Mechanism of the Molybdenum Mediated Cadogan Reaction

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1. Non-catalyzed reduction of nitro-styrene furnishing its nitroso analogous 14.

We have explored the possibility of phosphine reducing the nitro group of nitro-styrene to a nitroso group without the intervention of any catalyst. The reaction is feasible, but the barrier of the rate-limiting step (33.4 kcal/mol) is considerably higher than that found for the catalyzed alternatives, making it non-competitive in the presence of the molybdenum complex.

![Mechanism diagram](image)

**Figure S1** Mechanism proposed for the deoxygenation of nitrostyrene in the presence of PMe$_3$. Calculations were performed at the UB3PW91/Def2-SVPD(PCM,toluene) theoretical level. Gibbs Free Energies are reported in kcal/mol (1atm and 298K), relative to NS + PMe$_3$.

2. Energy analysis of the molybdenum mediated reduction of nitrostyrene to its homologous nitroso derivative, a different perspective.

In an attempt to facilitate the visual analysis of the energy values obtained from the computation of the proposed mechanistic alternatives for the catalyzed reduction of nitrostyrene to its nitroso derivative, we provide here the energy profiles associated with all the explored paths.
2. ENERGY ANALYSIS OF THE MOLYBDENUM MEDIATED REDUCTION OF NITROSTYRENE TO ITS HOMOLOGOUS NITROSO DERIVATIVE, A DIFFERENT PERSPECTIVE.

Figure S2 Lewis-acid-type path: available reaction pathways for the molybdenum-catalyzed OAT reaction between ArNO₂ and PMe₃ considering the Lewis acid character of the catalyst. Also, the enzymatic-type-mechanism is considered in this scheme. We have named all the possible alternative paths to simplify its location in the energy profiles depicted in Figure S3.
Figure 3 Energy profiles

Figure S3 Energy profiles of the available reaction pathways for the molybdenum-catalyzed OAT reaction between ArNO₂ and PMe₃ considering the Lewis acid character of the catalyst and also the enzymatic type mechanism.
The inspection of Figure S3 reveals that those paths involving TS11-7 and TS12-8 should be disregarded since these two transition state constitute the two points with highest energy. Nevertheless, for a more detailed analysis and identification of the rate determining state distinguishing between TS8-9 (rate determining state) and TS1-2 may not be illustrative enough, concluding with the need of reviewing also Figure S2.

3 Mechanisms explored for the transformation of nitrosostyrene 14 into indole 24.

As explained in the main text, there are different mechanistic proposals in the literature for the transformation of nitrosostyrene to indole with phosphine as a reductant. We have explored an ample set of alternatives for this transformation at the UB3PW91/Def2-SVPD(PCM, toluene) level, as collected in Figure S4. The preferred path is shown in Figure 4 in the main manuscript.

The difficulties in optimizing a transition structure between 20 and 21, led us to run a NEB calculation between them, and use the results to estimate the barrier corresponding to this step. In Figure S5 we display the energy profiles thus obtained.
Figure S4 Full perspective of the mechanisms explored for the reduction of nitrosostyrene 14 into indole 24. The values annotated correspond to relative Gibbs Free Energies (in kcal/mol) calculated at 1 atm and 298 K at the UB3PW91/Def2-SVPD(PCM,toluene) level.
Figure S5 Energy profiles obtained from the application of the NEB method to obtain an energetic and structural approximation for TS_{20–21}. The electronic Energy (a.u.) is plotted against the number of the interpolation point between the reactant and the product.
In an attempt to clarify the data contained in this two pictures, we have plotted the energy profiles for the different alternative mechanisms plus those profiles corresponding to the energetically most feasible alternative depicted in the Manuscript (Figure 4) in Figures S6 and S7, respectively.

**Figure S2-a-Energy profiles**

**Figure S2-b-Energy profiles**

*Figure S6* Energy profiles obtained from the energy analysis of the different mechanistic alternatives for the reduction of nitrosostyrene towards indole.
Figure S7 Energy profiles obtained from the energy analysis of the most energetically feasible mechanisms for the reduction of nitrosostyrene towards indole.
4 Isomerism: analysis of the structural isomers of complexes shown at Scheme 3.

In this manuscript most of the complexes from 6 onwards can \textit{a priori} present structural isomers. Acknowledging this fact, we have explored different stereoisomers for some of the key complexes:

1. Pentacoordination:
   The complexes with a coordination number of 5 could in principle be assigned a trigonal bipyramid geometry. Nevertheless, the apicophilicity of the oxygen induces a geometry more similar to a square pyramid (see scheme S8).

   In an attempt to identify the most stable geometries for the complexes studied, we optimized the possible stereoisomers of 11 and 7, finding that:

   - Structure 7 is more stable than 7-isomer by 1.6 kcal/mol. If equilibrium between these two isomers were established, it would be shifted towards 7. This result led us to discard alternative paths that would derive from 7-isomer.

   - The isomer of compound 11 is 0.9 kcal/mol more unstable, indicating again that an equilibrium would be slightly shifted towards 11. Despite that, due to the low energy gap between the two isomers, we also explored the reduction of 11-isomer. The corresponding transition state, TS\textsubscript{11-isomer-7}, has a relative energy of 29.5 kcal/mol, lower than the 32.2 kcal/mol of TS\textsubscript{11-7}. Irrespective of whether some molecules follow the path 11-11-isomer-TS\textsubscript{11-isomer-7}, it is expected that 7 would be the product, as 7-isomer would evolve towards the most stable stereoisomer (see scheme S8).

Moreover, all our attempts to locate the transition state corresponding to the reduction of 11 in the apical oxygen led to TS\textsubscript{11-7}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure_s8.png}
\caption{Study of the stereoisomers of complexes 7 and 11.}
\end{figure}
2. Hexacoordination:
On those complexes with a coordination number of 6, those isomers in which two oxo groups were located in trans-diaxial positions were discarded due to their high energies, induced by the strong trans effect caused by the oxo ligands. This first screening reduces the configurational space to those complexes in which the chlorine atoms are in trans-diaxial or adopt a cis disposition.

We explored such geometries for complexes 8 and 12. For complex 8, 3 isomers could be proposed \textit{a priori} as shown in scheme S9. However, 8-isom1 progresses into 7, and 8-isom2 turns out to be 0.6 kcal/mol less stable than 8. Moreover, all our attempts to locate the other isomer of compound 12 led towards 11.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{s9}
\caption{Study of the stereoisomers of complex 8.}
\end{figure}
5 Cartesian coordinates of all the stationary points computed.

The label identifying the computed stationary points is ended in -X, where X = -s, -t, which stand, for singlet and triplet, respectively. In some cases, we have calculated the energy of the singlet or triplet electronic state on a geometry optimized in a different potential energy surface, in order to estimate how far we are from the MECP between surfaces, for example. We have included in the following section the SCF energies thus calculated, with the labels name-SPS or name-SPT, denoting single point calculations to a singlet or triplet state, respectively.

Please note that nitrostyrene has been designated using the common name but also as 14 along the text. In order to avoid unnecessary repetition we have chosen the numeric name on this SI. We adopted the same rationale for the case of 24/indole.
5. **CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.**

| Ortho-nitrostyrene (A) | SCF Energy: -974.445952918 | Num. Imaginary Frequencies: 0 |
|------------------------|-------------------------------|-------------------------------|
| N 0.032310 | 0.358795 | -0.842825 |
| C 1.202183 | -0.201708 | -0.382493 |
| C 1.419059 | -1.577383 | -0.477076 |
| C 2.627026 | -2.140382 | -0.066745 |
| C 3.630333 | -1.321180 | 0.446812 |
| C 3.420157 | 0.053596 | 0.515666 |
| C 2.225695 | 0.662707 | 0.086731 |
| H 0.620853 | -2.194224 | -0.884127 |
| H 2.776808 | -3.218737 | -0.146395 |
| H 4.579230 | -1.744922 | 0.779917 |
| H 4.216093 | 0.697166 | 0.896798 |
| P 0.000048 | -0.000063 | -0.594654 |
| C -0.234962 | 1.621110 | 0.275031 |
| C -1.286597 | -1.013956 | 0.275079 |
| C 1.521490 | -0.607072 | 0.275119 |
| H 0.560875 | 2.318233 | -0.024756 |
| H -1.196368 | 2.063182 | -0.024137 |
| H -0.219292 | 1.515602 | 1.371651 |
| H -2.288145 | -0.673574 | -0.025348 |
| H -1.188497 | -2.067716 | -0.023557 |

| PMe3 | SCF Energy: -460.844449435 | Num. Imaginary Frequencies: 0 |
|------|-------------------------------|-------------------------------|
| P 0.000001 | 0.245734 | 0.000029 |
| C 1.971208 | -0.894149 | 0.000137 |
| C -1.971214 | -0.894141 | 0.000138 |
| O 0.000010 | 1.255536 | 1.329077 |
| O 0.000007 | 1.254475 | -1.329815 |

| OPMe3 | SCF Energy: -536.026776398 | Num. Imaginary Frequencies: 0 |
|-------|-------------------------------|-------------------------------|
| O 0.000049 | -0.000094 | 1.688664 |
| P 0.000087 | -0.000183 | 0.172730 |
| C -1.388530 | -0.929914 | -0.551067 |
| C 1.499942 | -0.736430 | -0.551654 |
| C -0.111923 | 1.667399 | -0.550103 |
| H 1.466707 | -0.713636 | -1.650000 |
| H 2.377725 | -0.176266 | -0.202221 |
| H 1.588339 | -1.777006 | -0.211356 |
| H -0.108361 | 1.628088 | -1.648483 |
| H -1.038958 | 2.145257 | -0.205646 |
| H 0.741842 | 2.265564 | -0.204192 |
| H -1.357794 | -0.904913 | -1.649433 |
| H -1.338609 | -1.972397 | -0.208815 |
| H 0.741842 | 2.265564 | -0.204192 |
| H -1.357794 | -0.904913 | -1.649433 |
| H -1.338609 | -1.972397 | -0.208815 |

| 1-s | SCF Energy: -1138.77058287 | Num. Imaginary Frequencies: 0 |
|-----|-------------------------------|-------------------------------|
| Mo -0.000001 | 0.245734 | 0.000029 |
| Cl 1.971208 | -0.894149 | 0.000137 |
| Cl -1.971214 | -0.894141 | 0.000138 |
| O 0.000010 | 1.255536 | 1.329077 |
| O 0.000007 | 1.254475 | -1.329815 |
### Cartesian Coordinates of All the Stationary Points Computed

| Code | SCF Energy | Num. Imaginary Frequencies |
|------|------------|---------------------------|
| 2-s  | -1599.64133134 | 0                         |
| 2-SPT| -1599.65019625 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | -0.692217 | -0.669475 | 0.432649 |
| Mo    | 1.216284  | 0.102876  | 0.373958 |
| Cl    | 2.278053  | -1.634433 | -0.829762 |
| O     | 1.876817  | 0.606290  | 1.819630 |
| P     | -2.154328 | -0.284710 | 0.046795 |
| C     | -3.249282 | -1.531307 | 0.754424 |
| H     | -4.292837 | -1.314516 | 0.488079 |
| H     | -3.141514 | -1.529290 | 1.846859 |
| H     | -2.969032 | -2.519083 | 0.366139 |
| C     | -2.632834 | 1.322891  | 0.708809 |
| H     | -3.684730 | 1.530552  | 0.468637 |
| H     | -2.500626 | 1.315670  | 1.798883 |
| H     | -1.987991 | 2.093033  | 0.266571 |
| C     | -2.392833 | -0.723966 | -1.739576 |
| H     | -3.442896 | -0.053348 | -1.977055 |
| H     | -2.123114 | -1.258816 | -2.143243 |
| H     | -1.740813 | 0.491837  | -2.178471 |
| Cl    | 0.503562  | 1.904646  | -1.035223 |

| 3-s  | -1063.57854479 | 0                         |
| 3-SPS| -1063.54490716 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 0.071330  | 1.932983 | 0.000000 |
| Mo    | -0.007508 | 0.284901 | 0.000000 |
| Cl    | -0.007508 | -0.806756 | 2.055414 |
| Cl    | -0.007508 | -0.806756 | -2.055414 |

| 4-s  | -1577.20038511 | 0                         |
| 4-SPT| -1577.20098013 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 1.887884  | 0.224857 | -0.299756 |
| Mo    | 1.981333  | 0.548952 | 1.975535 |
| Cl    | 2.362610  | 1.687076 | -0.903687 |
| Cl    | 3.405387  | -1.453403 | -0.785907 |
| N     | -0.815337 | -0.798259 | 0.249794 |
| C     | -2.221018 | -0.657959 | 0.101593 |
| C     | -2.955875 | -1.851511 | 0.082646 |
| C     | -4.331820 | -1.809927 | -0.090050 |
| C     | -4.972669 | -0.575426 | -0.232522 |
| C     | -4.236134 | 0.603915  | -0.179440 |
| C     | -2.841477 | 0.609688  | -0.009922 |
| H     | -2.423408 | -2.795894 | 0.185921 |
| H     | -4.902659 | -2.739005 | -0.116703 |
| H     | -6.055203 | -0.530884 | -0.361159 |
| H     | -4.755057 | 1.561633  | -0.227037 |
| C     | -2.112868 | 1.880050  | 0.133152 |
| C     | -2.460928 | 3.036251  | -0.447245 |
| C     | -3.303926 | 3.112580  | -1.137332 |
| H     | -1.233452 | 1.867495  | 0.780060 |
| H     | -1.890820 | 3.946671  | -0.259803 |
| O     | -0.053852 | 0.062885  | -0.406195 |
| O     | -0.283354 | -1.789162 | 0.760418 |

