Roles of Lewis Acid Catalysts in Diels-Alder Reactions between Cyclopentadiene and Methyl Acrylate

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Computational Details

The quantum chemical calculations were carried out with the Gaussian16\textsuperscript{S1} and GAMESS\textsuperscript{S2} program packages. Geometry optimization and analytical vibrational frequency analysis were performed by the M06-2X Kohn-Sham DFT method\textsuperscript{S3-S5} with the 6-311G\textit{(p,d)} basis set\textsuperscript{S6} and the \textit{ab initio} MP2 method\textsuperscript{S7} with the 6-311G\textit{(p,d)} basis set (M06-2X/6-311G\textit{(p,d)} and MP2/6-311G\textit{(p,d)}). In the numerical integration for the M06-2X Kohn-Sham DFT method, larger grid (ultrafinegrid) was used. For the structures optimized at the MP2/6-311G\textit{(p,d)}, the energies were calculated by using the CCSD(T) method\textsuperscript{S8} (CCSD(T)/6-311G\textit{(p,d)}/MP2/6-311G\textit{(p,d)}) and the SCS-MP2 method\textsuperscript{S9} (SCS-MP2/6-311++G(3\textit{df},3\textit{pd})//MP2/6-311G\textit{(p,d)}).

Population Analysis and Orbital Interactions

To estimate the electron population of atoms, we used both Mulliken population analysis\textsuperscript{S10} and natural population analysis (NPA).\textsuperscript{S11} The pairs of interaction orbitals were obtained by the singular value decomposition of the intermolecular submatrix of the LCMO-based bond-order matrix.\textsuperscript{S12}

The pairs of interaction orbitals show that electron delocalization from the diene fragment to (dienophile·AlCl\textsubscript{3}) fragment at TS\textsubscript{endo-1} is characterized by a pair of orbitals (\psi\textsuperscript{1}; \phi\textsuperscript{1}) (Figure S2). The orbital \psi\textsuperscript{1} that consists of the occupied Kohn-Sham orbitals is similar in shape to the highest occupied (HO) orbital of the diene. The orbital \phi\textsuperscript{1} is the \pi-type anti-bonding orbital localized on the C=C bond of dienophile, given by a linear combination of the unoccupied orbitals of the dienophile fragment with an AlCl\textsubscript{3} molecule. The orbital \phi\textsuperscript{1} and \psi\textsuperscript{1} are located at \(-7.53\) eV and \(-2.20\) eV in energy, respectively. The orbital \phi\textsuperscript{1} is located lower by 2.05 eV in energy compared with the orbital \phi''\textsuperscript{1} obtained for the system without AlCl\textsubscript{3} (Figure S3). The AlCl\textsubscript{3} molecule strengthens electron-accepting ability of the terminal carbon of the dienophile in two ways. Electron delocalization from the diene fragment to the dienophile fragment at TS\textsubscript{endo-1} is characterized by another pair of orbitals (\psi\textsuperscript{2}; \phi\textsuperscript{2}). The former looks very much like the LUMO of cyclopentadiene and \phi\textsuperscript{2} consists of the occupied orbitals of methylacrylate with AlCl\textsubscript{3}. It is essentially a \pi-type bonding orbital of the C\textsuperscript{6}–C\textsuperscript{7} bond, but shows a larger amplitude on the inner carbon
C₇, being polarized under the influence of the attached AlCl₃.

### Overlap populations

Total overlap population between two fragments at TS'_{endo-1} is calculated to be −0.432 as shown in Table S2. The antibonding term arising from the interaction of the occupied orbitals of the two fragments, (oc-oc), is −0.743, indicating an intervention of strong overlap repulsion. The contribution from the interaction between the diene occupied orbitals and the dienophile unoccupied orbitals, (oc-unoc), is +0.202 and that from the interaction between the dienophile occupied orbitals and the diene unoccupied orbitals, (unoc-oc), is bonding but much weaker, +0.095. Strengthening of electron delocalization from the diene to the dienophile at the cost of electron delocalization from the dienophile to the diene is the major difference between the catalyzed and non-catalyzed reaction systems. The antibonding term (oc-oc) between C² and C⁶ atoms is −0.276, but is reduced to −0.244 by an attachment of AlCl₃. The remarkably preceded formation of the C²–C⁶ bond in the catalyzed system is attributed to two sources, the reduction of overlap repulsion and the strengthening of electron delocalization. The formation of the C³–C⁷ bond is retarded in every respect by the presence of the catalyst. These results are in conformity with the changes in the pairs of interaction orbitals upon the attachment of AlCl₃. The same pattern is observed for total overlap population between two fragments at TS'_{exo-1} (Table S3).

### Interaction Energies

We applied the method proposed by Li and Su¹³ to the calculations of the M06-2X level interaction energies. We assumed first that the diene and the AlCl₃-attached dienophile come into the relative positions at the transition state, freezing their electron configurations in their separated state. Each of the two species has the geometry that is the same as the one in the transition state. Three types of interactions take place, the electrostatic interaction (E_{ES}), the exchange interaction (E_{EX}), and the overlap repulsion (E_{REP}). The electrostatic interaction is related to a classical concept of Coulombic attractions or repulsions between net charges on the atoms in diene and those in dienophile. The exchange interaction and the overlap repulsion
appear as a consequence of electron exchange between the diene part and the dienophile part. The $E^K$ at the RHF level of theory corresponds to the sum of $E^{EX}$ and $E^{REP}$. It becomes intense in the interaction at small distances where the occupied MOs of diene and those of dienophile strongly overlap. We allow next electrons of the reacting system to shift from one part to the other part, i.e., electron delocalization, and to promote from the occupied MOs to the unoccupied MOs within each part, i.e., polarization, yielding the electron distribution calculated for the transition state ($E^{POL}$). Finally, the DFT dispersion energy ($E^{DISP}$) is also considered. The difference in interaction energies between the reacting system with AlCl$_3$ and the system without AlCl$_3$ that are produced by removing the AlCl$_3$ part from TS'$_{endo-1}$ and TS'$_{exo-1}$, respectively, is shown in Figure S4.

