 | -0.820798 | 1.900825 | 0.043008 |
| 6 | -1.861806 | 1.584060 | 0.680594 |
| 8 | -2.112481 | 0.391452 | 1.066383 |
| 6 | -2.902356 | 2.671400 | 0.906196 |
| 30 | -2.785311 | -1.043713 | -0.234828 |
| 17 | -4.943220 | -1.115354 | -0.605669 |
| 17 | -1.167200 | -0.479747 | -1.939269 |
| 1 | 2.079358 | -1.297880 | 0.533798 |
| 8 | 2.577476 | -1.479733 | 1.807984 |
| 6 | 3.829571 | -1.315077 | 2.001068 |
| 8 | 4.604282 | -0.766699 | 1.193585 |
| 6 | 4.369044 | -1.824045 | 3.309406 |
| 1 | 4.054348 | -1.144748 | 4.109157 |
| 1 | 3.955512 | -2.809886 | 3.537779 |
| 1 | 5.459393 | -1.859260 | 3.284341 |
| 6 | 4.070431 | 3.614600 | -1.230800 |
| 1 | 3.894239 | 4.556050 | -1.764818 |
| 1 | 4.620540 | 3.844478 | -0.310945 |
| 1 | 4.705960 | 2.977283 | -1.852735 |
| 6 | 1.841861 | 3.912103 | -0.128959 |
| 1 | 2.319251 | 4.193455 | 0.817506 |
| 1 | 1.687989 | 4.827827 | -0.712949 |
| 1 | 0.865020 | 3.473873 | 0.094621 |
| 6 | 2.038697 | 2.578236 | -2.248432 |
| 1 | 2.622172 | 1.830678 | -2.802017 |
| 1 | 1.024327 | 2.187880 | -2.089621 |
| 1 | 1.957068 | 3.474076 | -2.876331 |
| 6 | -2.241671 | 4.040060 | 1.038758 |
| 1 | -3.013131 | 4.803808 | 1.194615 |
| 1 | -1.555760 | 4.072070 | 1.894439 |
| 1 | -1.674893 | 4.302756 | 0.139714 |
| 6 | -3.749110 | 2.360323 | 2.136266 |
| 1 | -4.507134 | 3.143044 | 2.261235 |
| 1 | -4.264324 | 1.399561 | 2.037105 |
| 1 | -3.140194 | 2.333743 | 3.048305 |
| 6 | -3.784493 | 2.635005 | -0.353837 |
| 1 | -3.194003 | 2.838157 | -1.255685 |
| 1 | -4.285876 | 1.664407 | -0.471505 |
| 1 | -4.561679 | 3.404631 | -0.270408 |
| 1 | 4.192119 | 0.218117 | 0.269853 |

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**(2b-3b)$_{p\text{-}p\text{-}s}$**$^{‡}$

---

Number of imaginary frequencies : 1

Electronic energy =-2568.604045
Zero-point correction= 0.538329
Thermal correction to Energy= 0.579118
Thermal correction to Enthalpy= 0.580062
Thermal correction to Gibbs Free Energy= 0.467526
Sum of electronic and zero-point Energies= -2568.065716
Sum of electronic and thermal Energies= -2568.024927
Sum of electronic and thermal Enthalpies= -2568.023983
Sum of electronic and thermal Free Energies= -2568.136519

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.894640 | -0.740066 | -1.139759 |
| 8 | 1.035303 | -0.965333 | -1.980382 |
| 6 | 2.024672 | -1.108140 | -1.217519 |
| 8 | 2.040079 | -0.854464 | 0.024571 |
| 6 | 3.290380 | -1.701804 | -1.832744 |
| 30 | 0.531422 | 0.146329 | 0.902907 |
| 8 | -1.030714 | -0.170212 | 2.122823 |
| 6 | -2.251469 | -0.384834 | 2.089875 |
| 7 | -3.053798 | 0.138018 | 3.038096 |
| 8 | 0.354525 | 1.883350 | -0.066303 |
| 8 | -0.922085 | 1.225016 | -1.796681 |
| 6 | -0.299795 | 2.097863 | -1.129150 |
| 6 | -0.251089 | 3.509297 | -1.705908 |
| 17 | -0.748912 | -2.956180 | -0.420692 |
| 8 | 1.852918 | 0.616047 | 2.395655 |
| 6 | 3.037648 | 0.869320 | 2.082457 |
| 7 | 4.035619 | 0.098906 | 2.543837 |
| 6 | 3.349985 | 2.029611 | 1.181838 |
| 1 | 3.714506 | 1.656034 | 0.215898 |
| 1 | 2.424238 | 2.581111 | 1.003092 |
| 1 | 4.102568 | 2.702893 | 1.603018 |
| 6 | 3.716097 | -1.113124 | 3.282657 |
| 1 | 4.474373 | -1.273585 | 4.055692 |
| 1 | 2.733951 | -1.012815 | 3.743294 |
| 1 | 3.703769 | -1.976330 | 2.603344 |
| 6 | 5.432706 | 0.251801 | 2.190016 |
| 1 | 6.045170 | 0.301787 | 3.098364 |
| 1 | 5.765560 | -0.609845 | 1.595731 |
| 1 | 5.604519 | 1.155434 | 1.605646 |
| 6 | -3.000329 | -1.129397 | 1.044818 |
| 6 | -3.976376 | -2.046888 | 1.400701 |
| 6 | -2.830680 | -0.707615 | -0.299928 |
| 6 | -4.783222 | -2.609246 | 0.408981 |

| | | | |
|---|---|---|---|
| 1 | -4.095780 | -2.345201 | 2.440800 |
| 6 | -3.702331 | -1.254270 | -1.258930 |
| 6 | -4.660417 | -2.202688 | -0.914239 |
| 1 | -5.523523 | -3.357528 | 0.681413 |
| 1 | -3.612291 | -0.929272 | -2.294454 |
| 1 | -5.308692 | -2.627906 | -1.676265 |
| 1 | -2.798274 | 0.649044 | -0.200556 |
| 17 | -3.043533 | 2.130781 | 0.425357 |
| 1 | -4.040796 | 0.248896 | 2.829406 |
| 8 | -2.548104 | 1.090060 | 3.876997 |
| 1 | -2.243843 | 1.803031 | 3.283028 |
| 6 | 4.521351 | -1.328788 | -1.013626 |
| 1 | 4.419347 | -1.664475 | 0.025187 |
| 1 | 5.413859 | -1.797422 | -1.447809 |
| 1 | 4.684515 | -0.241300 | -1.007254 |
| 6 | 3.079274 | -3.220813 | -1.792034 |
| 1 | 2.182441 | -3.503839 | -2.354580 |
| 1 | 3.947512 | -3.729389 | -2.230800 |
| 1 | 2.952755 | -3.573032 | -0.760716 |
| 6 | 3.455728 | -1.235761 | -3.275886 |
| 1 | 3.563707 | -0.145019 | -3.333291 |
| 1 | 4.354547 | -1.690077 | -3.712061 |
| 1 | 2.590825 | -1.518605 | -3.882343 |
| 6 | 1.091483 | 3.601992 | -2.443201 |
| 1 | 1.202360 | 4.597466 | -2.891691 |
| 1 | 1.929887 | 3.439584 | -1.753297 |
| 1 | 1.153243 | 2.855413 | -3.245381 |
| 6 | -0.301247 | 4.539590 | -0.580105 |
| 1 | -1.234871 | 4.448236 | -0.011901 |
| 1 | 0.535549 | 4.417172 | 0.115761 |
| 1 | -0.250695 | 5.549308 | -1.007662 |
| 6 | -1.402186 | 3.743296 | -2.677053 |
| 1 | -1.347925 | 4.766546 | -3.070482 |
| 1 | -1.363639 | 3.045518 | -3.519413 |
| 1 | -2.365724 | 3.612543 | -2.170421 |

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**(2b-3b)$_{p\text{-}c}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2280.923183
Zero-point correction= 0.404459
Thermal correction to Energy= 0.437739
Thermal correction to Enthalpy= 0.438683
Thermal correction to Gibbs Free Energy= 0.339660
Sum of electronic and zero-point Energies= -2280.518724

Sum of electronic and thermal Energies= -2280.485444
Sum of electronic and thermal Enthalpies= -2280.484500
Sum of electronic and thermal Free Energies= -2280.583524

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.515016 | -0.901975 | -0.971181 |
| 8 | 2.558809 | -0.527281 | -0.723454 |
| 6 | 2.978857 | 0.034322 | 0.326048 |
| 8 | 2.266667 | 0.510715 | 1.263639 |
| 6 | 4.495243 | 0.061772 | 0.512378 |
| 30 | 0.311794 | 0.285765 | 1.246672 |
| 8 | -1.474642 | -0.292530 | 2.047317 |
| 6 | -2.363547 | -1.001045 | 1.512141 |
| 7 | -3.517740 | -1.107578 | 2.179235 |
| 8 | -0.406518 | 2.052002 | 0.714915 |
| 8 | -2.093805 | 1.419586 | -0.633598 |
| 6 | -1.376675 | 2.292706 | -0.060771 |
| 6 | -1.676225 | 3.752496 | -0.381013 |
| 17 | 0.701329 | -2.331115 | 0.947346 |
| 6 | -2.310401 | -1.717638 | 0.213531 |
| 6 | -3.004167 | -2.914743 | 0.096644 |
| 6 | -1.663028 | -1.129050 | -0.912245 |
| 6 | -3.068846 | -3.571383 | -1.135510 |
| 1 | -3.464671 | -3.373057 | 0.970068 |
| 6 | -1.816653 | -1.784676 | -2.146669 |
| 6 | -2.494742 | -3.001696 | -2.258955 |
| 1 | -3.581404 | -4.527666 | -1.205673 |
| 1 | -1.386015 | -1.323411 | -3.033648 |
| 1 | -2.564906 | -3.499362 | -3.222865 |
| 1 | -4.388905 | -1.413049 | 1.770752 |
| 8 | -3.687355 | -0.436848 | 3.360094 |
| 1 | -2.850407 | 0.061172 | 3.442957 |
| 1 | -1.699534 | 0.206195 | -0.804471 |
| 17 | 0.460136 | 0.594273 | -2.747479 |
| 6 | -3.153236 | 3.945432 | -0.710429 |
| 1 | -3.790767 | 3.687573 | 0.144600 |
| 1 | -3.338296 | 4.997046 | -0.962846 |
| 1 | -3.457298 | 3.326008 | -1.559053 |
| 6 | -0.822848 | 4.073883 | -1.616714 |
| 1 | 0.243317 | 3.925058 | -1.409143 |
| 1 | -1.095073 | 3.430042 | -2.461114 |
| 1 | -0.979551 | 5.120554 | -1.907131 |
| 6 | -1.271265 | 4.656681 | 0.778219 |
| 1 | -1.466832 | 5.703275 | 0.513399 |

| | | | |
|---|---|---|---|
| 1 | -1.845601 | 4.426560 | 1.684618 |
| 1 | -0.208581 | 4.550837 | 1.014949 |
| 6 | 5.209095 | 0.132485 | -0.833747 |
| 1 | 4.946386 | 1.048276 | -1.376162 |
| 1 | 6.294338 | 0.131759 | -0.671663 |
| 1 | 4.951018 | -0.719116 | -1.469410 |
| 6 | 4.910319 | 1.236034 | 1.392295 |
| 1 | 4.443248 | 1.183709 | 2.380111 |
| 1 | 5.999851 | 1.225465 | 1.521354 |
| 1 | 4.632478 | 2.193650 | 0.936207 |
| 6 | 4.826522 | -1.263388 | 1.212797 |
| 1 | 4.532675 | -2.119400 | 0.593740 |
| 1 | 5.906714 | -1.321416 | 1.397176 |
| 1 | 4.306873 | -1.341747 | 2.175719 |

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**(2b-3b)$_{p\text{-}c\text{-}6\text{-}s}$‡**

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Number of imaginary frequencies : 1
Electronic energy =-2568.6207369
Zero-point correction= 0.538511
Thermal correction to Energy= 0.579496
Thermal correction to Enthalpy= 0.580440
Thermal correction to Gibbs Free Energy= 0.466607
Sum of electronic and zero-point Energies= -2568.082226
Sum of electronic and thermal Energies= -2568.041241
Sum of electronic and thermal Enthalpies= -2568.040297
Sum of electronic and thermal Free Energies= -2568.154129

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.647448 | 0.075407 | -1.085643 |
| 6 | -1.008132 | 2.576969 | 0.321053 |
| 6 | -2.111008 | 2.081659 | -0.419019 |
| 6 | -0.524604 | 3.861405 | 0.118272 |
| 6 | -2.704333 | 2.934580 | -1.362063 |
| 6 | -1.151721 | 4.689211 | -0.809680 |
| 1 | 0.357105 | 4.195154 | 0.659800 |
| 6 | -2.238158 | 4.230416 | -1.550419 |
| 1 | -3.542813 | 2.568166 | -1.951663 |
| 1 | -0.773580 | 5.695915 | -0.970673 |
| 1 | -2.706295 | 4.879933 | -2.285839 |
| 6 | -0.212455 | 1.641249 | 1.162399 |
| 8 | 1.032363 | 1.605920 | 1.073252 |
| 8 | -3.228269 | -0.948813 | -0.198860 |
| 6 | -3.875088 | -0.446780 | 0.754539 |

| | | | |
|---|---|---|---|
| 6 | -4.790876 | -1.348896 | 1.574159 |
| 8 | -3.761538 | 0.765307 | 1.129921 |
| 7 | -0.887377 | 0.795649 | 1.944161 |
| 1 | -1.904395 | 0.789024 | 2.013759 |
| 8 | -0.246542 | -0.248581 | 2.551145 |
| 1 | 0.098136 | -0.794526 | 1.807101 |
| 8 | -0.857968 | -1.821497 | -1.539694 |
| 6 | 0.179723 | -2.046980 | -0.869206 |
| 8 | 0.609053 | -1.272605 | 0.051497 |
| 6 | 1.021189 | -3.267645 | -1.216435 |
| 17 | 0.259853 | 0.989202 | -2.146296 |
| 1 | -2.954352 | 1.364936 | 0.269794 |
| 6 | 1.430037 | -3.991659 | 0.065598 |
| 1 | 2.109631 | -4.817852 | -0.180481 |
| 1 | 1.936608 | -3.310125 | 0.756856 |
| 1 | 0.558073 | -4.420167 | 0.576143 |
| 6 | 0.280048 | -4.208944 | -2.156158 |
| 1 | 0.917447 | -5.069865 | -2.394134 |
| 1 | -0.643713 | -4.581785 | -1.698928 |
| 1 | 0.009758 | -3.707474 | -3.090870 |
| 6 | 2.269789 | -2.706877 | -1.914342 |
| 1 | 2.003597 | -2.099452 | -2.789670 |
| 1 | 2.862905 | -2.083898 | -1.231478 |
| 1 | 2.906015 | -3.534213 | -2.253451 |
| 6 | -4.969242 | -2.705219 | 0.905420 |
| 1 | -5.429565 | -2.605636 | -0.083844 |
| 1 | -4.010234 | -3.216452 | 0.774885 |
| 1 | -5.618917 | -3.335228 | 1.525415 |
| 6 | -4.088776 | -1.519073 | 2.928605 |
| 1 | -3.999537 | -0.560182 | 3.451844 |
| 1 | -4.668724 | -2.202853 | 3.560406 |
| 1 | -3.083187 | -1.942948 | 2.805099 |
| 6 | -6.142864 | -0.665039 | 1.769162 |
| 1 | -6.778811 | -1.287930 | 2.410294 |
| 1 | -6.029210 | 0.316958 | 2.238408 |
| 1 | -6.661558 | -0.531096 | 0.811961 |
| 17 | 3.804369 | 0.993739 | -1.309411 |
| 8 | 3.074395 | -0.801175 | 1.232605 |
| 6 | 4.303928 | -0.627551 | 1.354676 |
| 6 | 5.252399 | -1.658111 | 0.813854 |
| 1 | 4.678701 | -2.558353 | 0.585021 |
| 1 | 5.688361 | -1.281253 | -0.120190 |
| 1 | 6.061901 | -1.910092 | 1.504953 |
| 7 | 4.804611 | 0.462110 | 1.964587 |
| 6 | 6.189148 | 0.877075 | 1.851208 |

| | | | |
|---|---|---|---|
| 1 | 6.288855 | 1.641178 | 1.067245 |
| 1 | 6.522762 | 1.304723 | 2.803356 |
| 1 | 6.842391 | 0.040751 | 1.602703 |
| 6 | 3.900899 | 1.502092 | 2.428670 |
| 1 | 4.304234 | 1.935487 | 3.350333 |
| 1 | 3.806562 | 2.292153 | 1.670738 |
| 1 | 2.911309 | 1.083572 | 2.617118 |
| 30 | 1.939312 | 0.277355 | -0.246245 |

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**(2b-3b)$_{p\text{-}c\text{-}N}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2280.9306861
Zero-point correction= 0.404781
Thermal correction to Energy= 0.437646
Thermal correction to Enthalpy= 0.438590
Thermal correction to Gibbs Free Energy= 0.340307
Sum of electronic and zero-point Energies= -2280.525905
Sum of electronic and thermal Energies= -2280.493040
Sum of electronic and thermal Enthalpies= -2280.492096
Sum of electronic and thermal Free Energies= -2280.590379

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.553932 | -0.026360 | -0.970843 |
| 6 | 0.519723 | -2.600412 | 0.417062 |
| 6 | 1.270767 | -2.065064 | -0.655605 |
| 6 | -0.053284 | -3.863334 | 0.332711 |
| 6 | 1.415704 | -2.845544 | -1.810787 |
| 6 | 0.124145 | -4.620789 | -0.824836 |
| 1 | -0.621649 | -4.279728 | 1.163571 |
| 6 | 0.852378 | -4.114188 | -1.896665 |
| 1 | 1.988603 | -2.445506 | -2.645298 |
| 1 | -0.316388 | -5.612494 | -0.888149 |
| 1 | 0.974319 | -4.708389 | -2.798377 |
| 6 | 0.283172 | -1.710139 | 1.578439 |
| 8 | 1.100571 | -1.007620 | 2.135618 |
| 8 | 2.161179 | 1.008375 | -0.261686 |
| 6 | 3.251986 | 0.438297 | 0.060143 |
| 6 | 4.305109 | 1.343757 | 0.706524 |
| 8 | 3.486434 | -0.786524 | -0.048403 |
| 7 | -1.086489 | -1.564710 | 1.923744 |
| 8 | -1.281066 | -0.805640 | 3.079399 |
| 1 | -0.404221 | -0.383040 | 3.199198 |
| 8 | -0.314715 | 1.850056 | -1.168933 |

| | | | |
|---|---|---|---|
| 6 | -1.176833 | 2.169734 | -0.307260 |
| 8 | -1.554455 | 1.426815 | 0.652550 |
| 6 | -1.875214 | 3.513204 | -0.479514 |
| 30 | -2.333916 | -0.366960 | 0.454339 |
| 17 | -4.348167 | -1.032412 | 1.041728 |
| 17 | -1.524322 | -0.993954 | -1.704198 |
| 1 | 2.284145 | -1.376518 | -0.381096 |
| 6 | -2.067597 | 4.182873 | 0.878950 |
| 1 | -2.616977 | 5.123120 | 0.746307 |
| 1 | -2.632514 | 3.543265 | 1.563102 |
| 1 | -1.103972 | 4.420341 | 1.346097 |
| 6 | -1.104642 | 4.429120 | -1.421841 |
| 1 | -1.640773 | 5.380418 | -1.527243 |
| 1 | -0.101270 | 4.642722 | -1.035406 |
| 1 | -0.992220 | 3.982833 | -2.414775 |
| 6 | -3.241502 | 3.159636 | -1.087446 |
| 1 | -3.122030 | 2.631075 | -2.042478 |
| 1 | -3.827501 | 2.527072 | -0.409023 |
| 1 | -3.810304 | 4.078500 | -1.275686 |
| 6 | 4.242209 | 2.754506 | 0.131578 |
| 1 | 4.469613 | 2.758041 | -0.941254 |
| 1 | 3.252359 | 3.199815 | 0.267661 |
| 1 | 4.983975 | 3.386813 | 0.635343 |
| 6 | 3.942010 | 1.364903 | 2.197384 |
| 1 | 3.930279 | 0.351221 | 2.616033 |
| 1 | 4.683971 | 1.959629 | 2.744965 |
| 1 | 2.953910 | 1.812714 | 2.354696 |
| 6 | 5.697451 | 0.753651 | 0.516392 |
| 1 | 6.435628 | 1.399454 | 1.008108 |
| 1 | 5.770115 | -0.249707 | 0.946206 |
| 1 | 5.960901 | 0.686794 | -0.545834 |
| 1 | -1.620695 | -2.430854 | 2.018005 |

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**(2b-3b)$_{p\text{-}c\text{-}s}$‡**

---

Number of imaginary frequencies : 1
Electronic energy =-2568.615219
Zero-point correction= 0.538214
Thermal correction to Energy= 0.579531
Thermal correction to Enthalpy= 0.580475
Thermal correction to Gibbs Free Energy= 0.465931
Sum of electronic and zero-point Energies= -2568.077005
Sum of electronic and thermal Energies= -2568.035688
Sum of electronic and thermal Enthalpies= -2568.034744
Sum of electronic and thermal Free Energies= -2568.149288

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.716564 | -1.637947 | -0.138600 |
| 8 | -1.196265 | -2.421974 | -0.011494 |
| 6 | -2.143101 | -1.593002 | 0.114475 |
| 8 | -2.061297 | -0.343077 | -0.016449 |
| 6 | -3.482001 | -2.184342 | 0.560919 |
| 30 | -0.382514 | 0.747862 | -0.578400 |
| 8 | 1.337920 | 1.772854 | -1.244198 |
| 6 | 2.517534 | 1.436424 | -1.458035 |
| 7 | 3.364507 | 2.410962 | -1.846659 |
| 8 | -0.016795 | 1.374383 | 1.298077 |
| 8 | 2.137679 | 0.844763 | 1.688219 |
| 6 | 1.016350 | 1.332104 | 2.019768 |
| 6 | 0.914837 | 1.871117 | 3.446578 |
| 17 | 0.177102 | -0.920076 | -2.385773 |
| 6 | 3.123490 | 0.091009 | -1.324142 |
| 6 | 4.175764 | -0.243728 | -2.170098 |
| 6 | 2.724440 | -0.776545 | -0.270844 |
| 6 | 4.863414 | -1.444969 | -1.993338 |
| 1 | 4.444406 | 0.413362 | -2.994989 |
| 6 | 3.492648 | -1.938258 | -0.079060 |
| 6 | 4.539920 | -2.280452 | -0.935975 |
| 1 | 5.662156 | -1.712417 | -2.681052 |
| 1 | 3.248137 | -2.584826 | 0.761231 |
| 1 | 5.092693 | -3.203252 | -0.777825 |
| 1 | 4.360622 | 2.367349 | -1.684930 |
| 8 | 2.895083 | 3.700962 | -1.886645 |
| 1 | 1.971849 | 3.592504 | -1.579049 |
| 1 | 2.253121 | -0.065084 | 0.736673 |
| 17 | 0.985019 | -2.293073 | 2.083716 |
| 8 | -1.633784 | 2.159379 | -1.341598 |
| 6 | -2.815333 | 2.232431 | -0.934269 |
| 6 | -3.101938 | 2.729665 | 0.453022 |
| 1 | -3.760012 | 3.604661 | 0.456101 |
| 1 | -3.568264 | 1.936053 | 1.048956 |
| 1 | -2.149317 | 2.986259 | 0.921273 |
| 7 | -3.824917 | 1.865647 | -1.737564 |
| 6 | -3.525964 | 1.222477 | -3.008429 |
| 1 | -2.524579 | 1.501193 | -3.335540 |
| 1 | -3.565736 | 0.130596 | -2.895435 |
| 1 | -4.263061 | 1.536611 | -3.754376 |
| 6 | -5.228069 | 1.908290 | -1.379821 |
| 1 | -5.651921 | 0.896149 | -1.405977 |

| | | | |
|---|---|---|---|
| 1 | -5.375200 | 2.313856 | -0.378701 |
| 1 | -5.779395 | 2.532287 | -2.094231 |
| 6 | -3.452896 | -2.099476 | 2.092621 |
| 1 | -3.352315 | -1.058572 | 2.426267 |
| 1 | -4.381776 | -2.510862 | 2.508646 |
| 1 | -2.606783 | -2.669816 | 2.493836 |
| 6 | -3.623074 | -3.637793 | 0.122856 |
| 1 | -4.580879 | -4.039065 | 0.478608 |
| 1 | -3.599126 | -3.728474 | -0.969716 |
| 1 | -2.814364 | -4.252982 | 0.526621 |
| 6 | -4.639597 | -1.356985 | 0.014552 |
| 1 | -4.653706 | -1.376519 | -1.084130 |
| 1 | -5.593255 | -1.766524 | 0.371757 |
| 1 | -4.565620 | -0.312508 | 0.337892 |
| 6 | 0.840217 | 0.637260 | 4.354354 |
| 1 | 1.728555 | 0.008873 | 4.230247 |
| 1 | 0.767583 | 0.952577 | 5.403496 |
| 1 | -0.035886 | 0.022312 | 4.112781 |
| 6 | -0.337127 | 2.720696 | 3.625194 |
| 1 | -0.386160 | 3.097569 | 4.654984 |
| 1 | -0.335672 | 3.584004 | 2.947239 |
| 1 | -1.242636 | 2.136459 | 3.427470 |
| 6 | 2.160186 | 2.686855 | 3.786689 |
| 1 | 2.238011 | 3.580102 | 3.153337 |
| 1 | 2.113154 | 3.019116 | 4.831675 |
| 1 | 3.067166 | 2.090987 | 3.649570 |

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**(2b-3b)$_{p\text{-}c\text{-}w}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2645.0100923
Zero-point correction= 0.562527
Thermal correction to Energy= 0.605321
Thermal correction to Enthalpy= 0.606265
Thermal correction to Gibbs Free Energy= 0.489068
Sum of electronic and zero-point Energies= -2644.447565
Sum of electronic and thermal Energies= -2644.404771
Sum of electronic and thermal Enthalpies= -2644.403827
Sum of electronic and thermal Free Energies= -2644.521025

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.656764 | 0.648956 | -0.689294 |
| 6 | -0.271498 | 3.007589 | 0.413015 |
| 6 | -1.592825 | 2.693565 | -0.012196 |

| | | | |
|---|---|---|---|
| 6 | 0.367042 | 4.158410 | -0.019881 |
| 6 | -2.216031 | 3.576917 | -0.910503 |
| 6 | -0.295563 | 5.024253 | -0.889536 |
| 1 | 1.390752 | 4.355450 | 0.288746 |
| 6 | -1.579583 | 4.735154 | -1.342961 |
| 1 | -3.216100 | 3.336790 | -1.269461 |
| 1 | 0.209269 | 5.923435 | -1.235047 |
| 1 | -2.072605 | 5.406101 | -2.042019 |
| 6 | 0.524713 | 2.004356 | 1.181740 |
| 8 | 1.701381 | 1.742132 | 0.847816 |
| 8 | -3.614120 | 0.094373 | -0.165437 |
| 6 | -3.904192 | -0.636377 | 0.818867 |
| 6 | -4.650687 | -1.943694 | 0.584006 |
| 8 | -3.609331 | -0.357964 | 2.025006 |
| 7 | -0.088735 | 1.357058 | 2.168946 |
| 1 | -1.050618 | 1.552460 | 2.470769 |
| 8 | 0.547889 | 0.323725 | 2.797890 |
| 1 | 0.576747 | -0.394046 | 2.132650 |
| 8 | -1.351304 | -1.410597 | -1.066820 |
| 6 | -0.285650 | -1.829978 | -0.538600 |
| 8 | 0.445528 | -1.134971 | 0.236265 |
| 6 | 0.195000 | -3.231229 | -0.904344 |
| 17 | 0.286965 | 1.074214 | -1.967975 |
| 1 | -2.325823 | 2.223972 | 0.964044 |
| 6 | 0.678902 | -3.949232 | 0.354417 |
| 1 | 1.131497 | -4.910875 | 0.079171 |
| 1 | 1.421686 | -3.343037 | 0.885475 |
| 1 | -0.151332 | -4.156273 | 1.042104 |
| 6 | -0.885882 | -4.037915 | -1.612535 |
| 1 | -0.488310 | -5.024316 | -1.883026 |
| 1 | -1.763875 | -4.191982 | -0.973073 |
| 1 | -1.222394 | -3.537280 | -2.526257 |
| 6 | 1.377630 | -3.010454 | -1.860005 |
| 1 | 1.092026 | -2.385879 | -2.716814 |
| 1 | 2.222012 | -2.525233 | -1.353838 |
| 1 | 1.726769 | -3.977610 | -2.243272 |
| 6 | -4.888216 | -2.175450 | -0.902125 |
| 1 | -5.505637 | -1.381999 | -1.337288 |
| 1 | -3.940600 | -2.202384 | -1.452377 |
| 1 | -5.405426 | -3.132695 | -1.045030 |
| 6 | -3.757496 | -3.057033 | 1.145753 |
| 1 | -3.616508 | -2.948501 | 2.225748 |
| 1 | -4.216119 | -4.033601 | 0.944577 |
| 1 | -2.771079 | -3.036513 | 0.662857 |
| 6 | -5.976104 | -1.909560 | 1.345895 |

| | | | |
|---|---|---|---|
| 1 | -6.487684 | -2.874163 | 1.236688 |
| 1 | -5.815296 | -1.721756 | 2.412519 |
| 1 | -6.642384 | -1.132052 | 0.951435 |
| 17 | 3.797042 | 0.085170 | -1.749043 |
| 8 | 3.069862 | -1.077633 | 1.163335 |
| 6 | 4.297210 | -1.266844 | 1.039320 |
| 6 | 4.797413 | -2.590179 | 0.535848 |
| 1 | 3.952381 | -3.280740 | 0.500116 |
| 1 | 5.185425 | -2.465281 | -0.482763 |
| 1 | 5.587838 | -3.016092 | 1.161615 |
| 7 | 5.192384 | -0.311758 | 1.349957 |
| 6 | 6.574304 | -0.360482 | 0.911179 |
| 1 | 6.667821 | 0.074071 | -0.094712 |
| 1 | 7.191135 | 0.218895 | 1.605544 |
| 1 | 6.955878 | -1.382290 | 0.891654 |
| 6 | 4.718200 | 1.007547 | 1.737448 |
| 1 | 5.384711 | 1.414069 | 2.505576 |
| 1 | 4.716117 | 1.680587 | 0.868250 |
| 1 | 3.700953 | 0.935941 | 2.125766 |
| 30 | 2.027601 | 0.066051 | -0.334547 |
| 1 | -3.224038 | 0.763014 | 2.110940 |
| 8 | -2.800908 | 1.887657 | 2.154784 |
| 1 | -3.439816 | 2.519715 | 2.498115 |