| 4-t  | -1577.20373491 | 0                         |
| 4-t   | -1577.20373491 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 0.071330  | 1.932983 | 0.000000 |
| Mo    | -0.007508 | 0.284901 | 0.000000 |
| Cl    | -0.007508 | -0.806756 | 2.055414 |
| Cl    | -0.007508 | -0.806756 | -2.055414 |

| 5-t  | -1577.20373491 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 0.071330  | 1.932983 | 0.000000 |
| Mo    | -0.007508 | 0.284901 | 0.000000 |
| Cl    | -0.007508 | -0.806756 | 2.055414 |
| Cl    | -0.007508 | -0.806756 | -2.055414 |

| Code | SCF Energy | Num. Imaginary Frequencies |
|------|------------|---------------------------|
| 3-t  | -1063.57854479 | 0                         |
| 4-SPT| -1063.54490716 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 0.071330  | 1.932983 | 0.000000 |
| Mo    | -0.007508 | 0.284901 | 0.000000 |
| Cl    | -0.007508 | -0.806756 | 2.055414 |
| Cl    | -0.007508 | -0.806756 | -2.055414 |

| 6-t  | -1577.20373491 | 0                         |

| Atoms | X    | Y    | Z    |
|-------|------|------|------|
| O     | 0.071330  | 1.932983 | 0.000000 |
| Mo    | -0.007508 | 0.284901 | 0.000000 |
| Cl    | -0.007508 | -0.806756 | 2.055414 |
| Cl    | -0.007508 | -0.806756 | -2.055414 |
## 5. Cartesian Coordinates of All the Stationary Points Computed.

| Element | x     | y     | z     | Element | x     | y     | z     |
|---------|-------|-------|-------|---------|-------|-------|-------|
| Mo      | 1.876081 | 0.299204 | -0.241154 | Mo      | -1.715993 | -0.048398 | -0.258446 |
| Cl      | 2.487642 | 0.241942 | 1.985623 | Cl      | -2.629898 | -1.271131 | 1.479478  |
| O       | 2.432895 | 1.693606 | -0.950496 | O       | -2.365123 | -0.665963 | -1.644999 |
| Cl      | 2.986309 | -1.506784 | -1.164551 | Cl      | -2.906027 | 1.879821 | 0.214306  |
| N       | -0.861808 | -0.841573 | 0.295322 | N       | 0.807458  | 0.155183 | -0.276101 |
| C       | -2.264319 | -0.634385 | 0.155043 | C       | 2.154676  | 0.385699 | -0.085074 |
| C       | -3.044804 | -1.798050 | 0.108035 | C       | 2.560473  | 1.739119 | -0.109495 |
| C       | -4.414537 | -1.699723 | -0.086809 | C       | 3.870960  | 2.072681 | 0.183228  |
| C       | -5.002637 | -0.438889 | -0.224198 | C       | 4.784737  | 1.067635 | 0.522961  |
| C       | -4.221728 | 0.709894  | -0.141230 | C       | 4.385480  | -0.265990 | 0.512131  |
| C       | -2.831366 | 0.659784  | 0.051552  | C       | 3.084669  | -0.665613 | 0.167813  |
| H       | -2.552587 | -2.764850 | 0.202341  | H       | 1.817391  | 2.505322 | -0.321443 |
| H       | -5.021242 | -2.604584 | -0.136288 | H       | 4.174544  | 3.120069 | 0.176025  |
| H       | -6.079719 | -0.349119 | -0.373346 | H       | 5.813205  | 1.323051 | 0.781393  |
| H       | -4.700204 | 1.688663  | -0.184057 | H       | 5.115257  | -1.045475 | 0.737944  |
| C       | -2.071094 | 1.908852  | 0.225251  | C       | 2.844395  | -2.108659 | 0.023138  |
| C       | -2.338341 | 3.058995  | -0.406611 | C       | 2.105942  | -2.714253 | -0.915800 |
| H       | -3.121056 | 3.138329  | -1.164073 | H       | 1.537342  | -2.163078 | -1.665710 |
| H       | -1.246217 | 1.885108  | 0.940107  | H       | 3.428842  | -2.732640 | 0.706472  |
| H       | -1.757255 | 3.957826  | -0.197959 | H       | 2.061224  | -3.802790 | -0.966001 |
| O       | -0.079475 | 0.073538  | 0.214676  | O       | 0.127946  | -0.892295 | 0.134735  |
| O       | -0.379503 | -1.857580 | 0.781434  | O       | -0.033516 | 1.099576  | -0.645859 |

**5-s**

SCF Energy: -1577.22310613  
Num. Imaginary Frequencies: 0

**5-t**

SCF Energy: -1577.22191107  
Num. Imaginary Frequencies: 0
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Mo      | -1.699245 | -0.03536 | -0.243767 |
| Cl      | -2.727576 | -1.299958 | 1.397149 |
| O       | -2.154685 | -0.645936 | -1.708398 |
| Cl      | -2.992065 | 1.849510  | 0.137416  |
| N       | 0.811068  | 0.192774  | -0.147297 |
| C       | 2.168811  | 0.392173  | -0.031452 |
| C       | 2.597746  | 1.739830  | -0.055027 |
| C       | 3.924784  | 2.045987  | 0.185114  |
| C       | 4.835208  | 1.019578  | 0.467291  |
| C       | 4.413450  | -0.307164 | 0.450590  |
| C       | 3.091866  | -0.679259 | 0.158991  |
| H       | 1.859876  | 2.521566  | -0.223946 |
| H       | 4.246404  | 3.087986  | 0.180297  |
| H       | 5.878698  | 1.253519  | 0.682171  |
| H       | 5.140208  | -1.102256 | 0.626238  |
| C       | 2.821616  | -2.114628 | -0.007953 |
| C       | 2.037384  | -2.684951 | -0.931748 |
| H       | 1.449073  | -2.106260 | -1.644904 |
| H       | 3.422014  | -2.763626 | 0.637133  |
| H       | 1.972657  | -3.771021 | -1.006917 |
| O       | 0.132509  | -0.859851 | 0.254592  |
| O       | -0.026501 | 1.157797  | -0.481533 |

**6-s**

SCF Energy: -1577.24886719  
Num. Imaginary Frequencies: 0

**6-t**

SCF Energy: -1577.22867105  
Num. Imaginary Frequencies: 0
### Cartesian Coordinates of All the Stationary Points Computed

| Element | X-Cartesian | Y-Cartesian | Z-Cartesian |
|---------|-------------|-------------|-------------|
| Mo      | -2.778939   | -0.147715   | -0.038064   |
| Cl      | -1.693733   | -0.851863   | 1.833749    |
| Cl      | -2.543944   | 2.061656    | -0.532033   |
| O       | -4.404699   | -0.453445   | 0.182708    |
| N       | 1.780358    | -0.200068   | -0.63704    |
| C       | 2.995017    | 0.269499    | -0.235621   |
| C       | 3.142032    | 1.654688    | 0.025119    |
| C       | 4.366386    | 2.158818    | 0.429847    |
| C       | 5.461811    | 1.298271    | 0.582919    |
| O       | 0.734875    | 0.388705    | -0.828228   |

**7-s**

SCF Energy: -2113.27489058

Num. Imaginary Frequencies: 0

**7-t**

SCF Energy: -2113.27284934

Num. Imaginary Frequencies: 0
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|     | X-Coord      | Y-Coord      | Z-Coord      |
|-----|--------------|--------------|--------------|
| Mo  | -0.775044    | 0.662188     | 0.477950     |
| Cl  | -0.857310    | 2.687411     | -0.715710    |
| Cl  | -0.367116    | -1.662515    | 0.260447     |
| O   | -2.555922    | 0.277567     | -0.457490    |
| N   | 2.060779     | 0.141258     | 1.117466     |
| C   | 3.068298     | -0.457336    | 0.328505     |
| C   | 3.473977     | -1.740942    | 0.731600     |
| C   | 4.400022     | -2.458401    | -0.012245    |
| C   | 4.929076     | -1.901694    | -1.180007    |
| C   | 4.555273     | -0.614910    | -1.553450    |
| O   | 1.175061     | 0.945635     | -0.035723    |
| O   | 1.828465     | -1.209453    | -1.809874    |
| C   | 1.439219     | -0.343378    | 0.957777     |
| H   | 2.670783     | 1.804870     | -1.757777    |
| H   | 4.571694     | 2.877767     | -0.553844    |
| H   | 5.538069     | 1.745467     | 1.468315     |
| H   | 6.561055     | 2.746325     | -1.782930    |
| O   | 0.621239     | -1.172142    | -0.533969    |
| O   | 1.384785     | -0.089374    | 1.103895     |
| P   | -0.798870    | -0.556000    | -0.054367    |
| C   | -2.012173    | 1.831637     | -0.054367    |
| H   | -3.644347    | 1.985157     | 0.236509     |
| H   | -3.240768    | 3.729318     | -0.421169    |
| H   | -2.762821    | 2.547640     | -1.684308    |
| C   | -0.514907    | 2.724746     | 2.001850     |
| H   | -0.511850    | 4.654978     | -0.202210    |
| H   | 0.816211     | 3.489318     | 0.111305     |
| H   | -0.020083    | 3.483841     | -1.470263    |

7-isom1-s
SCF Energy: -2113.27480684
Num. Imaginary Frequencies: 0
7-isom1-SPT
SCF Energy: -2113.27293544

8-s
SCF Energy: -2113.28849437
Num. Imaginary Frequencies: 0
8-s-SPT
SCF Energy: -2113.27534906
CONTENTS 5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| 8-s-isom2 | SCF Energy: -2113.29436994 | Num. Imaginary Frequencies: 0 |
|-----------|-----------------------------|-------------------------------|
| 9-SPT     | SCF Energy: -2113.26162120   | Num. Imaginary Frequencies: 0 |
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

Mo  -1.153390  -1.349233  -0.303682  Mo  1.260264  -0.126362  0.051564
O   -2.734576  -1.916801  -0.331697  Cl  1.622237  2.200668  -0.214395
O   -1.602354   0.521561  0.665855  Cl  0.132417  -2.482030  -0.212478
Cl  -1.255105   0.060995  -2.265227  O   1.847167  -0.347866  1.602808
O   0.988051  -0.139998  -0.191629  O   2.495620  -0.578743  -0.992837
N   1.991961  -0.810517  -0.001370
C   3.236718  -0.173862  0.040566
C   4.230901  -1.123054  0.366491
C   5.545513  -0.754373  0.600438
C   5.872769   0.600931  0.533384
C   4.904155   1.548201  0.469058
C   3.570157  -1.261307  -0.091629
C   3.904931  -2.160519  0.447808
H   6.297559  -1.503147  0.850078
H   6.893329   0.930979  0.736140
H   5.196737   2.598167  -0.060555
H   5.196737   2.598167  0.144473
C   2.737899   2.349161  -0.517745
C   1.661313   2.397309  -1.317330
H   1.160078   1.521835  -1.722456
H   3.157509   3.310338  -1.658738
H   1.259925   3.725897  -1.598969
O   -0.271275  -2.544539  -1.090340
P   -2.666864   1.638469  0.672182
C   -2.03535   1.160972  -0.146004
C   -3.066646   2.069975  2.380873
C   -2.053170   3.131118  -0.138520
H   -2.808131   3.927832  -0.095572
H   -1.137585  3.462582  -0.367985
H   -1.822937  2.891468  -1.184130
H   -4.939227   1.972630  -0.060555
H   -3.998905   0.953837  -1.203937
H   -4.597719   0.250201  0.326066
H   -3.795435   2.891177  2.411108
H   -3.483694   1.188299  2.884524
H   -2.147137   2.374327  2.897447
Cl  -0.526829  -1.950215  1.899541