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| Structure               | M06-2X/6-311G(p,d) (6d-type) | MP2/6-311G(p,d) (6d-type) | CCSD(T)/6-311G(p,d) //6-311G(p,d) (6d-type) | \( E \)       | \( G \)              | thermal free term \( E \)       | \( G \)              |
|------------------------|-------------------------------|----------------------------|---------------------------------------------|---------------|----------------------|-------------------------------|----------------------|
| cyclopentadiene        | −194.058628                   | −193.988825                 | −193.544396                                 | 0.069127      | −193.616929          | −193.547802                  |                     |
| methyl acrylate        | −306.423552                   | −306.354213                 | −305.721564                                 | 0.068902      | −305.797961          | −305.729059                  |                     |
| TS\(_{endo-1}\)        | −500.467275                   | −500.306560                 | −499.262998                                 | 0.159598      | −499.397140          | −499.237542                  |                     |
| TS\(_{endo-2}\)        | −500.455624                   | −500.294236                 | −499.250344                                 | 0.159893      | −499.384746          | −499.224853                  |                     |
| TS\(_{endo-3}\)        | −500.465334                   | −500.304291                 | −499.261091                                 | 0.159800      | −499.395146          | −499.235346                  |                     |
| TS\(_{exo-1}\)         | −500.466864                   | −500.305895                 | −499.262494                                 | 0.159914      | −499.396410          | −499.236496                  |                     |
| TS\(_{exo-2}\)         | −500.455411                   | −500.293912                 | −499.250034                                 | 0.160253      | −499.383961          | −499.223708                  |                     |
| TS\(_{exo-3}\)         | −500.464037                   | −500.303213                 | −499.259994                                 | 0.159839      | −499.393818          | −499.233979                  |                     |
| PR\(_{endo-1}\)        | −500.531168                   | −500.365373                 | −499.324788                                 | 0.165313      | −499.465467          | −499.300154                  |                     |
| PR\(_{exo-1}\)         | −500.531973                   | −500.365639                 | −499.325339                                 | 0.166130      | −499.466100          | −499.299970                  |                     |
| PR\(_{exo-3}\)         | −500.529324                   | −500.363428                 | −499.322879                                 | 0.165748      | −499.463606          | −499.297858                  |                     |
| AlCl\(_3\)             | −1623.217656                  | −1623.239126                | −1621.127962                                | −0.021299     | −1621.177180         | −1621.198479                 |                     |
| AlCl\(_3\)-attached     | −1929.703449                  | −1929.637914                | −1926.902362                                | 0.065800      | −1927.027678         | −1926.961878                 |                     |
| methyl acrylate        |                               |                            |                                            |               |                      |                               |                     |
| RC\(_{endo-1}\)         | −2123.779235                  | −2123.629799                | −2120.461882                                | 0.152720      | −2120.655543         | −2120.502823                 |                     |
| RC\(_{endo-3}\)         | −2123.778620                  | −2123.623493                | −2120.462243                                | 0.153427      | −2120.655544         | −2120.502117                 |                     |
| RC\(_{exo-1}\)         | −2123.778281                  | −2123.624376                | −2120.461603                                | 0.152873      | −2120.655496         | −2120.502623                 |                     |
| RC\(_{exo-3}\)         | −2123.778281                  | −2123.624376                | −2120.461603                                | 0.152870      | −2120.655497         | −2120.502627                 |                     |
| TS\(_{endo-1}\)         | −2123.764566                  | −2123.605877                | −2120.456751                                | 0.156927      | −2120.640438         | −2120.483511                 |                     |
| TS\(_{endo-2}\)         | −2123.758067                  | −2123.600054                | −2120.450178                                | 0.157290      | −2120.634909         | −2120.477619                 |                     |
| TS\(_{endo-3}\)         | −2123.764403                  | −2123.604894                | −2120.457487                                | 0.158062      | −2120.641067         | −2120.483005                 |                     |
| TS\(_{exo-1}\)         | −2123.760358                  | −2123.601202                | −2120.454612                                | 0.158597      | −2120.637503         | −2120.478906                 |                     |
| TS\(_{exo-2}\)         | −2123.754735                  | −2123.596474                | −2120.448438                                | 0.157863      | −2120.631511         | −2120.473648                 |                     |
| TS\(_{exo-3}\)         | −2123.760069                  | −2123.601333                | −2120.454631                                | 0.157394      | −2120.637650         | −2120.480256                 |                     |
| PR\(_{endo-1}\)         | −2123.815682                  | −2123.651634                | −2120.508839                                | 0.163380      | −2120.698142         | −2120.534762                 |                     |
| PR\(_{endo-3}\)         | −2123.815658                  | −2123.651939                | −2120.510684                                | 0.163697      | −2120.699927         | −2120.536230                 |                     |
| PR\(_{exo-1}\)         | −2123.813862                  | −2123.649707                | −2120.508048                                | 0.164147      | −2120.697751         | −2120.533604                 |                     |
| PR\(_{exo-3}\)         | −2123.814312                  | −2123.650065                | −2120.509334                                | 0.163915      | −2120.698831         | −2120.534916                 |                     |

\(^{a)}\) Gibbs free energies were obtained by adding the thermal free term at MP2/6-311G(p,d) level of theory to the electronic energy at CCSD(T)/6-311G(p,d)//MP2/6-311G(p,d) level.
### Table S2. Overlap population between diene and dienophile attached with AlCl$_3$ at TS$'_{\text{endo-1}}$

|       | total | C$^2$–C$^6$ bond | C$^3$–C$^7$ bond |     |
|-------|-------|-----------------|-----------------|-----|
|       | without AlCl$_3$ |                 |                 |     |
| oc-oc | $-0.743$ | $-0.740$ (+0.003) | $-0.244$ | $-0.276$ ($-0.032$) | $-0.065$ | $-0.059$ (+0.006) |
| oc-unoc | $0.202$ | $0.148$ ($-0.054$) | $0.293$ | $0.244$ ($-0.049$) | $0.086$ | $0.093$ (+0.007) |
| unoc-oc | $0.095$ | $0.122$ (+0.027) | $0.127$ | $0.155$ (+0.028) | $0.041$ | $0.054$ (+0.013) |
| unoc-unoc | $0.015$ | $0.014$ ($-0.001$) | $0.068$ | $0.048$ ($-0.020$) | $0.034$ | $0.039$ (+0.005) |
| total | $-0.432$ | $-0.455$ ($-0.023$) | $0.243$ | $0.171$ ($-0.072$) | $0.096$ | $0.127$ (+0.031) |

### Table S3. Overlap population between diene and dienophile attached with AlCl$_3$ at TS$'_{\text{exo-1}}$

|       | total | C$^2$–C$^6$ bond | C$^3$–C$^7$ bond |     |
|-------|-------|-----------------|-----------------|-----|
|       | without AlCl$_3$ |                 |                 |     |
| oc-oc | $-0.728$ | $-0.720$ (+0.008) | $-0.232$ | $-0.266$ ($-0.034$) | $-0.074$ | $-0.069$ (+0.005) |
| oc-unoc | $0.197$ | $0.154$ ($-0.043$) | $0.264$ | $0.219$ ($-0.045$) | $0.104$ | $0.110$ (+0.006) |
| unoc-oc | $0.100$ | $0.121$ (+0.021) | $0.097$ | $0.138$ (+0.041) | $0.046$ | $0.071$ (+0.025) |
| unoc-unoc | $0.014$ | $0.014$ ($-0.000$) | $0.082$ | $0.058$ ($-0.024$) | $0.035$ | $0.044$ (+0.009) |
| total | $-0.417$ | $-0.431$ ($-0.014$) | $0.210$ | $0.149$ ($-0.061$) | $0.111$ | $0.157$ (+0.046) |
Table S4. Components of the interaction energy between two fragments at the M06-2X/6-311G(d,p) level of theory (kcal/mol).