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**(2b-3b)$_{c\text{-}c}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2280.9368028
Zero-point correction= 0.404894
Thermal correction to Energy= 0.437912
Thermal correction to Enthalpy= 0.438856
Thermal correction to Gibbs Free Energy= 0.340390
Sum of electronic and zero-point Energies= -2280.531909
Sum of electronic and thermal Energies= -2280.498891
Sum of electronic and thermal Enthalpies= -2280.497947
Sum of electronic and thermal Free Energies= -2280.596413

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.239401 | 3.697845 | 0.044856 |
| 6 | 2.227314 | 4.433906 | 0.648931 |
| 6 | 1.037189 | 3.821071 | 1.042215 |
| 6 | 0.827336 | 2.468490 | 0.797208 |
| 6 | 1.880442 | 1.691117 | 0.251693 |
| 6 | 3.073166 | 2.326628 | -0.120050 |

| | | | |
|---|---|---|---|
| 1 | 4.161403 | 4.184101 | -0.262773 |
| 1 | 2.362689 | 5.497500 | 0.829415 |
| 1 | 0.291357 | 4.423401 | 1.557492 |
| 1 | 3.886675 | 1.718773 | -0.514053 |
| 6 | -0.474565 | 1.792657 | 1.089401 |
| 7 | -1.527015 | 2.602278 | 1.257253 |
| 1 | -1.486584 | 3.601652 | 1.112383 |
| 8 | -0.597710 | 0.551441 | 1.107917 |
| 8 | -2.758619 | 2.134157 | 1.592065 |
| 1 | -3.060185 | 1.569091 | 0.834529 |
| 46 | 1.344062 | 0.102542 | -1.126772 |
| 30 | -1.365976 | -0.441280 | -0.617913 |
| 17 | 0.076680 | -1.842695 | -1.928161 |
| 17 | -0.425491 | 1.444897 | -2.009404 |
| 8 | -3.317071 | 0.333402 | -0.333400 |
| 6 | -3.639841 | -0.807256 | 0.161882 |
| 8 | -2.785159 | -1.730842 | 0.181168 |
| 6 | -5.057938 | -1.034539 | 0.647955 |
| 8 | 2.833923 | -1.152533 | -0.526472 |
| 6 | 3.047203 | -1.261095 | 0.726822 |
| 8 | 2.598338 | -0.477186 | 1.593082 |
| 1 | 2.065120 | 0.604051 | 0.853365 |
| 6 | 3.842206 | -2.494518 | 1.156451 |
| 6 | 4.461250 | -2.279461 | 2.531452 |
| 1 | 4.997162 | -3.187297 | 2.835271 |
| 1 | 5.178692 | -1.450204 | 2.521484 |
| 1 | 3.699240 | -2.056260 | 3.284104 |
| 6 | 4.919379 | -2.831112 | 0.129847 |
| 1 | 5.452142 | -3.736895 | 0.445094 |
| 1 | 4.486200 | -3.007673 | -0.858810 |
| 1 | 5.655671 | -2.022633 | 0.041987 |
| 6 | 2.801974 | -3.622055 | 1.210401 |
| 1 | 2.020941 | -3.402682 | 1.948403 |
| 1 | 2.325916 | -3.761505 | 0.232832 |
| 1 | 3.293961 | -4.559431 | 1.498963 |
| 6 | -5.911036 | -1.237384 | -0.611522 |
| 1 | -5.567623 | -2.108437 | -1.183165 |
| 1 | -6.955182 | -1.410994 | -0.322604 |
| 1 | -5.873412 | -0.356708 | -1.262384 |
| 6 | -5.131917 | -2.273631 | 1.531363 |
| 1 | -6.168598 | -2.435795 | 1.851916 |
| 1 | -4.788709 | -3.164600 | 0.996737 |
| 1 | -4.509910 | -2.161356 | 2.426744 |
| 6 | -5.548182 | 0.194976 | 1.411046 |
| 1 | -4.925472 | 0.396857 | 2.292048 |

| | | | |
|---|---|---|---|
| 1 | -5.544891 | 1.087070 | 0.775538 |
| 1 | -6.575199 | 0.026692 | 1.757633 |

---

**(4b-7a$_1$)‡**

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Number of imaginary frequencies : 1
Electronic energy =-2756.7978928
Zero-point correction= 0.538768
Thermal correction to Energy= 0.582336
Thermal correction to Enthalpy= 0.583280
Thermal correction to Gibbs Free Energy= 0.460423
Sum of electronic and zero-point Energies= -2756.259125
Sum of electronic and thermal Energies= -2756.215557
Sum of electronic and thermal Enthalpies= -2756.214613
Sum of electronic and thermal Free Energies= -2756.337470

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.131877 | 0.304780 | -0.603203 |
| 6 | -1.668165 | -2.265141 | -0.455731 |
| 6 | -1.101735 | -1.305602 | -1.312455 |
| 6 | -2.561635 | -3.226581 | -0.943806 |
| 6 | -1.432807 | -1.342460 | -2.665642 |
| 6 | -2.897920 | -3.233827 | -2.290287 |
| 1 | -2.958249 | -3.981425 | -0.266378 |
| 6 | -2.329565 | -2.294552 | -3.147758 |
| 1 | -0.989847 | -0.620314 | -3.348893 |
| 1 | -3.583353 | -3.983911 | -2.675836 |
| 1 | -2.580767 | -2.306351 | -4.206096 |
| 6 | -1.260756 | -2.287214 | 0.958648 |
| 8 | -0.069043 | -2.166198 | 1.334578 |
| 7 | -2.205044 | -2.481106 | 1.883662 |
| 1 | -3.156608 | -2.161695 | 1.733841 |
| 8 | -1.843470 | -2.452824 | 3.208504 |
| 1 | -0.924811 | -2.121728 | 3.185357 |
| 30 | 1.392131 | -1.929724 | -0.098398 |
| 17 | 1.809561 | -0.268831 | -1.851879 |
| 8 | -1.866262 | 0.507656 | 0.553730 |
| 6 | -2.797024 | 1.287266 | 0.182015 |
| 7 | -2.565960 | 2.280909 | -0.653153 |
| 6 | -4.152454 | 0.991330 | 0.713659 |
| 6 | -4.648609 | -0.300742 | 0.518560 |
| 6 | -4.895787 | 1.921472 | 1.436802 |
| 6 | -5.881879 | -0.661446 | 1.048436 |
| 1 | -4.070756 | -1.000542 | -0.088108 |

| | | | |
|---|---|---|---|
| 6 | -6.117871 | 1.548565 | 1.985631 |
| 1 | -4.511475 | 2.929264 | 1.570537 |
| 6 | -6.611179 | 0.261471 | 1.794554 |
| 1 | -6.278200 | -1.659772 | 0.876373 |
| 1 | -6.691052 | 2.269667 | 2.563123 |
| 1 | -7.570354 | -0.021776 | 2.221271 |
| 8 | 0.869236 | 2.063801 | 0.134358 |
| 6 | 0.623866 | 3.169830 | -0.419881 |
| 6 | 1.682579 | 4.269010 | -0.316848 |
| 8 | -0.408837 | 3.424125 | -1.107535 |
| 8 | -3.636614 | 3.135710 | -0.906003 |
| 1 | -3.733686 | 3.118924 | -1.867266 |
| 17 | 2.302612 | -3.901611 | -0.719178 |
| 8 | 2.770684 | -1.140977 | 1.205098 |
| 6 | 3.984653 | -1.077350 | 0.981740 |
| 8 | 4.636109 | -1.982100 | 0.292208 |
| 1 | 4.028094 | -2.698612 | -0.020711 |
| 6 | 4.796765 | 0.121741 | 1.403755 |
| 6 | 2.666751 | 4.007864 | -1.464938 |
| 1 | 2.158763 | 4.070883 | -2.435165 |
| 1 | 3.467038 | 4.759239 | -1.447708 |
| 1 | 3.123734 | 3.014090 | -1.384578 |
| 6 | 1.051025 | 5.646198 | -0.491199 |
| 1 | 1.827613 | 6.419901 | -0.433162 |
| 1 | 0.543071 | 5.732359 | -1.456176 |
| 1 | 0.312338 | 5.847154 | 0.294280 |
| 6 | 2.409076 | 4.199047 | 1.023463 |
| 1 | 1.719004 | 4.378807 | 1.857149 |
| 1 | 2.874654 | 3.221539 | 1.179955 |
| 1 | 3.190616 | 4.969210 | 1.061003 |
| 6 | 4.214375 | 0.711725 | 2.684719 |
| 1 | 3.157385 | 0.966398 | 2.556611 |
| 1 | 4.302516 | 0.012609 | 3.524990 |
| 1 | 4.764181 | 1.624633 | 2.943459 |
| 6 | 4.595431 | 1.116788 | 0.246271 |
| 1 | 5.110954 | 2.056392 | 0.483920 |
| 1 | 5.001075 | 0.726065 | -0.695369 |
| 1 | 3.526310 | 1.323363 | 0.101544 |
| 6 | 6.274602 | -0.209827 | 1.573868 |
| 1 | 6.711153 | -0.600739 | 0.649803 |
| 1 | 6.817828 | 0.701146 | 1.851839 |
| 1 | 6.432067 | -0.951715 | 2.365732 |
| 1 | -1.491554 | 2.738699 | -0.882622 |

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**($6a_1$-7a)‡**

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Number of imaginary frequencies : 1
Electronic energy =-2756.8257006
Zero-point correction= 0.546929 (Hartree/Particle)
Thermal correction to Energy= 0.588238
Thermal correction to Enthalpy= 0.589183
Thermal correction to Gibbs Free Energy= 0.474380
Sum of electronic and zero-point Energies= -2756.278771
Sum of electronic and thermal Energies= -2756.237462
Sum of electronic and thermal Enthalpies= -2756.236518
Sum of electronic and thermal Free Energies= -2756.351321

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.486146 | 0.229766 | -0.603686 |
| 6 | -2.114921 | -2.160016 | 0.071296 |
| 6 | -2.061331 | -0.985739 | -0.682149 |
| 6 | -3.249341 | -2.975454 | 0.037422 |
| 6 | -3.129233 | -0.655711 | -1.510956 |
| 6 | -4.324992 | -2.623093 | -0.766722 |
| 1 | -3.273560 | -3.885502 | 0.634616 |
| 6 | -4.256118 | -1.472887 | -1.549448 |
| 1 | -3.096527 | 0.251447 | -2.111832 |
| 1 | -5.211255 | -3.251854 | -0.793196 |
| 1 | -5.092535 | -1.198786 | -2.189152 |
| 6 | -0.897544 | -2.569974 | 0.818679 |
| 8 | 0.045657 | -3.203222 | 0.275548 |
| 7 | -0.826674 | -2.186439 | 2.081947 |
| 1 | -1.497131 | -1.528918 | 2.501971 |
| 8 | 0.321544 | -2.368363 | 2.803547 |
| 1 | 1.045144 | -2.088887 | 2.204423 |
| 30 | 1.358991 | -2.420942 | -0.986982 |
| 17 | 0.434971 | -0.896930 | -2.528523 |
| 8 | 1.261726 | 1.676081 | -0.705455 |
| 6 | 1.184685 | 2.870210 | -0.414631 |
| 8 | 0.274915 | 3.357984 | 0.398817 |
| 17 | 3.243297 | -3.329371 | -1.711232 |
| 8 | 2.111318 | -1.239043 | 0.647743 |
| 6 | 3.059725 | -0.447648 | 0.653001 |
| 8 | 3.638728 | -0.025305 | -0.447879 |
| 1 | 3.215950 | -0.403745 | -1.239912 |
| 7 | -1.045134 | 1.110602 | 1.238645 |
| 1 | -0.301595 | 2.615414 | 0.745460 |
| 6 | -2.264958 | 0.789507 | 1.773310 |
| 8 | -2.353796 | 0.141139 | 2.834069 |

| | | | |
|---|---|---|---|
| 6 | -3.462030 | 1.273835 | 1.051614 |
| 6 | -3.412654 | 2.322924 | 0.128981 |
| 6 | -4.678178 | 0.643297 | 1.318651 |
| 6 | -4.566660 | 2.717451 | -0.534843 |
| 1 | -2.470828 | 2.831878 | -0.066109 |
| 6 | -5.829389 | 1.035796 | 0.649039 |
| 1 | -4.693068 | -0.165892 | 2.044671 |
| 6 | -5.774131 | 2.069982 | -0.281488 |
| 1 | -4.526630 | 3.537417 | -1.247935 |
| 1 | -6.772391 | 0.533384 | 0.850922 |
| 1 | -6.675812 | 2.379734 | -0.805116 |
| 8 | -0.011548 | 0.733650 | 2.127633 |
| 1 | -0.501146 | 0.396691 | 2.908445 |
| 6 | 3.670441 | 0.128360 | 1.911089 |
| 6 | 2.099509 | 3.915637 | -1.022797 |
| 6 | 1.248787 | 4.668691 | -2.057914 |
| 1 | 0.403040 | 5.178246 | -1.583809 |
| 1 | 1.869391 | 5.422192 | -2.557497 |
| 1 | 0.862495 | 3.985728 | -2.824766 |
| 6 | 3.275476 | 3.243042 | -1.721812 |
| 1 | 3.900584 | 2.676920 | -1.020125 |
| 1 | 2.933950 | 2.545381 | -2.494299 |
| 1 | 3.902012 | 4.007182 | -2.196670 |
| 6 | 2.590430 | 4.893525 | 0.044798 |
| 1 | 3.228383 | 5.651823 | -0.425218 |
| 1 | 1.757149 | 5.401573 | 0.539521 |
| 1 | 3.185394 | 4.386357 | 0.814419 |
| 6 | 5.191112 | -0.053006 | 1.852533 |
| 1 | 5.629075 | 0.327264 | 2.782803 |
| 1 | 5.466336 | -1.110059 | 1.757138 |
| 1 | 5.633356 | 0.493604 | 1.014180 |
| 6 | 3.319431 | 1.621470 | 1.955228 |
| 1 | 2.237264 | 1.762931 | 2.059111 |
| 1 | 3.813555 | 2.077543 | 2.821661 |
| 1 | 3.665278 | 2.133980 | 1.050009 |
| 6 | 3.102513 | -0.567354 | 3.140387 |
| 1 | 3.324968 | -1.641535 | 3.138523 |
| 1 | 3.553678 | -0.134452 | 4.040383 |
| 1 | 2.018413 | -0.430465 | 3.206325 |

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**$(7a\text{-}9)_3^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2756.7802813
Zero-point correction= 0.543145

Thermal correction to Energy= 0.586290
Thermal correction to Enthalpy= 0.587234
Thermal correction to Gibbs Free Energy= 0.466020
Sum of electronic and zero-point Energies= -2756.237136
Sum of electronic and thermal Energies= -2756.193992
Sum of electronic and thermal Enthalpies= -2756.193047
Sum of electronic and thermal Free Energies= -2756.314261

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 0.127571 | -0.053117 | -0.743825 |
| 6 | -1.245239 | -2.639715 | 0.017264 |
| 6 | -1.248642 | -1.527884 | -0.853102 |
| 6 | -1.664735 | -3.888078 | -0.476298 |
| 6 | -1.701156 | -1.692815 | -2.176843 |
| 6 | -2.086738 | -4.046780 | -1.783487 |
| 1 | -1.603334 | -4.753828 | 0.180942 |
| 6 | -2.100544 | -2.936547 | -2.632168 |
| 1 | -1.747684 | -0.825259 | -2.832325 |
| 1 | -2.390606 | -5.024525 | -2.145822 |
| 1 | -2.432496 | -3.041542 | -3.662738 |
| 8 | -2.127920 | 1.509065 | -1.708491 |
| 6 | -2.671437 | 0.857773 | -0.802509 |
| 7 | -1.884647 | 0.009617 | -0.058029 |
| 8 | -2.388246 | -0.400785 | 1.163079 |
| 1 | -1.939558 | 0.193117 | 1.810106 |
| 6 | -4.129354 | 0.928725 | -0.573283 |
| 6 | -4.781095 | 2.125967 | -0.879655 |
| 6 | -4.873996 | -0.190274 | -0.186649 |
| 6 | -6.161232 | 2.216275 | -0.765983 |
| 1 | -4.188403 | 2.976566 | -1.206929 |
| 6 | -6.256599 | -0.102122 | -0.099770 |
| 1 | -4.367835 | -1.127428 | 0.032012 |
| 6 | -6.899282 | 1.101543 | -0.377408 |
| 1 | -6.664198 | 3.154001 | -0.988786 |
| 1 | -6.837058 | -0.975385 | 0.187701 |
| 1 | -7.981669 | 1.169458 | -0.295525 |
| 6 | -0.804736 | -2.567253 | 1.419702 |
| 8 | 0.186564 | -1.952914 | 1.886447 |
| 30 | 1.073724 | -0.127032 | 1.694510 |
| 17 | 3.282936 | -0.039852 | 1.891673 |
| 17 | -0.357081 | 1.322931 | 2.717383 |
| 8 | 2.040672 | -1.126174 | -1.144150 |
| 8 | 1.401454 | 1.890864 | -0.820607 |
| 6 | 3.221285 | -0.795107 | -1.265234 |

| | | | |
|---|---|---|---|
| 6 | 0.953110 | 3.017740 | -0.573012 |
| 6 | 1.827048 | 4.133843 | -0.046626 |
| 6 | 4.329705 | -1.827257 | -1.304144 |
| 8 | 3.614397 | 0.444147 | -1.454089 |
| 1 | 2.859727 | 1.061592 | -1.311867 |
| 8 | -0.313524 | 3.307376 | -0.697690 |
| 1 | -0.839112 | 2.547206 | -1.068905 |
| 7 | -1.505057 | -3.319587 | 2.281533 |
| 1 | -2.467376 | -3.578588 | 2.117041 |
| 8 | -1.184587 | -3.290454 | 3.615826 |
| 1 | -0.459865 | -2.635226 | 3.646861 |
| 6 | 1.361580 | 5.489239 | -0.573233 |
| 1 | 2.011653 | 6.273629 | -0.168135 |
| 1 | 1.417902 | 5.537029 | -1.667535 |
| 1 | 0.332341 | 5.707758 | -0.273771 |
| 6 | 1.691429 | 4.083831 | 1.484360 |
| 1 | 0.653804 | 4.223785 | 1.806788 |
| 1 | 2.046373 | 3.124641 | 1.881436 |
| 1 | 2.305360 | 4.882343 | 1.918434 |
| 6 | 3.281029 | 3.875764 | -0.432147 |
| 1 | 3.411618 | 3.836455 | -1.521101 |
| 1 | 3.905533 | 4.690332 | -0.047776 |
| 1 | 3.651458 | 2.938413 | -0.002195 |
| 6 | 3.928470 | -3.023861 | -0.445322 |
| 1 | 3.807539 | -2.725414 | 0.603304 |
| 1 | 2.985580 | -3.462047 | -0.787704 |
| 1 | 4.711364 | -3.789920 | -0.500813 |
| 6 | 5.651177 | -1.241797 | -0.812732 |
| 1 | 5.985872 | -0.410496 | -1.441221 |
| 1 | 5.559044 | -0.877025 | 0.217026 |
| 1 | 6.420564 | -2.023337 | -0.837015 |
| 6 | 4.455050 | -2.252456 | -2.774767 |
| 1 | 5.236546 | -3.016352 | -2.867894 |
| 1 | 3.513572 | -2.676756 | -3.144239 |
| 1 | 4.730693 | -1.402943 | -3.411513 |

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**(7a-9)$_{3\text{-}s\text{-}PivOH}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2583.6509553
Zero-point correction= 0.663180
Thermal correction to Energy= 0.711854
Thermal correction to Enthalpy= 0.712798
Thermal correction to Gibbs Free Energy= 0.583121
Sum of electronic and zero-point Energies= -2582.987775

Sum of electronic and thermal Energies= -2582.939101
Sum of electronic and thermal Enthalpies= -2582.938157
Sum of electronic and thermal Free Energies= -2583.067835

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.218032 | 1.005685 | -1.425021 |
| 8 | -0.112056 | -1.111763 | -2.252684 |
| 6 | -0.887764 | -1.911041 | -1.697313 |
| 8 | -1.317123 | -1.817564 | -0.494952 |
| 30 | -1.335391 | -0.078588 | 0.497957 |
| 8 | -0.686013 | 1.575918 | 1.551112 |
| 6 | 0.275251 | 2.351273 | 1.674679 |
| 7 | 0.800357 | 2.519175 | 2.913100 |
| 8 | -3.135601 | -0.255764 | 1.471903 |
| 6 | -4.166847 | -0.022796 | 0.801457 |
| 7 | -4.788670 | 1.162401 | 0.887128 |
| 6 | -4.723984 | -1.080646 | -0.106165 |
| 1 | -4.759342 | -0.717030 | -1.139570 |
| 1 | -4.051393 | -1.940956 | -0.063237 |
| 1 | -5.733735 | -1.385384 | 0.190698 |
| 6 | -4.139510 | 2.255135 | 1.598469 |
| 1 | -4.903070 | 2.875343 | 2.078491 |
| 1 | -3.460654 | 1.852622 | 2.350126 |
| 1 | -3.555951 | 2.861441 | 0.892044 |
| 6 | -5.845730 | 1.558310 | -0.024635 |
| 1 | -6.486624 | 2.294362 | 0.470413 |
| 1 | -5.419145 | 2.011653 | -0.930925 |
| 1 | -6.466022 | 0.706516 | -0.308672 |
| 6 | 0.839744 | 3.199444 | 0.609615 |
| 6 | 0.918446 | 4.572264 | 0.867146 |
| 6 | 1.129707 | 2.703819 | -0.701650 |
| 6 | 1.228587 | 5.491992 | -0.124574 |
| 1 | 0.667442 | 4.919563 | 1.868635 |
| 6 | 1.403786 | 3.670116 | -1.708447 |
| 6 | 1.428534 | 5.024395 | -1.423526 |
| 1 | 1.266985 | 6.553831 | 0.099906 |
| 1 | 1.544442 | 3.331985 | -2.733373 |
| 1 | 1.604666 | 5.729360 | -2.234038 |
| 1 | 1.793880 | 2.713927 | 2.960117 |
| 8 | 0.405595 | 1.616747 | 3.879131 |
| 1 | 0.069020 | 0.851683 | 3.367146 |
| 7 | 2.229824 | 1.392157 | -0.891764 |
| 6 | -1.438840 | -3.069487 | -2.538201 |
| 17 | -2.292158 | 1.293773 | -1.385694 |

| | | | |
|---|---|---|---|
| 8 | -0.215157 | -1.035517 | 2.129017 |
| 6 | 0.578430 | -1.974520 | 2.206110 |
| 6 | 0.173490 | -3.431176 | 2.292162 |
| 8 | 1.876830 | -1.779445 | 2.222848 |
| 1 | 2.060532 | -0.819551 | 2.022718 |
| 6 | 2.736160 | 0.628948 | 0.124854 |
| 8 | 2.211139 | 0.672649 | 1.251289 |
| 6 | 3.888159 | -0.269618 | -0.134343 |
| 6 | 3.976296 | -1.049326 | -1.291769 |
| 6 | 4.822597 | -0.435875 | 0.890876 |
| 6 | 5.005604 | -1.972566 | -1.420632 |
| 1 | 3.224755 | -0.944823 | -2.070469 |
| 6 | 5.864837 | -1.340889 | 0.744605 |
| 1 | 4.720514 | 0.153275 | 1.799848 |
| 6 | 5.955522 | -2.110500 | -0.411768 |
| 1 | 5.064801 | -2.589831 | -2.313604 |
| 1 | 6.601082 | -1.454799 | 1.536463 |
| 1 | 6.764190 | -2.829238 | -0.523431 |
| 8 | 3.046598 | 1.517173 | -2.009084 |
| 1 | 3.384750 | 2.428958 | -1.952167 |
| 6 | -2.491132 | -2.426576 | -3.450116 |
| 1 | -2.938198 | -3.182987 | -4.108760 |
| 1 | -3.294003 | -1.970026 | -2.854869 |
| 1 | -2.041594 | -1.638415 | -4.063842 |
| 6 | -2.094570 | -4.149222 | -1.685685 |
| 1 | -2.497596 | -4.939211 | -2.333471 |
| 1 | -1.379957 | -4.612922 | -0.993957 |
| 1 | -2.917320 | -3.743808 | -1.085925 |
| 6 | -0.320495 | -3.674223 | -3.382849 |
| 1 | 0.447322 | -4.137302 | -2.748617 |
| 1 | -0.723173 | -4.452063 | -4.044844 |
| 1 | 0.163198 | -2.906326 | -3.993705 |
| 6 | -1.345242 | -3.549821 | 2.325343 |
| 1 | -1.792979 | -3.101031 | 1.432230 |
| 1 | -1.624055 | -4.610442 | 2.364790 |
| 1 | -1.765707 | -3.050496 | 3.206052 |
| 6 | 0.785111 | -4.045035 | 3.555945 |
| 1 | 0.503545 | -5.103575 | 3.612629 |
| 1 | 1.877719 | -3.978576 | 3.550160 |
| 1 | 0.411707 | -3.551003 | 4.461495 |
| 6 | 0.736176 | -4.134284 | 1.049441 |
| 1 | 0.421457 | -5.185739 | 1.055258 |
| 1 | 0.348875 | -3.663795 | 0.137472 |
| 1 | 1.830348 | -4.097343 | 1.027760 |

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**(7a-9)$_5^‡$**

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Number of imaginary frequencies : 1
Electronic energy =-2756.7731236
Zero-point correction= 0.542977
Thermal correction to Energy= 0.586208
Thermal correction to Enthalpy= 0.587153
Thermal correction to Gibbs Free Energy= 0.464001
Sum of electronic and zero-point Energies= -2756.230146
Sum of electronic and thermal Energies= -2756.186915
Sum of electronic and thermal Enthalpies= -2756.185971
Sum of electronic and thermal Free Energies= -2756.309122