SCF Energy:  -1652.37416470
Num. Imaginary Frequencies:  0

Mo  -2.249774   0.247888  -0.042991  Mo  -2.249774   0.247888  -0.042991
C   -1.910588  -1.972982  -0.554801  Cl  -1.910588  -1.972982  -0.554801
Cl  -1.688055   1.350445  1.898199  Cl  -1.688055   1.350445  1.898199
O   -3.916605   0.269740  0.071956  O   -3.916605   0.269740  0.071956
P   -2.808131   3.927832  -0.095572  O   -1.923628   1.226060  -1.355365
C   -1.137585   3.462582  -0.367985  N   1.095235   0.077627  -0.798011
C   -1.822937   2.891468  -1.184130  C   2.501651   0.222674  -0.419793
H   -4.939227   1.972630  -0.060555  C   3.173897   1.284910  -1.022853
H   -3.998905   0.953837  -1.203937  C   4.472777   1.578751  -0.621459
H   -4.597719   0.250201  0.326066  C   5.078558   0.801577  0.367789
H   -3.795435   2.891177  2.411108  C   4.398770  -0.275426  0.931213
H   -3.483694   1.188299  2.884524  C   3.090962  -0.613124  0.545663
H   -2.147137   2.374327  2.897447  H   2.661317   1.888671  -1.771651
C   -0.526829  -1.950215  1.899541  H   5.001265   2.420891  -1.069480
H   6.093762   1.029261  0.696307  H   4.895800  -0.899106  1.676334
H   4.895800  -0.899106  1.676334  C   2.475465  -1.831590  1.098217
C   1.765680  -2.727387  0.403334  C   1.765680  -2.727387  0.403334
H   1.560683  -2.613782  -0.663155  H   1.560683  -2.613782  -0.663155
H   2.692657  -2.025954  2.152812  H   2.692657  -2.025954  2.152812
H   1.376112  -3.625683  0.883242  O   0.277325   0.049880  0.124162
O   0.809485   0.055799  -1.971146
### 5. Cartesian Coordinates of All the Stationary Points Computed

| 11-s-isom | SCF Energy: -1652.37735070 | Num. Imaginary Frequencies: 0 |
|-----------|-----------------------------|-------------------------------|
| Mo        | 2.104487                    | -0.084093                    | 0.011954                     |
| Cl        | 1.443485                    | -2.073318                    | 1.070365                     |
| O         |                             |                              |                              |
| Cl        | -1.675320                   | -1.548766                    | 1.419073                     |
| O         | -1.704359                   | 1.769970                     | 0.383394                     |
| Mo        | -1.984226                   | 0.196828                     | -0.116304                    |
| Cl        | -4.275383                   | 0.093234                     | -0.101804                    |
| O         | -1.637577                   | 0.103773                     | -1.755595                    |
| N         | 1.081873                    | -0.724535                    | -0.375801                    |
| C         | 2.511718                    | -0.543962                    | -0.220211                    |
| C         | 3.269090                    | -1.720486                    | -0.238073                    |
| Cl        | 4.639923                    | -1.653076                    | -0.043068                    |
| Cl        | 5.241909                    | -0.405615                    | 0.149163                     |
| O         | 3.083260                    | 0.737522                     | -0.037593                    |
| C         | 4.972582                    | 1.723948                     | 0.227607                     |
| C         | 2.337916                    | 2.004717                     | -0.097111                    |
| H         | 5.235549                    | -2.566231                    | -0.040192                    |
| H         | 6.321266                    | -0.336764                    | 0.293886                     |
| H         | 4.972582                    | 1.723948                     | 0.227607                     |
| C         | 2.657972                    | 3.098987                     | 0.605703                     |
| C         | 3.474132                    | 3.109537                     | 1.331124                     |
| H         | 1.472869                    | 2.043526                     | -0.760277                    |
| H         | 2.080292                    | 4.017045                     | 0.495772                     |
| O         | 0.345766                    | 0.157600                     | 0.105526                     |
| O         | 0.656773                    | -1.708541                    | -0.929011                    |

| 12-s      | SCF Energy: -1652.37397199  | Num. Imaginary Frequencies: 0 |
|-----------|-----------------------------|-------------------------------|
| S         |                             |                              |                              |

| 13-s      | SCF Energy: -2113.24224361  | Num. Imaginary Frequencies: 0 |
|-----------|-----------------------------|-------------------------------|
| S         |                             |                              |                              |
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Mo      | 2.190775| -0.305995| -0.212442|
| Cl      | 1.431788| -0.777115| -2.383865|
| Cl      | 2.067190| 0.216587 | 2.147302 |
| O       | 3.070837| -1.723316| 0.007932 |
| O       | 3.270374| 0.924922 | -2.383865|
| O       | -1.214680| 1.463364| -1.027568|
| P       | -1.185479| 2.528613| 0.214877 |
| N       | -0.844911| 0.082944| -0.760636|
| C       | -2.207142| 3.851161| -0.451607|
| C       | -1.906376| 1.877959| 1.727776 |
| C       | 0.456241 | 3.179067| 0.536900 |
| O       | 0.160196 | 0.112054| 0.129459 |
| C       | -2.005226| -0.656994| 0.214877 |
| C       | -3.219264| -0.317784| -0.983699|
| C       | -1.926605| -1.810513| 0.457421 |
| C       | -4.368483| -1.072295| -0.778480|
| C       | -3.112269| -2.549233| 0.635102 |
| C       | -4.318948| -2.200788| 0.039089 |
| C       | -0.706709| -2.308717| 1.133240 |
| C       | -0.326896| -3.592810| 1.110227|
| H       | 0.350686 | 4.117192 | 1.100230 |
| H       | 1.039365 | 2.456844 | 1.122562|
| H       | 0.957175 | 3.381190 | -0.418421|
| H       | -1.918561| 2.688321 | 2.470989 |
| H       | -2.927911| 1.527443 | 1.538757 |
| H       | -1.281957| 1.054453 | 2.093407 |
| H       | -2.232453| 4.685986 | 0.261901 |
| H       | -1.771848| 4.195755 | -1.398605|
| H       | -3.224537| 3.480831 | -0.627245|
| H       | -3.246127| 0.535603 | -1.657791|
| H       | -5.297971| -0.779697| -1.269964|
| H       | -3.067819| -3.419645| 1.290898 |
| H       | -5.211069| -2.804112| 0.213779 |
| H       | -0.103541| -1.592611| 1.691749 |
| H       | -0.867132| -4.344951| 0.530317 |
| H       | 0.561350 | -3.922130| 1.650740 |

15-s
SCF Energy: -438.526940743
Num. Imaginary Frequencies: 0

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| N       | 0.828014| 1.798166| -0.168607|
| C       | -0.111307| 0.743306| -0.032401|
| C       | -1.418500| 1.262438| 0.038308 |
| C       | -2.529020| 0.437353| 0.117561 |
| C       | -2.333821| -0.944866| 0.060234 |
| C       | -1.049518| -1.468398| -0.056460|
| C       | 0.110937 | -0.668603| -0.072030|
| H       | -1.516581| 2.349158| 0.025332 |
| H       | -3.531516| 0.859733| 0.195583 |
| H       | -3.188420| -1.623445| 0.089917 |
| H       | -0.926653| -2.551210| -0.123304|
| C       | 1.370613 | -1.421125| -0.197923|
| C       | 2.603629 | -1.184733| 0.276823 |
| H       | 2.866906 | -0.291086| 0.834500 |
| H       | 1.222579 | -2.382898| -0.701491|
| H       | 3.383637 | -1.931936| 0.116749 |
| O       | 2.004485 | 1.556536| -0.007713|

14-s
SCF Energy: -438.460847826
Num. Imaginary Frequencies: 0

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
|   S     | 22      |         |         |

16-s
SCF Energy: -438.494012055
Num. Imaginary Frequencies: 0
CONTENTS  

5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|     | X Coords       | Y Coords       | Z Coords       |
|-----|----------------|----------------|----------------|
| N   | 1.493560       | -0.485227      | 0.000293       |
| C   | 0.161450       | -0.412767      | 0.000006       |
| C   | -0.773769      | -1.485611      | -0.000004      |
| C   | -2.099779      | -1.158603      | -0.000158      |
| C   | -2.544135      | 0.218966       | 0.000343       |
| C   | -1.667584      | 1.262774       | -0.000178      |
| C   | -0.254008      | 0.986007       | -0.000178      |
| H   | -0.420478      | -2.516393      | 0.000083       |
| H   | -2.852719      | -1.948771      | -0.000175      |
| H   | -3.617880      | 0.415570       | -0.000428      |
| H   | -2.019155      | 2.295686       | -0.000494      |
| C   | 0.858344       | 1.777438       | -0.000055      |
| C   | 2.048899       | 0.882232       | 0.000121       |
| H   | 2.691582       | 0.988407       | -0.887196      |
| H   | 0.905919       | 2.863618       | 0.000066       |
| H   | 2.691758       | 0.988724       | 0.887262       |
| O   | 2.223694       | -1.514109      | 0.000549       |

17-s  
SCF Energy: -438.520829527  
Num. Imaginary Frequencies: 0

|     | X Coords       | Y Coords       | Z Coords       |
|-----|----------------|----------------|----------------|
| N   | -1.565546      | -0.464338      | -0.000241      |
| C   | -0.125997      | -0.394926      | -0.157979      |
| C   | 0.758779       | -1.460271      | -0.177294      |
| C   | 2.118333       | -1.135349      | 0.133139       |
| C   | 2.539830       | 0.200810       | 0.133139       |
| C   | 1.616964       | 1.253842       | 0.000318       |
| C   | 0.261391       | 0.943141       | 0.000118       |
| H   | 0.394306       | -2.487315      | -0.000171      |
| H   | 2.862660       | -1.933551      | 0.000194       |
| H   | 3.608190       | 0.423964       | 0.000500       |
| H   | 1.957835       | 2.290948       | 0.000454       |
| C   | -0.982378      | 1.787418       | 0.000333       |
| C   | -2.060249      | 0.755794       | -0.000196      |
| H   | -3.136489      | 0.903915       | -0.000321      |
| H   | -1.040630      | 2.447660       | 0.882693       |
| O   | -2.175779      | -1.568189      | -0.000418      |

18-s  
SCF Energy: -438.468559052  
Num. Imaginary Frequencies: 0

|     | X Coords       | Y Coords       | Z Coords       |
|-----|----------------|----------------|----------------|
| S   | 1.568870       | -0.513641      | -0.278731      |

19-s  
SCF Energy: -899.320458821  
Num. Imaginary Frequencies: 0

S23
CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

N  -0.486476  0.335568  -0.396228
C   0.817284  -0.179094  -0.235812
C   1.046954  -1.552741  -0.395095
C   2.310528  -2.112232  -0.212719
C   3.381633  -1.280339   0.110949
C   3.168246   0.088313   0.253330
C   1.902355   0.682007   0.089581
H   0.215246  -2.188003  -0.703672
H   2.457746  -3.186044  -0.342559
H   4.382315  -1.693429   0.249686
H   4.009311  -2.188003   0.249686
C   1.797820   2.125127   0.337141
C   0.792014   2.958397  -0.023436
H  -0.076061   2.617646  -0.551361
H   2.677455   2.543696   0.839365
H   0.875306   4.014817   0.289171
O  -0.829251   1.011520  -1.565175
P  -1.890475  -0.284919   0.194348
C  -1.631652  -1.134225   1.774958
H  -0.990328  -2.013025   1.640694
H  -1.156715  -0.442548   2.482193
H  -2.604388  -1.452368   2.173680
C  -3.019712   1.094504   0.496428
H  -3.212768   1.600161  -0.455599
H  -3.956076   0.713443   0.926016
H  -2.544413   1.795769   1.193505
C  -2.732320  -1.411702  -0.955765
H  -2.586060  -0.991674  -1.959723
H  -2.287710  -2.413477  -0.902479
H  -3.805303  -1.475136  -0.732139

20-s
SCF Energy:  -899.323259992
Num. Imaginary Frequencies:  0

21-s
SCF Energy:  -899.334213133
Num. Imaginary Frequencies:  0
### 5. Cartesian Coordinates of All the Stationary Points Computed.

| N      | -0.131860 | 0.485852 | 0.706925 | N | 0.019072 | 2.312414 | 0.003874 |
|--------|-----------|----------|----------|---|-----------|----------|----------|
| C      | 1.016290  | -0.164435| 0.406580 | C | 0.407087 | 1.085186 | 0.026313 |
| C      | 1.198374  | -1.575262| 0.478437 | C | 1.829427 | 0.764309 | 0.093333 |
| C      | 2.405102  | -2.176452| 0.146177 | C | 2.276580 | -0.529001| -0.019485|
| C      | 3.496804  | -2.176452| -0.281293| C | 1.336867 | -1.584993| -0.035030|
| C      | 3.341561  | -0.031739| -0.350138| C | -0.036783| -1.351583| -0.021916|
| C      | 2.147602  | 0.632720 | -0.017772| C | -0.543011| -0.049112| -0.055123|
| H      | 0.366594  | -2.189329| 0.817106 | H | 2.513574 | 1.610836 | 0.168251 |
| H      | 2.494057  | -3.263199| 0.225100 | H | 3.344703 | -0.753445| -0.034808|
| H      | 4.445768  | -1.881701| -0.546108| H | 1.696968 | -2.616193| -0.049874|
| H      | 4.184880  | 0.583958 | -0.675238| H | -0.715919| -2.205135| -0.046064|
| C      | 2.146773  | 2.087641 | -0.127847| C | -1.954416| 0.275036 | -0.119388|
| C      | 1.196661  | 2.991992 | 0.186075 | C | -2.979988| -0.563868| 0.110732 |
| H      | 0.238530  | 2.695680 | 0.607501 | H | -4.010976| -0.232672| -0.020242|
| H      | 3.090193  | 2.485879 | -0.520435| H | -2.141264| 1.325588 | -0.372815|
| H      | 1.397573  | 4.056095 | 0.044057 | H | -2.835169| -1.591730| 0.451818 |
| O      | -1.196364 | -0.541638| 1.041595 | O | -1.844507| 1.928978 | -0.000057|
| P      | -2.240578 | -0.152935| -0.095339| P | 0.001934 | 0.925168 | -0.000012|
| C      | -2.847839 | 1.537403 | 0.044566 | C | -1.408906| 1.223630 | 0.000007 |
| H      | -3.220337 | 1.699061 | 1.064254 | C | -2.348643| 0.216249 | 0.000020 |
| H      | -2.032922 | 2.236474 | -0.167426| C | -1.935998| -1.129515| 0.000010 |
| H      | -3.667871 | 1.678669 | -0.673585| C | -0.577602| -1.447369| -0.000002|
| C      | -1.615111 | -0.445214| -1.758816| C | 0.425888 | -0.470548| 0.000014 |
| H      | -1.199740 | -1.459539| -1.812083| H | -1.701262| 2.274249 | 0.000006 |
| H      | -2.447663 | -0.350642| -2.469542| H | -3.411473| 0.464023 | 0.000030 |
| H      | -0.832032 | 0.283759 | -1.992875| H | -2.678188| -1.929253| 0.000001 |
| C      | -3.641884 | -1.259340| 0.189728 | C | 1.819640 | -0.892847| -0.000042|
| H      | -3.323564 | -2.300880| 0.054519 | C | 2.925417 | -0.126220| 0.000054 |
| H      | -4.005699 | -1.122112| 1.216186 | H | 3.912723 | -0.590476| -0.000039|
| H      | -4.451153 | -1.030814| -0.516760 | H | 1.952227 | -1.979802| -0.000134|