| Component         | TS’endo-1 with AlCl3 | TS’endo-1 without AlCl3 | TS’exo-1 with AlCl3 | TS’exo-1 without AlCl3 |
|-------------------|----------------------|-------------------------|---------------------|------------------------|
| Electrostatic (Eₚ) | −58.0                | −55.9 (+2.1)            | −56.1               | −54.8                  |
| Exchange (Eₓ)     | −82.1                | −84.1 (−2.0)            | −85.1               | −79.3                  |
| Repulsion (Eᵣ)   | 218.1                | 218.3 (+0.2)            | 217.1               | 209.5                  |
| Polarization (Eₚ) | −65.8                | −60.4 (+5.4)            | −58.2               | −62.4                  |
| Dispersion (Eᵈ)   | −37.5                | −30.9 (+6.6)            | −31.8               | −36.1                  |
| Interaction (I)   | −25.3                | −13.0 (+12.3)           | −14.1               | −23.1                  |

Table S5. Components of the interaction energy between two fragments at the RHF/6-311G(d,p) level of theory (kcal/mol).

| Component         | TS’endo-1 with AlCl3 | TS’endo-1 without AlCl3 | TS’exo-1 with AlCl3 | TS’exo-1 without AlCl3 |
|-------------------|----------------------|-------------------------|---------------------|------------------------|
| Electrostatic (Eₚ) | −67.2                | −68.4 (−1.2)            | −66.2               | −70.0 (−3.8)           |
| Exchange (Eₓ)     | 137.0                | 144.9 (+7.9)            | 137.3               | 146.9 (+9.6)           |
| Delocalization-Polarization (D-P) | −81.4 | −72.2 (+9.2) | −81.4 | −73.1 (+8.3) |
| Interaction (I)   | −11.6                | 4.3 (+15.9)             | −10.3               | 3.8 (+14.1)            |

Table S6. Components of the interaction energy between two fragments at the M06-2X/6-311G(d,p) level of theory (kcal/mol).

| Component         | TS’endo-3 with AlCl3 | TS’endo-3 without AlCl3 | TS’exo-3 with AlCl3 | TS’exo-3 without AlCl3 |
|-------------------|----------------------|-------------------------|---------------------|------------------------|
| Electrostatic (Eₚ) | −57.8                | −55.9 (+1.9)            | −56.4               | −53.3                  |
| Exchange (Eₓ)     | −81.5                | −83.5 (−2.0)            | −85.5               | −77.1                  |
| Repulsion (Eᵣ)   | 217.1                | 217.6 (+0.5)            | 217.9               | 204.4                  |
| Polarization (Eₚ) | −65.7                | −56.7 (+9.0)            | −57.8               | −61.3                  |
| Dispersion (Eᵈ)   | −38.1                | −30.9 (+7.2)            | −32.1               | −35.5                  |
| Interaction (I)   | −26.0                | −9.4 (+16.6)            | −14.0               | −22.9                  |

Table S7. Components of the interaction energy between two fragments at the RHF/6-311G(d,p) level of theory (kcal/mol).

| Component         | TS’endo-3 with AlCl3 | TS’endo-3 without AlCl3 | TS’exo-3 with AlCl3 | TS’exo-3 without AlCl3 |
|-------------------|----------------------|-------------------------|---------------------|------------------------|
| Electrostatic (Eₚ) | −65.2                | −66.9 (−1.7)            | −62.6               | −65.2 (−2.6)           |
| Exchange (Eₓ)     | 131.8                | 140.8 (+9.0)            | 129.1               | 137.7 (+8.6)           |
| Delocalization-Polarization (D-P) | −77.5 | −65.9 (+11.6) | −75.8 | −63.8 (+12.0) |
| Interaction (I)   | −10.8                | 8.0 (+18.8)             | −9.3                | 8.8 (+18.1)            |

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Figure S1. Transition state structures, TS\textsubscript{endo-4}, TS\textsubscript{′endo-4}, TS\textsubscript{endo-5}, and TS\textsubscript{′exo-4}, at the M06-2X/6-311G(d,p) level of theory. Bond distances are in Å.
**Figure S2.** Pairs of interacting orbitals of $\text{TS}'_{\text{endo-1}}$ ($\phi'_1; \psi'_1$) and ($\phi'_2; \psi'_2$), calculated at the M06-2X/6-311G(d,p) level of theory. The orbital expectation values of $\phi'_1$, $\psi'_1$, $\phi'_2$, and $\psi'_2$ are $-2.20$, $-7.53$, $-11.32$, and $+1.58$ eV, respectively.

**Figure S3.** Pairs of interacting orbitals of $\text{TS}'_{\text{endo-1}}$ ($\phi''_1; \psi''_1$) and ($\phi''_2; \psi''_2$), calculated at the M06-2X/6-311G(d,p) level of theory. The orbital expectation values of $\phi''_1$, $\psi''_1$, $\phi''_2$, and $\psi''_2$ are $-0.15$, $-7.54$, $-9.53$, and $+1.18$ eV, respectively.
**Figure S4.** (a) The difference in interaction energies between the reacting system with AlCl\(_3\) and the system without AlCl\(_3\) that are produced by removing the AlCl\(_3\) part from TS\(_{\text{endo-1}}\) and TS\(_{\text{exo-1}}\), respectively. (b) The difference in (a) between TS\(_{\text{endo-1}}\) and TS\(_{\text{exo-1}}\).

**Figure S5.** (a) The difference in interaction energies between the reacting system with AlCl\(_3\) and the system without AlCl\(_3\) that are produced by removing the AlCl\(_3\) part from TS\(_{\text{endo-3}}\) and TS\(_{\text{exo-3}}\), respectively, at the M06-2X level of theory. (b) The difference in (a) between TS\(_{\text{endo-3}}\) and TS\(_{\text{exo-3}}\).
Figure S6.  (a) The difference in interaction energies between the reacting system with AlCl$_3$ and the system without AlCl$_3$ that are produced by removing the AlCl$_3$ part from TS$'_{endo-1}$ and TS$'_{exo-1}$, respectively, at the B3LYP/6-311G(d,p)//M06-2X/6-311G(d,p) level of theory.  (b) The difference in (a) between TS$'_{endo-1}$ and TS$'_{exo-1}$.

Figure S7.  (a) The difference in interaction energies between the reacting system with AlCl$_3$ and the system without AlCl$_3$ that are produced by removing the AlCl$_3$ part from TS$'_{endo-3}$ and TS$'_{exo-1}$, respectively, at the B3LYP/6-311G(d,p)//M06-2X/6-311G(d,p) level of theory.  (b) The difference in (a) between TS$'_{endo-3}$ and TS$'_{exo-3}$. 
Figure S8. The electrostatic potential maps on the isodensity (0.0004 e au\(^{-3}\)) surfaces of the reactants at the M06-2X/6-311G(d,p) level of theory. Negative value regions are described in red and positive regions are in blue.