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| 46 | 0.744208 | 0.151081 | 1.182709 |
| 6 | 0.214204 | -2.781694 | 0.551453 |
| 6 | 1.061439 | -1.827103 | 1.172046 |
| 6 | 0.026666 | -4.049387 | 1.137735 |
| 6 | 1.750373 | -2.227768 | 2.341253 |
| 6 | 0.646755 | -4.388352 | 2.320405 |
| 1 | -0.669416 | -4.744920 | 0.666403 |
| 6 | 1.526839 | -3.464502 | 2.908689 |
| 1 | 2.462635 | -1.537979 | 2.791689 |
| 1 | 0.463708 | -5.352151 | 2.786690 |
| 1 | 2.047974 | -3.726761 | 3.827519 |
| 6 | -0.370795 | -2.508818 | -0.750408 |
| 8 | -0.961947 | -1.477384 | -1.124001 |
| 8 | 0.412851 | 2.413305 | 1.253517 |
| 6 | 0.850200 | 3.253098 | 0.471356 |
| 6 | 0.316247 | 4.672309 | 0.419949 |
| 8 | 1.855097 | 3.032533 | -0.350880 |
| 7 | -0.306414 | -3.517580 | -1.689961 |
| 1 | -0.558665 | -3.212071 | -2.626057 |
| 8 | 0.851752 | -4.291630 | -1.730088 |
| 1 | 0.607349 | -5.144114 | -1.344277 |
| 17 | -1.532610 | -0.076337 | 2.187933 |
| 8 | 2.648016 | 0.556921 | 0.307709 |
| 6 | 3.175810 | -0.460660 | -0.277897 |
| 7 | 2.469143 | -1.570762 | -0.277149 |
| 8 | 3.132581 | -2.748003 | -0.588087 |
| 1 | 2.429554 | -3.315432 | -0.952524 |
| 6 | 4.508320 | -0.263333 | -0.896183 |
| 6 | 5.020510 | -1.091003 | -1.901524 |
| 6 | 5.253439 | 0.847094 | -0.481303 |

| | | | |
|---|---|---|---|
| 6 | 6.255297 | -0.810419 | -2.471706 |
| 1 | 4.447684 | -1.952218 | -2.226280 |
| 6 | 6.491709 | 1.116630 | -1.046936 |
| 1 | 4.846832 | 1.493285 | 0.291791 |
| 6 | 6.995677 | 0.287774 | -2.044324 |
| 1 | 6.642437 | -1.456070 | -3.256503 |
| 1 | 7.063424 | 1.978360 | -0.710864 |
| 1 | 7.965303 | 0.497770 | -2.490447 |
| 30 | -1.710669 | 0.122618 | -0.109888 |
| 17 | -1.710321 | 1.961865 | -1.458227 |
| 8 | -3.704122 | -0.491531 | -0.368203 |
| 6 | -4.694925 | -0.017389 | -0.927341 |
| 8 | -4.668733 | 1.074710 | -1.651592 |
| 1 | -3.753044 | 1.455651 | -1.678549 |
| 6 | -6.071206 | -0.636811 | -0.802884 |
| 1 | 2.212441 | 2.117245 | -0.214264 |
| 6 | 0.159377 | 5.133821 | -1.029547 |
| 1 | -0.533144 | 4.483091 | -1.576662 |
| 1 | -0.244779 | 6.153978 | -1.038720 |
| 1 | 1.118125 | 5.138443 | -1.556968 |
| 6 | -1.022407 | 4.740538 | 1.144889 |
| 1 | -1.759963 | 4.088999 | 0.661688 |
| 1 | -0.927914 | 4.423734 | 2.188397 |
| 1 | -1.397802 | 5.771178 | 1.122980 |
| 6 | 1.348045 | 5.554046 | 1.136842 |
| 1 | 2.321113 | 5.514548 | 0.634481 |
| 1 | 1.001518 | 6.594984 | 1.137350 |
| 1 | 1.480062 | 5.240703 | 2.180152 |
| 6 | -6.910198 | 0.313232 | 0.063435 |
| 1 | -6.465887 | 0.440139 | 1.058165 |
| 1 | -7.007708 | 1.298884 | -0.403521 |
| 1 | -7.913584 | -0.109859 | 0.193210 |
| 6 | -5.968567 | -2.000502 | -0.131746 |
| 1 | -6.971131 | -2.432210 | -0.029152 |
| 1 | -5.357152 | -2.691307 | -0.723326 |
| 1 | -5.520140 | -1.925399 | 0.863943 |
| 6 | -6.705262 | -0.769464 | -2.189288 |
| 1 | -6.109546 | -1.420510 | -2.840680 |
| 1 | -7.701515 | -1.216548 | -2.088594 |
| 1 | -6.810790 | 0.203325 | -2.679073 |

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**(7a-9)$_7^‡$**

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Number of imaginary frequencies : 1
Electronic energy =-2756.7823715

Zero-point correction= 0.543859
Thermal correction to Energy= 0.586479
Thermal correction to Enthalpy= 0.587423
Thermal correction to Gibbs Free Energy= 0.468864
Sum of electronic and zero-point Energies= -2756.238513
Sum of electronic and thermal Energies= -2756.195893
Sum of electronic and thermal Enthalpies= -2756.194948
Sum of electronic and thermal Free Energies= -2756.313508

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 0.376131 | 0.158997 | -1.167754 |
| 6 | 0.549376 | -2.832511 | -0.889556 |
| 6 | -0.210194 | -1.748624 | -1.397432 |
| 6 | 0.677054 | -3.999595 | -1.670285 |
| 6 | -0.808118 | -1.884779 | -2.671966 |
| 6 | 0.112747 | -4.104725 | -2.923516 |
| 1 | 1.201713 | -4.856192 | -1.250684 |
| 6 | -0.621997 | -3.024308 | -3.427861 |
| 1 | -1.428302 | -1.074795 | -3.050569 |
| 1 | 0.211918 | -5.022678 | -3.495308 |
| 1 | -1.080877 | -3.089353 | -4.412321 |
| 8 | -1.795522 | 0.649857 | -1.176347 |
| 6 | -2.424685 | -0.255904 | -0.570280 |
| 7 | -1.687789 | -1.322558 | -0.149839 |
| 8 | -2.398431 | -2.476347 | 0.136870 |
| 1 | -2.389194 | -2.544628 | 1.120369 |
| 6 | -3.851253 | -0.065529 | -0.248160 |
| 6 | -4.227972 | 1.223394 | 0.151446 |
| 6 | -4.811266 | -1.079283 | -0.328076 |
| 6 | -5.547551 | 1.489345 | 0.484525 |
| 1 | -3.471728 | 2.002079 | 0.227664 |
| 6 | -6.136133 | -0.793350 | -0.022417 |
| 1 | -4.518567 | -2.076486 | -0.636762 |
| 6 | -6.504767 | 0.482563 | 0.390685 |
| 1 | -5.830015 | 2.484996 | 0.816560 |
| 1 | -6.884364 | -1.578109 | -0.100475 |
| 1 | -7.541159 | 0.693552 | 0.643711 |
| 6 | 1.240222 | -2.760063 | 0.391931 |
| 8 | 0.955140 | -2.020600 | 1.368150 |
| 30 | -0.539257 | -0.674614 | 1.665192 |
| 17 | 0.203280 | 1.439986 | 1.842347 |
| 17 | -1.995854 | -1.668696 | 3.093096 |
| 8 | 2.546370 | -0.348446 | -0.758379 |
| 8 | 0.814266 | 2.512095 | -1.165064 |

| | | | |
|---|---|---|---|
| 6 | 3.384067 | 0.436206 | -0.309115 |
| 6 | 0.044253 | 3.396060 | -0.778582 |
| 6 | 0.499074 | 4.740260 | -0.249089 |
| 6 | 4.637277 | -0.038666 | 0.401027 |
| 8 | 3.260261 | 1.741197 | -0.333666 |
| 1 | 2.377741 | 2.034624 | -0.673808 |
| 8 | -1.259793 | 3.273123 | -0.846573 |
| 1 | -1.514011 | 2.356233 | -1.110068 |
| 7 | 2.260756 | -3.624314 | 0.589494 |
| 1 | 2.843149 | -3.943932 | -0.171221 |
| 8 | 2.975356 | -3.527557 | 1.764954 |
| 1 | 2.425813 | -2.912376 | 2.290402 |
| 6 | 5.780566 | 0.961570 | 0.249560 |
| 1 | 6.071866 | 1.081314 | -0.800970 |
| 1 | 5.509591 | 1.945860 | 0.641612 |
| 1 | 6.654615 | 0.597408 | 0.802732 |
| 6 | 4.231320 | -0.152836 | 1.879463 |
| 1 | 3.384728 | -0.840380 | 1.995403 |
| 1 | 5.076748 | -0.542104 | 2.459881 |
| 1 | 3.941626 | 0.820275 | 2.292319 |
| 6 | 5.060235 | -1.404691 | -0.126437 |
| 1 | 4.287885 | -2.155077 | 0.061286 |
| 1 | 5.268182 | -1.372957 | -1.202532 |
| 1 | 5.972506 | -1.726050 | 0.389638 |
| 6 | 2.001578 | 4.727394 | -0.001687 |
| 1 | 2.275794 | 3.989583 | 0.761375 |
| 1 | 2.562209 | 4.501694 | -0.916273 |
| 1 | 2.318101 | 5.714568 | 0.354541 |
| 6 | 0.152399 | 5.787365 | -1.316871 |
| 1 | -0.924205 | 5.814988 | -1.514694 |
| 1 | 0.464120 | 6.777836 | -0.964218 |
| 1 | 0.675840 | 5.584514 | -2.259666 |
| 6 | -0.244498 | 5.054610 | 1.052533 |
| 1 | -1.322348 | 5.145031 | 0.888186 |
| 1 | -0.076915 | 4.274023 | 1.804554 |
| 1 | 0.124664 | 6.007291 | 1.451545 |

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**(7a-9)$_{p\text{-}p\text{-}s}$‡**

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Number of imaginary frequencies : 1
Electronic energy =-2122.8489307
Zero-point correction= 0.651907
Thermal correction to Energy= 0.697153
Thermal correction to Enthalpy= 0.698098
Thermal correction to Gibbs Free Energy= 0.577542

Sum of electronic and zero-point Energies= -2122.197023
Sum of electronic and thermal Energies= -2122.151777
Sum of electronic and thermal Enthalpies= -2122.150833
Sum of electronic and thermal Free Energies= -2122.271388

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.944665 | 0.610903 | -1.467456 |
| 8 | 0.172338 | -1.534609 | -2.109774 |
| 6 | -0.807243 | -1.876344 | -1.423433 |
| 8 | -1.037729 | -1.511698 | -0.215074 |
| 6 | -1.824241 | -2.841550 | -2.048640 |
| 30 | 0.245067 | -0.374828 | 0.856332 |
| 8 | 1.254876 | 1.051091 | 2.149088 |
| 6 | 2.208693 | 1.604268 | 1.551257 |
| 7 | 3.472054 | 1.225816 | 1.814455 |
| 8 | 2.016072 | -1.416813 | 0.888063 |
| 8 | 2.848787 | -0.389727 | -0.931553 |
| 6 | 2.877233 | -1.277526 | -0.050839 |
| 6 | 4.057908 | -2.252832 | -0.089490 |
| 8 | -0.916329 | -0.786315 | 2.497479 |
| 6 | -1.702517 | -1.758940 | 2.476118 |
| 7 | -3.029918 | -1.564507 | 2.499694 |
| 6 | -1.161679 | -3.160808 | 2.450699 |
| 1 | -1.557002 | -3.724933 | 1.599109 |
| 1 | -0.075094 | -3.101144 | 2.356533 |
| 1 | -1.405898 | -3.702139 | 3.371756 |
| 6 | -3.577393 | -0.222282 | 2.384396 |
| 1 | -4.178035 | -0.145804 | 1.467790 |
| 1 | -4.220289 | -0.005096 | 3.246063 |
| 1 | -2.766439 | 0.505984 | 2.345250 |
| 6 | -4.010710 | -2.629385 | 2.451782 |
| 1 | -4.815878 | -2.412728 | 3.163353 |
| 1 | -4.447383 | -2.705351 | 1.446070 |
| 1 | -3.572430 | -3.591756 | 2.717635 |
| 6 | 2.035017 | 2.624154 | 0.512347 |
| 6 | 2.832126 | 3.776791 | 0.519505 |
| 6 | 1.082132 | 2.418645 | -0.523871 |
| 6 | 2.664950 | 4.767879 | -0.431569 |
| 1 | 3.566169 | 3.896294 | 1.316126 |
| 6 | 0.886147 | 3.468842 | -1.448939 |
| 6 | 1.678458 | 4.602394 | -1.410165 |
| 1 | 3.272503 | 5.667846 | -0.403333 |
| 1 | 0.123917 | 3.356289 | -2.217289 |
| 1 | 1.524326 | 5.377468 | -2.158921 |

| | | | |
|---|---|---|---|
| 1 | 4.199169 | 1.381673 | 1.124426 |
| 8 | 3.704416 | 0.168216 | 2.656347 |
| 1 | 3.080811 | -0.528644 | 2.352180 |
| 7 | -0.592588 | 1.822360 | 0.285903 |
| 6 | -1.548921 | 1.670791 | -0.669559 |
| 8 | -0.953892 | 2.521197 | 1.433516 |
| 1 | -0.335621 | 2.136104 | 2.086387 |
| 8 | -1.158438 | 1.257402 | -1.785615 |
| 6 | -2.999455 | 1.844810 | -0.433687 |
| 6 | -3.564694 | 2.789401 | 0.428239 |
| 6 | -3.834776 | 0.975898 | -1.147869 |
| 6 | -4.947057 | 2.846428 | 0.577278 |
| 1 | -2.925832 | 3.474389 | 0.973521 |
| 6 | -5.210555 | 1.020259 | -0.974152 |
| 1 | -3.376131 | 0.267602 | -1.834256 |
| 6 | -5.770154 | 1.959375 | -0.109703 |
| 1 | -5.382782 | 3.591174 | 1.239235 |
| 1 | -5.847335 | 0.330451 | -1.523616 |
| 1 | -6.849077 | 2.005518 | 0.020890 |
| 6 | -3.095099 | -2.957824 | -1.213434 |
| 1 | -2.890240 | -3.386155 | -0.223647 |
| 1 | -3.564803 | -1.976508 | -1.058727 |
| 1 | -3.817074 | -3.611105 | -1.721822 |
| 6 | -2.169688 | -2.341707 | -3.450635 |
| 1 | -1.266796 | -2.252911 | -4.061413 |
| 1 | -2.866723 | -3.033987 | -3.941252 |
| 1 | -2.642568 | -1.350823 | -3.412861 |
| 6 | -1.142649 | -4.209286 | -2.141147 |
| 1 | -0.235058 | -4.148449 | -2.751048 |
| 1 | -0.861677 | -4.576661 | -1.144076 |
| 1 | -1.821436 | -4.944225 | -2.593927 |
| 6 | 5.353999 | -1.443208 | -0.003533 |
| 1 | 5.410981 | -0.709266 | -0.814353 |
| 1 | 5.420697 | -0.918502 | 0.959558 |
| 1 | 6.220682 | -2.112230 | -0.078716 |
| 6 | 4.002572 | -3.261076 | 1.051146 |
| 1 | 3.074354 | -3.842396 | 1.027358 |
| 1 | 4.847353 | -3.957132 | 0.968168 |
| 1 | 4.068745 | -2.772302 | 2.030640 |
| 6 | 3.988300 | -2.983540 | -1.433605 |
| 1 | 4.817654 | -3.698086 | -1.513804 |
| 1 | 3.047392 | -3.540362 | -1.530797 |
| 1 | 4.048415 | -2.276201 | -2.266349 |

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**(7a-9)$_{p\text{-}c\text{-}3\text{-}PivoH}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2295.972946
Zero-point correction= 0.530463
Thermal correction to Energy= 0.570797
Thermal correction to Enthalpy= 0.571741
Thermal correction to Gibbs Free Energy= 0.456890
Sum of electronic and zero-point Energies= -2295.442483
Sum of electronic and thermal Energies= -2295.402149
Sum of electronic and thermal Enthalpies= -2295.401205
Sum of electronic and thermal Free Energies= -2295.516056

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.838638 | -0.528935 | -1.761964 |
| 8 | -0.011726 | 1.596085 | -2.326925 |
| 6 | 0.827002 | 2.120222 | -1.587790 |
| 8 | 1.664107 | 1.449431 | -0.856507 |
| 30 | 1.666649 | -0.552291 | -0.896648 |
| 8 | 1.004140 | -1.264877 | 0.888034 |
| 6 | -0.059151 | -1.733805 | 1.329572 |
| 7 | -0.271528 | -1.708942 | 2.668397 |
| 6 | -1.115852 | -2.436194 | 0.566976 |
| 6 | -1.416125 | -3.737973 | 0.982958 |
| 6 | -1.780453 | -1.887079 | -0.577251 |
| 6 | -2.308168 | -4.547422 | 0.293124 |
| 1 | -0.885530 | -4.135833 | 1.846969 |
| 6 | -2.670305 | -2.744517 | -1.279993 |
| 6 | -2.905530 | -4.044638 | -0.860429 |
| 1 | -2.499883 | -5.563206 | 0.625281 |
| 1 | -3.106283 | -2.394243 | -2.214445 |
| 1 | -3.559696 | -4.678404 | -1.456213 |
| 1 | -1.229464 | -1.734743 | 2.999066 |
| 8 | 0.554930 | -0.929915 | 3.437667 |
| 1 | 0.558771 | -0.063696 | 2.989634 |
| 7 | -2.480776 | -0.308247 | -0.413923 |
| 6 | 0.862904 | 3.638156 | -1.425809 |
| 17 | 1.202428 | -1.742443 | -2.790157 |
| 6 | -2.291394 | 0.478391 | 0.704551 |
| 8 | -1.157830 | 0.579022 | 1.177069 |
| 6 | -3.435779 | 1.185075 | 1.346624 |
| 6 | -4.724717 | 0.658709 | 1.470045 |
| 6 | -3.136279 | 2.403133 | 1.965230 |
| 6 | -5.695186 | 1.346931 | 2.186299 |
| 1 | -4.971185 | -0.297552 | 1.019361 |

| | | | |
|---|---|---|---|
| 6 | -4.115578 | 3.103612 | 2.655661 |
| 1 | -2.120766 | 2.785684 | 1.897121 |
| 6 | -5.398059 | 2.575915 | 2.768243 |
| 1 | -6.691049 | 0.922142 | 2.287355 |
| 1 | -3.875271 | 4.059278 | 3.115198 |
| 1 | -6.165939 | 3.118579 | 3.314612 |
| 8 | -3.715945 | -0.223626 | -1.033801 |
| 1 | -4.108402 | -1.111347 | -0.919516 |
| 6 | 0.035344 | 3.923448 | -0.165008 |
| 1 | -0.978859 | 3.515913 | -0.273782 |
| 1 | 0.495926 | 3.469788 | 0.721626 |
| 1 | -0.040072 | 5.006193 | -0.001723 |
| 6 | 2.286426 | 4.157618 | -1.243384 |
| 1 | 2.764359 | 3.751355 | -0.345248 |
| 1 | 2.916008 | 3.909176 | -2.106484 |
| 1 | 2.269783 | 5.250419 | -1.144578 |
| 6 | 0.213082 | 4.313306 | -2.628107 |
| 1 | -0.816438 | 3.970855 | -2.766194 |
| 1 | 0.206246 | 5.401186 | -2.483880 |
| 1 | 0.762882 | 4.093576 | -3.550726 |
| 8 | 3.573819 | -0.599904 | -0.084914 |
| 6 | 3.918306 | 0.130727 | 0.852019 |
| 6 | 4.904449 | -0.321410 | 1.904501 |
| 8 | 3.423444 | 1.326550 | 1.053103 |
| 1 | 2.757751 | 1.559725 | 0.339938 |
| 6 | 5.579191 | -1.614915 | 1.466961 |
| 1 | 6.276548 | -1.942921 | 2.246787 |
| 1 | 4.845448 | -2.409747 | 1.300223 |
| 1 | 6.142608 | -1.478693 | 0.537078 |
| 6 | 4.067440 | -0.569451 | 3.170254 |
| 1 | 3.629643 | 0.363202 | 3.543456 |
| 1 | 3.250681 | -1.277717 | 2.981386 |
| 1 | 4.713031 | -0.986183 | 3.952702 |
| 6 | 5.946145 | 0.765257 | 2.169324 |
| 1 | 6.630145 | 0.424368 | 2.955873 |
| 1 | 6.543686 | 0.974073 | 1.273663 |
| 1 | 5.482254 | 1.699634 | 2.499345 |

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**(7a-9)$_{c\text{-3-PivOH}}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2756.7755854
Zero-point correction= 0.542938
Thermal correction to Energy= 0.585673
Thermal correction to Enthalpy= 0.586617

Thermal correction to Gibbs Free Energy= 0.467981
Sum of electronic and zero-point Energies= -2756.232647
Sum of electronic and thermal Energies= -2756.189912
Sum of electronic and thermal Enthalpies= -2756.188968
Sum of electronic and thermal Free Energies= -2756.307605

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.299846 | 0.211962 | -1.494448 |
| 8 | 1.553086 | -1.298521 | -1.738943 |
| 6 | 2.666921 | -0.873699 | -1.987358 |
| 8 | 2.917088 | 0.406817 | -2.276269 |
| 30 | -2.259708 | -1.664317 | -0.440120 |
| 8 | -2.638432 | -0.038851 | 0.742076 |
| 6 | -2.678833 | 1.206145 | 0.782037 |
| 7 | -3.147405 | 1.777814 | 1.913556 |
| 6 | -2.359366 | 2.141538 | -0.310844 |
| 6 | -3.310832 | 3.132214 | -0.589257 |
| 6 | -1.211871 | 2.013909 | -1.148986 |
| 6 | -3.191122 | 3.986408 | -1.674501 |
| 1 | -4.193578 | 3.183547 | 0.045958 |
| 6 | -1.123663 | 2.881264 | -2.267957 |
| 6 | -2.102082 | 3.827265 | -2.528940 |
| 1 | -3.953472 | 4.733493 | -1.873545 |
| 1 | -0.302486 | 2.757088 | -2.971335 |
| 1 | -2.013633 | 4.444288 | -3.420853 |
| 1 | -2.752985 | 2.672411 | 2.179092 |
| 8 | -3.344964 | 0.962678 | 3.004993 |
| 1 | -2.855353 | 0.148168 | 2.780242 |
| 7 | 0.398787 | 1.872358 | -0.420186 |
| 6 | 3.929962 | -1.712759 | -1.962020 |
| 17 | -1.856069 | -1.365633 | -2.667990 |
| 8 | -0.529849 | -2.059946 | 0.675524 |
| 6 | -0.485833 | -2.152072 | 1.903843 |
| 6 | 0.791246 | -1.951375 | 2.690286 |
| 8 | -1.528713 | -2.461517 | 2.644005 |
| 1 | -2.299860 | -2.722993 | 2.074389 |
| 6 | 0.586733 | 1.798241 | 0.948569 |
| 8 | -0.335943 | 1.402092 | 1.657583 |
| 6 | 1.905795 | 2.142128 | 1.551324 |
| 6 | 3.132884 | 1.853642 | 0.944409 |
| 6 | 1.884958 | 2.608199 | 2.869243 |
| 6 | 4.315880 | 2.044348 | 1.646641 |
| 1 | 3.167118 | 1.452517 | -0.065058 |
| 6 | 3.070643 | 2.822813 | 3.558261 |

| | | | |
|---|---|---|---|
| 1 | 0.923119 | 2.785049 | 3.345019 |
| 6 | 4.289118 | 2.539132 | 2.947283 |
| 1 | 5.264562 | 1.801012 | 1.173238 |
| 1 | 3.044582 | 3.199266 | 4.577886 |
| 1 | 5.219088 | 2.694400 | 3.489459 |
| 8 | 1.367354 | 2.582044 | -1.134334 |
| 1 | 0.943256 | 3.433648 | -1.347974 |
| 1 | 2.099833 | 0.939140 | -2.200433 |
| 17 | -3.660979 | -3.190309 | 0.487554 |
| 6 | 1.169753 | -3.300031 | 3.316437 |
| 1 | 1.322517 | -4.069310 | 2.549449 |
| 1 | 2.108425 | -3.186162 | 3.872228 |
| 1 | 0.397535 | -3.649258 | 4.009551 |
| 6 | 0.547006 | -0.918860 | 3.797073 |
| 1 | 1.487213 | -0.748193 | 4.336667 |
| 1 | 0.211738 | 0.038757 | 3.379763 |
| 1 | -0.199924 | -1.276520 | 4.513573 |
| 6 | 1.897273 | -1.488117 | 1.749116 |
| 1 | 2.795581 | -1.239958 | 2.330249 |
| 1 | 2.145937 | -2.267818 | 1.018889 |
| 1 | 1.598581 | -0.602068 | 1.178097 |
| 6 | 3.567606 | -3.175648 | -1.741426 |
| 1 | 4.481820 | -3.781019 | -1.729056 |
| 1 | 3.042244 | -3.323246 | -0.791836 |
| 1 | 2.915455 | -3.548182 | -2.538563 |
| 6 | 4.685111 | -1.552664 | -3.284010 |
| 1 | 4.969133 | -0.511450 | -3.465114 |
| 1 | 5.598518 | -2.159343 | -3.255568 |
| 1 | 4.080404 | -1.897866 | -4.131289 |
| 6 | 4.795020 | -1.197567 | -0.803147 |
| 1 | 4.250007 | -1.230052 | 0.150660 |
| 1 | 5.686346 | -1.829284 | -0.705945 |
| 1 | 5.121717 | -0.166092 | -0.979353 |

---

**(7a-9)$_{c\text{-}3\text{-}S\text{-}PivOH}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2697.5907197
Zero-point correction= 0.526629
Thermal correction to Energy= 0.569077
Thermal correction to Enthalpy= 0.570021
Thermal correction to Gibbs Free Energy= 0.450011
Sum of electronic and zero-point Energies= -2697.064091
Sum of electronic and thermal Energies= -2697.021642
Sum of electronic and thermal Enthalpies= -2697.020698

Sum of electronic and thermal Free Energies= -2697.140708

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.603808 | 0.292004 | -1.375745 |
| 30 | -1.432897 | 0.123894 | 0.264386 |
| 8 | -0.509117 | 1.161265 | 1.684791 |
| 6 | 0.270247 | 2.132803 | 1.602553 |
| 7 | 0.792635 | 2.646959 | 2.740072 |
| 6 | 0.653866 | 2.853646 | 0.376709 |
| 6 | 0.533554 | 4.251593 | 0.383401 |
| 6 | 1.125412 | 2.185204 | -0.790067 |
| 6 | 0.832508 | 5.013391 | -0.733520 |
| 1 | 0.148563 | 4.731925 | 1.282162 |
| 6 | 1.439031 | 2.989093 | -1.914538 |
| 6 | 1.270771 | 4.361361 | -1.889297 |
| 1 | 0.706063 | 6.091838 | -0.715042 |
| 1 | 1.780998 | 2.500990 | -2.825520 |
| 1 | 1.482150 | 4.935349 | -2.789605 |
| 1 | 1.669537 | 3.147879 | 2.649606 |
| 8 | 0.712335 | 1.890907 | 3.881060 |
| 1 | 1.098587 | 1.033601 | 3.621422 |
| 7 | 2.450999 | 0.949516 | -0.582397 |
| 17 | -1.892968 | 0.476543 | -1.976531 |
| 8 | -3.400357 | 0.357222 | 0.926228 |
| 6 | -4.327066 | -0.405025 | 0.635775 |
| 8 | -4.150399 | -1.685936 | 0.408456 |
| 6 | 2.885780 | 0.397216 | 0.599310 |
| 8 | 2.258219 | 0.564099 | 1.649403 |
| 6 | 4.122313 | -0.431140 | 0.577883 |
| 6 | 4.320721 | -1.420893 | -0.390388 |
| 6 | 5.022338 | -0.294207 | 1.635627 |
| 6 | 5.434463 | -2.247668 | -0.301168 |
| 1 | 3.585829 | -1.557283 | -1.184716 |
| 6 | 6.148047 | -1.104866 | 1.701514 |
| 1 | 4.828512 | 0.454758 | 2.400594 |
| 6 | 6.354218 | -2.082052 | 0.731372 |
| 1 | 5.585322 | -3.024817 | -1.046749 |
| 1 | 6.861131 | -0.981484 | 2.513373 |
| 1 | 7.231776 | -2.722894 | 0.784442 |
| 8 | 3.366668 | 0.955079 | -1.629192 |
| 1 | 3.703615 | 1.866199 | -1.649072 |
| 6 | -5.736227 | 0.095535 | 0.428097 |
| 1 | -3.193655 | -1.919749 | 0.528436 |
| 17 | 0.870870 | -2.153142 | -1.906290 |

| | | | |
|---|---|---|---|
| 8 | -1.490879 | -1.848139 | 0.821501 |
| 6 | -0.542493 | -2.693570 | 0.844769 |
| 6 | 0.723674 | -2.380169 | 1.571135 |
| 1 | 1.585991 | -2.531816 | 0.912336 |
| 1 | 0.712800 | -1.336702 | 1.898362 |
| 1 | 0.832455 | -3.026218 | 2.450757 |
| 7 | -0.715381 | -3.877488 | 0.270038 |
| 6 | -1.840339 | -4.031944 | -0.648503 |
| 1 | -1.894990 | -3.159479 | -1.310582 |
| 1 | -1.665367 | -4.917053 | -1.262292 |
| 1 | -2.783542 | -4.161518 | -0.105893 |
| 6 | 0.367799 | -4.843367 | 0.159241 |
| 1 | 0.990076 | -4.835585 | 1.055833 |
| 1 | -0.059153 | -5.843662 | 0.051067 |
| 1 | 0.981282 | -4.593320 | -0.717972 |
| 6 | -6.772267 | -0.993613 | 0.686969 |
| 1 | -7.774747 | -0.584826 | 0.513117 |
| 1 | -6.632288 | -1.852033 | 0.023241 |
| 1 | -6.729206 | -1.351556 | 1.722546 |
| 6 | -5.991819 | 1.304605 | 1.322878 |
| 1 | -5.258355 | 2.095650 | 1.142672 |
| 1 | -6.992561 | 1.702286 | 1.117209 |
| 1 | -5.946435 | 1.033380 | 2.384371 |
| 6 | -5.774843 | 0.523126 | -1.049904 |
| 1 | -6.768379 | 0.925521 | -1.281350 |
| 1 | -5.025507 | 1.296235 | -1.256874 |
| 1 | -5.580781 | -0.325680 | -1.716264 |

---

**(7a-9)$_{c\text{-5-PivOH}}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2756.7731236
Zero-point correction= 0.542977
Thermal correction to Energy= 0.586208
Thermal correction to Enthalpy= 0.587153
Thermal correction to Gibbs Free Energy= 0.464001
Sum of electronic and zero-point Energies= -2756.230146
Sum of electronic and thermal Energies= -2756.186915
Sum of electronic and thermal Enthalpies= -2756.185971
Sum of electronic and thermal Free Energies= -2756.309122