**22-s**

SCF Energy: -363.306364596
Num. Imaginary Frequencies: 0

**22-t**

SCF Energy: -363.321378862
Num. Imaginary Frequencies: 0

**23-s**

SCF Energy: -363.394812128
Num. Imaginary Frequencies: 0
### 5. Cartesian Coordinates of All the Stationary Points Computed.

|   | X          | Y          | Z               |   | X          | Y          | Z               |
|---|------------|------------|-----------------|---|------------|------------|-----------------|
| N | 1.496246   | 1.213399   | -0.000031       | N | -1.564986  | -1.077111  | 0.000031        |
| C | 0.290281   | 0.718308   | 0.000154        | C | -0.251199  | -0.671285  | -0.000025       |
| C | -0.956170  | 1.445713   | 0.000077        | C | 0.931923   | -1.419952  | -0.000156       |
| C | -2.118617  | 0.736380   | -0.000120       | C | 2.133512   | -0.720909  | -0.000195       |
| C | -2.147357  | -0.713192  | -0.000274       | C | 2.159657   | 0.690078   | -0.000101       |
| C | -1.002841  | -1.451425  | 0.000123        | C | 0.984161   | 1.429770   | 0.000034        |
| C | 0.257802   | -0.759287  | 0.000347        | C | -0.250168  | 0.753206   | 0.000073        |
| H | -0.943724  | 2.536268   | 0.000451        | H | 0.913458   | -2.511486  | -0.000218       |
| H | -3.073279  | 1.267351   | 0.000038        | H | 3.074842   | -1.274207  | -0.000298       |
| H | -3.118577  | -1.211659  | -0.000441       | H | 3.122164   | 1.205257   | -0.000136       |
| H | -1.033989  | -2.542547  | 0.000322        | H | 1.016075   | 2.521347   | 0.000110        |
| C | 1.560568   | -1.160173  | 0.000120        | C | -1.624720  | 1.168952   | 0.000190        |
| C | 2.387118   | 0.079573   | -0.000188       | C | -2.386327  | 0.026325   | 0.000155        |
| H | 3.062001   | 0.129733   | 0.875369        | H | -3.467245  | -0.091247  | 0.000220        |
| H | 1.948146   | -2.178329  | -0.000606       | H | -2.003603  | 2.187563   | 0.000271        |
| H | 3.060998   | 0.130004   | -0.876347       | H | -1.881824  | -2.034552  | -0.000021       |

#### 23-t

**SCF Energy:** -363.344515298  
**Num. Imaginary Frequencies:** 0

#### 27-s

**SCF Energy:** -363.426592726  
**Num. Imaginary Frequencies:** 0

#### 24-s

**SCF Energy:** -363.447768089  
**Num. Imaginary Frequencies:** 0

#### 29-s

**SCF Energy:** -899.356857460  
**Num. Imaginary Frequencies:** 0
### 5. Cartesian Coordinates of All the Stationary Points Computed

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| N    | -0.072577 | -0.686629 | -1.211652 |
| C    | -1.295953 | -0.468087 | -0.542880 |
| C    | -2.207041 | -1.436487 | -0.123143 |
| C    | -3.390676 | 0.358575  | 0.660253  |
| C    | -3.655745 | 0.358575  | 0.660253  |
| C    | -2.725015 | 1.319496  | 0.246918  |
| C    | -1.541121 | 0.899213  | -0.351367 |
| H    | -1.988700 | -2.496021 | -0.259243 |
| H    | -4.120977 | -1.742981 | 0.818047  |
| C    | -0.361113 | 1.686450  | -0.865764 |
| C    | 0.658034  | 0.569005  | -1.135094 |
| H    | -0.005231 | 2.448803  | -0.158335 |
| H    | -0.601590 | 2.213383  | -1.802769 |
| O    | 0.818691  | -1.560417 | -0.568470 |
| H    | 1.282277  | 0.745825  | -2.024114 |
| P    | 1.848644  | -0.036128 | 0.216622  |
| C    | 2.654356  | 1.610280  | 0.614003  |
| H    | 1.921656  | 2.316215  | 1.029693  |
| H    | 3.460879  | 1.487008  | 1.350343  |
| H    | 3.082465  | 2.056886  | -0.296060 |
| C    | 3.366217  | -0.955651 | -0.219627 |
| H    | 4.210248  | -0.639611 | 0.406725  |
| H    | 3.180288  | -2.029934 | -0.116873 |
| H    | 3.606389  | -0.749219 | -1.271613 |
| C    | 1.236517  | -0.450756 | 1.889086  |
| H    | 1.889350  | -0.028345 | 2.664532  |
| C    | 0.227653  | -0.032298 | 2.002149  |
| H    | 1.165146  | -1.539367 | 1.981410  |
| Mo   | -1.243252 | -0.162992 | 0.226752  |
| Cl   | -2.933937 | 1.121427  | -0.737645 |
| Cl   | 0.015631  | -1.742465 | -0.874843 |
| O    | -1.498360 | -0.744367 | 1.769066  |
| O    | 0.249497  | 0.808884  | 0.333294  |
| P    | 2.156935  | 0.296179  | -0.066163 |
| C    | 2.639859  | 0.600052  | 1.677322  |
| H    | 2.058556  | 0.743829  | 2.307653  |
| H    | 2.420902  | -0.971766 | 1.983697  |
| H    | 3.713490  | 0.255096  | 1.814578  |
| H    | 3.304027  | -1.764793 | -0.693699 |
| H    | 3.214829  | -0.632741 | -2.068766 |
| H    | 4.426376  | -0.362493 | -0.771844 |
| C    | 2.641471  | 2.005345  | -0.484241 |
| H    | 2.499937  | 2.174002  | -1.560569 |
| H    | 2.011103  | 2.710541  | 0.070286  |
| H    | 3.697851  | 2.180492  | -0.233238 |

**TS1-2-s**

SCF Energy: -1599.59738652

Num. Imaginary Frequencies: 1

Imaginary Frequency: -254.5016

**TS1-2-SPT**

SCF Energy: -1599.56189294

Num. Imaginary Frequencies: 1

Imaginary Frequency: -254.5016

**TS2-3-t**

SCF Energy: -1599.63798593

Num. Imaginary Frequencies: 1

Imaginary Frequency: -103.2230

**TS3-4-t**

SCF Energy: -1577.18564708

Num. Imaginary Frequencies: 1

Imaginary Frequency: -44.2544

**TS3-4-t-SPS**
### 5. Cartesian Coordinates of All the Stationary Points Computed.

| Atom | SCF Energy: -1577.17343529 | O | -2.366870 | 1.704083 | -0.862750 |
|------|-----------------------------|---|------------|----------|-----------|
| Mo   | 2.922110 | 0.007855 | 0.067231 | Mo | -1.887416 | 0.231658 | -0.289515 |
| Cl   | 2.893952 | -1.820524 | -1.365136 | O  | 0.058918 | 0.089737 | -0.416409 |
| O    | 3.730819 | -0.138892 | 1.497828 | N  | 0.807371 | -0.816122 | 0.182404 |
| Cl   | 2.079689 | 2.104374 | -0.467237 | O  | 0.260362 | -1.833098 | 0.623834 |
| N    | -1.690329 | -0.953126 | 1.025047 | Cl | -1.948808 | 0.526400 | 1.993217 |
| C    | -2.500149 | 0.115916 | 0.438805 | Cl | -3.402605 | -1.449847 | -0.769144 |
| C    | -2.028355 | 1.417343 | 0.620642 | C  | 2.214081 | -0.663319 | 0.080979 |
| C    | -2.771133 | 2.490435 | 0.145584 | C  | 2.829381 | 0.609973 | -0.008304 |
| C    | -3.969970 | 2.246350 | -0.528860 | C  | 4.227600 | 0.614244 | -0.142442 |
| C    | -4.412100 | 0.942275 | -0.726971 | C  | 4.974416 | -0.559332 | -0.181078 |
| C    | -3.704050 | -0.171281 | -0.240452 | C  | 4.338849 | -1.798720 | -0.059426 |
| H    | -1.089190 | 1.568546 | 1.149473 | C  | 2.959243 | -1.851332 | 0.076020 |
| H    | -2.413652 | 3.509470 | 0.297060 | C  | 2.096565 | 1.880204 | 0.120175 |
| H    | -4.557460 | 3.078765 | -0.919845 | C  | 2.437103 | 3.025688 | -0.485112 |
| H    | -5.320594 | 0.764949 | -1.303091 | H  | 2.431571 | -2.800181 | 0.159906 |
| C    | -4.198384 | -1.531291 | -0.514947 | H  | 4.917090 | -2.723449 | -0.073850 |
| C    | -5.493775 | -1.861828 | -0.593343 | H  | 6.059499 | -0.506069 | -0.281957 |
| H    | -6.292157 | -1.143023 | -0.395976 | H  | 4.739247 | 1.576588 | -0.173400 |
| H    | -3.448335 | -2.310021 | -0.663509 | H  | 1.224069 | 1.877310 | 0.776425 |
| H    | -5.794592 | -2.882925 | -0.830413 | H  | 1.867941 | 3.939056 | -0.309144 |
| O    | -0.493850 | -0.746732 | 1.168310 | H  | 3.271775 | 3.088371 | -1.186677 |
| O    | -2.245059 | 1.983970 | 1.360721 |

**TS4-5-s**

| SCF Energy: -1577.20092000 | Num. Imaginary Frequencies: 1 |
|----------------------------|--------------------------------|
| Imaginary Frequency: -97.6070 |

**TS4-5-SPT**

| SCF Energy: -1577.2002573 |
|---------------------------|

**TS4-5-t**

| SCF Energy: -1577.20385785 | Num. Imaginary Frequencies: 1 |
|-----------------------------|--------------------------------|
| Imaginary Frequency: -53.8983 |

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## 5. Cartesian Coordinates of All the Stationary Points Computed.

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| O       | -2.644665| 1.827373 | 0.162888 |
| Mo      | -1.830136| 0.393628 | -0.028082|
| O       | 0.162279 | 0.852911 | -0.184382|
| N       | 0.718660 | -0.327655| -0.289360|
| O       | -0.139847| -1.247339| -0.388675|
| Cl      | -2.304149| -0.724872| 1.926241 |
| Cl      | -3.155606| -0.879152| -1.424899|
| C       | 2.091539 | -0.537410| -0.192915|
| C       | 3.034525 | 0.529743 | -0.177317|
| C       | 4.377736 | 0.159360 | -0.002812|
| C       | 4.777360 | -1.165441| 0.143657 |
| C       | 3.828496 | -2.194025| 0.098263 |
| C       | 2.491003 | -1.884330| -0.070839|
| C       | 2.692828 | 1.946037 | -0.380654|
| C       | 3.331660 | 2.968382 | 0.205711 |
| H       | 1.726479 | -2.658636| -0.088774|
| H       | 4.133148 | -3.236216| 0.199985 |
| H       | 5.834857 | -1.390032| 0.274715 |
| H       | 5.131868 | 0.946328 | -0.020928|
| H       | 1.871804 | 2.165062 | -1.063573|
| H       | 3.054653 | 3.999344 | -0.016895|
| H       | 4.125089 | 2.815314 | 0.940413 |
| Mo      | -1.589809| 0.267014 | -0.138282|
| Cl      | -2.494215| -1.844549| -0.603727|
| Cl      | -2.486965| 0.312334 | 1.988498 |
| O       | 2.553197 | 1.286195 | -1.025592|
| O       | -0.080590| 1.175394 | 0.325921 |
| N       | 0.881264 | 0.383602 | -0.872657|
| Cl      | 1.950884 | -0.280759| -0.302223|
| C       | 1.926421 | -1.686802| -0.172722|
| C       | 3.034128 | -2.365313| 0.299166 |
| C       | 4.178936 | -1.640280| 0.658907 |
| C       | 4.206718 | -0.255106| 0.537839 |
| C       | 3.111641 | 0.480679 | 0.050840 |
| C       | 1.023296 | -2.217446| 0.468889 |
| H       | 3.014411 | -3.451579| 0.391464 |
| H       | 5.058853 | -2.163062| 1.037480 |
| H       | 5.110065 | 0.287349 | 0.820648 |
| C       | 3.283526 | 1.927931 | -0.055720|
| C       | 2.407452 | 2.882934 | -0.413779|
| H       | 1.372014 | 2.680257 | -0.673885|
| H       | 4.296344 | 2.252414 | 0.200972 |
| H       | 2.738674 | 3.922037 | -0.441258|
| H       | 3.207927 | -0.404314| 1.313457 |