Figure S9. Atomic charges obtained by the natural population analysis at the M06-2X/6-311G(d,p) level of theory.
Figure S10. The AlCl₃-catalyzed reaction between 1,3-butadiene and methyl acrylate. (a) Structures of TS''ₐndo-1, TS''ₐxo-1, TS''ₐndo-3, and TS''ₐxo-3 at the M06-2X/6-311G(d,p) level of theory. (b) The difference in interaction energies between the reacting system with AlCl₃ and the system without AlCl₃ that are produced by removing the AlCl₃ part from TS''ₐndo-1 and TS''ₐxo-1, respectively. (c) The difference in (b) between TS''ₐndo-1 and TS''ₐxo-1. (d) The difference in interaction energies between the reacting system with AlCl₃ and the system without AlCl₃ that are produced by removing the AlCl₃ part from TS''ₐndo-3 and TS''ₐxo-3, respectively. (e) The difference in (d) between TS''ₐndo-3 and TS''ₐxo-3.
Cartesian coordinates of stationary points at the M06-2X/6-311G\((p,d)\) level of theory are given below:

**cyclopentadiene** (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |   6           |   0         | -0.000000   0.000000   1.213826 |
|               |   6           |   0         | 0.000000     1.176051   0.280151 |
|               |   6           |   0         | -0.000000  -1.176051   0.280151 |
|               |   6           |   0         | 0.000000     0.735203  -0.986862 |
|               |   6           |   0         | -0.000000  -0.735203  -0.986862 |
|               |   6           |   0         | 0.000000     0.735203  -0.986862 |
|               |   6           |   0         | -0.000000  -0.735203  -0.986862 |
|               |   1           |   0         | 0.878592     0.000000   1.869949 |
|               |   1           |   0         | -0.878592  -0.000000   1.869949 |
|               |   1           |   0         | 0.000000     2.206712   0.605979 |
|               |   1           |   0         | -0.000000  -2.206712   0.605979 |
|               |   1           |   0         | 0.000000   1.349759  -1.877136 |

**methyl acrylate** (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |   6           |   0         | 2.320545     0.854020   0.000000 |
|               |   6           |   0         | 1.461941    -0.156600   0.000000 |
|               |   6           |   0         | 0.000000    0.116800   0.000000 |
|               |   8           |   0         | -0.507679   1.205500   0.000000 |
|               |   1           |   0         | 1.951256   1.873786   0.000000 |
|               |   1           |   0         | 3.391142   0.692156   0.000000 |
|               |   1           |   0         | 1.767749   -1.195406   0.000000 |
|               |   8           |   0         | -0.701517  -1.027739   0.000000 |
|               |   6           |   0         | -2.120327  -0.863607   0.000000 |
|               |   1           |   0         | -2.534910  -1.217889   0.000000 |
|               |   1           |   0         | -2.347210  -0.314210   0.886895 |
|               |   1           |   0         | -2.437310  -0.314210  -0.886895 |

**TS\textsubscript{endo-1}** (NIMAG=1, 461.1i cm\(^{-1}\))

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |   6           |   0         | 2.214020  -0.357799  -1.034830 |
|               |   6           |   0         | 2.399431    0.279847    0.321312 |
|               |   6           |   0         | 0.949394  -1.129548  -0.791177 |
|               |   6           |   0         | 1.768934  -0.557112   1.244120 |
|               |   6           |   0         | 0.881616  -1.404156   0.564684 |
|               |   1           |   0         | 3.029289  -1.080545   -1.179690 |
|               |   1           |   0         | 2.199470    0.322937  -1.883635 |
|               |   1           |   0         | 3.247725    0.907693    0.564180 |
|               |   1           |   0         | 0.399987  -1.652763  -1.562705 |
|               |   1           |   0         | 1.846147   -0.471269   2.319363 |
| Center Number | Atomic Number | Atomic Type | X    | Y    | Z    |
|---------------|---------------|-------------|------|------|------|
| 11            | 1             | 0           | 0.161514 | -2.056243 | 1.039448 |
| 12            | 6             | 0           | 0.882751 | 1.691532 | -0.031914 |
| 13            | 6             | 0           | -0.097857 | 0.979234 | -0.702408 |
| 14            | 6             | 0           | -1.251828 | 0.499670 | 0.062033 |
| 15            | 8             | 0           | -1.351968 | 0.528812 | 1.265157 |
| 16            | 1             | 0           | 1.536108 | 2.350786 | -0.590580 |
| 17            | 1             | 0           | 0.690952 | 1.969385 | 0.996139 |
| 18            | 1             | 0           | -0.189442 | 0.984920 | -0.031914 |
| 19            | 8             | 0           | -2.206003 | -0.027875 | 0.736202 |
| 20            | 6             | 0           | -3.341891 | -0.544158 | -0.048165 |
| 21            | 1             | 0           | -4.018296 | -0.905147 | 0.818879 |
| 22            | 1             | 0           | -3.049008 | -1.358642 | 0.616383 |
| 23            | 1             | 0           | -3.818107 | 0.236338 | 0.546260 |

**TS\text{endo-2} (NIMAG=1, 453.9i cm\textsuperscript{-1})**

| Center Number | Atomic Number | Atomic Type | X    | Y    | Z    |
|---------------|---------------|-------------|------|------|------|
| 1             | 6             | 0           | -1.868020 | -1.328623 | 0.264357 |
| 2             | 6             | 0           | -2.273453 | 0.120027 | 0.413535 |
| 3             | 6             | 0           | -0.786299 | -1.194711 | 0.767099 |
| 4             | 6             | 0           | -1.948398 | 0.748956 | 0.792945 |
| 5             | 6             | 0           | -1.033829 | -0.047555 | 0.792021 |
| 6             | 1             | 0           | -2.709174 | 1.868565 | 0.192038 |
| 7             | 1             | 0           | -1.587792 | 0.840150 | 1.183352 |
| 8             | 1             | 0           | 3.099522 | 0.432932 | 1.040405 |
| 9             | 1             | 0           | -0.150694 | 2.010826 | 0.984920 |
| 10            | 1             | 0           | -2.243713 | 1.750137 | -0.031914 |
| 11            | 1             | 0           | -0.502266 | 0.259440 | 2.368602 |
| 12            | 6             | 0           | -0.657655 | 0.604026 | 1.586296 |
| 13            | 6             | 0           | -1.422912 | -0.055709 | 0.015215 |
| 14            | 6             | 0           | -1.250749 | 0.714910 | 0.078729 |
| 15            | 8             | 0           | 1.935766 | 1.807582 | 0.319617 |
| 16            | 1             | 0           | -1.093334 | 0.202852 | 2.494073 |
| 17            | 1             | 0           | -0.703776 | 1.678816 | 1.471560 |
| 18            | 1             | 0           | 0.751725 | -1.009971 | 1.398193 |
| 19            | 8             | 0           | 2.390959 | 0.159786 | 0.409141 |
| 20            | 6             | 0           | 2.852108 | -1.082496 | 0.092296 |
| 21            | 1             | 0           | 3.890005 | -1.279606 | 0.422111 |
| 22            | 1             | 0           | 3.037581 | -1.036140 | 1.168447 |
| 23            | 1             | 0           | -2.148472 | 1.890815 | -0.124520 |