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.744208 | 0.151081 | 1.182709 |
| 6 | 0.214204 | -2.781694 | 0.551453 |

| | | | |
|---|---|---|---|
| 6 | 1.061439 | -1.827103 | 1.172046 |
| 6 | 0.026666 | -4.049387 | 1.137735 |
| 6 | 1.750373 | -2.227768 | 2.341253 |
| 6 | 0.646755 | -4.388352 | 2.320405 |
| 1 | -0.669416 | -4.744920 | 0.666403 |
| 6 | 1.526839 | -3.464502 | 2.908689 |
| 1 | 2.462635 | -1.537979 | 2.791689 |
| 1 | 0.463708 | -5.352151 | 2.786690 |
| 1 | 2.047974 | -3.726761 | 3.827519 |
| 6 | -0.370795 | -2.508818 | -0.750408 |
| 8 | -0.961947 | -1.477384 | -1.124001 |
| 8 | 0.412851 | 2.413305 | 1.253517 |
| 6 | 0.850200 | 3.253098 | 0.471356 |
| 6 | 0.316247 | 4.672309 | 0.419949 |
| 8 | 1.855097 | 3.032533 | -0.350880 |
| 7 | -0.306414 | -3.517580 | -1.689961 |
| 1 | -0.558665 | -3.212071 | -2.626057 |
| 8 | 0.851752 | -4.291630 | -1.730088 |
| 1 | 0.607349 | -5.144114 | -1.344277 |
| 17 | -1.532610 | -0.076337 | 2.187933 |
| 8 | 2.648016 | 0.556921 | 0.307709 |
| 6 | 3.175810 | -0.460660 | -0.277897 |
| 7 | 2.469143 | -1.570762 | -0.277149 |
| 8 | 3.132581 | -2.748003 | -0.588087 |
| 1 | 2.429554 | -3.315432 | -0.952524 |
| 6 | 4.508320 | -0.263333 | -0.896183 |
| 6 | 5.020510 | -1.091003 | -1.901524 |
| 6 | 5.253439 | 0.847094 | -0.481303 |
| 6 | 6.255297 | -0.810419 | -2.471706 |
| 1 | 4.447684 | -1.952218 | -2.226280 |
| 6 | 6.491709 | 1.116630 | -1.046936 |
| 1 | 4.846832 | 1.493285 | 0.291791 |
| 6 | 6.995677 | 0.287774 | -2.044324 |
| 1 | 6.642437 | -1.456070 | -3.256503 |
| 1 | 7.063424 | 1.978360 | -0.710864 |
| 1 | 7.965303 | 0.497770 | -2.490447 |
| 30 | -1.710669 | 0.122618 | -0.109888 |
| 17 | -1.710321 | 1.961865 | -1.458227 |
| 8 | -3.704122 | -0.491531 | -0.368203 |
| 6 | -4.694925 | -0.017389 | -0.927341 |
| 8 | -4.668733 | 1.074710 | -1.651592 |
| 1 | -3.753044 | 1.455651 | -1.678549 |
| 6 | -6.071206 | -0.636811 | -0.802884 |
| 1 | 2.212441 | 2.117245 | -0.214264 |
| 6 | 0.159377 | 5.133821 | -1.029547 |

| | | | |
|---|---|---|---|
| 1 | -0.533144 | 4.483091 | -1.576662 |
| 1 | -0.244779 | 6.153978 | -1.038720 |
| 1 | 1.118125 | 5.138443 | -1.556968 |
| 6 | -1.022407 | 4.740538 | 1.144889 |
| 1 | -1.759963 | 4.088999 | 0.661688 |
| 1 | -0.927914 | 4.423734 | 2.188397 |
| 1 | -1.397802 | 5.771178 | 1.122980 |
| 6 | 1.348045 | 5.554046 | 1.136842 |
| 1 | 2.321113 | 5.514548 | 0.634481 |
| 1 | 1.001518 | 6.594984 | 1.137350 |
| 1 | 1.480062 | 5.240703 | 2.180152 |
| 6 | -6.910198 | 0.313232 | 0.063435 |
| 1 | -6.465887 | 0.440139 | 1.058165 |
| 1 | -7.007708 | 1.298884 | -0.403521 |
| 1 | -7.913584 | -0.109859 | 0.193210 |
| 6 | -5.968567 | -2.000502 | -0.131746 |
| 1 | -6.971131 | -2.432210 | -0.029152 |
| 1 | -5.357152 | -2.691307 | -0.723326 |
| 1 | -5.520140 | -1.925399 | 0.863943 |
| 6 | -6.705262 | -0.769464 | -2.189288 |
| 1 | -6.109546 | -1.420510 | -2.840680 |
| 1 | -7.701515 | -1.216548 | -2.088594 |
| 1 | -6.810790 | 0.203325 | -2.679073 |

---

**(7a-9)$_{c\text{-}s\text{-}p\text{-}7}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -2697.6068495
Zero-point correction= 0.528556
Thermal correction to Energy= 0.570025
Thermal correction to Enthalpy= 0.570969
Thermal correction to Gibbs Free Energy= 0.455799
Sum of electronic and zero-point Energies= -2697.078293
Sum of electronic and thermal Energies= -2697.036824
Sum of electronic and thermal Enthalpies= -2697.035880
Sum of electronic and thermal Free Energies= -2697.151050

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.583577 | 0.994244 | -0.769364 |
| 30 | -0.015910 | -0.296365 | 1.270878 |
| 8 | -1.678828 | -1.795073 | 1.701198 |
| 6 | -2.805696 | -1.467802 | 1.290631 |
| 7 | -3.776903 | -1.062876 | 2.127761 |
| 8 | 0.975970 | -1.718238 | 2.394391 |

| | | | |
|---|---|---|---|
| 6 | 2.125265 | -1.480860 | 2.832784 |
| 7 | 3.213241 | -1.979119 | 2.228380 |
| 6 | 2.295900 | -0.635249 | 4.060486 |
| 1 | 2.844661 | 0.280398 | 3.813031 |
| 1 | 1.303279 | -0.361116 | 4.423090 |
| 1 | 2.833960 | -1.162521 | 4.855581 |
| 6 | 3.086106 | -2.638884 | 0.937676 |
| 1 | 3.393913 | -1.952498 | 0.135655 |
| 1 | 3.724901 | -3.528775 | 0.917062 |
| 1 | 2.048014 | -2.926900 | 0.769543 |
| 6 | 4.558430 | -1.555959 | 2.568515 |
| 1 | 5.258928 | -2.354252 | 2.304455 |
| 1 | 4.827404 | -0.650015 | 2.006412 |
| 1 | 4.659845 | -1.357003 | 3.636514 |
| 6 | -3.174719 | -1.457802 | -0.140509 |
| 6 | -4.359502 | -2.053153 | -0.582799 |
| 6 | -2.341397 | -0.810695 | -1.077397 |
| 6 | -4.688353 | -2.071357 | -1.932622 |
| 1 | -5.009675 | -2.532221 | 0.148217 |
| 6 | -2.639721 | -0.889061 | -2.446249 |
| 6 | -3.824241 | -1.490205 | -2.858745 |
| 1 | -5.601646 | -2.557957 | -2.263667 |
| 1 | -1.943424 | -0.471177 | -3.170879 |
| 1 | -4.063630 | -1.518700 | -3.919677 |
| 1 | -4.568793 | -0.543809 | 1.764396 |
| 8 | -3.489460 | -0.830831 | 3.441132 |
| 1 | -2.813272 | -0.116345 | 3.408924 |
| 7 | -0.356517 | -1.411416 | -0.686237 |
| 6 | 0.461249 | -0.930476 | -1.659094 |
| 8 | -0.257487 | -2.777004 | -0.424982 |
| 1 | -0.652286 | -2.827726 | 0.469212 |
| 8 | 0.193647 | 0.210415 | -2.108727 |
| 6 | 1.671773 | -1.636775 | -2.139569 |
| 6 | 1.745190 | -3.018639 | -2.341735 |
| 6 | 2.787892 | -0.835236 | -2.413031 |
| 6 | 2.927392 | -3.586116 | -2.805907 |
| 1 | 0.880375 | -3.641488 | -2.142698 |
| 6 | 3.970727 | -1.413518 | -2.851128 |
| 1 | 2.719012 | 0.237121 | -2.248802 |
| 6 | 4.041675 | -2.790382 | -3.051011 |
| 1 | 2.975974 | -4.659177 | -2.975467 |
| 1 | 4.837897 | -0.786814 | -3.044432 |
| 1 | 4.966159 | -3.241896 | -3.404394 |
| 17 | -1.591598 | 1.307818 | 2.020745 |
| 17 | 1.937774 | 0.902621 | 0.840407 |

| | | | |
|---|---|---|---|
| 8 | -0.691421 | 3.082222 | -0.714570 |
| 6 | 0.459976 | 3.401644 | -0.991307 |
| 8 | 1.196281 | 2.777503 | -1.892373 |
| 1 | 0.770380 | 1.927954 | -2.143345 |
| 6 | 1.122799 | 4.610184 | -0.359614 |
| 6 | 2.643894 | 4.497575 | -0.392603 |
| 1 | 3.080390 | 5.373432 | 0.103914 |
| 1 | 2.977271 | 3.595569 | 0.133693 |
| 1 | 3.026352 | 4.457453 | -1.417706 |
| 6 | 0.666371 | 5.830617 | -1.169563 |
| 1 | 1.099446 | 6.740947 | -0.736418 |
| 1 | 0.997071 | 5.759710 | -2.213563 |
| 1 | -0.425524 | 5.927994 | -1.154408 |
| 6 | 0.634584 | 4.721874 | 1.084068 |
| 1 | -0.454054 | 4.822986 | 1.129186 |
| 1 | 0.909887 | 3.828441 | 1.659372 |
| 1 | 1.092118 | 5.600233 | 1.556484 |

---

**(7a-9)$_{p\text{-}p\text{-}s\text{-}7}$‡**

---

Number of imaginary frequencies : 1
Electronic energy = -2122.8489307
Zero-point correction= 0.651907
Thermal correction to Energy= 0.697153
Thermal correction to Enthalpy= 0.698098
Thermal correction to Gibbs Free Energy= 0.577542
Sum of electronic and zero-point Energies= -2122.197023
Sum of electronic and thermal Energies= -2122.151777
Sum of electronic and thermal Enthalpies= -2122.150833
Sum of electronic and thermal Free Energies= -2122.271388

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.944665 | 0.610903 | -1.467456 |
| 8 | 0.172338 | -1.534609 | -2.109774 |
| 6 | -0.807243 | -1.876344 | -1.423433 |
| 8 | -1.037729 | -1.511698 | -0.215074 |
| 6 | -1.824241 | -2.841550 | -2.048640 |
| 30 | 0.245067 | -0.374828 | 0.856332 |
| 8 | 1.254876 | 1.051091 | 2.149088 |
| 6 | 2.208693 | 1.604268 | 1.551257 |
| 7 | 3.472054 | 1.225816 | 1.814455 |
| 8 | 2.016072 | -1.416813 | 0.888063 |
| 8 | 2.848787 | -0.389727 | -0.931553 |
| 6 | 2.877233 | -1.277526 | -0.050839 |

| | | | |
|---|---|---|---|
| 6 | 4.057908 | -2.252832 | -0.089490 |
| 8 | -0.916329 | -0.786315 | 2.497479 |
| 6 | -1.702517 | -1.758940 | 2.476118 |
| 7 | -3.029918 | -1.564507 | 2.499694 |
| 6 | -1.161679 | -3.160808 | 2.450699 |
| 1 | -1.557002 | -3.724933 | 1.599109 |
| 1 | -0.075094 | -3.101144 | 2.356533 |
| 1 | -1.405898 | -3.702139 | 3.371756 |
| 6 | -3.577393 | -0.222282 | 2.384396 |
| 1 | -4.178035 | -0.145804 | 1.467790 |
| 1 | -4.220289 | -0.005096 | 3.246063 |
| 1 | -2.766439 | 0.505984 | 2.345250 |
| 6 | -4.010710 | -2.629385 | 2.451782 |
| 1 | -4.815878 | -2.412728 | 3.163353 |
| 1 | -4.447383 | -2.705351 | 1.446070 |
| 1 | -3.572430 | -3.591756 | 2.717635 |
| 6 | 2.035017 | 2.624154 | 0.512347 |
| 6 | 2.832126 | 3.776791 | 0.519505 |
| 6 | 1.082132 | 2.418645 | -0.523871 |
| 6 | 2.664950 | 4.767879 | -0.431569 |
| 1 | 3.566169 | 3.896294 | 1.316126 |
| 6 | 0.886147 | 3.468842 | -1.448939 |
| 6 | 1.678458 | 4.602394 | -1.410165 |
| 1 | 3.272503 | 5.667846 | -0.403333 |
| 1 | 0.123917 | 3.356289 | -2.217289 |
| 1 | 1.524326 | 5.377468 | -2.158921 |
| 1 | 4.199169 | 1.381673 | 1.124426 |
| 8 | 3.704416 | 0.168216 | 2.656347 |
| 1 | 3.080811 | -0.528644 | 2.352180 |
| 7 | -0.592588 | 1.822360 | 0.285903 |
| 6 | -1.548921 | 1.670791 | -0.669559 |
| 8 | -0.953892 | 2.521197 | 1.433516 |
| 1 | -0.335621 | 2.136104 | 2.086387 |
| 8 | -1.158438 | 1.257402 | -1.785615 |
| 6 | -2.999455 | 1.844810 | -0.433687 |
| 6 | -3.564694 | 2.789401 | 0.428239 |
| 6 | -3.834776 | 0.975898 | -1.147869 |
| 6 | -4.947057 | 2.846428 | 0.577278 |
| 1 | -2.925832 | 3.474389 | 0.973521 |
| 6 | -5.210555 | 1.020259 | -0.974152 |
| 1 | -3.376131 | 0.267602 | -1.834256 |
| 6 | -5.770154 | 1.959375 | -0.109703 |
| 1 | -5.382782 | 3.591174 | 1.239235 |
| 1 | -5.847335 | 0.330451 | -1.523616 |
| 1 | -6.849077 | 2.005518 | 0.020890 |

| | | | |
|---|---|---|---|
| 6 | -3.095099 | -2.957824 | -1.213434 |
| 1 | -2.890240 | -3.386155 | -0.223647 |
| 1 | -3.564803 | -1.976508 | -1.058727 |
| 1 | -3.817074 | -3.611105 | -1.721822 |
| 6 | -2.169688 | -2.341707 | -3.450635 |
| 1 | -1.266796 | -2.252911 | -4.061413 |
| 1 | -2.866723 | -3.033987 | -3.941252 |
| 1 | -2.642568 | -1.350823 | -3.412861 |
| 6 | -1.142649 | -4.209286 | -2.141147 |
| 1 | -0.235058 | -4.148449 | -2.751048 |
| 1 | -0.861677 | -4.576661 | -1.144076 |
| 1 | -1.821436 | -4.944225 | -2.593927 |
| 6 | 5.353999 | -1.443208 | -0.003533 |
| 1 | 5.410981 | -0.709266 | -0.814353 |
| 1 | 5.420697 | -0.918502 | 0.959558 |
| 1 | 6.220682 | -2.112230 | -0.078716 |
| 6 | 4.002572 | -3.261076 | 1.051146 |
| 1 | 3.074354 | -3.842396 | 1.027358 |
| 1 | 4.847353 | -3.957132 | 0.968168 |
| 1 | 4.068745 | -2.772302 | 2.030640 |
| 6 | 3.988300 | -2.983540 | -1.433605 |
| 1 | 4.817654 | -3.698086 | -1.513804 |
| 1 | 3.047392 | -3.540362 | -1.530797 |
| 1 | 4.048415 | -2.276201 | -2.266349 |

## Cartesian Coordinates for the Formation of Pd-Zn Heterobimetallic Complexes when Pivalate as Ligand

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**Pd-Zn-1**

---

Number of imaginary frequencies : 0
The smallest frequency is : 12.7812 cm(-1)
Electronic energy = -1805.1224126
Zero-point correction= 0.275861
Thermal correction to Energy= 0.300110
Thermal correction to Enthalpy= 0.301054
Thermal correction to Gibbs Free Energy= 0.217512
Sum of electronic and zero-point Energies= -1804.846551
Sum of electronic and thermal Energies= -1804.822303
Sum of electronic and thermal Enthalpies= -1804.821359
Sum of electronic and thermal Free Energies= -1804.904900

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -1.523744 | -0.010866 | -0.191102 |
| 17 | 0.167380 | 1.661657 | -0.357688 |
| 17 | 0.150153 | -1.705618 | -0.310737 |
| 30 | 1.776665 | -0.028861 | -0.196327 |
| 8 | -3.255377 | 1.089430 | -0.023340 |
| 8 | -3.275276 | -1.078421 | 0.003091 |
| 8 | 3.327491 | 0.001089 | 1.135164 |
| 8 | 3.622698 | -0.037844 | -1.041813 |
| 6 | -3.937973 | 0.012627 | 0.064353 |
| 6 | 4.112186 | -0.010825 | 0.135888 |
| 6 | 5.616725 | 0.024823 | 0.313228 |
| 6 | -5.420372 | 0.026563 | 0.296919 |
| 6 | -6.059213 | -1.190175 | -0.368851 |
| 1 | -5.630311 | -2.124908 | 0.005883 |
| 1 | -7.135045 | -1.193751 | -0.157027 |
| 1 | -5.927016 | -1.166381 | -1.456710 |
| 6 | -5.605159 | -0.050338 | 1.820834 |
| 1 | -5.131984 | 0.803724 | 2.319738 |
| 1 | -6.675844 | -0.036033 | 2.057214 |
| 1 | -5.175031 | -0.974285 | 2.224334 |
| 6 | -6.019203 | 1.323713 | -0.238967 |
| 1 | -5.884433 | 1.408984 | -1.323298 |
| 1 | -7.094792 | 1.339294 | -0.026789 |
| 1 | -5.561645 | 2.201061 | 0.229215 |
| 6 | 6.216754 | -1.170097 | -0.431845 |
| 1 | 5.957190 | -1.144043 | -1.494792 |
| 1 | 7.309438 | -1.148655 | -0.336756 |
| 1 | 5.861791 | -2.119779 | -0.012662 |
| 6 | 6.117443 | 1.328029 | -0.319068 |
| 1 | 5.692660 | 2.203702 | 0.187418 |
| 1 | 7.209222 | 1.383204 | -0.227359 |
| 1 | 5.852156 | 1.377711 | -1.380023 |
| 6 | 5.993431 | -0.024257 | 1.787937 |
| 1 | 5.560590 | 0.817735 | 2.338198 |
| 1 | 5.638315 | -0.946739 | 2.260199 |
| 1 | 7.084914 | 0.017716 | 1.889544 |

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**Pd-Zn-2**

---

Number of imaginary frequencies : 0
The smallest frequency is : 28.6984 cm(-1)
Electronic energy = -2380.5031314
Zero-point correction= 0.543493
Thermal correction to Energy= 0.583496

Thermal correction to Enthalpy= 0.584440
Thermal correction to Gibbs Free Energy= 0.472362
Sum of electronic and zero-point Energies= -2379.959639
Sum of electronic and thermal Energies= -2379.919636
Sum of electronic and thermal Enthalpies= -2379.918692
Sum of electronic and thermal Free Energies= -2380.030770

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | -0.907628 | -0.589011 | -1.601159 |
| 8 | 1.056000 | -0.365063 | -2.246906 |
| 6 | 1.986100 | -0.394164 | -1.401247 |
| 8 | 1.845478 | -0.339711 | -0.142691 |
| 6 | 3.400776 | -0.587996 | -1.942828 |
| 30 | 0.106504 | -0.092547 | 0.838363 |
| 8 | -0.783063 | -1.576772 | 1.813325 |
| 6 | -1.953906 | -2.024296 | 1.878020 |
| 6 | -2.218231 | -3.433285 | 1.459730 |
| 1 | -1.257333 | -3.940216 | 1.366791 |
| 1 | -2.868850 | -3.972653 | 2.153953 |
| 1 | -2.675261 | -3.414794 | 0.461659 |
| 7 | -2.947486 | -1.263915 | 2.357613 |
| 6 | -2.668874 | 0.118165 | 2.713104 |
| 1 | -2.674836 | 0.759084 | 1.819388 |
| 1 | -3.440654 | 0.462224 | 3.407889 |
| 1 | -1.692765 | 0.194685 | 3.199181 |
| 6 | -4.354893 | -1.587403 | 2.215829 |
| 1 | -4.868492 | -1.445231 | 3.173779 |
| 1 | -4.801868 | -0.927651 | 1.460692 |
| 1 | -4.496598 | -2.616058 | 1.886641 |
| 8 | -0.716815 | 1.719071 | 0.550728 |
| 8 | -1.183025 | 1.479346 | -1.637634 |
| 6 | -1.130528 | 2.144952 | -0.573377 |
| 6 | -1.679965 | 3.570024 | -0.622242 |
| 17 | -0.522667 | -2.870764 | -1.525345 |
| 8 | 1.254664 | 0.393491 | 2.506743 |
| 6 | 2.358249 | 0.956690 | 2.357296 |
| 7 | 3.501035 | 0.311860 | 2.652344 |
| 6 | 2.418099 | 2.367401 | 1.843952 |
| 1 | 3.045985 | 2.434726 | 0.948408 |
| 1 | 1.398752 | 2.668892 | 1.590495 |
| 1 | 2.816767 | 3.057996 | 2.595144 |
| 6 | 3.470050 | -1.101167 | 2.991459 |
| 1 | 4.035042 | -1.671379 | 2.242514 |
| 1 | 3.924062 | -1.263975 | 3.976397 |

| | | | |
|---|---|---|---|
| 1 | 2.436731 | -1.447742 | 3.003163 |
| 6 | 4.823907 | 0.897477 | 2.578309 |
| 1 | 5.343499 | 0.756584 | 3.534283 |
| 1 | 5.414608 | 0.411050 | 1.790426 |
| 1 | 4.779387 | 1.965572 | 2.365966 |
| 17 | -3.113675 | -0.793036 | -0.883299 |
| 6 | 3.540678 | 0.004330 | -3.340727 |
| 1 | 4.553817 | -0.179503 | -3.720374 |
| 1 | 2.821407 | -0.442087 | -4.032688 |
| 1 | 3.371491 | 1.088037 | -3.333989 |
| 6 | 3.595966 | -2.109266 | -1.997775 |
| 1 | 4.594006 | -2.341231 | -2.391587 |
| 1 | 3.502053 | -2.554738 | -0.999279 |
| 1 | 2.844951 | -2.574213 | -2.646845 |
| 6 | 4.427637 | 0.031545 | -1.000690 |
| 1 | 4.287538 | 1.118215 | -0.913424 |
| 1 | 4.347742 | -0.403677 | 0.002070 |
| 1 | 5.440484 | -0.146788 | -1.383978 |
| 6 | -1.695137 | 4.100303 | -2.051714 |
| 1 | -2.308909 | 3.470980 | -2.702434 |
| 1 | -2.103863 | 5.118687 | -2.061312 |
| 1 | -0.684789 | 4.133314 | -2.476016 |
| 6 | -3.117228 | 3.465493 | -0.095773 |
| 1 | -3.699204 | 2.748838 | -0.688880 |
| 1 | -3.130818 | 3.141553 | 0.952045 |
| 1 | -3.606461 | 4.446049 | -0.158294 |
| 6 | -0.862993 | 4.495178 | 0.274611 |
| 1 | 0.181989 | 4.551134 | -0.058166 |
| 1 | -1.280029 | 5.509491 | 0.235718 |
| 1 | -0.874978 | 4.157906 | 1.316166 |

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**Pd-Zn-3**

---

Number of imaginary frequencies : 0
The smallest frequency is : 31.9327 cm(-1)
Electronic energy = -2380.457665
Zero-point correction= 0.543739
Thermal correction to Energy= 0.582865
Thermal correction to Enthalpy= 0.583810
Thermal correction to Gibbs Free Energy= 0.474887
Sum of electronic and zero-point Energies= -2379.913926
Sum of electronic and thermal Energies= -2379.874800
Sum of electronic and thermal Enthalpies= -2379.873855
Sum of electronic and thermal Free Energies= -2379.982778
.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.985229 | -0.006350 | -0.527915 |
| 8 | -0.125643 | 1.591847 | -1.153867 |
| 6 | -1.291464 | 1.837405 | -0.681263 |
| 8 | -1.883073 | 1.178157 | 0.187219 |
| 6 | -1.988554 | 3.080255 | -1.245661 |
| 30 | -1.793790 | -0.185828 | 1.727292 |
| 8 | -1.256362 | -1.773770 | 0.505404 |
| 8 | -0.440186 | -1.136924 | -1.469528 |
| 6 | -1.309828 | -1.730761 | -0.741992 |
| 6 | -2.474263 | -2.378472 | -1.483531 |
| 17 | 0.053483 | 0.338825 | 2.946627 |
| 17 | -3.892708 | -0.574785 | 2.353403 |
| 7 | 2.097622 | -1.882368 | -0.083941 |
| 7 | 2.442699 | 1.632370 | 0.001974 |
| 6 | 1.612580 | -2.998613 | -0.944697 |
| 1 | 2.294291 | -3.853871 | -0.835221 |
| 1 | 0.623440 | -3.301290 | -0.598815 |
| 1 | 1.546248 | -2.698913 | -1.991642 |
| 6 | 1.870234 | -2.253361 | 1.335998 |
| 1 | 2.260210 | -1.481382 | 1.997205 |
| 1 | 0.794284 | -2.343622 | 1.488985 |
| 1 | 2.380112 | -3.199672 | 1.554507 |
| 6 | 1.746493 | 2.655418 | 0.830336 |
| 1 | 0.952933 | 3.096526 | 0.227618 |
| 1 | 1.299555 | 2.199692 | 1.718383 |
| 1 | 2.458532 | 3.443073 | 1.112629 |
| 6 | 2.768828 | 2.198632 | -1.330311 |
| 1 | 1.835103 | 2.489671 | -1.813967 |
| 1 | 3.426191 | 3.069475 | -1.212450 |
| 1 | 3.290221 | 1.453995 | -1.932988 |
| 6 | 3.652976 | 1.157759 | 0.662390 |
| 6 | 3.521368 | -1.693811 | -0.359374 |
| 6 | 3.889551 | -1.424608 | -1.787857 |
| 1 | 3.070837 | -0.989396 | -2.369601 |
| 1 | 4.751936 | -0.753427 | -1.780928 |
| 1 | 4.193435 | -2.363596 | -2.265754 |
| 6 | 3.574289 | 0.909444 | 2.133866 |
| 1 | 2.579838 | 0.608247 | 2.479038 |
| 1 | 4.323760 | 0.154447 | 2.380251 |
| 1 | 3.837105 | 1.834869 | 2.661712 |
| 8 | 4.321871 | -1.782458 | 0.532931 |
| 8 | 4.657570 | 1.009716 | 0.011191 |
| 6 | -1.137611 | 3.801061 | -2.283997 |

| | | | |
|---|---|---|---|
| 1 | -1.687709 | 4.669320 | -2.667449 |
| 1 | -0.196111 | 4.166143 | -1.854576 |
| 1 | -0.892821 | 3.149452 | -3.130110 |
| 6 | -2.274738 | 4.010632 | -0.063284 |
| 1 | -2.780785 | 4.915072 | -0.423189 |
| 1 | -2.915126 | 3.523044 | 0.677822 |
| 1 | -1.348494 | 4.323690 | 0.437102 |
| 6 | -3.309139 | 2.627147 | -1.872386 |
| 1 | -3.929276 | 2.096161 | -1.142656 |
| 1 | -3.864499 | 3.502785 | -2.230936 |
| 1 | -3.135345 | 1.967107 | -2.732468 |
| 6 | -3.034023 | -3.526805 | -0.649131 |
| 1 | -3.377403 | -3.176308 | 0.329033 |
| 1 | -3.881729 | -3.981083 | -1.176761 |
| 1 | -2.279159 | -4.307906 | -0.488084 |
| 6 | -2.050355 | -2.873861 | -2.862376 |
| 1 | -1.260960 | -3.634213 | -2.788384 |
| 1 | -2.908711 | -3.335393 | -3.365576 |
| 1 | -1.679850 | -2.058579 | -3.491430 |
| 6 | -3.531066 | -1.271548 | -1.617925 |
| 1 | -3.836369 | -0.887571 | -0.634783 |
| 1 | -3.151997 | -0.436249 | -2.221042 |
| 1 | -4.419012 | -1.680035 | -2.116495 |

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**Pd-Zn-4**

---

Number of imaginary frequencies : 0
Electronic energy =-2380.4899839
Zero-point correction= 0.544070
Thermal correction to Energy= 0.583810
Thermal correction to Enthalpy= 0.584755
Thermal correction to Gibbs Free Energy= 0.473297
Sum of electronic and zero-point Energies= -2379.945914
Sum of electronic and thermal Energies= -2379.906173
Sum of electronic and thermal Enthalpies= -2379.905229
Sum of electronic and thermal Free Energies= -2380.016686