**TS5-6-s**
SCF Energy: -1577.19266624  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -473.2883

**TS6-1-s**
SCF Energy: -1577.23948392  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -75.7359
### 5. Cartesian Coordinates of all the Stationary Points Computed.

|  |  |  |  
|---|---|---|---|
| O  | 0.966385 | 0.195559 | -0.132347 |
| Mo | -2.519112 | -0.123164 | -0.136338 |
| O  | -1.850450 | -1.651364 | -0.097534 |
| O  | -1.985442 | 0.595435 | -1.545890 |
| Cl | -4.783594 | -0.349405 | -0.252726 |
| N  | 1.621417 | -0.822688 | -0.042228 |
| C  | 3.031454 | -0.694149 | -0.034649 |
| C  | 3.772001 | 0.499046 | -0.270905 |
| C  | 5.167479 | 0.397069 | -0.173845 |
| C  | 5.801089 | -0.801941 | 0.154652 |
| C  | 5.058895 | -1.965648 | 0.374020 |
| C  | 3.676365 | -1.904979 | 0.266723 |
| C  | 3.156674 | 1.780049 | -0.648159 |
| C  | 3.604983 | 2.977298 | -0.243064 |
| H  | 3.127792 | 3.897296 | -0.583020 |
| H  | 4.431076 | 3.077916 | 0.464862 |
| H  | 2.281487 | 1.734301 | -1.297830 |
| H  | 5.770897 | 1.279058 | -0.393199 |
| H  | 6.890505 | -0.829419 | 0.220991 |
| H  | 5.556018 | -2.905411 | 0.617437 |
| H  | 3.048015 | -2.782709 | 0.426692 |

**TS7-8-s**

- **SCF Energy:** -2113.27124127
- **Num. Imaginary Frequencies:** 1
- **Imaginary Frequency:** -92.5015
- **TS7-8-SPT**
- **SCF Energy:** -2113.26080900

**TS7-11-s**

- **SCF Energy:** -2113.20831798
- **Num. Imaginary Frequencies:** 1
- **Imaginary Frequency:** -180.3802
- **TS7-11-SPT**
- **SCF Energy:** -2113.17623009
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Atom | X     | Y     | Z     |
|------|-------|-------|-------|
| Mo   | 0.849278 | -0.706859 | -0.346895 |
| Cl   | 0.225733 | -2.050993 | 1.533903 |
| Cl   | 1.181282 | 1.533869 | -0.887503 |
| N    | -1.955645 | 0.427190 | 0.568742 |
| C    | -3.60438 | 0.689712 | 0.308103 |
| Cl   | -3.811333 | 1.940428 | 0.743759 |
| O    | -1.955645 | 0.427190 | 0.568742 |
| C    | -5.102679 | 2.350313 | 0.442762 |
| C    | -5.931907 | 1.505423 | -0.298427 |
| H    | -3.124600 | 2.587897 | 1.287001 |
| Cl   | -5.41255 | 3.331009 | 0.767669 |
| O    | -5.931907 | 1.505423 | -0.298427 |
| C    | -4.186623 | -0.213401 | -0.396441 |
| H    | -2.869284 | -2.71982 | 0.998355 |
| H    | -4.263172 | -1.917666 | -1.737533 |
| C    | -3.30187 | -0.228965 | -0.281385 |
| O    | -1.429626 | 0.907702 | 1.548769 |
| P    | 4.083464 | 0.703332 | -0.019715 |
| C    | 4.095286 | 1.008068 | 1.784647 |
| C    | 5.389394 | -0.554098 | -0.276155 |
| C    | 4.874733 | 2.235910 | -0.699803 |
| H    | 5.104407 | 1.270996 | 2.135397 |
| H    | 3.407750 | 1.830449 | 2.024197 |
| H    | 3.753566 | 0.102925 | 2.301645 |
| H    | 5.875669 | 2.393827 | -0.266583 |
| H    | 4.963070 | 2.146126 | -1.790723 |
| H    | 4.236780 | 3.099982 | -0.472955 |
| H    | 6.339215 | -0.238862 | 0.181557 |
| H    | 5.065537 | -1.503214 | 0.167501 |
| H    | 5.546140 | -0.705387 | -1.353009 |

TS8-5-s
SCF Energy: -2113.23719869
Num. Imaginary Frequencies: 1
Imaginary Frequency: -53.4008

TS8-9-s
SCF Energy: -2113.22493114
Num. Imaginary Frequencies: 1
Imaginary Frequency: -372.4014
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Element | x       | y       | z       |
|---------|---------|---------|---------|
| Mo      | 0.563830| -0.069236| 0.450173|
| O       | 1.123855| -0.223902| 2.047992|
| O       | 2.192578| -0.395341| -0.688635|
| Cl      | 1.588845| 2.204809 | 0.571087|
| O       | -0.646263| 0.772673 | -0.599066|
| N       | -2.062625| 0.600952 | 0.771967|
| C       | -3.118063| -0.070092| 0.203144|
| C       | -3.255801| -1.470780| 0.360494|
| C       | -4.389847| -2.113538| -0.092276|
| C       | -5.405153| -1.362174| -0.706687|
| H       | -2.451366| -2.006885| 0.860709|
| C       | -4.500188| -3.191192| 0.033320|
| C       | -6.310331| -1.860054| -1.059559|
| C       | -6.073599| -0.571417| -1.362725|
| C       | -4.080532| 2.145729 | -0.699931|
| C       | -3.011708| 2.961941 | -0.699688|
| C       | -5.053551| 2.575275 | -0.958466|
| C       | -3.150480| 4.019792 | -0.929831|
| O       | -1.242364| -0.104450| 1.469566|
| P       | 3.742446 | -0.202270| -0.643741|
| C       | 4.368095 | -0.026364| 1.033465|
| C       | 4.489674 | -1.666335| -1.385040|
| C       | 4.224377 | 1.232587 | -1.618638|
| H       | 5.318907 | 1.327942 | -1.622958|
| H       | 3.860256 | 1.105130 | -2.646292|
| H       | 3.764012 | 2.124045 | -1.175287|
| H       | 5.461011 | 0.082414 | 1.003286|
| H       | 3.909892 | 0.859669 | 1.490588|
| H       | 4.099683 | -0.916233 | 1.617035|
| H       | 5.581766 | -1.554168 | -1.420851|
| H       | 4.227712 | -2.548813 | -0.787450|
| H       | 4.099769 | -1.792214 | -2.403374|
| Cl      | 0.170791 | -2.332366 | -0.163106|

TS6-9-s
SCF Energy: -2113.27859575
Num. Imaginary Frequencies: 1
Imaginary Frequency: -39.0904

TS9-10-s
SCF Energy: -2113.29831170
Num. Imaginary Frequencies: 1
Imaginary Frequency: -69.5289
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Mo      | 1.708114  | -1.305405 | 0.026437  |
| Cl      | 2.519585  | -0.339675 | -2.030262 |
| Cl      | 0.399774  | -1.448419 | 2.003487  |
| O       | 3.116106  | -2.049435 | 0.538975  |
| O       | 1.788844  | 0.686818  | 0.623055  |
| P       | 2.064453  | 2.180173  | 0.301943  |
| N       | -1.729953 | 0.896505  | -0.437535 |
| C       | 3.813786  | 2.465331  | -0.033197 |
| C       | 1.094062  | 2.783225  | -1.08817  |
| C       | 1.610534  | 3.147581  | 1.756999  |
| O       | -1.117708 | -0.135698 | -0.626092 |
| N       | -3.123962 | 0.797549  | -0.238907 |
| C       | -3.766789 | 2.047158  | -0.280505 |
| C       | -3.856856 | -0.406749 | -0.031312 |
| C       | -5.145020 | 2.140438  | -0.160178 |
| C       | -5.246434 | -0.270689 | 0.110858  |
| C       | -5.882310 | 0.967744  | 0.033457  |
| C       | -3.231278 | -1.729954 | 0.093563  |
| C       | -3.794886 | -2.868083 | -0.337982 |
| H       | 1.829076  | 4.211351  | 1.592392  |
| H       | 0.538453  | 3.017163  | 1.952771  |
| H       | 2.180533  | 2.784182  | 2.621798  |
| H       | 1.231960  | 3.868536  | -1.190523 |
| H       | 1.418225  | 2.274075  | -2.004045 |
| H       | 0.036239  | 2.551506  | -0.900811 |
| H       | 3.990742  | 3.533946  | -0.217469 |
| H       | 4.404662  | 2.138654  | 0.832377  |
| H       | 4.109469  | 1.880897  | -0.914739 |
| H       | -3.145322 | 2.931139  | -0.431234 |
| H       | -5.642921 | 3.109594  | -0.206744 |
| H       | -5.837674 | -1.163222 | 0.319492  |
| H       | -6.967015 | 1.018840  | 0.146235  |
| H       | -2.246902 | -1.771936 | 0.562007  |
| H       | -4.742079 | -2.879021 | -0.882247 |
| H       | -3.294139 | -3.825793 | -0.192827 |

TS11-7-s
SCF Energy: -2113.20831798
Num. Imaginary Frequencies: 1
Imaginary Frequency: -180.3802
TS11-7-SPT
SCF Energy: -2113.17623009
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Mo   | 0.849278   | -0.706859  | -0.346895  |
| Cl   | 0.225733   | -2.050993  | 1.533903   |
| Cl   | 1.181282   | 1.533869   | -0.887503  |
| O    | 0.753857   | -1.575042  | -1.765893  |
| N    | -1.955645  | 0.427190   | 0.568742   |
| C    | -3.360438  | 0.689712   | 0.308103   |
| C    | -3.811333  | 1.940428   | 0.743759   |
| C    | -5.102679  | 2.350313   | 0.442762   |
| C    | -5.931907  | 1.505423   | -0.298427  |
| C    | -5.476772  | 0.253482   | -0.701506  |
| C    | -4.186623  | -0.213401  | -0.396441  |
| H    | -3.124600  | 2.587897   | 1.287001   |
| H    | -5.451255  | 3.331009   | 0.767669   |
| H    | -6.944763  | 1.819163   | -0.555914  |
| H    | -6.146443  | -0.411884  | -1.248928  |
| C    | -3.868071  | -1.604810  | -0.766043  |
| C    | -3.257142  | -2.508634  | 0.006390   |
| H    | -2.869284  | -2.271982  | 0.998355   |
| H    | -4.263172  | -1.917666  | -1.73533   |
| H    | -3.120825  | -3.533322  | -0.340994  |
| O    | -1.330187  | -0.228965  | -0.281381  |
| O    | -1.429626  | 0.907702   | 1.548769   |
| P    | 4.083464   | 0.703332   | -0.019715  |
| C    | 4.095286   | 1.008068   | 1.784647   |
| C    | 5.389394   | -0.554098  | -0.276155  |
| C    | 4.874733   | 2.235910   | -0.699803  |
| H    | 5.104407   | 1.270996   | 2.135397   |
| H    | 3.407750   | 1.830449   | 2.024197   |
| H    | 3.753566   | 0.102925   | 2.301645   |
| H    | 5.875669   | 2.393827   | -0.266583  |
| H    | 4.963070   | 2.146126   | -1.790723  |
| H    | 4.236780   | 3.099892   | -0.472955  |
| H    | 6.339215   | -0.238862  | 0.181557   |
| H    | 5.065537   | -1.503214  | 0.167501   |
| H    | 5.546140   | -0.705387  | -1.353009  |

TS11-12-s
SCF Energy: -1652.3792745
Num. Imaginary Frequencies: 1
Imaginary Frequency: -41.7346

TS11-13-s
SCF Energy: -2113.21193375
Num. Imaginary Frequencies: 1
Imaginary Frequency: -162.2520
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5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Mo   | 2.272040   | -0.168385  | -0.190249  |
| Cl   | 1.392090   | -0.781518  | -0.190249  |
| Cl   | 2.271626   | -0.132537  | 2.189579   |
| O    | 3.611654   | -1.180481  | -0.296923  |
| O    | 2.806659   | 1.385925   | -0.528327  |
| O    | -0.982578  | 1.042987   | -0.958892  |
| P    | -1.428564  | 2.751978   | 0.260623   |
| N    | -0.840132  | -0.086841  | -0.435579  |
| C    | -1.814601  | 3.802661   | -1.170421  |
| C    | -2.672001  | 3.132826   | 1.552752   |
| O    | 0.171370   | 3.321003   | 0.908309   |
| O    | 0.202617   | -0.260792  | 0.335653   |
| N    | -1.975128  | -0.907098  | -0.232574  |
| C    | -3.187361  | -0.429758  | -0.759054  |
| C    | -1.907389  | -2.169539  | 0.415682   |
| C    | -4.353418  | -1.175592  | -0.641821  |
| C    | -3.110496  | -2.889249  | 0.506932   |
| C    | -4.315232  | -2.416218  | -0.006769  |
| C    | -0.692954  | -2.776521  | 0.998956   |
| C    | -3.361695  | -4.063691  | 0.830415   |
| H    | 0.143163   | 4.403137   | 1.105810   |
| H    | 0.401152   | 2.784325   | 1.837733   |
| H    | 0.960998   | 3.102318   | 0.178149   |
| H    | -2.643803  | 4.205444   | 1.803279   |
| H    | -3.673854  | 2.866697   | 1.192897   |
| H    | -2.447958  | 2.544700   | 2.451968   |
| H    | -1.713280  | 4.867001   | -0.914075  |
| H    | -1.121121  | 3.560499   | -1.986501  |
| H    | -2.840873  | 3.609008   | -1.509437  |
| H    | -3.190614  | 0.520008   | -1.287543  |
| H    | -5.286399  | -0.788607  | -1.054044  |
| H    | -3.088924  | -3.846477  | 1.028628   |
| H    | -5.221573  | -3.015022  | 0.945355   |
| H    | -0.054278  | -2.136383  | 1.606087   |
| H    | -0.940811  | -4.732489  | 0.189340   |
| H    | 0.525296   | -4.478884  | 1.310884   |