**TS\text{endo-3} (NIMAG=1, 466.8i cm\textsuperscript{-1})**

| Center Number | Atomic Number | Atomic Type | X    | Y    | Z    |
|---------------|---------------|-------------|------|------|------|
| 1             | 6             | 0           | -2.393273 | -0.543872 | 0.430440 |
| 2             | 6             | 0           | -2.176712 | 0.500640 | 0.637479 |
| 3             | 6             | 0           | -1.174003 | -0.309722 | 1.275151 |
| 4             | 6             | 0           | -1.414616 | 1.513466 | 0.053254 |
| 5             | 6             | 0           | -0.796990 | 1.013759 | 1.101534 |
| Center Number | Atomic Number | Atomic Type | X         | Y         | Z         |
|---------------|---------------|-------------|-----------|-----------|-----------|
| 1             | 6             | 0           | -1.257206 | -0.044587 | 1.331862  |
| 2             | 6             | 0           | -2.270215 | -0.689333 | 0.423595  |
| 3             | 6             | 0           | -0.887852 | 1.152479  | 0.508778  |
| 4             | 6             | 0           | -2.816053 | 0.330604  | -0.360270 |
| 5             | 6             | 0           | -1.962755 | 1.441398  | -0.321495 |
| 6             | 1             | 0           | -1.795199 | 0.318244  | 2.219762  |
| 7             | 1             | 0           | -0.430710 | -0.673395 | 1.655039  |
| 8             | 1             | 0           | -2.797730 | -1.598773 | 0.682633  |
| 9             | 1             | 0           | -0.097908 | 1.845778  | 0.768530  |
| 10            | 1             | 0           | -3.682618 | 0.229073  | -1.000345 |
| 11            | 1             | 0           | -2.061505 | 2.329940  | -0.930407 |
| 12            | 6             | 0           | -0.757665 | -1.393758 | -0.892716 |
| 13            | 6             | 0           | 0.143387  | -0.344559 | -0.973400 |
| 14            | 6             | 0           | 1.380055  | -0.388500 | -0.181800 |
| 15            | 8             | 0           | 1.625749  | -1.163202 | 0.713011  |
| 16            | 1             | 0           | -0.491035 | -2.237439 | -0.265550 |
| 17            | 1             | 0           | -1.406304 | -1.610134 | -1.729521 |
| 18            | 1             | 0           | 0.140607  | 0.347290  | -1.802812 |
| 19            | 8             | 0           | 2.246576  | 0.575089  | -0.559950 |
| 20            | 6             | 0           | 3.476503  | 0.592860  | 0.161152  |
| 21            | 1             | 0           | 4.059504  | 1.404358  | -0.266781 |
| 22            | 1             | 0           | 3.295524  | 0.767648  | 1.222591  |
| 23            | 1             | 0           | 3.999583  | -0.357309 | 0.048133  |

TS<sub>exo-1</sub> (NIMAG=1, 460.9i cm<sup>-1</sup>)

TS<sub>exo-2</sub> (NIMAG=1, 460.8i cm<sup>-1</sup>)
Center     Atomic      Atomic       Coordinates (Angstroms)
Number     Number       Type         X           Y           Z

1          6           0        1.027765  -0.707262  -1.152623
2          6           0        1.966298  -1.130161  -0.053317
3          6           0        1.057861   0.781424  -0.967550
4          6           0        2.838439  -0.059946   0.160421
5          6           0        2.274989   1.103192  -0.380925
6          1           0        1.521276  -0.931035  -2.109542
7          1           0        0.044948  -1.170528  -1.146073
8          1           0        2.223543  -2.164751   0.136263
9          1           0        0.421034   1.473409  -1.503700
10         1           0        3.735253  -0.098151   0.764733
11         1           0        2.660732   2.105593  -0.253226
12         6           0        0.505744  -0.721003   1.450743
13         6           0        -0.089036   0.458091   1.028762
14         6           0        -1.414780   0.514524   0.391444
15         8           0        -2.032051   1.525976   0.171841
16         1           0        -0.029496  -1.651903   1.307387
17         1           0        1.194892  -0.699424   2.283126
18         1           0        0.211910   1.412397   1.436320
19         8           0        -1.897356  -0.707919   0.056748
20         6           0        -3.177811  -0.692850  -0.570997
21         1           0        -3.425526  -1.733295  -0.766058
22         1           0        -3.918347  -0.238462   0.087518
23         1           0        -3.141776  -0.124359  -1.501213

TS_{exo-3} (NIMAG=1, 468.3i \text{ cm}^{-1})
### PR\textsubscript{endo-1} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z          |
| 1             | 6             | 0           | 2.241459    | -0.643885  | -0.853183  |
| 2             | 6             | 0           | 2.285643    | 0.469424   | 0.212260   |
| 3             | 6             | 0           | 0.775536    | -1.008520  | -0.559693  |
| 4             | 6             | 0           | 1.716875    | -0.274288  | 1.407615   |
| 5             | 6             | 0           | 0.825901    | -1.156241  | 0.951669   |
| 6             | 1             | 0           | 2.925409    | -1.465457  | -0.638269  |
| 7             | 1             | 0           | 2.399570    | -0.272300  | -1.869160  |
| 8             | 1             | 0           | 3.236142    | 0.975890   | 0.367125   |
| 9             | 1             | 0           | 0.326751    | -1.827174  | -1.116196  |
| 10            | 1             | 0           | 1.923824    | -0.032000  | 2.441883   |
| 11            | 1             | 0           | 0.158377    | -1.777396  | 1.534648   |
| 12            | 6             | 0           | 1.141579    | 1.396386   | -0.304533  |
| 13            | 6             | 0           | 0.094695    | 0.381686   | -0.823151  |
| 14            | 6             | 0           | -1.249706   | 0.497959   | -0.146110  |
| 15            | 8             | 0           | -1.606593   | 1.379143   | 0.585537   |
| 16            | 1             | 0           | 1.504101    | 2.033203   | -1.113304  |
| 17            | 1             | 0           | 0.726664    | 2.030990   | 0.477181   |
| 18            | 1             | 0           | -0.079659   | 0.493963   | -1.897095  |
| 19            | 8             | 0           | -2.036964   | -0.545291  | -0.470520  |
| 20            | 6             | 0           | -3.333419   | -0.532335  | 0.128141   |
| 21            | 1             | 0           | -3.248164   | -0.543966  | 1.215231   |
| 22            | 1             | 0           | -3.881797   | 0.360996   | -0.172121  |
| 23            | 1             | 0           | -3.834049   | -1.428672  | -0.228146  |