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.826418 | 0.476816 | -1.483121 |
| 8 | -1.231103 | 2.226433 | -0.458021 |
| 6 | -0.766204 | 2.416190 | 0.698385 |
| 8 | -0.100621 | 1.581586 | 1.376392 |
| 6 | -0.989096 | 3.798760 | 1.314166 |
| 30 | 0.070788 | -0.395832 | 1.230301 |

| | | | |
|---|---|---|---|
| 17 | 0.817628 | -1.388952 | 3.142895 |
| 8 | 1.810993 | -0.813792 | 0.126511 |
| 6 | 2.261703 | -1.958826 | 0.381863 |
| 6 | 1.515314 | -3.171824 | -0.082397 |
| 1 | 0.762679 | -2.855417 | -0.813116 |
| 1 | 2.165032 | -3.925443 | -0.537432 |
| 1 | 1.011916 | -3.629480 | 0.780247 |
| 7 | 3.401719 | -2.106563 | 1.077105 |
| 6 | 4.011217 | -0.952748 | 1.722721 |
| 1 | 5.101177 | -1.017616 | 1.627265 |
| 1 | 3.650081 | -0.035347 | 1.257239 |
| 1 | 3.729645 | -0.935131 | 2.783595 |
| 6 | 3.800990 | -3.381734 | 1.649356 |
| 1 | 4.884285 | -3.377919 | 1.803799 |
| 1 | 3.303125 | -3.527716 | 2.618361 |
| 1 | 3.554848 | -4.215542 | 0.991303 |
| 8 | -1.633496 | -1.360769 | 0.804931 |
| 8 | -2.606490 | -0.283214 | -0.911517 |
| 6 | -2.596920 | -1.133591 | 0.031243 |
| 6 | -3.842766 | -2.003472 | 0.165223 |
| 17 | -0.545952 | -1.507042 | -2.678870 |
| 8 | 1.004662 | 1.412848 | -1.916782 |
| 6 | 2.129724 | 0.915251 | -2.144677 |
| 7 | 3.179645 | 1.377650 | -1.442683 |
| 6 | 2.371051 | -0.123022 | -3.190789 |
| 1 | 3.256238 | 0.111353 | -3.790729 |
| 1 | 2.524855 | -1.100756 | -2.716622 |
| 1 | 1.489444 | -0.206121 | -3.826236 |
| 6 | 2.897996 | 2.306069 | -0.354006 |
| 1 | 2.324884 | 1.808808 | 0.440616 |
| 1 | 3.841533 | 2.683994 | 0.046233 |
| 1 | 2.302319 | 3.146255 | -0.721099 |
| 6 | 4.489716 | 0.759021 | -1.541740 |
| 1 | 4.892104 | 0.818940 | -2.558648 |
| 1 | 5.179604 | 1.286519 | -0.879737 |
| 1 | 4.459845 | -0.296543 | -1.236514 |
| 6 | -5.051764 | -1.364521 | -0.507749 |
| 1 | -4.873058 | -1.191840 | -1.573182 |
| 1 | -5.919164 | -2.028299 | -0.402820 |
| 1 | -5.302483 | -0.401782 | -0.047063 |
| 6 | -3.473713 | -3.306694 | -0.558965 |
| 1 | -4.326490 | -3.996732 | -0.529556 |
| 1 | -3.216467 | -3.109876 | -1.607155 |
| 1 | -2.614672 | -3.791468 | -0.080121 |
| 6 | -4.135704 | -2.282735 | 1.636159 |

| | | | |
|---|---|---|---|
| 1 | -3.278845 | -2.745300 | 2.134438 |
| 1 | -4.384687 | -1.360084 | 2.174922 |
| 1 | -4.995893 | -2.959497 | 1.715363 |
| 6 | -2.078235 | 4.565279 | 0.572994 |
| 1 | -2.213283 | 5.550391 | 1.037402 |
| 1 | -1.822696 | 4.709187 | -0.481378 |
| 1 | -3.036144 | 4.034555 | 0.612976 |
| 6 | -1.359625 | 3.646664 | 2.788289 |
| 1 | -0.586292 | 3.104054 | 3.339627 |
| 1 | -1.484395 | 4.639061 | 3.239771 |
| 1 | -2.305680 | 3.104065 | 2.905566 |
| 6 | 0.342987 | 4.546841 | 1.190387 |
| 1 | 0.240274 | 5.555852 | 1.609488 |
| 1 | 1.140225 | 4.028266 | 1.736299 |
| 1 | 0.638119 | 4.648099 | 0.137192 |

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**Pd-Zn-5**

---

Number of imaginary frequencies : 0
The smallest frequency is : 28.1176 cm(-1)
Electronic energy =-2092.8127377
Zero-point correction= 0.410434
Thermal correction to Energy= 0.442160
Thermal correction to Enthalpy= 0.443104
Thermal correction to Gibbs Free Energy= 0.347678
Sum of electronic and zero-point Energies= -2092.402304
Sum of electronic and thermal Energies= -2092.370578
Sum of electronic and thermal Enthalpies= -2092.369633
Sum of electronic and thermal Free Energies= -2092.465060

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | -0.348051 | -0.716099 | -0.741874 |
| 8 | -1.901867 | -1.692080 | 0.316269 |
| 6 | -2.746512 | -0.939305 | -0.267651 |
| 6 | -4.225723 | -1.211543 | -0.138466 |
| 8 | -2.289897 | 0.005638 | -0.997986 |
| 8 | 1.267287 | -1.841369 | -0.274028 |
| 6 | 2.347711 | -1.438422 | 0.260950 |
| 8 | 2.665274 | -0.249369 | 0.505832 |
| 6 | 3.328286 | -2.532136 | 0.690276 |
| 30 | 1.909399 | 1.480160 | -0.111827 |
| 17 | 3.018340 | 3.386201 | -0.247933 |
| 17 | 0.902091 | 0.691359 | -2.168452 |
| 8 | 0.271570 | 1.623452 | 1.105591 |

| | | | |
|---|---|---|---|
| 6 | -0.796718 | 2.229420 | 0.857045 |
| 6 | -0.878391 | 3.226209 | -0.254353 |
| 1 | -1.142193 | 2.695969 | -1.180362 |
| 1 | -1.611935 | 4.016610 | -0.080626 |
| 1 | 0.110462 | 3.676856 | -0.394623 |
| 7 | -1.884548 | 1.956540 | 1.591043 |
| 6 | -3.191092 | 2.510245 | 1.273379 |
| 1 | -3.379895 | 2.477372 | 0.195498 |
| 1 | -3.957420 | 1.902274 | 1.762095 |
| 1 | -3.299270 | 3.542349 | 1.629857 |
| 6 | -1.770699 | 0.967649 | 2.658685 |
| 1 | -2.574455 | 1.130382 | 3.381388 |
| 1 | -1.834031 | -0.054184 | 2.259130 |
| 1 | -0.807546 | 1.076856 | 3.159953 |
| 6 | -4.476963 | -2.570211 | -0.807500 |
| 1 | -3.892728 | -3.360357 | -0.325239 |
| 1 | -5.540970 | -2.824440 | -0.730892 |
| 1 | -4.210724 | -2.542463 | -1.871031 |
| 6 | -4.586723 | -1.300363 | 1.345593 |
| 1 | -4.427612 | -0.341297 | 1.857545 |
| 1 | -5.646757 | -1.561222 | 1.450858 |
| 1 | -3.989210 | -2.063252 | 1.855501 |
| 6 | -5.045398 | -0.131542 | -0.833339 |
| 1 | -6.110074 | -0.388086 | -0.775355 |
| 1 | -4.909800 | 0.849400 | -0.362563 |
| 1 | -4.768911 | -0.037820 | -1.888548 |
| 6 | 2.931474 | -3.897919 | 0.144574 |
| 1 | 3.658697 | -4.647262 | 0.481390 |
| 1 | 1.938402 | -4.199263 | 0.492900 |
| 1 | 2.917903 | -3.902956 | -0.950921 |
| 6 | 4.727908 | -2.155899 | 0.204172 |
| 1 | 5.039781 | -1.184687 | 0.599363 |
| 1 | 5.445113 | -2.915801 | 0.538749 |
| 1 | 4.771939 | -2.111968 | -0.890778 |
| 6 | 3.299935 | -2.553061 | 2.223064 |
| 1 | 4.003302 | -3.310138 | 2.591793 |
| 1 | 3.588552 | -1.580673 | 2.635924 |
| 1 | 2.300786 | -2.809658 | 2.597285 |

---

**Pd-Zn-6**

---

Number of imaginary frequencies : 0
Electronic energy =-2380.4922523
Zero-point correction= 0.542405
Thermal correction to Energy= 0.583199

Thermal correction to Enthalpy= 0.584143
Thermal correction to Gibbs Free Energy= 0.467931
Sum of electronic and zero-point Energies= -2379.949848
Sum of electronic and thermal Energies= -2379.909053
Sum of electronic and thermal Enthalpies= -2379.908109
Sum of electronic and thermal Free Energies= -2380.024321

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 1.471848 | 0.148129 | -0.524640 |
| 8 | 0.879011 | 2.058608 | -0.061702 |
| 6 | -0.143780 | 2.355976 | 0.629605 |
| 8 | -1.007320 | 1.554705 | 1.059976 |
| 6 | -0.354364 | 3.843287 | 0.921823 |
| 30 | -1.715022 | -0.116317 | 0.208560 |
| 17 | -0.430904 | -0.229189 | -1.853181 |
| 8 | -0.521498 | -1.375570 | 1.330324 |
| 6 | -0.136326 | -2.537839 | 1.075439 |
| 6 | -0.819227 | -3.371627 | 0.036078 |
| 1 | -0.236190 | -3.316372 | -0.892863 |
| 1 | -0.919355 | -4.419696 | 0.329886 |
| 1 | -1.814480 | -2.956959 | -0.146099 |
| 7 | 0.918192 | -3.027158 | 1.750997 |
| 6 | 1.644041 | -4.224100 | 1.376175 |
| 1 | 2.599836 | -3.945574 | 0.910781 |
| 1 | 1.837130 | -4.839217 | 2.262992 |
| 1 | 1.084471 | -4.816879 | 0.653005 |
| 6 | 1.610556 | -2.130760 | 2.665886 |
| 1 | 0.887156 | -1.574308 | 3.263947 |
| 1 | 2.247894 | -2.729685 | 3.323551 |
| 1 | 2.224117 | -1.406116 | 2.110172 |
| 17 | 2.412344 | -1.907147 | -1.157289 |
| 8 | -3.414385 | -1.318509 | 0.267931 |
| 6 | -4.085280 | -0.385042 | -0.285325 |
| 6 | -5.566896 | -0.601401 | -0.552960 |
| 8 | -3.528947 | 0.711485 | -0.560926 |
| 8 | 3.173709 | 0.438218 | 0.736839 |
| 6 | 4.302163 | 0.104365 | 0.301919 |
| 6 | 5.113027 | -0.860926 | 1.111901 |
| 1 | 6.182228 | -0.634644 | 1.130585 |
| 1 | 4.721158 | -0.853211 | 2.130792 |
| 1 | 4.963038 | -1.867044 | 0.697552 |
| 7 | 4.802252 | 0.605552 | -0.837404 |
| 6 | 5.880618 | -0.022058 | -1.580344 |
| 1 | 5.463477 | -0.554420 | -2.445936 |

| | | | |
|---|---|---|---|
| 1 | 6.581992 | 0.740028 | -1.937139 |
| 1 | 6.426273 | -0.740573 | -0.969177 |
| 6 | 4.026338 | 1.574554 | -1.596273 |
| 1 | 4.717221 | 2.173030 | -2.198122 |
| 1 | 3.312951 | 1.068831 | -2.264922 |
| 1 | 3.471268 | 2.229313 | -0.920871 |
| 6 | 0.859461 | 4.678640 | 0.535372 |
| 1 | 0.661277 | 5.735759 | 0.754343 |
| 1 | 1.750168 | 4.374431 | 1.097924 |
| 1 | 1.086388 | 4.584864 | -0.531839 |
| 6 | -0.661645 | 4.018597 | 2.408709 |
| 1 | -0.875765 | 5.074614 | 2.617400 |
| 1 | -1.529001 | 3.421286 | 2.704604 |
| 1 | 0.191574 | 3.718887 | 3.030180 |
| 6 | -1.569850 | 4.263894 | 0.087142 |
| 1 | -2.454056 | 3.676380 | 0.356427 |
| 1 | -1.785667 | 5.326325 | 0.258215 |
| 1 | -1.380623 | 4.122479 | -0.984508 |
| 6 | -6.274143 | -0.487097 | 0.802515 |
| 1 | -7.353797 | -0.638371 | 0.673961 |
| 1 | -5.898535 | -1.239277 | 1.505341 |
| 1 | -6.120912 | 0.506427 | 1.242722 |
| 6 | -5.786428 | -1.999008 | -1.128202 |
| 1 | -6.858475 | -2.171183 | -1.289950 |
| 1 | -5.277885 | -2.115419 | -2.093459 |
| 1 | -5.406412 | -2.767640 | -0.448310 |
| 6 | -6.104161 | 0.456457 | -1.508271 |
| 1 | -5.594836 | 0.410568 | -2.477790 |
| 1 | -7.177580 | 0.297329 | -1.674896 |
| 1 | -5.957128 | 1.463613 | -1.105702 |

---

**Pd-Zn-7**

---

Number of imaginary frequencies : 0
The smallest frequency is : 15.1142 cm(-1)
Electronic energy = -2380.4747124
Zero-point correction= 0.541589
Thermal correction to Energy= 0.582957
Thermal correction to Enthalpy= 0.583901
Thermal correction to Gibbs Free Energy= 0.464528
Sum of electronic and zero-point Energies= -2379.933123
Sum of electronic and thermal Energies= -2379.891756
Sum of electronic and thermal Enthalpies= -2379.890812
Sum of electronic and thermal Free Energies= -2380.010184

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.893535 | 0.324584 | -0.310571 |
| 8 | 3.639363 | -0.689132 | -0.995446 |
| 6 | 2.945498 | -1.600174 | -0.540860 |
| 6 | 3.453331 | -3.049094 | -0.471765 |
| 8 | 1.728673 | -1.482765 | -0.113274 |
| 8 | 0.103186 | 2.220366 | -0.502296 |
| 6 | -1.050260 | 2.570773 | -0.119522 |
| 8 | -1.946157 | 1.807576 | 0.331381 |
| 6 | -1.393164 | 4.056965 | -0.232517 |
| 30 | -1.911468 | -0.182702 | 0.340375 |
| 17 | -0.742219 | -0.653563 | -1.729578 |
| 8 | -3.866505 | -0.536440 | -0.182957 |
| 6 | -4.429184 | -1.651166 | -0.157466 |
| 6 | -3.646160 | -2.912666 | -0.359642 |
| 1 | -3.280074 | -3.267232 | 0.612979 |
| 1 | -4.213505 | -3.707351 | -0.849036 |
| 1 | -2.765331 | -2.679125 | -0.964861 |
| 7 | -5.754890 | -1.730546 | 0.058966 |
| 6 | -6.477656 | -2.985223 | 0.173757 |
| 1 | -5.858242 | -3.763571 | 0.623450 |
| 1 | -7.336716 | -2.829501 | 0.833118 |
| 1 | -6.849964 | -3.335316 | -0.798182 |
| 6 | -6.547096 | -0.520768 | 0.209409 |
| 1 | -7.400997 | -0.552401 | -0.477298 |
| 1 | -6.922821 | -0.436692 | 1.236236 |
| 1 | -5.927515 | 0.346078 | -0.017160 |
| 8 | 2.300141 | 1.068850 | 1.047340 |
| 6 | 3.394280 | 1.446326 | 0.556142 |
| 6 | 3.446813 | 2.359808 | -0.629691 |
| 1 | 3.842362 | 1.809496 | -1.489841 |
| 1 | 2.434035 | 2.702772 | -0.855650 |
| 1 | 4.083570 | 3.230188 | -0.439714 |
| 7 | 4.541310 | 1.077066 | 1.150284 |
| 6 | 4.512113 | 0.028879 | 2.157380 |
| 1 | 4.861642 | -0.915243 | 1.713057 |
| 1 | 5.172374 | 0.295846 | 2.989458 |
| 1 | 3.493176 | -0.103824 | 2.520402 |
| 6 | 5.827575 | 1.249454 | 0.499376 |
| 1 | 6.616598 | 1.187997 | 1.254898 |
| 1 | 5.974614 | 0.454477 | -0.246328 |
| 1 | 5.905935 | 2.220945 | 0.008325 |
| 6 | -0.179642 | 4.878090 | -0.649976 |

| | | | |
|---|---|---|---|
| 1 | -0.457400 | 5.937783 | -0.715432 |
| 1 | 0.634862 | 4.781272 | 0.077500 |
| 1 | 0.202640 | 4.560292 | -1.626155 |
| 6 | -2.499985 | 4.187376 | -1.283148 |
| 1 | -3.383428 | 3.607714 | -0.996168 |
| 1 | -2.790619 | 5.240806 | -1.384257 |
| 1 | -2.158516 | 3.834687 | -2.264394 |
| 6 | -1.910101 | 4.537003 | 1.124619 |
| 1 | -2.189996 | 5.596137 | 1.058789 |
| 1 | -2.786317 | 3.961573 | 1.438217 |
| 1 | -1.140600 | 4.438943 | 1.900296 |
| 6 | 4.965082 | -3.071614 | -0.660570 |
| 1 | 5.477460 | -2.533255 | 0.148701 |
| 1 | 5.326114 | -4.108307 | -0.657164 |
| 1 | 5.253438 | -2.600035 | -1.605425 |
| 6 | 2.774190 | -3.802019 | -1.620374 |
| 1 | 1.684293 | -3.776011 | -1.511497 |
| 1 | 3.033713 | -3.356247 | -2.588995 |
| 1 | 3.101720 | -4.850064 | -1.628788 |
| 6 | 3.075846 | -3.692124 | 0.861207 |
| 1 | 3.434402 | -4.729814 | 0.888686 |
| 1 | 3.532569 | -3.157919 | 1.704948 |
| 1 | 1.992541 | -3.689010 | 1.012450 |
| 17 | -1.557666 | -1.462796 | 2.134812 |

**Nucleophilic Addition Elimination**
**Concerted Pathway**

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**$(9\text{-}P)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1179.3427693
Zero-point correction= 0.304229
Thermal correction to Energy= 0.325897
Thermal correction to Enthalpy= 0.326842
Thermal correction to Gibbs Free Energy= 0.252673
Sum of electronic and zero-point Energies= -1179.038540
Sum of electronic and thermal Energies= -1179.016872
Sum of electronic and thermal Enthalpies= -1179.015928
Sum of electronic and thermal Free Energies= -1179.090096

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.671998 | 3.316574 | -0.366550 |
| 6 | 0.671553 | 1.927072 | -0.357797 |

| | | | |
|---|---|---|---|
| 6 | -0.517905 | 1.196088 | -0.480482 |
| 6 | -1.726256 | 1.880768 | -0.623483 |
| 6 | -1.716154 | 3.271161 | -0.613809 |
| 6 | -0.533137 | 3.997144 | -0.488760 |
| 1 | 1.619336 | 3.845820 | -0.287603 |
| 1 | -2.658639 | 1.344622 | -0.765869 |
| 1 | -2.660206 | 3.797695 | -0.732989 |
| 1 | -0.551201 | 5.083008 | -0.504661 |
| 6 | 1.924649 | 1.162738 | -0.185038 |
| 8 | 3.011306 | 1.272896 | -0.651721 |
| 7 | 1.963851 | 0.568330 | 1.393858 |
| 1 | 1.268830 | 1.049056 | 1.968458 |
| 7 | -0.303077 | -0.191601 | -0.509293 |
| 6 | -1.189756 | -1.255389 | -0.656637 |
| 8 | -0.830380 | -2.300910 | -1.161757 |
| 6 | -2.548515 | -1.090505 | -0.070108 |
| 6 | -2.760120 | -0.507738 | 1.181217 |
| 6 | -3.622872 | -1.648269 | -0.764160 |
| 6 | -4.040152 | -0.459364 | 1.718795 |
| 1 | -1.916255 | -0.099738 | 1.735055 |
| 6 | -4.904965 | -1.581226 | -0.234405 |
| 1 | -3.431509 | -2.135587 | -1.717259 |
| 6 | -5.114528 | -0.986578 | 1.007019 |
| 1 | -4.200138 | -0.014698 | 2.698110 |
| 1 | -5.741848 | -2.003900 | -0.784889 |
| 1 | -6.116857 | -0.942112 | 1.426546 |
| 8 | 0.997262 | -0.448539 | -0.886847 |
| 8 | 3.192230 | 0.796301 | 1.983343 |
| 1 | 1.791048 | -0.458109 | 1.364621 |
| 1 | 3.758551 | 0.049980 | 1.646457 |
| 8 | 2.200444 | -1.968015 | 0.499566 |
| 1 | 1.546093 | -1.512799 | -0.241713 |
| 6 | 3.472078 | -1.893720 | 0.124611 |
| 8 | 4.320032 | -1.378598 | 0.839792 |
| 6 | 3.775541 | -2.447956 | -1.231162 |
| 1 | 4.851705 | -2.464118 | -1.406836 |
| 1 | 3.342385 | -3.445440 | -1.346197 |
| 1 | 3.297389 | -1.800660 | -1.977685 |

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**$(9\text{-}P)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-1179.3594292
Zero-point correction= 0.302795
Thermal correction to Energy= 0.323926

Thermal correction to Enthalpy= 0.324871
Thermal correction to Gibbs Free Energy= 0.252554
Sum of electronic and zero-point Energies= -1179.056634
Sum of electronic and thermal Energies= -1179.035503
Sum of electronic and thermal Enthalpies= -1179.034559
Sum of electronic and thermal Free Energies= -1179.106875

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -2.317569 | 2.757721 | -0.503030 |
| 6 | -1.821381 | 1.555062 | -0.002773 |
| 6 | -0.445520 | 1.355227 | 0.189901 |
| 6 | 0.431991 | 2.395779 | -0.146229 |
| 6 | -0.074776 | 3.574857 | -0.671784 |
| 6 | -1.443655 | 3.773469 | -0.855360 |
| 1 | -3.394836 | 2.882378 | -0.600337 |
| 1 | 1.499217 | 2.296447 | 0.019665 |
| 1 | 0.622228 | 4.370890 | -0.923358 |
| 1 | -1.818854 | 4.713443 | -1.249146 |
| 6 | -2.755751 | 0.473020 | 0.344116 |
| 8 | -3.741604 | 0.489966 | 1.035486 |
| 7 | -2.794205 | -0.613285 | -0.763034 |
| 1 | -3.170595 | -0.155994 | -1.604003 |
| 7 | -0.103858 | 0.145232 | 0.789661 |
| 6 | 1.128202 | -0.210540 | 1.375488 |
| 8 | 1.187264 | -0.788471 | 2.437141 |
| 6 | 2.328506 | 0.048473 | 0.536092 |
| 6 | 2.310247 | -0.147946 | -0.848111 |
| 6 | 3.518905 | 0.392085 | 1.178748 |
| 6 | 3.477885 | 0.023580 | -1.582738 |
| 1 | 1.384631 | -0.451529 | -1.337110 |
| 6 | 4.676670 | 0.584859 | 0.436745 |
| 1 | 3.515787 | 0.501014 | 2.260772 |
| 6 | 4.656129 | 0.401207 | -0.943964 |
| 1 | 3.468946 | -0.140194 | -2.657683 |
| 1 | 5.600385 | 0.868973 | 0.935140 |
| 1 | 5.565547 | 0.543856 | -1.523338 |
| 8 | -1.208334 | -0.502013 | 1.309160 |
| 8 | -3.658398 | -1.629652 | -0.388096 |
| 1 | -1.810236 | -1.113215 | -1.018804 |
| 1 | -4.165699 | -1.208685 | 0.343636 |
| 8 | -0.748629 | -1.934984 | -1.450822 |
| 6 | -0.382208 | -2.794310 | -0.607668 |
| 8 | -0.631786 | -2.735426 | 0.638281 |
| 1 | -1.001178 | -1.667006 | 0.998543 |

| | | | |
|---|---|---|---|
| 6 | 0.444875 | -3.957379 | -1.064521 |
| 1 | 1.498279 | -3.732291 | -0.860606 |
| 1 | 0.187184 | -4.851894 | -0.492709 |
| 1 | 0.322219 | -4.126173 | -2.135707 |

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**$(9a'\text{-}P)_8^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy =-2165.2592518
Zero-point correction= 0.306232
Thermal correction to Energy= 0.333372
Thermal correction to Enthalpy= 0.334316
Thermal correction to Gibbs Free Energy= 0.244813
Sum of electronic and zero-point Energies= -2164.953020
Sum of electronic and thermal Energies= -2164.925880
Sum of electronic and thermal Enthalpies= -2164.924936
Sum of electronic and thermal Free Energies= -2165.014438

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.148239 | -2.973888 | -0.489865 |
| 6 | 0.257289 | -1.655038 | -0.394337 |
| 6 | 1.605728 | -1.304111 | -0.388540 |
| 6 | 2.598020 | -2.269930 | -0.478867 |
| 6 | 2.184540 | -3.601645 | -0.551839 |
| 6 | 0.838439 | -3.957838 | -0.555005 |
| 1 | -1.211829 | -3.215853 | -0.530926 |
| 1 | 3.652030 | -2.013293 | -0.504796 |
| 1 | 2.943509 | -4.376364 | -0.628629 |
| 1 | 0.556020 | -5.004225 | -0.629357 |
| 6 | -0.609657 | -0.430300 | -0.316021 |
| 8 | -1.665498 | -0.315786 | -1.015122 |
| 7 | -0.841865 | 0.011468 | 1.133573 |
| 1 | -1.054421 | 1.835967 | 0.886205 |
| 7 | 1.699938 | 0.111790 | -0.304715 |
| 6 | 2.719583 | 1.052560 | -0.429659 |
| 8 | 2.467530 | 2.173750 | -0.824212 |
| 6 | 4.066541 | 0.630582 | 0.027666 |
| 6 | 4.264402 | -0.147430 | 1.170835 |
| 6 | 5.164723 | 1.134083 | -0.672213 |
| 6 | 5.554893 | -0.443699 | 1.591822 |
| 1 | 3.408535 | -0.511168 | 1.736329 |
| 6 | 6.452369 | 0.820484 | -0.258850 |
| 1 | 4.988639 | 1.770651 | -1.535724 |
| 6 | 6.647786 | 0.031054 | 0.871579 |

| | | | |
|---|---|---|---|
| 1 | 5.708776 | -1.040377 | 2.487295 |
| 1 | 7.306684 | 1.199042 | -0.814042 |
| 1 | 7.656909 | -0.207616 | 1.198677 |
| 8 | 0.454008 | 0.611191 | -0.745298 |
| 8 | -1.948130 | -0.692158 | 1.652564 |
| 1 | -1.773036 | -1.654290 | 1.605843 |
| 1 | 0.077696 | 1.839398 | -0.285757 |
| 30 | -3.426565 | -0.529352 | -0.078035 |
| 17 | -4.424753 | 1.430738 | 0.264921 |
| 17 | -3.913077 | -2.703757 | 0.119068 |
| 8 | -0.528022 | 2.504140 | 0.346374 |
| 1 | -0.038847 | -0.225695 | 1.722009 |
| 6 | -1.151638 | 3.678060 | -0.222761 |
| 6 | -2.231321 | 4.184174 | 0.652630 |
| 1 | -3.058216 | 3.457641 | 0.665617 |
| 1 | -1.865319 | 4.304224 | 1.676994 |
| 1 | -2.587205 | 5.137238 | 0.261583 |
| 8 | -0.712028 | 4.079000 | -1.244248 |

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**(9a'-P)$_{10}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy =-2165.2897993
Zero-point correction= 0.308196
Thermal correction to Energy= 0.334353
Thermal correction to Enthalpy= 0.335298
Thermal correction to Gibbs Free Energy= 0.250347
Sum of electronic and zero-point Energies= -2164.981604
Sum of electronic and thermal Energies= -2164.955446
Sum of electronic and thermal Enthalpies= -2164.954502
Sum of electronic and thermal Free Energies= -2165.039452

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.371310 | 3.058663 | -0.099014 |
| 6 | 0.027914 | 1.736497 | -0.361793 |
| 6 | -1.298398 | 1.342118 | -0.560287 |
| 6 | -2.309181 | 2.302535 | -0.518231 |
| 6 | -1.960554 | 3.619502 | -0.239947 |
| 6 | -0.638528 | 4.007966 | -0.024684 |
| 1 | 1.418731 | 3.318823 | 0.046215 |
| 1 | -3.343540 | 2.039207 | -0.712491 |
| 1 | -2.749107 | 4.367330 | -0.209200 |
| 1 | -0.398868 | 5.046982 | 0.180241 |
| 6 | 1.049052 | 0.680717 | -0.445475 |

| | | | |
|---|---|---|---|
| 8 | 2.091882 | 0.697989 | -1.076621 |
| 7 | 1.140539 | -0.101427 | 0.907631 |
| 1 | 1.575486 | 0.563875 | 1.579407 |
| 7 | -1.425942 | -0.021632 | -0.854312 |
| 6 | -2.532546 | -0.840628 | -1.076182 |
| 8 | -2.424963 | -1.877902 | -1.698077 |
| 6 | -3.789846 | -0.412220 | -0.410692 |
| 6 | -3.811342 | -0.102241 | 0.951569 |
| 6 | -4.969899 | -0.409394 | -1.154721 |
| 6 | -5.012903 | 0.248104 | 1.554726 |
| 1 | -2.891536 | -0.155907 | 1.532413 |
| 6 | -6.163880 | -0.036370 | -0.549734 |
| 1 | -4.935909 | -0.693281 | -2.204164 |
| 6 | -6.183575 | 0.296525 | 0.802526 |
| 1 | -5.036931 | 0.483393 | 2.615783 |
| 1 | -7.082049 | -0.013263 | -1.131288 |
| 1 | -7.119852 | 0.583812 | 1.275272 |
| 8 | -0.196435 | -0.539895 | -1.255912 |
| 8 | 2.082782 | -1.127982 | 0.809640 |
| 1 | 0.218575 | -0.548117 | 1.270828 |
| 1 | 1.566672 | -1.892548 | 0.415642 |
| 8 | -0.857241 | -1.622589 | 1.668859 |
| 6 | -0.738684 | -2.612377 | 0.923991 |
| 8 | 0.085172 | -2.628334 | -0.087862 |
| 1 | -0.089204 | -1.593783 | -0.769869 |
| 30 | 3.849042 | 0.017285 | -0.077232 |
| 17 | 3.702871 | 1.522520 | 1.601522 |
| 17 | 5.226229 | -1.305738 | -1.104931 |
| 6 | -1.582644 | -3.827004 | 1.105189 |
| 1 | -0.973276 | -4.729835 | 1.012608 |
| 1 | -2.111392 | -3.802843 | 2.058967 |
| 1 | -2.303281 | -3.840929 | 0.277660 |