TS12-8-s
SCF Energy: -2113.20934527
Num. Imaginary Frequencies: 1
Imaginary Frequency: -175.9627

TS13-6-s
SCF Energy: -2113.27886107
Num. Imaginary Frequencies: 1
Imaginary Frequency: -24.8974
TS14-16-s
SCF Energy: -438.449089876
Num. Imaginary Frequencies: 1
Imaginary Frequency: -464.1834

TS14-19-s
SCF Energy: -899.307727777
Num. Imaginary Frequencies: 1
Imaginary Frequency: -110.1055
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|      |          |          |          |          |          |          |          |
|------|----------|----------|----------|----------|----------|----------|----------|
| N    | 0.254249 | -0.497901| -1.216971| N        | -0.398417| 1.779701 | -0.403611|
| C    | -0.996414| -0.348085| -0.495313| O        | 0.905214 | 0.780395 | -1.091803|
| C    | -1.793605| -1.475352| -0.265231| P        | 1.668903 | -0.292259| -0.158932|
| C    | -3.040257| -1.360730| 0.341917 | C        | 2.847590 | -0.731848| -1.557491|
| C    | -3.513397| -1.022151| 0.722304 | C        | 1.094514 | -2.002505| 0.189640 |
| C    | -2.733477| 1.023199  | 0.474179 | C        | 2.964950 | 0.239840 | 1.033408 |
| C    | -1.474913| 0.947614  | 0.35194  | C        | 0.162973 | 1.858126 | 0.934809 |
| H    | -1.400517| -2.439754| -0.585457| H        | 0.074964 | 0.420330 | 1.405834 |
| H    | -3.645235| -2.253064| 0.515914 | H        | -1.175030| -0.003196| 0.837119 |
| H    | -4.489294| 0.003908 | 1.199106 | H        | -1.418021| 0.845902 | -0.282091|
| H    | -3.108934| 2.008746 | 0.759706 | C        | -2.495259| 0.660920 | -1.154562|
| C    | -0.770932| 2.209066 | -0.378756| C        | -3.390109| -0.364133| -0.870009|
| C    | 0.346221 | 2.448743 | -1.091624| C        | -3.180276| -1.200191| 0.246660 |
| H    | 0.848943 | 1.662096 | -1.651870| H        | -2.086999| -1.045328| 1.094863 |
| H    | -1.251921| 3.068306 | 0.101268 | H        | 3.455417 | 1.132920 | 0.623038 |
| H    | 0.727684 | 3.468754 | -1.169059| H        | 3.712172 | -0.563761| 1.084223 |
| O    | 0.523919 | -1.680961| -1.551465| H        | 2.584787 | 0.453898 | 2.035436 |
| P    | 1.731680 | -0.103253| 0.387627 | H        | 3.348728 | 0.174112 | -1.922434|
| C    | 3.217155 | -0.062634| -0.668594| H        | 2.274644 | -1.168964| -2.386750|
| C    | 3.052467 | -0.754093| -1.505504| H        | 3.607269 | -1.457200| -1.229933|
| H    | 3.361303 | 0.950992 | -1.065282| H        | 0.883090 | -2.132592| 1.256407 |
| H    | 4.114973 | -0.365838| -0.111709| H        | 1.852628 | -2.723635| -0.141222|
| C    | 2.077726 | 1.058308 | 1.774235 | H        | 0.168611 | -2.176496| -0.373869|
| H    | 1.199384 | 1.106146 | 2.431681 | H        | 0.344508 | 0.137930 | 2.426886 |
| H    | 2.949206 | 0.724489 | 2.357828 | H        | -1.950943| -1.716187| 1.945556 |
| H    | 2.265855 | 2.060096 | 1.369578 | H        | -3.901463| -1.995139| 0.453282 |
| C    | 1.728964 | -1.752618| 1.162796 | H        | -4.263931| -0.522170| -1.504100|
| H    | 1.123506 | -1.722867| 2.077995 | H        | -2.625630| 1.317481 | -2.015919|
| H    | 1.278614 | -2.456085| 0.445359 | H        | 1.150393 | 2.334189 | 0.914636 |
| H    | 2.745243 | -2.090179| 1.407012 | H        | -0.522396| 2.520929 | 1.497366 |

TS16-23-s
SCF Energy: -899.312518714
Num. Imaginary Frequencies: 1
Imaginary Frequency: -577.5796

TS17-27-s
SCF Energy: -899.297399977
Num. Imaginary Frequencies: 1
Imaginary Frequency: -757.5952

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5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|      |          |          |          |      |          |          |          |
|------|----------|----------|----------|------|----------|----------|----------|
| N    | 0.557846 | 0.881561 | -0.624433| N    | -0.427228| 0.394809 | -0.059951|
| C    | 1.605636 | -0.023586| -0.355904| C    | 0.853601 | -0.179801| -0.058954|
| C    | 1.615284 | -1.397065| -0.563954| C    | 1.012806 | -1.570075| -0.155361|
| C    | 2.785329 | -2.079727| -0.221249| C    | 2.268718 | -2.170068| -0.104057|
| C    | 3.890786 | -1.400649| 0.307394 | C    | 3.403477 | -1.370212| 0.024374 |
| C    | 3.860700 | -0.015548| 0.510617 | C    | 3.258166 | 0.011242 | 0.108865 |
| C    | 2.701994 | 0.674627 | 0.174156 | C    | 2.003187 | 0.648716 | 0.078217 |
| H    | 0.738650 | -1.896765| -0.974622| H    | 0.131171 | -2.195790| -0.295014|
| H    | 2.840505 | -3.159844| -0.368663| H    | 2.357559 | -3.255346| -0.179919|
| H    | 4.790732 | -1.961854| 0.565504 | H    | 4.398051 | -1.818147| 0.058382 |
| H    | 4.728544 | 0.502791 | 0.923202 | H    | 4.147865 | 0.635492 | 0.218510 |
| C    | 2.309147 | 2.123337 | 0.251656 | C    | 1.989394 | 2.105529 | 0.256104 |
| C    | 0.911959 | 2.076680 | -0.295036| C    | 0.985592 | 2.975761 | 0.059889 |
| H    | 0.238430 | 2.923252 | -0.429772| H    | 0.019230 | 2.665594 | -0.344329|
| H    | 2.949979 | 2.781716 | -0.358963| H    | 2.951127 | 2.505427 | 0.596619 |
| O    | -0.965771| 0.324877 | -0.881428| H    | 1.156577 | 4.036172 | 0.257877 |
| P    | -2.789598| -0.212614| -0.181091| O    | -0.923412| 1.050275 | -1.247577|
| C    | -4.512335| -0.929885| -0.403482| P    | -1.942199| -0.215685| 0.096361 |
| C    | -2.250702| -1.222093| 1.267649 | C    | -2.542767| -1.231209| -1.287042|
| C    | -3.249829| 1.377424 | 0.636182 | H    | -3.235293| -0.647860| -1.903796|
| H    | -5.095580| -0.932050| 0.532782 | H    | -1.682726| -1.503158| -1.909832|
| H    | -5.054054| -0.342249| -1.158517| H    | -3.042393| -2.134616| -0.913247|
| H    | -4.430016| -1.962073| -0.773218| C    | -2.022980| -1.286643| 1.586384 |
| H    | -2.991689| -1.208632| 2.081950 | H    | -1.688377| -0.713663| 2.461535 |
| H    | -2.095450| -2.263848| 0.952080 | H    | -3.057559| -1.617849| 1.751198 |
| H    | -1.294796| -0.832350| 1.640165 | H    | -1.382815| -2.170466| 1.477443 |
| H    | -3.710847| 2.049717 | -0.101646| C    | -3.125858| 1.099579 | 0.484687 |
| H    | -3.954932| 1.230038 | 1.469054 | H    | -2.664052| 1.765475 | 1.224958 |
| H    | -2.338660| 1.858320 | 1.014521 | H    | -3.363917| 1.667711 | -0.418733|
| H    | 2.336585 | 2.532006 | 1.276805 | H    | -4.033594| 0.653517 | 0.914562 |

TS19-20-s
SCF Energy: -899.318260869
Num. Imaginary Frequencies: 1
Imaginary Frequency: -97.0319

TS19-20-s
SCF Energy: -899.315340492
Num. Imaginary Frequencies: 1
Imaginary Frequency: -403.8336
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

N  -0.060781  0.334567  -0.601957
C  -1.233443  -0.221183  -0.314996
C  -1.500045  -1.304203  -0.399041
C  -2.746677  -2.144954   0.110672
C  -3.811610  -1.304203  0.252151
C  -3.585320   0.064107  0.326271
H  -0.668946  -2.273539  -0.665328
H  -2.899091  -3.225165  -0.171244
H  -4.797695   1.74782   0.473918
H  -4.407020  -3.225165  -0.171244
C  -2.332838   0.650847   0.071355
H  -0.668946  -2.273539  -0.665328
H  -2.899091  -3.225165  -0.171244
H  -4.797695   1.74782   0.473918
H  -4.407020  -3.225165  -0.171244
C  -2.218530   2.097554   0.182476
H  -0.370756  -2.525157  -0.795245
H  -3.074236   2.569816  0.678074
H  -1.284786  -0.62680   0.951822
O  1.257403  -1.088918  -0.295575
P  2.476529  -0.206027   0.077292
C  2.952201   0.948017  -1.232550
H  3.172725   0.379490  -2.145398
H  2.111101   1.622606  -1.425716
H  3.839364   1.522948  -0.932998
C  2.225656   0.755681   1.589042
H  1.998538   0.068432   2.417471
H  3.128031   1.334534   1.829303
H  1.373410   1.428388   1.436002
C  3.902868  -1.286692   0.366192
H  3.674264  -1.975863   1.189421
H  4.102936  -1.868682  -0.542848
H  4.791274  -0.629860   0.622690

TS22-23-t
SCF Energy: -363.289404202
Num. Imaginary Frequencies: 1
Imaginary Frequency: -630.1248

N  -1.324772  -1.469527  -0.206832
C  -0.185385  -0.769129  -0.074466
C  1.099755  -1.371522  -0.027575
C  2.226185  -0.561083   0.064734
C  2.109376   0.836499   0.073471
C  0.848338   1.452871   0.008496
C  -0.293857   0.667891  -0.035937
H  1.183656  -2.458469  -0.069672
H  3.216379  -1.018420   0.111403
H  3.008904   1.452314   0.127634
H  0.768686   2.541770   0.002777
C  -1.701717   1.035895  -0.179666
C  -2.579488   0.091396   0.325045
H  -3.609738   0.041828  -0.037389
H  -2.011845   1.771270  -0.926719
H  -2.421872  -0.340516  1.315174

TS22-23-s
SCF Energy: -363.298186472
Num. Imaginary Frequencies: 1
Imaginary Frequency: -500.9974

TS23-14-s
SCF Energy: -363.359075266
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1424.6949
### 5. Cartesian Coordinates of All the Stationary Points Computed

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| N    | 1.524938   | -1.195494  | -0.074459  |
| C    | 0.267467   | -0.690796  | -0.031980  |
| C    | -0.943682  | -1.427337  | 0.002403   |
| C    | -2.126401  | -0.724088  | 0.008567   |
| C    | -2.144779  | 0.703185   | -0.031980  |
| C    | -0.982939  | 1.439714   | 0.000885   |
| C    | 0.259214   | 0.746971   | -0.022369  |
| H    | -0.922362  | -2.517948  | 0.001510   |
| H    | -3.076247  | -1.262665  | 0.012049   |
| H    | -3.108901  | 1.215703   | 0.016846   |
| C    | 1.602050   | 1.156686   | -0.002058  |
| C    | 2.373351   | -0.023445  | -0.009242  |
| H    | 3.429689   | -0.132900  | -0.257106  |
| H    | 1.988775   | 2.173182   | 0.018944   |
| H    | 2.199791   | -0.723203  | 0.999146   |

**TS16-25-s**
- SCF Energy: -899.312518714
- Num. Imaginary Frequencies: 1
- Imaginary Frequency: -577.5796

**TS27-23-s**
- SCF Energy: -363.359075158
- Num. Imaginary Frequencies: 1
- Imaginary Frequency: -1424.9276

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CONTENTS 5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