### PR\textsubscript{exo-1} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z          |
| 1             | 6             | 0           | -1.302144   | -0.320322  | 1.319927   |
| 2             | 6             | 0           | -2.102991   | -0.864554  | 0.121894   |
| 3             | 6             | 0           | -0.742024   | 0.876138   | 0.527959   |
| 4             | 6             | 0           | -2.824521   | 0.395213   | -0.323716  |
| 5             | 6             | 0           | -2.015237   | 1.428184   | -0.086264  |
| 6             | 1             | 0           | -1.939996   | -0.005901  | 2.146232   |
| 7             | 1             | 0           | -0.530306   | -1.010477  | 1.666583   |
| 8             | 1             | 0           | -2.722518   | -1.742288  | 0.293511   |
| 9             | 1             | 0           | -0.104458   | 1.586255   | 1.051351   |
| 10            | 1             | 0           | -3.772962   | 0.415808   | -0.844985  |
| 11            | 1             | 0           | -2.161976   | 2.460707   | -0.375112  |
| 12            | 6             | 0           | -0.947631   | -1.089219  | -0.903851  |
| 13            | 6             | 0           | -0.011945   | 0.116968   | -0.647481  |
| 14            | 6             | 0           | 1.367660    | -0.286829  | -0.187211  |
| 15            | 8             | 0           | 1.677192    | -1.341803  | 0.299193   |
| 16            | 1             | 0           | -0.422602   | -2.020025  | -0.686064  |
| 17            | 1             | 0           | -1.309981   | -1.117675  | -1.931025  |
| 18            | 1             | 0           | 0.099459    | 0.778002   | -1.506193  |
| 19            | 8             | 0           | 2.237009    | 0.727905   | -0.336396  |
| 20            | 6             | 0           | 3.560022    | 0.466718   | 0.135100   |
### PR\(_{ex-3}\) (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1             | 6             | 0           | -1.096485               | -0.881258 | 1.076508 |
| 2             | 6             | 0           | -1.810088               | -1.093816 | -0.271559 |
| 3             | 6             | 0           | -2.885782               | 0.625674  | 0.839086  |
| 4             | 6             | 0           | -2.388864               | 0.021636  | -0.217234 |
| 5             | 6             | 0           | -2.290861               | 1.042512  | 0.443214  |
| 6             | 1             | 0           | -1.746216               | -1.074287 | 1.930478  |
| 7             | 1             | 0           | -0.164928               | -1.441488 | 1.162838  |
| 8             | 1             | 0           | -2.188962               | -2.091452 | -0.484204 |
| 9             | 1             | 0           | -0.407617               | 1.208486  | 1.624355  |
| 10            | 1             | 0           | -3.792939               | 0.011641  | -0.728296 |
| 11            | 1             | 0           | -2.698399               | 2.035991  | 0.577264  |
| 12            | 6             | 0           | -0.695156               | -0.613415 | 1.253698  |
| 13            | 6             | 0           | -0.081924               | 0.610077  | -0.519959 |
| 14            | 6             | 0           | 1.403454                | 0.560790  | -0.252933 |
| 15            | 8             | 0           | 2.115896                | 1.527327  | 0.228327  |
| 16            | 1             | 0           | -1.096160               | -0.341046 | -2.229652 |
| 17            | 1             | 0           | 0.049825                | 1.397715  | -1.387985 |
| 18            | 1             | 0           | -0.244652               | 1.546886  | -1.050376 |
| 19            | 8             | 0           | 1.859143                | -0.679172 | 0.012564  |
| 20            | 6             | 0           | 3.249073                | -0.754785 | 0.334619  |
| 21            | 1             | 0           | 3.465479                | -0.158052 | 1.221023  |
| 22            | 1             | 0           | 3.849776                | -0.382564 | -0.495377 |
| 23            | 1             | 0           | 3.454278                | -1.806132 | 0.517771  |

### AlCl\(_3\) (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1             | 13            | 0           | 0.000000                | 0.000000 | 0.000000 |
| 2             | 17            | 0           | -0.000000               | 2.065740 | 0.000000 |
| 3             | 17            | 0           | 1.788983                | -1.032870 | 0.000000 |
| 4             | 17            | 0           | -1.788983               | -1.032870 | 0.000000 |