## Nucleophilic Addition Elimination via stepwise Pathway

## C–O bond Formation

---

**$(9\text{-}11)_6^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1179.3303188
Zero-point correction= 0.301367
Thermal correction to Energy= 0.322812
Thermal correction to Enthalpy= 0.323757
Thermal correction to Gibbs Free Energy= 0.249603

Sum of electronic and zero-point Energies= -1179.028952
Sum of electronic and thermal Energies= -1179.007506
Sum of electronic and thermal Enthalpies= -1179.006562
Sum of electronic and thermal Free Energies= -1179.080716

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.954590 | 3.220991 | 0.716850 |
| 6 | 0.854620 | 1.953454 | 0.161338 |
| 6 | -0.378882 | 1.447611 | -0.250764 |
| 6 | -1.526770 | 2.224934 | -0.137784 |
| 6 | -1.416870 | 3.497178 | 0.417680 |
| 6 | -0.191207 | 3.999808 | 0.841961 |
| 1 | 1.927476 | 3.583348 | 1.038996 |
| 1 | -2.491728 | 1.855422 | -0.465688 |
| 1 | -2.312342 | 4.107339 | 0.507034 |
| 1 | -0.126967 | 4.998724 | 1.265015 |
| 6 | 2.007232 | 1.023072 | 0.018734 |
| 8 | 2.388743 | 0.377527 | 1.038299 |
| 7 | 3.003717 | 1.277091 | -0.989172 |
| 1 | 2.573167 | 1.734310 | -1.790778 |
| 7 | -0.280429 | 0.123459 | -0.785055 |
| 6 | -0.948643 | -0.999328 | -0.286442 |
| 8 | -0.360298 | -2.047333 | -0.094075 |
| 6 | -2.416407 | -0.873116 | -0.117442 |
| 6 | -3.002222 | -1.437150 | 1.016424 |
| 6 | -3.220448 | -0.326392 | -1.119982 |
| 6 | -4.381507 | -1.404227 | 1.171660 |
| 1 | -2.362528 | -1.895215 | 1.766962 |
| 6 | -4.602496 | -0.314680 | -0.971021 |
| 1 | -2.756326 | 0.072918 | -2.020236 |
| 6 | -5.181501 | -0.842342 | 0.179535 |
| 1 | -4.835991 | -1.825476 | 2.064881 |
| 1 | -5.228893 | 0.100614 | -1.756620 |
| 1 | -6.262243 | -0.826078 | 0.298699 |
| 8 | 1.055258 | -0.111150 | -1.092826 |
| 8 | 3.861534 | 2.262416 | -0.426400 |
| 1 | 4.628502 | 1.746065 | -0.148904 |
| 1 | 2.689824 | -0.760369 | 0.615511 |
| 8 | 2.511322 | -1.659817 | -0.105922 |
| 6 | 2.612166 | -2.934281 | 0.357769 |
| 8 | 3.126196 | -3.166325 | 1.418776 |
| 1 | 1.584180 | -1.138319 | -0.666249 |
| 6 | 2.076606 | -3.944229 | -0.606414 |
| 1 | 1.002270 | -3.781622 | -0.735919 |

| | | | |
|---|---|---|---|
| 1 | 2.553468 | -3.817137 | -1.583707 |
| 1 | 2.263509 | -4.948751 | -0.224829 |

---

**$(9\text{-}11)_8^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1179.3512684
Zero-point correction= 0.301565
Thermal correction to Energy= 0.323180
Thermal correction to Enthalpy= 0.324124
Thermal correction to Gibbs Free Energy= 0.249365
Sum of electronic and zero-point Energies= -1179.049704
Sum of electronic and thermal Energies= -1179.028088
Sum of electronic and thermal Enthalpies= -1179.027144
Sum of electronic and thermal Free Energies= -1179.101904

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.596406 | 3.317953 | -0.354692 |
| 6 | -0.604448 | 1.935977 | -0.293340 |
| 6 | 0.579757 | 1.202904 | -0.420386 |
| 6 | 1.789262 | 1.854048 | -0.632375 |
| 6 | 1.787817 | 3.247378 | -0.681955 |
| 6 | 0.613615 | 3.981094 | -0.545223 |
| 1 | -1.535868 | 3.856494 | -0.254764 |
| 1 | 2.712330 | 1.301162 | -0.774665 |
| 1 | 2.729951 | 3.763344 | -0.851593 |
| 1 | 0.639871 | 5.066037 | -0.598815 |
| 6 | -1.818049 | 1.108458 | -0.037447 |
| 8 | -2.892506 | 1.262518 | -0.654683 |
| 7 | -1.943708 | 0.568216 | 1.313928 |
| 1 | -1.021099 | 0.357071 | 1.694657 |
| 7 | 0.332460 | -0.195651 | -0.356582 |
| 6 | 1.166041 | -1.285408 | -0.606778 |
| 8 | 0.742296 | -2.288687 | -1.143197 |
| 6 | 2.550126 | -1.184207 | -0.071484 |
| 6 | 3.566656 | -1.814629 | -0.790585 |
| 6 | 2.837826 | -0.582048 | 1.155982 |
| 6 | 4.868376 | -1.807002 | -0.307451 |
| 1 | 3.313586 | -2.311339 | -1.724202 |
| 6 | 4.137467 | -0.592633 | 1.645961 |
| 1 | 2.039720 | -0.113702 | 1.728945 |
| 6 | 5.154318 | -1.196620 | 0.911204 |
| 1 | 5.660837 | -2.287563 | -0.875887 |
| 1 | 4.357040 | -0.133029 | 2.606526 |

| | | | |
|---|---|---|---|
| 1 | 6.172205 | -1.198902 | 1.294130 |
| 8 | -0.989678 | -0.378414 | -0.752265 |
| 8 | -2.383188 | 1.678799 | 2.091660 |
| 1 | -3.328710 | 1.508896 | 2.184121 |
| 1 | -3.618482 | 0.136163 | -0.440274 |
| 8 | -4.217598 | -0.763840 | -0.274550 |
| 6 | -3.658236 | -1.889831 | -0.038329 |
| 8 | -2.429325 | -2.136603 | -0.032962 |
| 1 | -1.607747 | -1.295923 | -0.335897 |
| 6 | -4.599831 | -3.020404 | 0.227246 |
| 1 | -4.079623 | -3.841584 | 0.721902 |
| 1 | -5.449493 | -2.676051 | 0.821003 |
| 1 | -4.991523 | -3.379391 | -0.730739 |

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**$(9\text{-}11)_8$,‡**

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Number of imaginary frequencies : 1
Electronic energy = -1408.3503969
Zero-point correction= 0.368779
Thermal correction to Energy= 0.395002
Thermal correction to Enthalpy= 0.395946
Thermal correction to Gibbs Free Energy= 0.311760
Sum of electronic and zero-point Energies= -1407.981618
Sum of electronic and thermal Energies= -1407.955395
Sum of electronic and thermal Enthalpies= -1407.954451
Sum of electronic and thermal Free Energies= -1408.038637

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.510656 | 3.466393 | -1.136637 |
| 6 | 0.128568 | 2.225739 | -0.621262 |
| 6 | 1.015202 | 1.131943 | -0.648331 |
| 6 | 2.263074 | 1.307164 | -1.262811 |
| 6 | 2.624396 | 2.544056 | -1.770900 |
| 6 | 1.762197 | 3.637539 | -1.704558 |
| 1 | -0.199656 | 4.290692 | -1.100087 |
| 1 | 2.945079 | 0.468436 | -1.350749 |
| 1 | 3.598059 | 2.650378 | -2.243165 |
| 1 | 2.055200 | 4.600941 | -2.110824 |
| 6 | -1.249984 | 2.111826 | -0.105398 |
| 8 | -2.226627 | 1.931380 | -0.935406 |
| 7 | -1.493152 | 2.495222 | 1.130603 |
| 1 | -0.738683 | 2.659141 | 1.788044 |
| 7 | 0.576932 | -0.068151 | -0.086842 |

| | | | |
|---|---|---|---|
| 6 | 1.272526 | -1.220184 | 0.267567 |
| 8 | 0.679793 | -2.277295 | 0.400034 |
| 6 | 2.730963 | -1.117160 | 0.547328 |
| 6 | 3.559040 | -2.136882 | 0.076059 |
| 6 | 3.262612 | -0.110629 | 1.356406 |
| 6 | 4.916904 | -2.122884 | 0.369109 |
| 1 | 3.120011 | -2.936748 | -0.515573 |
| 6 | 4.615996 | -0.112995 | 1.669037 |
| 1 | 2.610884 | 0.666723 | 1.750908 |
| 6 | 5.446253 | -1.111193 | 1.165358 |
| 1 | 5.562163 | -2.909866 | -0.013374 |
| 1 | 5.024812 | 0.663591 | 2.310921 |
| 1 | 6.507012 | -1.106471 | 1.404713 |
| 8 | -0.771217 | -0.122735 | 0.091681 |
| 8 | -2.765982 | 2.681353 | 1.565132 |
| 1 | -3.035470 | 1.812802 | 2.014392 |
| 1 | -3.042159 | 1.675530 | -0.440393 |
| 8 | -3.647382 | 0.015223 | 0.351472 |
| 6 | -3.289072 | -0.451504 | 1.539753 |
| 8 | -3.216744 | 0.312055 | 2.497394 |
| 1 | -1.348779 | -0.744198 | -0.749608 |
| 8 | -2.275285 | -1.226109 | -1.351583 |
| 6 | -2.375055 | -2.515877 | -1.642835 |
| 8 | -3.401616 | -3.140873 | -1.460281 |
| 1 | -3.346717 | -0.617444 | -0.394602 |
| 6 | -2.962363 | -1.903218 | 1.635739 |
| 1 | -3.060521 | -2.230265 | 2.671732 |
| 1 | -3.575211 | -2.509940 | 0.961959 |
| 1 | -1.913734 | -2.018919 | 1.326911 |
| 6 | -1.121504 | -3.122580 | -2.211461 |
| 1 | -0.742152 | -2.508124 | -3.034746 |
| 1 | -0.354427 | -3.137022 | -1.426943 |
| 1 | -1.314138 | -4.140047 | -2.556362 |

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**$(9\text{-}11)_{10}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy = -1408.3519101
Zero-point correction= 0.368193
Thermal correction to Energy= 0.395638
Thermal correction to Enthalpy= 0.396583
Thermal correction to Gibbs Free Energy= 0.308117
Sum of electronic and zero-point Energies= -1407.983717
Sum of electronic and thermal Energies= -1407.956272
Sum of electronic and thermal Enthalpies= -1407.955328

Sum of electronic and thermal Free Energies= -1408.043793

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.361181 | 3.490323 | 0.825826 |
| 6 | -0.088648 | 2.239350 | 0.276810 |
| 6 | -1.117390 | 1.387143 | -0.148625 |
| 6 | -2.440055 | 1.847409 | -0.064007 |
| 6 | -2.696560 | 3.088189 | 0.498156 |
| 6 | -1.672747 | 3.915977 | 0.959524 |
| 1 | 0.470206 | 4.120085 | 1.137213 |
| 1 | -3.261251 | 1.247964 | -0.439116 |
| 1 | -3.729327 | 3.423414 | 0.561536 |
| 1 | -1.897424 | 4.885973 | 1.393253 |
| 6 | 1.313827 | 1.819244 | 0.082552 |
| 8 | 1.976032 | 1.301373 | 1.083977 |
| 7 | 1.987166 | 2.494969 | -0.863256 |
| 1 | 1.494979 | 2.768588 | -1.705640 |
| 7 | -0.679674 | 0.194182 | -0.709231 |
| 6 | -1.349514 | -0.934189 | -1.176193 |
| 8 | -0.776211 | -1.755438 | -1.864198 |
| 6 | -2.769938 | -1.112409 | -0.761569 |
| 6 | -3.138872 | -1.136240 | 0.585730 |
| 6 | -3.716323 | -1.367464 | -1.754084 |
| 6 | -4.463921 | -1.382587 | 0.926385 |
| 1 | -2.380256 | -0.967624 | 1.348878 |
| 6 | -5.043513 | -1.589146 | -1.407096 |
| 1 | -3.398468 | -1.387403 | -2.794408 |
| 6 | -5.417842 | -1.594292 | -0.065867 |
| 1 | -4.754041 | -1.409110 | 1.974249 |
| 1 | -5.785133 | -1.768600 | -2.182068 |
| 1 | -6.455317 | -1.774768 | 0.207225 |
| 8 | 0.688570 | 0.157126 | -0.846152 |
| 8 | 3.350142 | 2.418415 | -0.974321 |
| 1 | 3.586403 | 1.486274 | -1.169614 |
| 1 | 2.819374 | 0.905796 | 0.767663 |
| 8 | 3.884577 | -0.107547 | -0.380025 |
| 6 | 4.380909 | -1.230470 | -0.483315 |
| 8 | 3.831551 | -2.309396 | -0.000729 |
| 1 | 1.053921 | -0.787327 | -0.063638 |
| 8 | 1.430030 | -1.596108 | 0.646521 |
| 6 | 0.739025 | -1.685015 | 1.770552 |
| 8 | -0.260765 | -1.033627 | 1.999273 |
| 1 | 2.900629 | -2.095158 | 0.329364 |
| 6 | 1.313925 | -2.692795 | 2.729676 |

| | | | |
|---|---|---|---|
| 1 | 1.232940 | -3.695844 | 2.296857 |
| 1 | 2.379355 | -2.499362 | 2.896854 |
| 1 | 0.776274 | -2.661150 | 3.678325 |
| 6 | 5.671220 | -1.483634 | -1.194637 |
| 1 | 6.289187 | -2.177109 | -0.618364 |
| 1 | 5.456734 | -1.965581 | -2.154477 |
| 1 | 6.202943 | -0.547864 | -1.370343 |

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**$(9\text{-}11)_{12}^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -1408.3531939
Zero-point correction= 0.367283
Thermal correction to Energy= 0.393982
Thermal correction to Enthalpy= 0.394927
Thermal correction to Gibbs Free Energy= 0.309472
Sum of electronic and zero-point Energies= -1407.985911
Sum of electronic and thermal Energies= -1407.959212
Sum of electronic and thermal Enthalpies= -1407.958267
Sum of electronic and thermal Free Energies= -1408.043722

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.328124 | 3.297460 | 0.790981 |
| 6 | -0.186128 | 2.031988 | 0.217745 |
| 6 | -1.261625 | 1.124918 | 0.189372 |
| 6 | -2.465471 | 1.513386 | 0.803393 |
| 6 | -2.585432 | 2.772318 | 1.367051 |
| 6 | -1.530595 | 3.685375 | 1.355681 |
| 1 | 0.531257 | 3.966182 | 0.795496 |
| 1 | -3.305135 | 0.829666 | 0.847721 |
| 1 | -3.530032 | 3.043511 | 1.833042 |
| 1 | -1.642403 | 4.671086 | 1.797453 |
| 6 | 1.174538 | 1.657785 | -0.226845 |
| 8 | 2.018143 | 1.273126 | 0.678737 |
| 7 | 1.583729 | 2.130150 | -1.396955 |
| 1 | 0.901996 | 2.306442 | -2.124398 |
| 7 | -1.018154 | -0.095218 | -0.439813 |
| 6 | -1.762506 | -1.279240 | -0.367301 |
| 8 | -1.202015 | -2.357308 | -0.295697 |
| 6 | -3.241317 | -1.178110 | -0.485620 |
| 6 | -4.022133 | -2.075341 | 0.244602 |
| 6 | -3.850761 | -0.295924 | -1.381328 |
| 6 | -5.404934 | -2.057808 | 0.116998 |
| 1 | -3.526521 | -2.781217 | 0.906743 |

| | | | |
|---|---|---|---|
| 6 | -5.232410 | -0.294705 | -1.522864 |
| 1 | -3.233099 | 0.384699 | -1.964017 |
| 6 | -6.010373 | -1.167221 | -0.765793 |
| 1 | -6.012854 | -2.745014 | 0.700419 |
| 1 | -5.704546 | 0.386383 | -2.226749 |
| 1 | -7.092801 | -1.158811 | -0.871103 |
| 8 | 0.280119 | -0.242297 | -0.829939 |
| 8 | 2.885271 | 2.152822 | -1.808456 |
| 1 | 3.267978 | 1.250875 | -1.689522 |
| 1 | 2.866844 | 0.874045 | 0.316822 |
| 8 | 3.997446 | 0.118905 | -0.580692 |
| 6 | 4.746251 | -0.872686 | -0.544233 |
| 8 | 4.846265 | -1.687409 | 0.444432 |
| 1 | 0.981425 | -1.141628 | -0.188273 |
| 8 | 1.853941 | -1.645533 | 0.278746 |
| 6 | 1.924851 | -1.527152 | 1.558351 |
| 8 | 3.016732 | -1.569381 | 2.151049 |
| 1 | 4.090754 | -1.591933 | 1.173594 |
| 6 | 0.651109 | -1.317314 | 2.322558 |
| 1 | 0.292254 | -0.297042 | 2.134212 |
| 1 | -0.113631 | -2.012940 | 1.962702 |
| 1 | 0.823223 | -1.438251 | 3.392921 |
| 6 | 5.619263 | -1.213472 | -1.711908 |
| 1 | 5.134802 | -2.014621 | -2.280867 |
| 1 | 5.756665 | -0.348815 | -2.363159 |
| 1 | 6.582382 | -1.596081 | -1.366142 |

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**$(11\text{-}P)_6^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -1179.3524333
Zero-point correction= 0.306000
Thermal correction to Energy= 0.327292
Thermal correction to Enthalpy= 0.328236
Thermal correction to Gibbs Free Energy= 0.252960
Sum of electronic and zero-point Energies= -1179.046433
Sum of electronic and thermal Energies= -1179.025142
Sum of electronic and thermal Enthalpies= -1179.024198
Sum of electronic and thermal Free Energies= -1179.099473

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.651756 | 2.871206 | -0.537347 |
| 6 | -0.400129 | 1.519871 | -0.390625 |
| 6 | 0.887062 | 1.014217 | -0.261398 |

| | | | |
|---|---|---|---|
| 6 | 1.987848 | 1.865032 | -0.278533 |
| 6 | 1.731928 | 3.227268 | -0.424678 |
| 6 | 0.438309 | 3.735428 | -0.550132 |
| 1 | -1.674487 | 3.223035 | -0.645391 |
| 1 | 3.004670 | 1.495785 | -0.197630 |
| 1 | 2.576851 | 3.911293 | -0.450378 |
| 1 | 0.286816 | 4.804929 | -0.665226 |
| 6 | -1.345870 | 0.380682 | -0.360430 |
| 8 | -2.392884 | 0.410094 | -1.138848 |
| 7 | -1.855354 | 0.183209 | 1.165718 |
| 1 | -1.058684 | 0.151649 | 1.806023 |
| 7 | 0.795050 | -0.394905 | -0.121575 |
| 6 | 1.735893 | -1.361938 | -0.552136 |
| 8 | 1.409558 | -2.315876 | -1.215079 |
| 6 | 3.113809 | -1.145828 | -0.043558 |
| 6 | 4.169875 | -1.579431 | -0.847691 |
| 6 | 3.373809 | -0.618659 | 1.224291 |
| 6 | 5.478461 | -1.449639 | -0.403823 |
| 1 | 3.942785 | -2.018287 | -1.816189 |
| 6 | 4.684140 | -0.505399 | 1.671839 |
| 1 | 2.547464 | -0.311202 | 1.861977 |
| 6 | 5.735886 | -0.911849 | 0.855058 |
| 1 | 6.300721 | -1.774166 | -1.036366 |
| 1 | 4.885271 | -0.105375 | 2.662471 |
| 1 | 6.760928 | -0.817943 | 1.205674 |
| 8 | -0.522355 | -0.766513 | -0.499744 |
| 8 | -2.713083 | 1.181101 | 1.586155 |
| 1 | -3.583123 | 0.793364 | 1.271421 |
| 1 | -3.232303 | -0.102371 | -0.712139 |
| 1 | -2.392822 | -0.705118 | 1.167688 |
| 8 | -5.928620 | -1.310317 | 1.286819 |
| 6 | -5.248737 | -1.163646 | 0.291621 |
| 8 | -4.094142 | -0.525799 | 0.289750 |
| 6 | -5.653714 | -1.702625 | -1.061735 |
| 1 | -5.736424 | -0.882266 | -1.783614 |
| 1 | -4.885314 | -2.384929 | -1.441968 |
| 1 | -6.608882 | -2.226208 | -0.992100 |

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**$(11\text{-}P)_8^{\ddagger}$**

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Number of imaginary frequencies : 1
Electronic energy = -1179.3718636
Zero-point correction= 0.306315
Thermal correction to Energy= 0.327430
Thermal correction to Enthalpy= 0.328374

Thermal correction to Gibbs Free Energy= 0.253936
Sum of electronic and zero-point Energies= -1179.065549
Sum of electronic and thermal Energies= -1179.044434
Sum of electronic and thermal Enthalpies= -1179.043489
Sum of electronic and thermal Free Energies= -1179.117928

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -0.663830 | 2.976089 | -0.476775 |
| 6 | -0.452750 | 1.615266 | -0.364406 |
| 6 | 0.817483 | 1.069329 | -0.235936 |
| 6 | 1.940915 | 1.890361 | -0.214858 |
| 6 | 1.726064 | 3.263198 | -0.325170 |
| 6 | 0.449391 | 3.810317 | -0.453064 |
| 1 | -1.675749 | 3.358042 | -0.582822 |
| 1 | 2.946045 | 1.491911 | -0.130690 |
| 1 | 2.590607 | 3.922855 | -0.319849 |
| 1 | 0.328436 | 4.886429 | -0.539843 |
| 6 | -1.433691 | 0.501452 | -0.375371 |
| 8 | -2.437479 | 0.612182 | -1.216182 |
| 7 | -2.005629 | 0.294214 | 1.070261 |
| 1 | -1.246236 | 0.135165 | 1.737207 |
| 7 | 0.685784 | -0.339582 | -0.139574 |
| 6 | 1.600182 | -1.321042 | -0.587080 |
| 8 | 1.254301 | -2.249100 | -1.277025 |
| 6 | 2.980464 | -1.163176 | -0.061253 |
| 6 | 4.027999 | -1.616115 | -0.865863 |
| 6 | 3.247080 | -0.676934 | 1.221153 |
| 6 | 5.335985 | -1.546347 | -0.407021 |
| 1 | 3.793622 | -2.023007 | -1.846519 |
| 6 | 4.556323 | -0.623380 | 1.683355 |
| 1 | 2.425762 | -0.354414 | 1.857872 |
| 6 | 5.600597 | -1.049279 | 0.866949 |
| 1 | 6.151798 | -1.886325 | -1.039928 |
| 1 | 4.762181 | -0.255485 | 2.685457 |
| 1 | 6.624909 | -1.002683 | 1.229114 |
| 8 | -0.639993 | -0.665494 | -0.533171 |
| 8 | -2.737632 | 1.396652 | 1.494032 |
| 1 | -3.652691 | 1.038250 | 1.444928 |
| 1 | -3.099407 | -0.184951 | -1.160716 |
| 1 | -2.768857 | -0.498792 | 1.075772 |
| 8 | -4.136716 | -1.230638 | -0.989307 |
| 6 | -4.687061 | -1.327106 | 0.128984 |
| 8 | -4.235437 | -0.824180 | 1.213766 |
| 6 | -5.976316 | -2.098027 | 0.242813 |

| | | | |
|---|---|---|---|
| 1 | -6.287710 | -2.489945 | -0.726800 |
| 1 | -5.848514 | -2.918085 | 0.956379 |
| 1 | -6.754655 | -1.444393 | 0.649992 |

## Effect of Solvent Coordination on Lewis Acid in Nucleophilic addition Elimination

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**(9a'-P)$_{6s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2452.9433058
Zero-point correction= 0.439253
Thermal correction to Energy= 0.474211
Thermal correction to Enthalpy= 0.475155
Thermal correction to Gibbs Free Energy= 0.370714
Sum of electronic and zero-point Energies= -2452.504053
Sum of electronic and thermal Energies= -2452.469095
Sum of electronic and thermal Enthalpies= -2452.468150
Sum of electronic and thermal Free Energies= -2452.572592

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.942527 | 2.922618 | -0.426742 |
| 6 | -1.244732 | 1.580508 | -0.262195 |
| 6 | -2.523099 | 1.083829 | -0.509106 |
| 6 | -3.538464 | 1.931498 | -0.938084 |
| 6 | -3.232623 | 3.282606 | -1.091576 |
| 6 | -1.956408 | 3.782081 | -0.841411 |
| 1 | 0.070788 | 3.272847 | -0.230367 |
| 1 | -4.532447 | 1.560166 | -1.165589 |
| 1 | -4.014480 | 3.956328 | -1.433967 |
| 1 | -1.748796 | 4.838949 | -0.983344 |
| 6 | -0.271411 | 0.537368 | 0.180887 |
| 8 | 0.877152 | 0.409011 | -0.272620 |
| 7 | -0.411706 | 0.260102 | 1.692641 |
| 1 | -0.566354 | -1.110884 | 1.777369 |
| 7 | -2.554246 | -0.318202 | -0.298664 |
| 6 | -3.514625 | -1.281433 | -0.626612 |
| 8 | -3.187889 | -2.388860 | -0.994968 |
| 6 | -4.926767 | -0.887289 | -0.383691 |
| 6 | -5.311348 | -0.135406 | 0.728937 |
| 6 | -5.894988 | -1.381480 | -1.259089 |
| 6 | -6.654991 | 0.139960 | 0.948443 |
| 1 | -4.557207 | 0.223471 | 1.426523 |
| 6 | -7.235716 | -1.088315 | -1.046966 |

| | | | |
|---|---|---|---|
| 1 | -5.577762 | -1.995753 | -2.098294 |
| 6 | -7.615663 | -0.327792 | 0.055751 |
| 1 | -6.954341 | 0.716331 | 1.820265 |
| 1 | -7.987565 | -1.461605 | -1.737714 |
| 1 | -8.666608 | -0.106254 | 0.226192 |
| 8 | -1.231865 | -0.771793 | -0.436256 |
| 8 | 0.775906 | 0.416490 | 2.402261 |
| 1 | 1.063764 | 1.361431 | 2.326923 |
| 1 | -1.008678 | -1.705046 | 0.337651 |
| 30 | 2.735374 | 0.833734 | 0.453705 |
| 17 | 3.903350 | -0.913992 | 1.294340 |
| 17 | 2.296760 | 2.860038 | 1.455449 |
| 8 | -0.631620 | -2.164200 | 1.364738 |
| 1 | -1.136333 | 0.857891 | 2.096907 |
| 6 | 0.596978 | -2.810244 | 1.232284 |
| 6 | 1.328126 | -2.914353 | 2.524028 |
| 1 | 2.161320 | -3.609208 | 2.415004 |
| 1 | 1.742853 | -1.926843 | 2.766461 |
| 1 | 0.654956 | -3.223643 | 3.328553 |
| 8 | 0.943533 | -3.203869 | 0.156350 |
| 8 | 3.694781 | 1.075206 | -1.331479 |
| 6 | 4.546911 | 0.213161 | -1.655705 |
| 6 | 6.002489 | 0.532841 | -1.494842 |
| 1 | 6.606055 | 0.266077 | -2.367252 |
| 1 | 6.091143 | 1.602845 | -1.302519 |
| 1 | 6.387115 | -0.010232 | -0.622175 |
| 7 | 4.182995 | -0.985767 | -2.129422 |
| 6 | 5.093839 | -2.113752 | -2.204045 |
| 1 | 5.038770 | -2.695169 | -1.272943 |
| 1 | 4.802357 | -2.756344 | -3.040856 |
| 1 | 6.123921 | -1.792760 | -2.360948 |
| 6 | 2.771976 | -1.347780 | -2.194062 |
| 1 | 2.603321 | -1.948517 | -3.093551 |
| 1 | 2.486435 | -1.938476 | -1.312662 |
| 1 | 2.153643 | -0.450976 | -2.230539 |

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**$(9a'\text{-}P)_{8s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2452.9729893
Zero-point correction= 0.441627
Thermal correction to Energy= 0.476367
Thermal correction to Enthalpy= 0.477311
Thermal correction to Gibbs Free Energy= 0.373843
Sum of electronic and zero-point Energies= -2452.531363