TS16-17-s
SCF Energy: -438.456682666
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1304.9646

TS17-29
SCF Energy: -899.326486790
Num. Imaginary Frequencies: 1
Imaginary Frequency: -561.1304

TS18-24-s
SCF Energy: -899.292530143
Num. Imaginary Frequencies: 1
Imaginary Frequency: -551.6319

N 1.524911 -1.195479 -0.074396 N 0.786375 1.137658 -1.170670
C 0.267385 -0.690792 -0.031814 C 1.628950 0.106004 -0.649236
C -0.943758 -1.427341 0.002498 C 1.746461 -1.203973 -1.080918
C -2.126454 -0.724070 0.008463 C 2.615460 -2.032152 -0.361673
C -2.144825 0.703212 0.007181 C 3.322967 -1.547153 0.746681
C -0.982991 1.439743 0.000916 C 3.190721 -0.220656 1.166463
C 0.259168 0.746997 -0.022355 C 2.335088 0.620350 0.452274
H -0.922456 -2.517954 0.001755 H 1.177445 -1.574836 -1.933627
H -3.076310 -1.262630 0.011911 H 2.737934 -3.073099 -0.665443
H -3.108952 1.215724 0.016634 H 3.988932 -2.218932 1.291142
H -1.011074 2.530979 0.008996 H 3.749079 0.148859 2.028213
C 1.602215 1.156655 -0.001880 C 1.967638 2.025981 0.572631
C 2.373407 -0.023467 -0.009487 C 1.095879 2.313511 -0.416941
H 3.429604 -0.132825 -0.257987 H 0.570399 3.229965 -0.665690
H 2.200673 -0.723592 0.998831 H 2.316248 2.720369 1.333030
H 1.989261 2.173030 0.019502 O -0.762750 0.805792 -0.988337
H 0.812848 1.251959 -2.182233 P -2.690797 -0.050512 -0.117788
C -0.452686 -0.400601 -0.033197 C -2.447113 0.644150 1.577254
Imaginary Frequency: -1304.9646
N 1.536693 -0.453535 -1.170670 H -2.871794 -0.005184 2.359200
C 1.628950 0.106004 -0.649236 H -1.371209 0.771168 1.750513
C 1.746461 -1.471719 0.012180 H -2.923848 1.633006 1.640833
C 2.615460 -2.032152 -0.361673 H -4.806029 -0.986692 0.857845
C 3.322967 -1.547153 0.746681 H -5.078136 0.550300 -0.019120
C 3.190721 -0.220656 1.166463 H -4.833137 -0.954549 -0.932097
H 2.335088 0.620350 0.452274 H -2.479207 -2.252250 1.013257
O -0.762750 0.805792 -0.988337 H -2.308593 -2.377621 -0.762874
H 0.812848 1.251959 -2.182233 P -2.690797 -0.050512 -0.117788
H 1.251959 -2.182233 C -2.447113 0.644150 1.577254
H 2.359200 -2.182233 C -2.447113 0.644150 1.577254
H 2.359200 -2.182233 C -2.447113 0.644150 1.577254
H 2.359200 -2.182233 C -2.447113 0.644150 1.577254
O -0.762750 0.805792 -0.988337 H -2.308593 -2.377621 -0.762874
H 0.812848 1.251959 -2.182233 P -2.690797 -0.050512 -0.117788
H 1.251959 -2.182233 C -2.447113 0.644150 1.577254
5. **Cartesian Coordinates of All the Stationary Points Computed.**

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| N | -0.158256 | -0.353086 | -1.204924 |
| C | -1.410173 | -0.369711  | -0.561494 |
| C | -2.275677 | -1.460792  | 0.461410  |
| C | -3.497570 | -1.267715  | 0.181195  |
| C | -3.497570 | -1.267715  | 0.181195  |
| C | -3.841795 | -0.013128  | 0.705704  |
| C | -2.969128 | -1.073319  | 0.597561  |
| H | -1.989707 | -2.432129  | -0.865764 |
| C | -4.196350 | -2.101070  | 0.276761  |
| C | -4.06014 | 0.115265   | 1.201719  |
| C | -2.486333 | 2.047638   | 1.004672  |
| C | -0.624276 | 1.838745   | -0.348969 |
| C | 0.393835  | 0.915512   | -1.030867 |
| H | -0.273168 | 2.361629   | 0.555151  |
| H | -0.951585 | 2.629545   | -1.045048 |
| O | 0.846619  | -1.263568  | -0.46239 |
| H | 0.867718  | 1.308048   | -1.937402 |
| P | 1.988381  | -0.137385  | 0.167184  |
| C | 3.171154  | 0.201743   | -1.91304  |
| H | 3.215209  | 1.280714   | -1.382817 |
| H | 4.172027  | -0.179352  | -0.952025 |
| H | 2.801293  | -0.299599  | -2.094944 |
| C | 3.016470  | -1.341198  | 1.166061  |
| H | 3.974118  | -0.870450  | 1.434076  |
| H | 2.485961  | -1.621719  | 2.085115  |
| H | 3.208172  | -2.249551  | 0.582317  |
| C | 1.998540  | 1.226712   | 1.401040  |
| H | 2.883185  | 1.153076   | 2.046723  |
| H | 1.979193  | 2.199175   | 0.896087  |
| H | 1.100890  | 1.136180   | 2.028265  |

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**TS18-15-s**
SCF Energy: -438.433862006
Num. Imaginary Frequencies: 1
Imaginary Frequency: -1567.8138

**TS15-24**
SCF Energy: -899.325564123
Num. Imaginary Frequencies: 1
Imaginary Frequency: -500.6771
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|    |     |     |     |     |    |    |     |
|----|-----|-----|-----|-----|----|----|-----|
| N  | -0.794819 | -1.018206 | -1.018085 |     | P  | 2.129213 | -0.253462 | 0.278696 |
| C  | -1.670875 | -0.062771 | -0.544975 |     | O  | 0.838323 | 0.277261  | -1.200592 |
| C  | -1.703620 | 1.313551  | -0.788658 |     | N  | -0.119838 | -0.558383 | -1.438271 |
| C  | -2.743188 | 2.055324  | -0.228935 |     | C  | -1.280407 | -0.329690 | -0.709292 |
| C  | -3.739797 | 1.436846  | 0.549952  |     | C  | -2.195445 | -1.409105 | -0.778379 |
| C  | -3.710295 | 0.065295  | 0.796157  |     | C  | -3.327021 | -1.474691 | 0.016217  |
| C  | -2.658987 | -0.697915 | 0.267045  |     | C  | -3.573538 | -0.453473 | 0.943536  |
| H  | -0.936731 | 1.790489  | -1.401181 |     | O  | 0.956707 | 0.109511  | -0.052506 |
| H  | -2.791368 | 3.132268  | -0.404402 |     | N  | -0.119838 | -0.558383 | -1.438271 |
| H  | -4.549184 | 2.042601  | 0.963010  |     | C  | -0.968316 | 2.114019  | 0.180601  |
| H  | -4.494515 | -0.405964 | 1.393520  |     | C  | -3.97853 | 2.809219  | -0.81436 |
| C  | -2.282557 | -2.087416 | 0.328380  |     | H  | -1.942927 | -2.221390 | -1.462923 |
| C  | -1.133969 | -2.208509 | -0.420390 |     | H  | -4.000402 | -2.330815 | -0.059711 |
| H  | -0.538182 | -3.100582 | -0.607579 |     | H  | -4.438630 | -0.499519 | 1.607489  |
| H  | -2.816143 | -2.892525 | 0.829800  |     | H  | -2.936174 | 1.453556 | 1.686262  |
| O  | 0.956707 | -0.571833 | -0.775940 |     | H  | -1.127703 | 2.643282  | 1.127589  |
| H  | 1.140199 | -0.576181 | -1.725507 |     | H  | -0.091655 | 3.844433 | -0.650834 |
| P  | 2.821393 | 0.109511 | -0.052506 |     | H  | -0.223150 | 2.386187 | 1.802603  |
| C  | 2.743567 | -0.861508 | 1.493790  |     | C  | 2.480354 | 0.174748 | 2.038864 |
| C  | 4.641372 | 0.245671 | -0.368556 |     | C  | 1.900774 | -2.051273 | 0.210849 |
| C  | 2.361414 | 1.803559 | 0.464797  |     | C  | 3.655334 | 0.178545 | -0.614052 |
| H  | 2.960268 | 2.138570 | 1.324518  |     | H  | 4.544991 | -0.227476 | -0.111543 |
| H  | 2.515581 | 2.500342 | -0.370566 |     | H  | 3.590536 | -0.216966 | 1.635167 |
| H  | 1.297722 | 1.814449 | 0.735287  |     | H  | 3.743375 | 1.272687 | -0.670366 |
| H  | 3.350514 | -0.402244 | 2.287358  |     | H  | 1.084512 | -2.224094 | -0.516632 |
| H  | 1.697639 | -0.921538 | 1.820680  |     | H  | 2.806507 | -2.570257 | -0.129189 |
| H  | 3.107188 | -1.881404 | 1.307975  |     | H  | 1.598575 | -2.437600 | 1.191849 |
| H  | 5.167753 | 0.649824 | 0.510815  |     | H  | 3.383734 | -0.342159 | 2.401155 |
| H  | 5.045334 | -0.747828 | -0.605221 |     | H  | 2.625922 | 1.259781 | 2.124077  |
| H  | 4.814727 | 0.906398 | -1.228439 |     | H  | 1.620339 | -0.114382 | 2.656527 |

TS14-21-s
SCF Energy: -899.283143719
Num. Imaginary Frequencies: 1
Imaginary Frequency: -261.6227

TS17-29
SCF Energy: -899.297399977
Num. Imaginary Frequencies: 1
Imaginary Frequency: -757.5952
### CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| N       | 0.557846 | 0.881561 | -0.624433|
| C       | 1.605636 | -0.023586| -0.355904|
| C       | 1.615284 | -1.397065| -0.563954|
| C       | 2.785329 | -2.079727| -0.221249|
| C       | 3.890786 | -1.400649| 0.307394 |
| C       | 3.860700 | -0.015548| 0.510617 |
| C       | 2.701994 | 0.674627 | 0.174156 |
| H       | 0.738650 | -1.896765| -0.974622|
| H       | 2.840505 | -3.159844| -0.368663|
| H       | 4.790732 | -1.961854| 0.565504 |
| C       | 0.124823 | -0.367243| -0.104527|
| C       | -0.728800| -1.458488| -0.101599|
| C       | -2.096335| -1.184081| -0.011988|
| C       | -2.568208| 0.135061 | 0.065388 |
| C       | -1.690012| 1.220189 | 0.073744 |
| C       | -0.317290| 0.965327 | 0.001369 |
| H       | 0.343545 | -2.476687| -0.152925|
| H       | 2.808655 | -2.010744| -0.000190|
| H       | 3.642969 | 0.314117 | 0.128462 |
| H       | 2.066612 | 2.242099 | 0.143156 |
| C       | 0.238430 | 2.923252 | -0.429772|
| C       | 2.309147 | 2.123337 | 0.251656 |
| C       | 0.911959 | 2.076680 | -0.295036|
| H       | 0.021627 | 0.123202 | 0.000190 |
| C       | 3.018237 | 1.226446 | -0.059939|
| H       | 2.093743 | -1.037710| -0.881800|
| O       | -0.965771| 0.324877 | -0.881428|
| P       | -2.789598| -0.212614| -0.181091|
| C       | -4.512335| -0.929885| -0.403482|
| C       | -2.250702| -1.222093| 1.267649 |
| C       | -3.249829| 1.377424 | 0.636182 |
| H       | -5.095580| -0.932050| 0.532782 |
| H       | -5.054054| -0.342249| -1.158517|
| H       | -4.430016| -1.962073| -0.773218|
| H       | -2.991689| -1.208632| 2.081950 |
| H       | -2.095450| -2.263848| 0.952080 |
| H       | -1.294796| -0.832350| 1.640165 |
| H       | -3.710847| 2.049717 | -0.101646|
| H       | -3.954932| 1.230038 | 1.469054 |
| H       | -2.338660| 1.858320 | 1.014521 |
| H       | 2.336585 | 2.532006 | 1.276805 |

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**TS16-18-s**
SCF Energy: -438.433862006  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -1567.8138