### AlCl\(_3\)-attached methyl acrylate (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X       | Y       | Z       |
|---------------|---------------|-------------|-------------------------|---------|---------|---------|
| 1             | 6             | 0           | -1.529999               | -2.491514 | 0.166440 |
| 2             | 6             | 0           | -2.363052               | -1.471241 | -0.022685 |
| 3             | 6             | 0           | -1.913908               | -0.089292 | 0.140199 |
| Center Number | Atomic Number | Atomic Type | X         | Y         | Z         |
|---------------|---------------|-------------|-----------|-----------|-----------|
| 1             | 6             | 0           | -3.918581 | -0.481537 | 0.148574  |
| 2             | 6             | 0           | -2.964914 | -1.640960 | 0.087082  |
| 3             | 6             | 0           | -3.195161 | 0.503657  | 1.019914  |
| 4             | 6             | 0           | -1.899331 | -1.385139 | 0.868017  |
| 5             | 6             | 0           | -2.047597 | -0.049714 | 1.454878  |
| 6             | 1             | 0           | -4.859030 | -0.786337 | 0.626154  |
| 7             | 1             | 0           | -4.186370 | -0.081135 | -0.834286 |
| 8             | 1             | 0           | -3.152787 | -2.552531 | -0.463600 |
| 9             | 1             | 0           | -3.586089 | 1.474845  | 1.291594  |
| 10            | 1             | 0           | -1.064132 | -2.047967 | 1.054112  |
| 11            | 1             | 0           | -1.338642 | 0.389759  | 2.145293  |
| 12            | 6             | 0           | -1.698577 | -0.171819 | -2.316135 |
| 13            | 6             | 0           | -1.663709 | 1.034786  | -1.751444 |
| 14            | 6             | 0           | -0.585294 | 1.355725  | -0.823401 |
| 15            | 8             | 0           | 0.316630  | 0.551878  | -0.548919 |
| 16            | 1             | 0           | -2.492099 | -0.444050 | -3.001460 |
| 17            | 1             | 0           | -0.930464 | -0.909551 | -2.109763 |
| 18            | 1             | 0           | -2.401753 | 1.807532  | -1.920001 |
| 19            | 8             | 0           | -0.613785 | 2.552121  | -0.318930 |
| 20            | 6             | 0           | 0.427853  | 2.901086  | 0.620745  |
| 21            | 1             | 0           | 0.376529  | 2.236248  | 1.483014  |
| 22            | 1             | 0           | 1.401937  | 2.817820  | 0.138933  |
| 23            | 1             | 0           | 0.218695  | 3.926881  | 0.904741  |
| 24            | 13            | 0           | 1.722434  | -0.458342 | 0.044254  |
| 25            | 17            | 0           | 1.417087  | -2.336722 | -0.879149 |
| 26            | 17            | 0           | 1.480436  | -0.473053 | 2.153258  |
| 27            | 17            | 0           | 3.412575  | 0.627328  | -0.615087 |
| Center | Atomic Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|-------|---------------|---------------|-------------|-------------------------|
|       |               |               |             | X      | Y      | Z      |
| 2     | 6             | 0             | 3.838246    | -0.786360 | 0.136682 |
| 3     | 6             | 0             | 1.690931    | -1.456966 | 0.820136 |
| 4     | 6             | 0             | 3.360314    | 0.102512  | 1.027309 |
| 5     | 6             | 0             | 2.022290    | -0.316792 | 1.455701 |
| 6     | 1             | 0             | 3.236918    | -2.844723 | 0.297895 |
| 7     | 1             | 0             | 2.537655    | -2.038694 | -1.094719|
| 8     | 1             | 0             | 4.807705    | -0.760552 | -0.342182|
| 9     | 1             | 0             | 0.779590    | -2.024439 | 0.948685 |
| 10    | 1             | 0             | 3.874252    | -0.985046 | 1.385803 |
| 11    | 1             | 0             | 1.410617    | 0.188716  | 2.192942 |
| 12    | 6             | 0             | 2.435043    | 0.732357  | -2.137311|
| 13    | 6             | 0             | 1.188772    | 0.450167  | -1.760155|
| 14    | 6             | 0             | 0.520174    | 1.230537  | -0.723683|
| 15    | 8             | 0             | -2.050035   | 1.298997  | 0.830323 |
| 16    | 6             | 0             | 3.327256    | 1.538179  | 0.081373 |
| 17    | 6             | 0             | 2.430543    | 0.732357  | -2.137311|
| 18    | 1             | 0             | 1.188772    | 0.107374  | 1.323797 |
| 19    | 1             | 0             | 0.520174    | 1.230537  | -0.723683|
|       |               |               |             | X      | Y      | Z      |
| 20    | 1             | 0             | 0.292686    | 2.304877  | 1.644338 |
| 21    | 1             | 0             | 1.278256    | 3.718880  | 1.135736 |
| 22    | 1             | 0             | 2.397422    | 1.760457  | 1.818677 |
| 23    | 1             | 0             | -0.360499   | 3.569487  | 2.466624 |
| 24    | 1             | 0             | 3.569487    | 2.304877  | 1.644338 |
| 25    | 1             | 0             | 3.569487    | 2.304877  | 1.644338 |
| 26    | 1             | 0             | 2.397422    | 1.760457  | 1.818677 |
| 27    | 1             | 0             | -0.360499   | 3.569487  | 2.466624 |

RC'_{exo-1} (NIMAG=0)
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
| 1      | 6             | 0           | X: -2.050032 Y: -1.298991 Z: 0.830313 |
| 2      | 6             | 0           | X: -3.327239 Y: -1.538189 Z: 0.081344 |
| 3      | 6             | 0           | X: -2.203316 Y: 0.107371 Z: 1.323804 |
| 4      | 6             | 0           | X: -4.104241 Y: -0.443532 Z: 0.163943 |
| 5      | 6             | 0           | X: -3.402831 Y: 0.583894 Z: 0.939137 |
| 6      | 1             | 0           | X: 1.771318 Y: -0.477600 Z: 0.068976 |
| 7      | 1             | 0           | X: 3.545437 Y: 0.571294 Z: -0.387889 |
| 8      | 1             | 0           | X: 1.281271 Y: -0.504832 Z: 2.135350 |
| 9      | 1             | 0           | X: 1.513623 Y: -2.342054 Z: -0.896186 |

**RC’exo-3 (NIMAG=0)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
| 1      | 6             | 0           | X: -3.840155 Y: -0.327518 Z: 0.156069 |
| 2      | 6             | 0           | X: -2.852175 Y: -1.399137 Z: -0.254006 |
| 3      | 6             | 0           | X: -2.980844 Y: 0.526492 Z: 1.031940 |
| 4      | 6             | 0           | X: -1.855894 Y: -1.413833 Z: 0.729825 |
| 5      | 6             | 0           | X: -1.919753 Y: -0.222006 Z: 1.481596 |
| 6      | 1             | 0           | X: -4.595652 Y: -0.804621 Z: 0.796324 |
| 7      | 1             | 0           | X: -4.357484 Y: 0.188602 Z: -0.650146 |
| 8      | 1             | 0           | X: -3.150110 Y: -2.294786 Z: -0.785221 |
| 9      | 1             | 0           | X: -3.267267 Y: 1.503460 Z: 1.398939 |
| 10     | 1             | 0           | X: -1.095237 Y: -2.177013 Z: 0.836226 |

**TS’endo-1 (NIMAG=1, 384.6i cm⁻¹)**
| Center Number | Atomic Number | Atomic Type | X  | Y  | Z  |
|---------------|---------------|-------------|----|----|----|
| 11            | 1             | 0           | -1.192138 | 0.076183 | 2.224119 |
| 12            | 6             | 0           | -1.989174 | -0.359318 | -1.736928 |
| 13            | 6             | 0           | -1.876323 | 0.965691 | -1.310540 |
| 14            | 6             | 0           | -0.677919 | 1.379799 | -0.678784 |
| 15            | 8             | 0           | 0.254436  | 0.575691 | -0.425717  |
| 16            | 1             | 0           | -2.764465 | -0.588339 | -2.459155 |
| 17            | 1             | 0           | -1.085070 | -0.947237 | -1.841212 |
| 18            | 1             | 0           | -2.618855 | 1.723931 | -1.510871 |
| 19            | 8             | 0           | 0.568258  | 2.645294 | -0.341687 |
| 20            | 6             | 0           | 0.642671  | 3.044398 | 0.327002  |
| 21            | 1             | 0           | 0.764331  | 2.478638 | 1.251943  |
| 22            | 1             | 0           | 1.502536  | 2.881473 | -0.322325 |
| 23            | 1             | 0           | 0.513870  | 4.101275 | 0.538163  |
| 24            | 13            | 0           | 1.670328  | -0.450892 | 0.008900  |
| 25            | 17            | 0           | 1.281187  | -2.327441 | -0.914192 |
| 26            | 17            | 0           | 1.600811  | -0.542155 | 2.134831  |
| 27            | 17            | 0           | 3.367370  | 0.562796 | -0.745951 |