Sum of electronic and thermal Energies= -2452.496623
Sum of electronic and thermal Enthalpies= -2452.495678
Sum of electronic and thermal Free Energies= -2452.599146

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.546355 | 2.981064 | -0.365492 |
| 6 | 0.874491 | 1.682033 | 0.011632 |
| 6 | 2.154035 | 1.345769 | 0.468312 |
| 6 | 3.120310 | 2.349586 | 0.566655 |
| 6 | 2.790538 | 3.639977 | 0.169970 |
| 6 | 1.519059 | 3.968214 | -0.298473 |
| 1 | -0.464301 | 3.194240 | -0.710514 |
| 1 | 4.108203 | 2.137775 | 0.960824 |
| 1 | 3.548987 | 4.414941 | 0.251386 |
| 1 | 1.286433 | 4.987929 | -0.590378 |
| 6 | -0.134078 | 0.613178 | -0.064975 |
| 8 | -1.258785 | 0.624226 | 0.396570 |
| 7 | 0.036573 | -0.230013 | -1.343343 |
| 1 | -0.308698 | 0.382405 | -2.116322 |
| 7 | 2.281216 | 0.008870 | 0.859535 |
| 6 | 3.375277 | -0.740881 | 1.281838 |
| 8 | 3.223714 | -1.764021 | 1.919905 |
| 6 | 4.710214 | -0.278363 | 0.815670 |
| 6 | 4.953301 | -0.012044 | -0.534073 |
| 6 | 5.750692 | -0.217659 | 1.743187 |
| 6 | 6.232180 | 0.346305 | -0.942403 |
| 1 | 4.144914 | -0.110849 | -1.257069 |
| 6 | 7.021598 | 0.164202 | 1.332006 |
| 1 | 5.547481 | -0.469658 | 2.781650 |
| 6 | 7.261301 | 0.448821 | -0.009994 |
| 1 | 6.427805 | 0.544149 | -1.993523 |
| 1 | 7.829023 | 0.231210 | 2.057047 |
| 1 | 8.258170 | 0.740505 | -0.332494 |
| 8 | 1.035591 | -0.577269 | 1.037239 |
| 8 | -0.869677 | -1.285462 | -1.359515 |
| 1 | 1.027733 | -0.623250 | -1.515107 |
| 1 | -0.421344 | -2.010646 | -0.853070 |
| 8 | 2.254839 | -1.626454 | -1.684313 |
| 6 | 2.056566 | -2.634394 | -0.981912 |
| 8 | 1.106596 | -2.698162 | -0.096003 |
| 1 | 1.078879 | -1.650796 | 0.540117 |
| 30 | -2.953888 | 0.011001 | -0.817650 |
| 17 | -2.315521 | 1.225104 | -2.655174 |
| 17 | -3.987794 | -1.953045 | -0.427016 |

| | | | |
|---|---|---|---|
| 6 | 2.943942 | -3.830838 | -1.076170 |
| 1 | 2.347441 | -4.746672 | -1.055451 |
| 1 | 3.572171 | -3.788989 | -1.967066 |
| 1 | 3.573851 | -3.838621 | -0.177931 |
| 8 | -4.198157 | 1.226252 | 0.290005 |
| 6 | -5.178976 | 0.710929 | 0.873607 |
| 6 | -6.526141 | 0.735910 | 0.217677 |
| 1 | -6.757812 | -0.270626 | -0.153321 |
| 1 | -7.328780 | 1.054864 | 0.889138 |
| 1 | -6.471888 | 1.414689 | -0.634455 |
| 7 | -5.039266 | 0.131535 | 2.076287 |
| 6 | -6.030943 | -0.766908 | 2.639115 |
| 1 | -5.813244 | -1.800135 | 2.333317 |
| 1 | -5.997105 | -0.704569 | 3.731369 |
| 1 | -7.038912 | -0.508081 | 2.314033 |
| 6 | -3.702757 | -0.001990 | 2.638005 |
| 1 | -3.776654 | -0.020550 | 3.729298 |
| 1 | -3.240220 | -0.936120 | 2.288139 |
| 1 | -3.083578 | 0.838738 | 2.323560 |

---

**$(9a'\text{-}11a')_{6s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2681.9237836
Zero-point correction= 0.499374
Thermal correction to Energy= 0.541902
Thermal correction to Enthalpy= 0.542846
Thermal correction to Gibbs Free Energy= 0.416573
Sum of electronic and zero-point Energies= -2681.424410
Sum of electronic and thermal Energies= -2681.381882
Sum of electronic and thermal Enthalpies= -2681.380938
Sum of electronic and thermal Free Energies= -2681.507211

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -0.471791 | -0.842808 | 2.334878 |
| 6 | -0.811247 | -0.399461 | 1.053812 |
| 6 | -1.847809 | 0.524754 | 0.840447 |
| 6 | -2.569672 | 0.965079 | 1.960521 |
| 6 | -2.226242 | 0.520014 | 3.226859 |
| 6 | -1.174311 | -0.373911 | 3.432928 |
| 1 | 0.350538 | -1.550768 | 2.448658 |
| 1 | -3.414055 | 1.634757 | 1.837008 |
| 1 | -2.810512 | 0.868206 | 4.075396 |
| 1 | -0.918610 | -0.709623 | 4.433561 |

| | | | |
|---|---|---|---|
| 6 | -0.062304 | -0.992687 | -0.070390 |
| 8 | -0.184020 | -2.210660 | -0.438398 |
| 7 | 1.005009 | -0.323787 | -0.498717 |
| 1 | 1.378704 | 0.510407 | -0.047743 |
| 7 | -2.091052 | 0.894926 | -0.480233 |
| 6 | -3.064558 | 1.778244 | -0.979467 |
| 8 | -3.614440 | 1.561828 | -2.035798 |
| 6 | -3.302839 | 3.032124 | -0.210148 |
| 6 | -4.590761 | 3.569378 | -0.234415 |
| 6 | -2.273279 | 3.730487 | 0.424636 |
| 6 | -4.855383 | 4.774075 | 0.404608 |
| 1 | -5.369852 | 3.029436 | -0.767126 |
| 6 | -2.536126 | 4.944516 | 1.046906 |
| 1 | -1.263706 | 3.324407 | 0.418082 |
| 6 | -3.828672 | 5.462123 | 1.045570 |
| 1 | -5.862729 | 5.183106 | 0.394927 |
| 1 | -1.730725 | 5.490706 | 1.532385 |
| 1 | -4.034168 | 6.409645 | 1.538528 |
| 8 | -1.600132 | -0.003611 | -1.396236 |
| 8 | 1.914720 | -0.965939 | -1.307793 |
| 1 | 1.703280 | -0.747921 | -2.230650 |
| 1 | -1.051903 | -2.613579 | -0.082265 |
| 30 | 3.790887 | -1.047780 | -0.130554 |
| 17 | 3.126914 | -2.147334 | 1.658239 |
| 17 | 5.399530 | -0.907368 | -1.662236 |
| 8 | 3.361935 | 0.999148 | 0.196757 |
| 6 | 4.170170 | 1.798167 | -0.346940 |
| 6 | 3.761862 | 2.516798 | -1.594728 |
| 1 | 4.001724 | 3.583547 | -1.583247 |
| 1 | 4.274703 | 2.054337 | -2.448371 |
| 1 | 2.685010 | 2.394068 | -1.729692 |
| 7 | 5.391694 | 1.984177 | 0.160850 |
| 6 | 6.470251 | 2.619829 | -0.579354 |
| 1 | 6.092305 | 3.354017 | -1.291011 |
| 1 | 7.134239 | 3.132066 | 0.122933 |
| 1 | 7.042802 | 1.856669 | -1.124087 |
| 6 | 5.819856 | 1.194332 | 1.308674 |
| 1 | 6.366104 | 0.303124 | 0.968034 |
| 1 | 6.484269 | 1.801667 | 1.930159 |
| 1 | 4.953460 | 0.888274 | 1.897363 |
| 8 | -2.498317 | -3.006474 | 0.230862 |
| 1 | -3.091314 | -2.444427 | -0.483539 |
| 8 | -3.430535 | -1.537261 | -1.427114 |
| 1 | -2.500936 | -0.738074 | -1.569080 |
| 6 | -3.201127 | -3.721886 | 1.115870 |

| | | | |
|---|---|---|---|
| 6 | -4.175984 | -1.819902 | -2.499189 |
| 8 | -4.397127 | -3.868515 | 1.031797 |
| 8 | -3.936405 | -1.389351 | -3.602430 |
| 6 | -2.338060 | -4.292470 | 2.203798 |
| 1 | -1.499120 | -4.851355 | 1.776409 |
| 1 | -1.915494 | -3.473486 | 2.798170 |
| 1 | -2.931132 | -4.942329 | 2.848239 |
| 6 | -5.358823 | -2.693499 | -2.170630 |
| 1 | -5.145148 | -3.387633 | -1.350678 |
| 1 | -6.179575 | -2.049207 | -1.835106 |
| 1 | -5.688216 | -3.226998 | -3.064654 |

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**(9a'-11a')$_{8's}$‡**

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Number of imaginary frequencies : 1
Electronic energy =-2452.994046
Zero-point correction= 0.439399
Thermal correction to Energy= 0.474584
Thermal correction to Enthalpy= 0.475528
Thermal correction to Gibbs Free Energy= 0.371009
Sum of electronic and zero-point Energies= -2452.554647
Sum of electronic and thermal Energies= -2452.519462
Sum of electronic and thermal Enthalpies= -2452.518518
Sum of electronic and thermal Free Energies= -2452.623037

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.726578 | -3.445028 | 0.420654 |
| 6 | 1.502692 | -2.131122 | 0.039671 |
| 6 | 2.504095 | -1.166034 | 0.137372 |
| 6 | 3.759030 | -1.506661 | 0.639330 |
| 6 | 3.975565 | -2.828990 | 1.015665 |
| 6 | 2.978932 | -3.798176 | 0.910793 |
| 1 | 0.921406 | -4.171413 | 0.331806 |
| 1 | 4.545202 | -0.766746 | 0.748754 |
| 1 | 4.949619 | -3.102785 | 1.414099 |
| 1 | 3.178153 | -4.820636 | 1.218730 |
| 6 | 0.204037 | -1.616075 | -0.492779 |
| 8 | -0.876607 | -1.712975 | 0.213965 |
| 7 | 0.052717 | -1.872174 | -1.856770 |
| 1 | 0.850277 | -1.555151 | -2.403389 |
| 7 | 2.029466 | 0.089392 | -0.297643 |
| 6 | 2.586475 | 1.365093 | -0.241201 |
| 8 | 1.894083 | 2.344941 | -0.046231 |
| 6 | 4.045741 | 1.456830 | -0.506211 |

| | | | |
|---|---|---|---|
| 6 | 4.767355 | 2.439389 | 0.173652 |
| 6 | 4.677880 | 0.674314 | -1.475666 |
| 6 | 6.121463 | 2.609058 | -0.082691 |
| 1 | 4.246785 | 3.063510 | 0.895986 |
| 6 | 6.028569 | 0.858343 | -1.742294 |
| 1 | 4.106757 | -0.071477 | -2.024938 |
| 6 | 6.752299 | 1.818442 | -1.039898 |
| 1 | 6.684955 | 3.365935 | 0.457173 |
| 1 | 6.517096 | 0.256324 | -2.504329 |
| 1 | 7.810859 | 1.957750 | -1.246538 |
| 8 | 0.637555 | 0.069372 | -0.312072 |
| 8 | -1.093699 | -1.264893 | -2.375256 |
| 1 | -0.646891 | -1.573984 | 1.578540 |
| 1 | -1.721349 | -1.990142 | -2.570385 |
| 30 | -2.628408 | -0.730942 | -0.475834 |
| 17 | -3.932600 | -2.112595 | -1.714967 |
| 17 | -3.317075 | 0.055442 | 1.604708 |
| 8 | -2.226346 | 1.125502 | -1.255608 |
| 6 | -2.530816 | 2.171821 | -0.640877 |
| 7 | -3.804958 | 2.598982 | -0.596929 |
| 6 | -4.272728 | 3.574317 | 0.369168 |
| 1 | -5.102574 | 4.144035 | -0.061730 |
| 1 | -4.624705 | 3.060397 | 1.275413 |
| 1 | -3.482809 | 4.273667 | 0.644809 |
| 6 | -4.850269 | 1.772725 | -1.183197 |
| 1 | -5.244449 | 1.067677 | -0.437675 |
| 1 | -5.660962 | 2.420977 | -1.530555 |
| 1 | -4.451871 | 1.207054 | -2.026603 |
| 6 | -1.460369 | 2.956311 | 0.052712 |
| 1 | -1.528870 | 4.032621 | -0.132017 |
| 1 | -1.544048 | 2.782346 | 1.133757 |
| 1 | -0.481323 | 2.590529 | -0.270806 |
| 1 | 0.246458 | 0.416593 | 0.933986 |
| 8 | -0.542024 | -1.333892 | 2.612109 |
| 6 | -0.383250 | -0.089440 | 2.822615 |
| 8 | 0.028036 | 0.746504 | 1.962366 |
| 6 | -0.713797 | 0.416321 | 4.175010 |
| 1 | -0.548917 | -0.357764 | 4.926410 |
| 1 | -0.159951 | 1.328056 | 4.402517 |
| 1 | -1.787584 | 0.644003 | 4.150646 |

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**$(9a'\text{-}11a')_{8s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2681.9237836

Zero-point correction= 0.499374
Thermal correction to Energy= 0.541902
Thermal correction to Enthalpy= 0.542846
Thermal correction to Gibbs Free Energy= 0.416573
Sum of electronic and zero-point Energies= -2681.424410
Sum of electronic and thermal Energies= -2681.381882
Sum of electronic and thermal Enthalpies= -2681.380938
Sum of electronic and thermal Free Energies= -2681.507211

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | -0.471791 | -0.842808 | 2.334878 |
| 6 | -0.811247 | -0.399461 | 1.053812 |
| 6 | -1.847809 | 0.524754 | 0.840447 |
| 6 | -2.569672 | 0.965079 | 1.960521 |
| 6 | -2.226242 | 0.520014 | 3.226859 |
| 6 | -1.174311 | -0.373911 | 3.432928 |
| 1 | 0.350538 | -1.550768 | 2.448658 |
| 1 | -3.414055 | 1.634757 | 1.837008 |
| 1 | -2.810512 | 0.868206 | 4.075396 |
| 1 | -0.918610 | -0.709623 | 4.433561 |
| 6 | -0.062304 | -0.992687 | -0.070390 |
| 8 | -0.184020 | -2.210660 | -0.438398 |
| 7 | 1.005009 | -0.323787 | -0.498717 |
| 1 | 1.378704 | 0.510407 | -0.047743 |
| 7 | -2.091052 | 0.894926 | -0.480233 |
| 6 | -3.064558 | 1.778244 | -0.979467 |
| 8 | -3.614440 | 1.561828 | -2.035798 |
| 6 | -3.302839 | 3.032124 | -0.210148 |
| 6 | -4.590761 | 3.569378 | -0.234415 |
| 6 | -2.273279 | 3.730487 | 0.424636 |
| 6 | -4.855383 | 4.774075 | 0.404608 |
| 1 | -5.369852 | 3.029436 | -0.767126 |
| 6 | -2.536126 | 4.944516 | 1.046906 |
| 1 | -1.263706 | 3.324407 | 0.418082 |
| 6 | -3.828672 | 5.462123 | 1.045570 |
| 1 | -5.862729 | 5.183106 | 0.394927 |
| 1 | -1.730725 | 5.490706 | 1.532385 |
| 1 | -4.034168 | 6.409645 | 1.538528 |
| 8 | -1.600132 | -0.003611 | -1.396236 |
| 8 | 1.914720 | -0.965939 | -1.307793 |
| 1 | 1.703280 | -0.747921 | -2.230650 |
| 1 | -1.051903 | -2.613579 | -0.082265 |
| 30 | 3.790887 | -1.047780 | -0.130554 |
| 17 | 3.126914 | -2.147334 | 1.658239 |

| | | | |
|---|---|---|---|
| 17 | 5.399530 | -0.907368 | -1.662236 |
| 8 | 3.361935 | 0.999148 | 0.196757 |
| 6 | 4.170170 | 1.798167 | -0.346940 |
| 6 | 3.761862 | 2.516798 | -1.594728 |
| 1 | 4.001724 | 3.583547 | -1.583247 |
| 1 | 4.274703 | 2.054337 | -2.448371 |
| 1 | 2.685010 | 2.394068 | -1.729692 |
| 7 | 5.391694 | 1.984177 | 0.160850 |
| 6 | 6.470251 | 2.619829 | -0.579354 |
| 1 | 6.092305 | 3.354017 | -1.291011 |
| 1 | 7.134239 | 3.132066 | 0.122933 |
| 1 | 7.042802 | 1.856669 | -1.124087 |
| 6 | 5.819856 | 1.194332 | 1.308674 |
| 1 | 6.366104 | 0.303124 | 0.968034 |
| 1 | 6.484269 | 1.801667 | 1.930159 |
| 1 | 4.953460 | 0.888274 | 1.897363 |
| 8 | -2.498317 | -3.006474 | 0.230862 |
| 1 | -3.091314 | -2.444427 | -0.483539 |
| 8 | -3.430535 | -1.537261 | -1.427114 |
| 1 | -2.500936 | -0.738074 | -1.569080 |
| 6 | -3.201127 | -3.721886 | 1.115870 |
| 6 | -4.175984 | -1.819902 | -2.499189 |
| 8 | -4.397127 | -3.868515 | 1.031797 |
| 8 | -3.936405 | -1.389351 | -3.602430 |
| 6 | -2.338060 | -4.292470 | 2.203798 |
| 1 | -1.499120 | -4.851355 | 1.776409 |
| 1 | -1.915494 | -3.473486 | 2.798170 |
| 1 | -2.931132 | -4.942329 | 2.848239 |
| 6 | -5.358823 | -2.693499 | -2.170630 |
| 1 | -5.145148 | -3.387633 | -1.350678 |
| 1 | -6.179575 | -2.049207 | -1.835106 |
| 1 | -5.688216 | -3.226998 | -3.064654 |

---

**$(9a'\text{-}11a')_{10s}^{\ddagger}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2681.9648001
Zero-point correction= 0.507022
Thermal correction to Energy= 0.546785
Thermal correction to Enthalpy= 0.547729
Thermal correction to Gibbs Free Energy= 0.435419
Sum of electronic and zero-point Energies= -2681.457778
Sum of electronic and thermal Energies= -2681.418015
Sum of electronic and thermal Enthalpies= -2681.417071
Sum of electronic and thermal Free Energies= -2681.529381

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -1.204053 | 3.285742 | 1.071542 |
| 6 | -1.289151 | 2.190526 | 0.226059 |
| 6 | -2.515268 | 1.744230 | -0.253157 |
| 6 | -3.684231 | 2.423501 | 0.071192 |
| 6 | -3.587838 | 3.535862 | 0.901130 |
| 6 | -2.365263 | 3.971817 | 1.405582 |
| 1 | -0.234956 | 3.581786 | 1.472433 |
| 1 | -4.653391 | 2.092850 | -0.284688 |
| 1 | -4.498245 | 4.069377 | 1.163408 |
| 1 | -2.321203 | 4.838224 | 2.059465 |
| 6 | -0.125178 | 1.341779 | -0.148876 |
| 8 | 0.429579 | 0.595342 | 0.726751 |
| 7 | 0.704413 | 1.998747 | -1.131447 |
| 1 | 1.027131 | 2.884067 | -0.738030 |
| 7 | -2.377924 | 0.548188 | -1.019374 |
| 6 | -3.110666 | -0.623595 | -0.826312 |
| 8 | -2.553341 | -1.706148 | -0.718066 |
| 6 | -4.581375 | -0.483041 | -0.908236 |
| 6 | -5.376319 | -1.259409 | -0.064698 |
| 6 | -5.176312 | 0.323868 | -1.881357 |
| 6 | -6.758755 | -1.198874 | -0.166188 |
| 1 | -4.896868 | -1.898917 | 0.671355 |
| 6 | -6.561099 | 0.369258 | -1.991190 |
| 1 | -4.547002 | 0.905467 | -2.552366 |
| 6 | -7.351398 | -0.385147 | -1.128860 |
| 1 | -7.378020 | -1.790779 | 0.503019 |
| 1 | -7.023833 | 0.990159 | -2.754167 |
| 1 | -8.434891 | -0.344466 | -1.211806 |
| 8 | -1.018383 | 0.323716 | -1.206709 |
| 8 | 1.890993 | 1.249962 | -1.313156 |
| 1 | 1.748185 | 0.729691 | -2.117099 |
| 1 | -0.587592 | -0.538555 | 1.520158 |
| 1 | -0.501253 | -0.813654 | -1.152245 |
| 30 | 2.470368 | 0.106682 | 0.532329 |
| 17 | 3.762853 | 1.820432 | 1.316852 |
| 17 | 2.323364 | -1.937054 | 1.538731 |
| 8 | 3.798284 | -0.635279 | -1.113113 |
| 6 | 4.988625 | -0.539160 | -0.742441 |
| 6 | 5.568826 | -1.524216 | 0.231498 |
| 1 | 5.764298 | -1.026755 | 1.190180 |
| 1 | 4.828460 | -2.306209 | 0.413158 |
| 1 | 6.506426 | -1.960279 | -0.129208 |

| | | | |
|---|---|---|---|
| 7 | 5.772109 | 0.455622 | -1.202582 |
| 6 | 7.023217 | 0.828099 | -0.567716 |
| 1 | 7.512742 | -0.034533 | -0.114500 |
| 1 | 7.700773 | 1.247487 | -1.318781 |
| 1 | 6.842452 | 1.582271 | 0.211436 |
| 6 | 5.164643 | 1.490539 | -2.025132 |
| 1 | 4.654201 | 2.227679 | -1.390123 |
| 1 | 5.948270 | 1.981484 | -2.610164 |
| 1 | 4.435127 | 1.040394 | -2.699312 |
| 8 | 0.372046 | -1.558613 | -1.365378 |
| 6 | 0.548599 | -2.703967 | -0.882873 |
| 8 | -0.213411 | -3.248145 | 0.000630 |
| 1 | -0.798949 | -2.581995 | 0.439095 |
| 8 | -1.051166 | -1.380668 | 1.786811 |
| 6 | -2.328247 | -1.170413 | 2.132780 |
| 8 | -2.885976 | -0.102621 | 2.024846 |
| 6 | 1.673648 | -3.522220 | -1.393995 |
| 1 | 1.819243 | -4.407820 | -0.775776 |
| 1 | 1.467928 | -3.806556 | -2.431706 |
| 1 | 2.571413 | -2.893777 | -1.380262 |
| 6 | -2.960010 | -2.434298 | 2.633361 |
| 1 | -3.967534 | -2.229239 | 2.999575 |
| 1 | -3.003500 | -3.164403 | 1.815270 |
| 1 | -2.349680 | -2.874441 | 3.427141 |

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**(9a'-11a')$_{12s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2681.9837996
Zero-point correction= 0.505040
Thermal correction to Energy= 0.544906
Thermal correction to Enthalpy= 0.545850
Thermal correction to Gibbs Free Energy= 0.432757
Sum of electronic and zero-point Energies= -2681.478760
Sum of electronic and thermal Energies= -2681.438893
Sum of electronic and thermal Enthalpies= -2681.437949
Sum of electronic and thermal Free Energies= -2681.551043

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 0.574680 | -2.816565 | 0.754837 |
| 6 | 0.963861 | -1.817647 | -0.121931 |
| 6 | 2.301616 | -1.587268 | -0.417428 |
| 6 | 3.301221 | -2.376621 | 0.145055 |
| 6 | 2.903095 | -3.398512 | 1.005858 |

| | | | |
|---|---|---|---|
| 6 | 1.561799 | -3.625055 | 1.312769 |
| 1 | -0.479434 | -2.930660 | 1.013060 |
| 1 | 4.352723 | -2.212836 | -0.064698 |
| 1 | 3.668883 | -4.032025 | 1.447895 |
| 1 | 1.288212 | -4.426682 | 1.993411 |
| 6 | 0.110849 | -0.748221 | -0.736093 |
| 8 | -0.398480 | 0.146609 | 0.109970 |
| 7 | -0.852154 | -1.340857 | -1.668731 |
| 1 | -1.377952 | -2.043248 | -1.137689 |
| 7 | 2.396628 | -0.472389 | -1.292161 |
| 6 | 3.251874 | 0.618320 | -1.169027 |
| 8 | 2.854735 | 1.759264 | -1.340275 |
| 6 | 4.672577 | 0.293331 | -0.906780 |
| 6 | 5.342942 | 1.010559 | 0.085225 |
| 6 | 5.354649 | -0.651779 | -1.674988 |
| 6 | 6.685574 | 0.752895 | 0.330547 |
| 1 | 4.791974 | 1.751580 | 0.660263 |
| 6 | 6.703612 | -0.890609 | -1.438324 |
| 1 | 4.823134 | -1.191932 | -2.456605 |
| 6 | 7.365745 | -0.195397 | -0.430162 |
| 1 | 7.207055 | 1.297709 | 1.113782 |
| 1 | 7.239350 | -1.618530 | -2.042561 |
| 1 | 8.419086 | -0.388531 | -0.240662 |
| 8 | 1.099445 | -0.081766 | -1.639736 |
| 8 | -1.873929 | -0.374609 | -1.929438 |
| 1 | -1.543685 | 0.134119 | -2.681797 |
| 1 | 0.098165 | 0.131608 | 1.509224 |
| 30 | -2.463083 | 0.348562 | 0.129985 |
| 17 | -3.058937 | -1.807548 | 0.834986 |
| 17 | -2.472973 | 2.189706 | 1.485300 |
| 8 | -4.285467 | 0.720163 | -0.916394 |
| 6 | -5.269673 | 0.187223 | -0.362442 |
| 6 | -5.803432 | 0.733525 | 0.929616 |
| 1 | -5.627462 | 0.007672 | 1.733726 |
| 1 | -5.252116 | 1.646218 | 1.166534 |
| 1 | -6.876677 | 0.945378 | 0.882033 |
| 7 | -5.863167 | -0.894876 | -0.904219 |
| 6 | -6.808182 | -1.711325 | -0.165746 |
| 1 | -7.455904 | -1.102298 | 0.467400 |
| 1 | -7.441420 | -2.254297 | -0.874620 |
| 1 | -6.274108 | -2.438892 | 0.463064 |
| 6 | -5.216920 | -1.568074 | -2.019314 |
| 1 | -4.597904 | -2.395114 | -1.642453 |
| 1 | -5.980041 | -1.957632 | -2.701574 |
| 1 | -4.569165 | -0.863911 | -2.540551 |

| | | | |
|---|---|---|---|
| 8 | 0.229643 | 2.532052 | -1.407279 |
| 6 | 0.241867 | 3.242226 | -0.335226 |
| 8 | 0.901591 | 2.976338 | 0.699840 |
| 1 | 1.458456 | 2.046800 | 0.864575 |
| 8 | 0.616986 | -0.045912 | 2.393231 |
| 6 | 1.847558 | 0.311941 | 2.269065 |
| 8 | 2.261163 | 1.111802 | 1.404403 |
| 6 | -0.608388 | 4.451071 | -0.342972 |
| 1 | -0.184923 | 5.209684 | 0.316738 |
| 1 | -0.745639 | 4.826596 | -1.357932 |
| 1 | -1.579157 | 4.143118 | 0.072009 |
| 6 | 2.796919 | -0.311346 | 3.235132 |
| 1 | 2.577268 | 0.050189 | 4.245044 |
| 1 | 2.645547 | -1.395482 | 3.233897 |
| 1 | 3.826604 | -0.066896 | 2.967228 |
| 1 | 0.866358 | 1.764063 | -1.378009 |

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**(11a'-P)$_{6s}^{‡}$**

---

Number of imaginary frequencies : 1
Electronic energy =-2452.9755505
Zero-point correction= 0.442143
Thermal correction to Energy= 0.477255
Thermal correction to Enthalpy= 0.478199
Thermal correction to Gibbs Free Energy= 0.372084
Sum of electronic and zero-point Energies= -2452.533407
Sum of electronic and thermal Energies= -2452.498296
Sum of electronic and thermal Enthalpies= -2452.497351
Sum of electronic and thermal Free Energies= -2452.603466