**TSNS-A-s**
SCF Energy: -974.412646266  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -296.7916
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

| N  | 0.055576 | 0.628233 | -0.724869 |
| C  | 1.197896 | -0.173824 | -0.380032 |
| C  | 1.108655 | -1.553116 | -0.571647 |
| C  | 2.153917 | -2.391725 | -0.186391 |
| C  | 3.300680 | -1.841232 | 0.381826  |
| C  | 3.394981 | -0.459982 | 0.537679  |
| C  | 2.368472 | 0.421482  | 0.150416  |
| H  | 0.206067 | -1.954129 | -1.028051 |
| H  | 2.067694 | -3.469918 | -0.332514 |
| H  | 4.128897 | -2.480590 | 0.691898  |
| H  | 4.307275 | -0.032136 | 0.958758  |
| C  | 2.656052 | 1.858544  | 0.286455  |
| C  | 1.995610 | 2.932405  | -0.171618 |
| C  | 1.048165 | 2.875480  | -0.702766 |
| H  | 3.600704 | 2.048073  | 0.807033  |
| H  | 2.416977 | 3.926190  | -0.010878 |
| O  | -0.828068| 0.089797  | -1.485886 |
| P  | -2.263641| -0.140976 | 0.196755  |
| C  | -2.592319| -0.179360| 2.008915  |
| H  | -2.006907| -0.987561| 2.467582  |
| H  | -2.269378| 0.775597 | 2.446865  |
| H  | -3.660141| -0.343337| 2.221368  |
| C  | -3.368052| 1.164590 | -0.427652 |
| H  | -4.401045| 0.988843 | -0.095678 |
| H  | -3.019637| 2.135850 | -0.056547 |
| H  | -3.328311| 1.173561 | -1.523788 |
| C  | -3.071503| -1.699083| -0.369436 |
| H  | -3.024391| -1.748198| -1.464865 |
| H  | -2.532529| -2.562458| 0.043501  |
| H  | -4.122156| -1.746977| -0.044048 |
| O  | -0.510937| 1.241271 | 0.260109  |

TSA-14-s
SCF Energy: -974.438070907
Num. Imaginary Frequencies: 1
Imaginary Frequency: -375.7811

min2-PPh₃
SCF Energy: -2174.11174590
Num. Imaginary Frequencies: 0

S45
5. CARTESIAN COORDINATES OF ALL THE STATIONARY POINTS COMPUTED.

|       | X         | Y         | Z         |
|-------|-----------|-----------|-----------|
| O     | -0.552830 | -0.717060 | -0.022633 |
| Mo    | -2.608676 | -0.526345 | -0.33186  |
| Cl    | -3.219406 | -2.345467 | 1.051164  |
| O     | -3.238673 | -0.554852 | -1.896627 |
| P     | 0.845619  | -0.050920 | 0.008734  |
| C     | 2.022777  | -1.231922 | -0.693054 |
| C     | 0.894246  | 1.456235  | -0.988055 |
| C     | 1.343420  | 0.338798  | 1.702931  |
| Cl    | -2.698712 | 1.654171  | 0.625084  |
| C     | 2.037985  | 0.951212  | 4.338821  |
| C     | 0.786885  | 1.327330  | 3.841273  |
| C     | 0.433650  | 1.023841  | 2.526922  |
| H     | 3.302379  | -0.592206 | 1.575931  |
| H     | 3.917091  | -0.035697 | 3.912825  |
| H     | 2.308844  | 1.189625  | 5.372215  |
| H     | 0.076310  | 1.857887  | 4.482118  |
| H     | -0.549339 | 1.317588  | 2.142374  |
| C     | 1.418829  | 2.659320  | -0.496078 |
| C     | 1.421255  | 3.797401  | -1.304868 |
| C     | 0.898955  | 3.738338  | -2.598206 |
| C     | 0.374588  | 2.594247  | -3.090925 |
| C     | 0.372145  | 1.398656  | -2.291832 |
| H     | 1.818055  | 2.713797  | 0.520749  |
| H     | 1.825801  | 4.737021  | -0.916710 |
| H     | 0.895142  | 4.634228  | -3.226989 |
| H     | -0.041121 | 2.494395  | -4.102007 |
| H     | -0.046010 | 0.465237  | -2.682966 |
| C     | 3.221811  | -0.805576 | -1.282569 |
| C     | 4.116060  | -1.747231 | -1.793213 |
| C     | 3.813065  | -3.109699 | -1.722780 |
| C     | 2.615087  | -3.534430 | -1.142426 |
| C     | 1.717357  | -2.599817 | -0.625405 |
| H     | 3.456744  | 0.261335  | -1.353515 |
| H     | 5.050116  | -1.414328 | -2.255755 |
| H     | 4.513729  | -3.845815 | -2.129265 |
| H     | 2.374351  | -4.600827 | -1.094723 |
| H     | 0.774827  | -2.927675 | -0.177434 |

**min2-PPh₃-t**

- SCF Energy: -2174.12315437
- Num. Imaginary Frequencies: 0

**PPPh₃**

- SCF Energy: -1035.37456578
- Num. Imaginary Frequencies: 0
### 5. Cartesian Coordinates of All the Stationary Points Computed

| Atom | X   | Y   | Z   |
|------|-----|-----|-----|
| P    | -0.000027 | 0.000261 | -1.207485 |
| C    | 0.265491  | -1.641812 | -0.405258 |
| C    | -0.375644 | -2.746655 | -0.991814 |
| C    | -0.375644 | -2.746655 | -0.991814 |
| C    | 1.084993  | -1.855299 | 0.713231 |
| C    | -0.220439 | -4.027700 | -0.460734 |
| H    | -1.003058 | -2.601111 | -1.878626 |
| C    | 1.251272  | -3.140325 | 1.237161 |
| H    | 1.600764  | -1.010959 | 1.180598 |
| C    | 0.596963  | -4.228219 | 0.655248 |
| H    | -0.731405 | -4.875926 | -0.927953 |
| H    | 1.896375  | -3.204034 | 2.109191 |
| H    | 0.728290  | -5.234025 | 1.067237 |
| C    | 1.289465  | 1.051151  | -0.405444 |
| C    | 1.064105  | 1.869667  | -0.711429 |
| C    | 2.567556  | 1.046668  | -0.990498 |
| H    | 0.074675  | 1.895450  | 1.178024 |
| C    | 3.599115  | 1.822016  | 0.460380 |
| C    | 2.755451  | 0.428949  | -1.876565 |
| C    | 3.363534  | 2.632317  | 0.653939 |
| H    | 1.900775  | 3.292116  | 2.105436 |
| H    | 4.589578  | 1.802285  | -0.926709 |
| C    | 4.168877  | 3.249332  | 1.065467 |
| C    | -1.554759 | 0.590991  | -0.404890 |
| C    | -2.196245 | 1.693023  | -0.996241 |
| C    | -2.144190 | -0.007162 | 0.718958 |
| C    | -3.835655 | 2.198304  | -0.464938 |
| H    | -1.760501 | 2.159655  | -1.887104 |
| C    | -3.340351 | 0.490485  | 1.243254 |
| H    | -1.666539 | -0.871555 | 1.190177 |
| C    | -3.960758 | 1.595411  | 0.656246 |
| H    | -3.866953 | 3.060431  | -0.936043 |
| H    | -3.788873 | 0.010649  | 2.119448 |
| H    | -4.897706 | 1.983837  | 1.068427 |
| O    | 0.887197  | -0.444726 | 0.405477 |
| Mo   | 2.562387  | 0.071605  | 0.828056 |
| Cl   | 3.915337  | -1.720290 | 1.491177 |
| O    | 2.736760  | 1.378023  | 1.904904 |
| P    | -1.128892 | -0.050064 | 0.111165 |
| C    | -1.580348 | -1.654058 | -0.596173 |
| C    | -2.545589 | 0.550223  | 1.073179 |
| C    | 0.810198  | 1.147426  | -1.20746 |
| O    | -1.167804 | 0.882203  | -2.537464 |
| C    | -0.898953 | 1.824875  | -3.531628 |
| C    | -0.273494 | 3.030214  | -3.206406 |
| C    | 0.088386  | 3.295796  | -1.882668 |
| C    | -0.173113 | 2.357719  | -0.885098 |
| H    | -1.654760 | -0.061520 | -2.799656 |
| H    | -0.058917 | 3.764177  | -3.989333 |
| H    | 0.589315  | 4.233862  | -1.625538 |
| H    | 0.130378  | 2.566429  | 0.146166 |
| C    | -3.138632 | 1.806459  | 0.845543 |
| C    | -4.163063 | 2.257953  | 1.677971 |
| C    | -4.603393 | 1.473297  | 2.746734 |
| C    | -4.009445 | 0.229554  | 2.987826 |
| C    | -2.979943 | -0.225678 | 2.168376 |
| C    | -2.811693 | 2.425818  | 0.005911 |
| C    | -4.625403 | 3.230750  | 1.483399 |
| C    | -5.406687 | 1.832769  | 3.397146 |
| C    | -4.344599 | -0.386378 | 3.828063 |
| H    | -2.509635 | -1.192331 | 2.378099 |
| H    | -2.930442 | -2.040722 | -0.685983 |
| C    | -3.270805 | -3.286555 | -1.253934 |
| C    | -2.274693 | -4.119467 | -1.738882 |
| C    | -0.933101 | -3.738488 | -1.655650 |
| H    | -0.581871 | -2.514966 | -1.086277 |
| H    | -3.720363 | -1.380595 | -0.317865 |
| H    | -4.323992 | -3.558327 | -1.320131 |
| H    | -2.545080 | -5.082756 | -2.182656 |
| H    | -0.148191 | -4.015282 | -2.031973 |
| H    | 0.467392  | -2.222686 | -1.012403 |

**TS1-2-PPh₃-t**  
SCF Energy: -2174.05540304  
Num. Imaginary Frequencies: 1  
Imaginary Frequency: -49.0104

**min1-s-def2svpp**  
SCF Energy: -1138.71552689  
Num. Imaginary Frequencies: 0
### 5. Cartesian Coordinates of All the Stationary Points Computed.

| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| Mo      | 0.000000 | 0.243370 | 0.000000 |
| Cl      | -1.980159 | -0.897001 | 0.000002 |
| Cl      | 1.980159  | -0.897001 | 0.000002 |
| O       | 0.000000  | 1.267275  | -1.341413 |
| O       | 0.000000  | 1.267287  | 1.341404  |
| Mo      | -1.675180 | -0.032824 | -0.293537 |
| Cl      | -2.770655 | -1.477838 | 1.140169  |
| O       | -1.983956 | -0.492794 | -1.849365 |
| N       | 0.799863  | 0.233901  | -0.044403 |
| C       | 2.161369  | 0.409085  | -0.01805 |
| C       | 2.603272  | 1.754312  | -0.045938 |
| C       | 3.939535  | 2.050896  | 0.145034  |
| C       | 4.851400  | 1.017418  | 0.398103  |
| C       | 4.417689  | -0.305456 | 0.402201  |
| C       | 3.083509  | -0.670988 | 0.161359  |
| H       | 1.869163  | 2.543418  | -0.194397 |
| H       | 4.269775  | 3.090068  | 0.121924  |
| H       | 5.903877  | 1.243036  | 0.575621  |
| H       | 5.143492  | -1.105328 | 0.559567  |
| C       | 2.807267  | -2.109523 | 0.030993  |
| C       | 1.994431  | -2.705867 | -0.851069 |
| H       | 1.378468  | -2.149707 | -1.558086 |
| H       | 3.433047  | -2.741225 | 0.669631  |
| H       | 1.933677  | -3.794548 | -0.894282 |
| O       | 0.129006  | -0.851364 | 0.281392  |
| O       | -0.044973 | 1.225571  | -0.286334 |

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### 5. Cartesian Coordinates of all the Stationary Points Computed

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Mo      | -0.787072 | 0.639500 | 0.358893 |
| Cl      | 0.762664   | 2.514807  | -1.049899 |
| Cl      | -0.420210  | -1.696266 | 0.285604  |
| O       | -2.557911  | 0.223220  | -0.579849 |
| O       | 1.297293   | 1.124582  | 1.858726  |
| N       | 2.035161   | 0.094866  | 1.048424  |
| C       | 3.073556   | -0.478195 | 0.277480  |
| C       | 3.440772   | -1.789752 | 0.617774  |
| C       | 4.407484   | -2.466543 | -0.113897 |
| C       | 5.012999   | -1.839397 | -1.206514 |
| C       | 4.670044   | -0.527219 | -1.518649 |
| C       | 3.732149   | 0.213191  | -0.773757 |
| H       | 2.925209   | -2.266579 | 1.450069  |
| H       | 4.671614   | -3.489851 | 0.157586  |
| H       | 5.761152   | -2.364078 | -1.803721 |
| H       | 5.175326   | -0.023445 | -2.345392 |
| C       | 3.619515   | 1.641488  | -1.105188 |
| C       | 3.318807   | 2.662429  | -0.291037 |
| H       | 3.049800   | 2.528418  | 0.756477  |
| H       | 3.911189   | 1.879379  | -2.133164 |
| H       | 3.339102   | 3.686243  | -0.668076 |
| O       | 1.162874   | 0.897971  | 0.387407  |
| O       | 1.749888   | -0.302589 | 2.192471  |
| P       | -3.715083  | -0.821343 | -0.556715 |
| C       | -3.432256  | -2.138629 | -1.752185 |
| H       | -2.527151  | -2.692472 | -1.472859 |
| H       | -4.297165  | -2.816929 | -1.768072 |
| H       | -3.295762  | -1.693873 | -2.746731 |
| C       | -3.962955  | -1.548457 | 1.073229  |
| H       | -4.160458  | -0.748321 | 1.798906  |
| H       | -4.821208  | -2.234483 | 1.041447  |
| H       | -3.059726  | -2.096232 | 1.370036  |
| C       | -5.229231  | 0.040518  | -1.018992 |
| H       | -6.076335  | -0.659529 | -1.030004 |
| H       | -5.422034  | 0.841734  | -0.293499 |
| H       | -5.101805  | 0.480652  | -2.016553 |