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.057716 | 2.455268 | 0.565407 |
| 6 | 1.400589 | 1.119659 | 0.437913 |
| 6 | 2.703869 | 0.713502 | 0.173267 |
| 6 | 3.717993 | 1.649440 | 0.003694 |
| 6 | 3.365939 | 2.992500 | 0.119524 |
| 6 | 2.062938 | 3.400861 | 0.399948 |
| 1 | 0.033531 | 2.754707 | 0.778171 |
| 1 | 4.738739 | 1.361392 | -0.222221 |
| 1 | 4.139620 | 3.743407 | -0.021634 |
| 1 | 1.827095 | 4.457744 | 0.477166 |
| 6 | 0.572004 | -0.102915 | 0.527594 |
| 8 | -0.617826 | -0.095709 | -0.125658 |
| 7 | 0.275787 | -0.487584 | 2.009056 |

| | | | |
|---|---|---|---|
| 1 | 1.149569 | -0.806217 | 2.432481 |
| 7 | 2.737561 | -0.703722 | 0.144187 |
| 6 | 3.575418 | -1.537962 | -0.636657 |
| 8 | 3.130312 | -2.439009 | -1.304449 |
| 6 | 5.024773 | -1.262779 | -0.478548 |
| 6 | 5.852067 | -1.524047 | -1.572829 |
| 6 | 5.581206 | -0.843510 | 0.733007 |
| 6 | 7.222260 | -1.328813 | -1.467503 |
| 1 | 5.402186 | -1.879648 | -2.496566 |
| 6 | 6.954839 | -0.663858 | 0.838617 |
| 1 | 4.936880 | -0.666459 | 1.591633 |
| 6 | 7.773422 | -0.898179 | -0.262953 |
| 1 | 7.864061 | -1.518397 | -2.324008 |
| 1 | 7.388283 | -0.345614 | 1.783378 |
| 1 | 8.847736 | -0.751869 | -0.179914 |
| 8 | 1.387433 | -1.147336 | 0.076305 |
| 8 | -0.157992 | 0.575945 | 2.787884 |
| 1 | -1.057234 | 0.826327 | 2.444197 |
| 1 | -1.174128 | -0.915838 | 0.167737 |
| 1 | -0.509135 | -1.281647 | 1.945795 |
| 8 | -3.851780 | -1.961734 | 1.055137 |
| 6 | -2.839655 | -1.978840 | 1.743329 |
| 8 | -1.627352 | -1.898896 | 1.264457 |
| 30 | -2.122710 | 1.438760 | -0.573994 |
| 17 | -2.770831 | 1.686408 | 1.618814 |
| 17 | -1.392510 | 3.080635 | -1.856229 |
| 8 | -3.131714 | -0.050431 | -1.423779 |
| 6 | -4.282648 | -0.521374 | -1.254959 |
| 6 | -5.346787 | 0.257229 | -0.549937 |
| 1 | -6.284721 | 0.284047 | -1.112526 |
| 1 | -5.526322 | -0.206832 | 0.426703 |
| 1 | -5.001559 | 1.280030 | -0.383191 |
| 7 | -4.561007 | -1.735831 | -1.744281 |
| 6 | -3.436568 | -2.550627 | -2.184983 |
| 1 | -3.815842 | -3.387846 | -2.776374 |
| 1 | -2.757296 | -1.953115 | -2.793813 |
| 1 | -2.892496 | -2.928611 | -1.308238 |
| 6 | -5.750438 | -2.469011 | -1.346783 |
| 1 | -5.586710 | -2.951273 | -0.374392 |
| 1 | -6.617533 | -1.809936 | -1.276294 |
| 1 | -5.967362 | -3.228342 | -2.103524 |
| 6 | -2.905160 | -2.111127 | 3.247669 |
| 1 | -3.940657 | -2.140101 | 3.590515 |
| 1 | -2.385342 | -3.021846 | 3.565039 |
| 1 | -2.390954 | -1.261774 | 3.714936 |

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**$(11a'\text{-}P)_{8s}^{‡}$**

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Number of imaginary frequencies : 1
Electronic energy = -2453.0002798
Zero-point correction= 0.440082
Thermal correction to Energy= 0.474624
Thermal correction to Enthalpy= 0.475568
Thermal correction to Gibbs Free Energy= 0.373674
Sum of electronic and zero-point Energies= -2452.560198
Sum of electronic and thermal Energies= -2452.525656
Sum of electronic and thermal Enthalpies= -2452.524711
Sum of electronic and thermal Free Energies= -2452.626606

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 6 | 0.066171 | -1.996415 | -2.646487 |
| 6 | -0.220581 | -1.979852 | -1.289823 |
| 6 | -1.525029 | -1.837430 | -0.828245 |
| 6 | -2.591491 | -1.710308 | -1.702725 |
| 6 | -2.301150 | -1.729749 | -3.065784 |
| 6 | -0.998891 | -1.874875 | -3.536762 |
| 1 | 1.090480 | -2.080164 | -3.000286 |
| 1 | -3.609170 | -1.585283 | -1.347403 |
| 1 | -3.117856 | -1.629018 | -3.776341 |
| 1 | -0.808072 | -1.886305 | -4.606142 |
| 6 | 0.663868 | -1.965643 | -0.081189 |
| 8 | 1.357827 | -0.838183 | 0.120750 |
| 7 | 1.663999 | -3.076344 | 0.029785 |
| 1 | 1.215607 | -3.975425 | -0.151399 |
| 7 | -1.517545 | -1.824356 | 0.604902 |
| 6 | -1.845798 | -0.617197 | 1.294963 |
| 8 | -1.073681 | -0.067876 | 2.045317 |
| 6 | -3.240656 | -0.169714 | 1.070016 |
| 6 | -3.479433 | 1.200831 | 0.964234 |
| 6 | -4.306028 | -1.072377 | 1.033991 |
| 6 | -4.775700 | 1.664568 | 0.790629 |
| 1 | -2.630095 | 1.879624 | 0.988864 |
| 6 | -5.605159 | -0.601638 | 0.879768 |
| 1 | -4.109948 | -2.137858 | 1.139456 |
| 6 | -5.838194 | 0.764536 | 0.750193 |
| 1 | -4.960418 | 2.730550 | 0.683951 |
| 1 | -6.437186 | -1.301384 | 0.863379 |
| 1 | -6.853887 | 1.131086 | 0.620020 |
| 8 | -0.240531 | -2.289826 | 0.977750 |

| | | | |
|---|---|---|---|
| 8 | 2.633545 | -2.941263 | -0.976331 |
| 1 | 2.851588 | -1.983957 | -0.983984 |
| 1 | 1.722772 | -0.686762 | 1.410408 |
| 1 | 2.157039 | -2.957657 | 1.189047 |
| 8 | 2.070703 | -0.618851 | 2.443731 |
| 6 | 2.506207 | -1.709086 | 2.941333 |
| 8 | 2.583427 | -2.809858 | 2.336602 |
| 30 | 1.361904 | 0.789255 | -1.104500 |
| 17 | 2.946561 | 0.189493 | -2.591508 |
| 17 | -0.707954 | 1.702147 | -1.337944 |
| 8 | 2.179694 | 1.942890 | 0.402397 |
| 6 | 1.450803 | 2.825010 | 0.911175 |
| 6 | 0.775545 | 2.553484 | 2.217556 |
| 1 | 1.262872 | 1.692717 | 2.680589 |
| 1 | 0.784361 | 3.406018 | 2.902360 |
| 1 | -0.265617 | 2.262114 | 2.022417 |
| 7 | 1.256784 | 4.000155 | 0.286659 |
| 6 | 1.839621 | 4.202690 | -1.032638 |
| 1 | 1.132355 | 3.887737 | -1.813217 |
| 1 | 2.068883 | 5.265363 | -1.159786 |
| 1 | 2.756329 | 3.617823 | -1.125026 |
| 6 | 0.163761 | 4.895678 | 0.616965 |
| 1 | -0.101390 | 4.832133 | 1.672918 |
| 1 | 0.460705 | 5.926794 | 0.399281 |
| 1 | -0.720862 | 4.645425 | 0.013367 |
| 6 | 2.951328 | -1.640675 | 4.364160 |
| 1 | 2.095971 | -1.363191 | 4.988106 |
| 1 | 3.356643 | -2.598506 | 4.690802 |
| 1 | 3.699775 | -0.850863 | 4.475181 |

## Reactants

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**Benzohydroxamic Acid**

---

Number of imaginary frequencies : 0
Electronic energy = -475.8060846
Zero-point correction= 0.131937
Thermal correction to Energy= 0.140430
Thermal correction to Enthalpy= 0.141374
Thermal correction to Gibbs Free Energy= 0.098276
Sum of electronic and zero-point Energies= -475.674147
Sum of electronic and thermal Energies= -475.665654
Sum of electronic and thermal Enthalpies= -475.664710
Sum of electronic and thermal Free Energies= -475.707809

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.245110 | 0.315953 | -0.114785 |
| 6 | -0.218060 | 0.094850 | -0.061641 |
| 6 | -1.032994 | 1.212118 | 0.129067 |
| 6 | -2.410840 | 1.061919 | 0.203778 |
| 6 | -2.981156 | -0.202196 | 0.077041 |
| 6 | -2.173065 | -1.316201 | -0.132567 |
| 6 | -0.793296 | -1.170462 | -0.204744 |
| 1 | -0.560017 | 2.187418 | 0.215236 |
| 1 | -3.043634 | 1.932396 | 0.358141 |
| 1 | -4.061018 | -0.318507 | 0.132247 |
| 1 | -2.620741 | -2.299768 | -0.252453 |
| 1 | -0.166036 | -2.035919 | -0.409873 |
| 8 | 1.773735 | 1.393473 | -0.370447 |
| 7 | 2.030918 | -0.783402 | 0.122386 |
| 8 | 3.385483 | -0.513460 | 0.226097 |
| 1 | 3.402042 | 0.451231 | 0.047453 |
| 1 | 1.745047 | -1.449034 | 0.830455 |

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**Acetic Acid**

---

Number of imaginary frequencies : 0
Electronic energy = -228.963173
Zero-point correction= 0.062298
Thermal correction to Energy= 0.066775
Thermal correction to Enthalpy= 0.067719
Thermal correction to Gibbs Free Energy= 0.035423
Sum of electronic and zero-point Energies= -228.900875
Sum of electronic and thermal Energies= -228.896398
Sum of electronic and thermal Enthalpies= -228.895454
Sum of electronic and thermal Free Energies= -228.927750

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 1.386991 | -0.099259 | -0.000005 |
| 6 | -0.092514 | 0.124300 | -0.000012 |
| 8 | -0.762262 | -1.046488 | -0.000001 |
| 8 | -0.652650 | 1.192243 | 0.000005 |
| 1 | -1.703109 | -0.813484 | 0.000013 |
| 1 | 1.903370 | 0.860874 | -0.000729 |
| 1 | 1.676165 | -0.681196 | 0.880539 |
| 1 | 1.676005 | -0.682482 | -0.879747 |

---

**_N_, _N_-dimethyl acetamide**

---

Number of imaginary frequencies : 0
Electronic energy = -287.6386198
Zero-point correction= 0.129682
Thermal correction to Energy= 0.137483
Thermal correction to Enthalpy= 0.138427
Thermal correction to Gibbs Free Energy= 0.097633
Sum of electronic and zero-point Energies= -287.508938
Sum of electronic and thermal Energies= -287.501137
Sum of electronic and thermal Enthalpies= -287.500193
Sum of electronic and thermal Free Energies= -287.540987

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 7 | 0.591821 | 0.080042 | -0.024398 |
| 6 | -0.732149 | -0.290417 | -0.003522 |
| 6 | -1.758196 | 0.820933 | 0.002032 |
| 1 | -1.646120 | 1.482558 | 0.868160 |
| 1 | -1.697783 | 1.438378 | -0.901366 |
| 1 | -2.741693 | 0.350747 | 0.040552 |
| 6 | 1.087078 | 1.434410 | 0.006595 |
| 1 | 0.281552 | 2.161543 | -0.103391 |
| 1 | 1.612572 | 1.643924 | 0.950683 |
| 1 | 1.801260 | 1.597521 | -0.812825 |
| 6 | 1.608755 | -0.947777 | 0.003779 |
| 1 | 1.115662 | -1.920636 | -0.015324 |
| 1 | 2.274614 | -0.856190 | -0.865196 |
| 1 | 2.220171 | -0.866239 | 0.913650 |
| 8 | -1.074488 | -1.461850 | 0.005317 |

---

**$NH_2OH$**

---

Number of imaginary frequencies: 0
Electronic energy = -131.6422859
Zero-point correction= 0.040737
Thermal correction to Energy= 0.043941
Thermal correction to Enthalpy= 0.044885
Thermal correction to Gibbs Free Energy= 0.018290
Sum of electronic and zero-point Energies= -131.601549
Sum of electronic and thermal Energies= -131.598345
Sum of electronic and thermal Enthalpies= -131.597401
Sum of electronic and thermal Free Energies= -131.623996

.....

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 7 | -0.679410 | -0.000005 | 0.155202 |
| 1 | -1.038695 | 0.810483 | -0.348347 |
| 1 | -1.038694 | -0.810462 | -0.348398 |
| 8 | 0.715039 | 0.000006 | -0.140768 |
| 1 | 1.112947 | -0.000030 | 0.736469 |

---

**$Pd(PivOH)_2$**

---

Number of imaginary frequencies : 0
Electronic energy = -820.4083595
Zero-point correction= 0.295988
Thermal correction to Energy= 0.315422
Thermal correction to Enthalpy= 0.316366
Thermal correction to Gibbs Free Energy= 0.246324
Sum of electronic and zero-point Energies= -820.112371
Sum of electronic and thermal Energies= -820.092938
Sum of electronic and thermal Enthalpies= -820.091993
Sum of electronic and thermal Free Energies= -820.162036

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 46 | 0.000004 | -0.702768 | 0.000050 |
| 8 | 2.114031 | -0.672081 | -0.456092 |
| 8 | -2.113926 | -0.671722 | 0.456519 |
| 6 | 2.801075 | 0.154715 | 0.138284 |
| 6 | -2.801177 | 0.154212 | -0.138817 |
| 8 | 2.282100 | 1.006277 | 1.005829 |
| 1 | 1.307247 | 0.802579 | 1.034960 |
| 8 | -2.282539 | 1.004402 | -1.007915 |
| 1 | -1.307686 | 0.800724 | -1.037068 |
| 6 | 4.293850 | 0.301931 | -0.061719 |
| 6 | -4.293800 | 0.302029 | 0.061891 |
| 6 | -4.558233 | 1.695618 | 0.644383 |
| 1 | -5.636030 | 1.822693 | 0.803250 |
| 1 | -4.058167 | 1.823591 | 1.612164 |
| 1 | -4.213184 | 2.484580 | -0.031703 |
| 6 | -4.792082 | -0.770883 | 1.021307 |
| 1 | -5.872070 | -0.653757 | 1.170988 |
| 1 | -4.604483 | -1.775713 | 0.627760 |
| 1 | -4.295730 | -0.696949 | 1.994509 |
| 6 | -4.993600 | 0.168392 | -1.294118 |
| 1 | -6.076450 | 0.272817 | -1.154253 |

| | | | |
|---|---|---|---|
| 1 | -4.659907 | 0.938779 | -1.996413 |
| 1 | -4.806250 | -0.813952 | -1.744333 |
| 6 | 4.792267 | -0.771468 | -1.020532 |
| 1 | 4.296534 | -0.697570 | -1.994054 |
| 1 | 5.872401 | -0.654885 | -1.169582 |
| 1 | 4.603953 | -1.776110 | -0.626844 |
| 6 | 4.559327 | 1.695268 | -0.644258 |
| 1 | 4.214327 | 2.484502 | 0.031534 |
| 1 | 5.637273 | 1.821762 | -0.802569 |
| 1 | 4.059859 | 1.823393 | -1.612329 |
| 6 | 4.992669 | 0.168276 | 1.294820 |
| 1 | 4.804606 | -0.813888 | 1.745132 |
| 1 | 6.075657 | 0.272216 | 1.155674 |
| 1 | 4.658833 | 0.938985 | 1.996700 |

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**Isoxazolone**

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Number of imaginary frequencies : 0
Electronic energy = -818.7575592
Zero-point correction= 0.200360
Thermal correction to Energy= 0.213889
Thermal correction to Enthalpy= 0.214833
Thermal correction to Gibbs Free Energy= 0.158861
Sum of electronic and zero-point Energies= -818.557199
Sum of electronic and thermal Energies= -818.543670
Sum of electronic and thermal Enthalpies= -818.542726
Sum of electronic and thermal Free Energies= -818.598698

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | 3.309359 | 1.283398 | -0.184712 |
| 6 | 2.442755 | 0.220517 | 0.035732 |
| 6 | 1.060470 | 0.376814 | 0.025416 |
| 6 | 0.488638 | 1.625164 | -0.224195 |
| 6 | 1.362950 | 2.682537 | -0.446307 |
| 6 | 2.755443 | 2.530480 | -0.423824 |
| 1 | 4.382872 | 1.112413 | -0.169950 |
| 1 | -0.585115 | 1.776798 | -0.250907 |
| 1 | 0.941872 | 3.665500 | -0.645029 |
| 1 | 3.393614 | 3.391605 | -0.600322 |
| 6 | 2.740516 | -1.185313 | 0.258347 |
| 8 | 3.770221 | -1.792171 | 0.352241 |
| 7 | 0.486090 | -0.874865 | 0.297828 |
| 6 | -0.721454 | -1.424173 | -0.203429 |
| 8 | -0.766557 | -2.532022 | -0.677911 |

| | | | |
|---|---|---|---|
| 6 | -1.908425 | -0.553476 | -0.020080 |
| 6 | -2.077960 | 0.244097 | 1.114926 |
| 6 | -2.920039 | -0.629282 | -0.979487 |
| 6 | -3.246017 | 0.980353 | 1.272704 |
| 1 | -1.300643 | 0.274028 | 1.875790 |
| 6 | -4.077562 | 0.120990 | -0.826154 |
| 1 | -2.779833 | -1.284231 | -1.835943 |
| 6 | -4.239875 | 0.925835 | 0.299324 |
| 1 | -3.384881 | 1.591841 | 2.160658 |
| 1 | -4.859305 | 0.072755 | -1.579890 |
| 1 | -5.150998 | 1.506496 | 0.422977 |
| 8 | 1.512209 | -1.822157 | 0.369203 |

---

**$Pd(AcOH)_2$**

---

Number of imaginary frequencies : 0
Electronic energy = -584.7053031
Zero-point correction= 0.126374
Thermal correction to Energy= 0.138288
Thermal correction to Enthalpy= 0.139232
Thermal correction to Gibbs Free Energy= 0.085648
Sum of electronic and zero-point Energies= -584.578930
Sum of electronic and thermal Energies= -584.567016
Sum of electronic and thermal Enthalpies= -584.566071
Sum of electronic and thermal Free Energies= -584.619655

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.000009 | -0.503797 | -0.000027 |
| 8 | -2.080032 | -0.474238 | 0.593106 |
| 8 | 2.079930 | -0.474073 | -0.593223 |
| 6 | 2.814110 | 0.298262 | 0.014582 |
| 6 | -2.814125 | 0.298286 | -0.014551 |
| 6 | 4.276697 | 0.413193 | -0.246254 |
| 1 | 4.831890 | 0.144667 | 0.657980 |
| 1 | 4.562199 | -0.243544 | -1.067998 |
| 1 | 4.530330 | 1.450693 | -0.483413 |
| 6 | -4.276747 | 0.413105 | 0.246120 |
| 1 | -4.562299 | -0.243657 | 1.067828 |
| 1 | -4.530525 | 1.450584 | 0.483204 |
| 1 | -4.831786 | 0.144478 | -0.658180 |
| 8 | 2.377758 | 1.104230 | 0.965201 |
| 1 | 1.401719 | 0.924954 | 1.046963 |
| 8 | -2.377652 | 1.104587 | -0.964836 |
| 1 | -1.401600 | 0.925355 | -1.046519 |

---

**$ZnCl_2$ $(DMA)_2$ (O-coordination)**

---

Number of imaginary frequencies : 0
Electronic energy = -1561.250299
Zero-point correction= 0.266581
Thermal correction to Energy= 0.288454
Thermal correction to Enthalpy= 0.289398
Thermal correction to Gibbs Free Energy= 0.213844
Sum of electronic and zero-point Energies= -1560.983719
Sum of electronic and thermal Energies= -1560.961845
Sum of electronic and thermal Enthalpies= -1560.960901
Sum of electronic and thermal Free Energies= -1561.036455

Cartesian Coordinates

| | | | |
|---|---|---|---|
| 30 | -0.145159 | 0.511382 | 0.461313 |
| 17 | 0.363038 | 2.581948 | -0.252052 |
| 17 | -1.503103 | -0.179492 | 2.127241 |
| 8 | -1.042760 | -0.532699 | -1.126846 |
| 8 | 1.652784 | -0.479398 | 0.520368 |
| 6 | 2.549087 | -0.403375 | -0.345757 |
| 6 | -2.166921 | -1.033685 | -0.895665 |
| 7 | -3.264185 | -0.268487 | -0.787311 |
| 7 | 3.831161 | -0.635041 | -0.007292 |
| 6 | -2.287278 | -2.518454 | -0.727296 |
| 1 | -1.350229 | -2.969805 | -1.055690 |
| 1 | -2.423809 | -2.739760 | 0.338899 |
| 1 | -3.120678 | -2.954380 | -1.285892 |
| 6 | -4.500826 | -0.741886 | -0.192078 |
| 1 | -5.346154 | -0.227288 | -0.660247 |
| 1 | -4.632819 | -1.814706 | -0.334528 |
| 1 | -4.501327 | -0.524143 | 0.885059 |
| 6 | -3.132647 | 1.181690 | -0.830951 |
| 1 | -4.031597 | 1.605721 | -1.289419 |
| 1 | -3.023650 | 1.581227 | 0.187682 |
| 1 | -2.255173 | 1.464469 | -1.414932 |
| 6 | 2.211024 | -0.054942 | -1.763094 |
| 1 | 1.200006 | -0.419922 | -1.965031 |
| 1 | 2.178823 | 1.038684 | -1.860575 |
| 1 | 2.900689 | -0.470445 | -2.500339 |
| 6 | 4.948098 | -0.494786 | -0.924187 |
| 1 | 5.824295 | -0.166794 | -0.356143 |
| 1 | 5.195076 | -1.445225 | -1.416107 |
| 1 | 4.749041 | 0.262572 | -1.684449 |

| | | | |
|---|---|---|---|
| 6 | 4.170498 | -1.031586 | 1.349885 |
| 1 | 3.256664 | -1.238037 | 1.905873 |
| 1 | 4.796752 | -1.931009 | 1.322993 |
| 1 | 4.724737 | -0.230755 | 1.854143 |

---

**$ZnCl_2$ $(DMA)_2$ (N-coordination)**

---

Number of imaginary frequencies : 0
Electronic energy = -1561.2145726
Zero-point correction= 0.265923
Thermal correction to Energy= 0.287144
Thermal correction to Enthalpy= 0.288089
Thermal correction to Gibbs Free Energy= 0.215991
Sum of electronic and zero-point Energies= -1560.948649
Sum of electronic and thermal Energies= -1560.927428
Sum of electronic and thermal Enthalpies= -1560.926484
Sum of electronic and thermal Free Energies= -1560.998582

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 30 | 0.000034 | 0.000171 | -0.403914 |
| 17 | -0.283287 | -2.036847 | -1.281685 |
| 17 | 0.284914 | 2.037938 | -1.279253 |
| 7 | -1.847741 | 0.189731 | 0.875364 |
| 7 | 1.847706 | -0.190868 | 0.876195 |
| 6 | -2.948096 | -0.133562 | -0.019072 |
| 6 | -3.237596 | 0.865025 | -1.099038 |
| 1 | -3.854073 | 1.678862 | -0.697973 |
| 1 | -2.331757 | 1.314208 | -1.523169 |
| 1 | -3.807184 | 0.355840 | -1.877934 |
| 6 | 2.946974 | 0.133857 | -0.018927 |
| 6 | 3.237392 | -0.864669 | -1.098751 |
| 1 | 2.331825 | -1.314063 | -1.523275 |
| 1 | 3.807057 | -0.355192 | -1.877398 |
| 1 | 3.853898 | -1.678395 | -0.697531 |
| 6 | -1.913807 | 1.572428 | 1.396356 |
| 1 | -1.807253 | 2.295676 | 0.584564 |
| 1 | -2.853714 | 1.740990 | 1.940425 |
| 1 | -1.079713 | 1.730925 | 2.086904 |
| 6 | -1.754445 | -0.802173 | 1.959900 |
| 1 | -1.600329 | -1.795543 | 1.529912 |
| 1 | -0.909900 | -0.535225 | 2.604472 |
| 1 | -2.671814 | -0.821983 | 2.561220 |
| 6 | 1.914168 | -1.573884 | 1.396086 |
| 1 | 1.080322 | -1.733129 | 2.086769 |

| | | | |
|---|---|---|---|
| 1 | 1.807529 | -2.296526 | 0.583773 |
| 1 | 2.854259 | -1.742749 | 1.939743 |
| 6 | 1.754256 | 0.800223 | 1.961428 |
| 1 | 1.599852 | 1.793864 | 1.532168 |
| 1 | 0.909938 | 0.532524 | 2.606022 |
| 1 | 2.671702 | 0.819759 | 2.562673 |
| 8 | 3.556909 | 1.160554 | 0.131140 |
| 8 | -3.559678 | -1.159179 | 0.131760 |

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**$ZnCl_2$**

---

Number of imaginary frequencies : 0
Electronic energy = -985.873539
Zero-point correction= 0.002218
Thermal correction to Energy= 0.006746
Thermal correction to Enthalpy= 0.007690
Thermal correction to Gibbs Free Energy= -0.024340
Sum of electronic and zero-point Energies= -985.871321
Sum of electronic and thermal Energies= -985.866793
Sum of electronic and thermal Enthalpies= -985.865849
Sum of electronic and thermal Free Energies= -985.897879

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 30 | 0.000000 | 0.000000 | 0.000000 |
| 17 | 0.000000 | 0.000000 | 2.130599 |
| 17 | 0.000000 | 0.000000 | -2.130599 |

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**$Pd(OAc)_2$**

---

Number of imaginary frequencies : 0
Electronic energy = -583.4786288
Zero-point correction= 0.103282
Thermal correction to Energy= 0.113933
Thermal correction to Enthalpy= 0.114877
Thermal correction to Gibbs Free Energy= 0.065185
Sum of electronic and zero-point Energies= -583.375346
Sum of electronic and thermal Energies= -583.364696
Sum of electronic and thermal Enthalpies= -583.363752
Sum of electronic and thermal Free Energies= -583.413443

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 6 | -3.917123 | 0.000031 | 0.011669 |
| 6 | -2.433166 | 0.000028 | -0.015737 |

| | | | |
|---|---|---|---|
| 8 | -1.766514 | 1.085025 | -0.015884 |
| 46 | -0.000001 | -0.000014 | -0.000033 |
| 8 | 1.766523 | 1.084997 | 0.015815 |
| 6 | 2.433165 | -0.000011 | 0.015707 |
| 6 | 3.917130 | 0.000031 | -0.011398 |
| 8 | -1.766553 | -1.084998 | -0.015897 |
| 8 | 1.766541 | -1.085026 | 0.015824 |
| 1 | -4.301450 | 0.900528 | -0.472665 |
| 1 | -4.301443 | -0.899545 | -0.474392 |
| 1 | -4.254600 | -0.001055 | 1.053624 |
| 1 | 4.301364 | -0.900356 | 0.473227 |
| 1 | 4.254871 | 0.000944 | -1.053259 |
| 1 | 4.301294 | 0.899658 | 0.474699 |

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**$Pd(OPiv)_2$**

---

Number of imaginary frequencies : 0
Electronic energy =-819.1824017
Zero-point correction= 0.272056
Thermal correction to Energy= 0.290541
Thermal correction to Enthalpy= 0.291485
Thermal correction to Gibbs Free Energy= 0.222582
Sum of electronic and zero-point Energies= -818.910346
Sum of electronic and thermal Energies= -818.891861
Sum of electronic and thermal Enthalpies= -818.890917
Sum of electronic and thermal Free Energies= -818.959819

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 46 | 0.000000 | 0.000000 | -0.000061 |
| 8 | -1.757198 | -1.099736 | -0.000309 |
| 8 | -1.773448 | 1.067980 | -0.000266 |
| 8 | 1.773448 | -1.067980 | 0.000136 |
| 8 | 1.757198 | 1.099736 | 0.000188 |
| 6 | 2.437423 | 0.022226 | 0.000218 |
| 6 | 3.942068 | 0.011319 | 0.000084 |
| 6 | -2.437423 | -0.022226 | -0.000333 |
| 6 | 4.404444 | -0.739564 | -1.253088 |
| 1 | 5.499975 | -0.791770 | -1.261798 |
| 1 | 4.007228 | -1.759670 | -1.271712 |
| 1 | 4.082713 | -0.225716 | -2.166935 |
| 6 | 4.404967 | -0.742898 | 1.251018 |
| 1 | 4.007663 | -1.763008 | 1.267154 |
| 1 | 5.500496 | -0.795226 | 1.259068 |
| 1 | 4.083725 | -0.231455 | 2.166383 |

| | | | |
|---|---|---|---|
| 6 | 4.483265 | 1.435421 | 0.001815 |
| 1 | 4.152274 | 1.991104 | -0.882129 |
| 1 | 4.152516 | 1.988863 | 0.887260 |
| 1 | 5.579707 | 1.407310 | 0.001638 |
| 6 | -3.942068 | -0.011319 | -0.000029 |
| 6 | -4.483266 | -1.435419 | -0.002699 |
| 1 | -4.152153 | -1.991729 | 0.880804 |
| 1 | -5.579707 | -1.407308 | -0.002355 |
| 1 | -4.152638 | -1.988233 | -0.888583 |
| 6 | -4.405194 | 0.743837 | -1.250300 |
| 1 | -5.500724 | 0.796200 | -1.258093 |
| 1 | -4.007865 | 1.763945 | -1.265763 |
| 1 | -4.084153 | 0.233070 | -2.166112 |
| 6 | -4.404215 | 0.738624 | 1.253803 |
| 1 | -5.499745 | 0.790796 | 1.262769 |
| 1 | -4.082287 | 0.224099 | 2.167200 |
| 1 | -4.007022 | 1.758728 | 1.273102 |