**TS'_{endo-2} (NIMAG=1, 341.0i cm\(^{-1}\))**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X                      | Y                      | Z                      |
| 1             | 6             | 0           | -3.777321              | -0.492091              | 0.370727               |
| 2             | 6             | 0           | -3.033686              | -1.411110              | -0.573597              |
| 3             | 6             | 0           | -2.690711              | -0.106464              | 1.322285               |
| 4             | 6             | 0           | -1.880105              | -1.825502              | 0.095262               |
| 5             | 6             | 0           | -1.660337              | -1.000543              | 1.225982               |
| 6             | 1             | 0           | -4.506843              | -1.101258              | 0.922315               |
| 7             | 1             | 0           | -4.316459              | 0.335279               | -0.088003              |
| 8             | 1             | 0           | -3.541822              | -2.041542              | -1.292952              |
| 9             | 1             | 0           | -2.787498              | 0.663853               | 2.076505               |
| 10            | 1             | 0           | -1.199756              | -2.599154              | -0.238699              |
| 11            | 1             | 0           | -0.783034              | -1.034097              | 1.858117               |
| 12            | 6             | 0           | -2.293259              | -0.030231              | -1.827882              |
| 13            | 6             | 0           | -1.905093              | 1.090807               | -1.089988              |
| 14            | 6             | 0           | -0.578123              | 1.138838               | -0.603565              |
| 15            | 8             | 0           | 0.189310               | 0.145053               | -0.759963              |
| 16            | 1             | 0           | -3.208210              | 0.042842               | -2.404910              |
| 17            | 1             | 0           | -1.514752              | -0.633556              | -2.276188              |
| 18            | 1             | 0           | -2.576199              | 1.918639               | -0.922574              |
| 19            | 8             | 0           | -0.058746              | 2.169771               | 0.027856               |
| 20            | 6             | 0           | -0.861065              | 3.313056               | 0.311167               |
| 21            | 1             | 0           | -1.200321              | 3.780399               | -0.614645              |
| 22            | 1             | 0           | -1.712836              | 3.031157               | 0.933456               |
| 23            | 1             | 0           | -0.211818              | 3.991630               | 0.855645               |
| 24            | 13            | 0           | 1.805645               | -0.303384              | -0.011447              |
| 25            | 17            | 0           | 1.769651               | -2.420711              | -0.243828              |
| 26            | 17            | 0           | 1.699764               | 0.247935               | 2.047481               |
| 27            | 17            | 0           | 3.302341               | 0.702813               | -1.108637              |

**TS'_{endo-3} (NIMAG=1, 380.5i cm\(^{-1}\))**
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 2.811391   | -1.778053 | 0.188939  |
| 2             | 6             | 0           | 3.685026   | -0.569610 | -0.067726 |
| 3             | 6             | 0           | 1.684085   | -1.166699 | 0.952171  |
| 4             | 6             | 0           | 3.335103   | 0.379726  | 0.899354  |
| 5             | 6             | 0           | 2.096902   | 0.034404  | 1.477889  |
| 6             | 1             | 0           | 3.354945   | -2.437514 | -0.067726 |
| 7             | 1             | 0           | 0.188939   | -2.368250 | -0.067726 |
| 8             | 1             | 0           | 4.691075   | -0.651299 | -0.460922 |
| 9             | 1             | 0           | 0.761901   | -1.680156 | 1.190948  |
| 10            | 1             | 0           | 3.885121   | 1.290172  | 1.099848  |
| 11            | 1             | 0           | 1.523851   | 0.639128  | 2.167978  |
| 12            | 6             | 0           | 2.717039   | 0.117870  | -1.684061 |
| 13            | 6             | 0           | 1.351148   | -0.084973 | -1.480131 |
| 14            | 6             | 0           | 0.541293   | 0.933526  | -0.926661 |
| 15            | 8             | 0           | 0.714401   | 0.869270  | -0.780126 |
| 16            | 1             | 0           | 3.221443   | -0.554054 | -2.369260 |
| 17            | 1             | 0           | 3.092691   | 1.132286  | -1.689535 |
| 18            | 1             | 0           | 0.837521   | -0.980729 | -1.798517 |
| 19            | 1             | 0           | 1.153501   | 2.042991  | 0.562273  |
| 20            | 6             | 0           | 0.353823   | 3.033624  | 0.115002  |
| 21            | 1             | 0           | -0.431636  | 3.390750  | -0.543572 |
| 22            | 1             | 0           | -0.080750  | 2.604418  | 1.016129  |
| 23            | 1             | 0           | 1.050863   | 3.833355  | 0.359676  |
| 24            | 13            | 0           | -1.919429  | -0.245169 | 0.001597  |
| 25            | 17            | 0           | -1.449326  | -2.225778 | -0.634416 |
| 26            | 17            | 0           | -3.816045  | 0.454178  | 0.579503  |
| 27            | 17            | 0           | -1.468211  | 0.022901  | 2.078305  |

**TS'exo-1 (NIMAG=1, 397.3 i cm⁻¹)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | -1.984348  | -1.091799 | 0.675326  |
| 2             | 6             | 0           | -3.052037  | -1.296312 | -0.366688 |
| 3             | 6             | 0           | -2.369012  | 0.234718  | 1.231754  |
| 4             | 6             | 0           | -4.136392  | -0.498651 | 0.018142  |
| 5             | 6             | 0           | -3.703307  | 0.457627  | 0.953221  |
| 6             | 1             | 0           | -2.455173  | -1.835937 | 1.469564  |
| 7             | 1             | 0           | -0.195968  | -1.207693 | 0.340004  |
| 8             | 1             | 0           | -3.162870  | -2.224917 | -0.912608 |
| 9             | 1             | 0           | -1.752677  | 0.800768  | 1.918758  |
| 10            | 1             | 0           | -5.124148  | -0.542008 | -0.417460 |
| 11            | 1             | 0           | -4.296982  | 1.277652  | 1.332811  |
| 12            | 6             | 0           | -2.172732  | -0.121315 | -1.774687 |
| 13            | 6             | 0           | -1.789097  | 1.065558  | -1.151253 |
| 14            | 6             | 0           | -0.448723  | 1.308334  | -0.748342 |
| 15            | 8             | 0           | 0.474899   | 0.450375  | -0.842167 |
| 16            | 1             | 0           | -3.003276  | -0.091358 | -2.466759 |
| 17            | 1             | 0           | -1.391757  | -0.833899 | -2.023030 |
| 18            | 1             | 0           | -2.445838  | 1.921547  | -1.101182 |
| 19            | 8             | 0           | -0.200158  | 2.522191  | -0.314077 |
| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
| 20            | 6             | 0           | 1.158129 | 2.883647 | -0.001562 |
| 21            | 1             | 0           | 1.815127 | 2.636314 | -0.834327 |
| 22            | 1             | 0           | 1.130674 | 3.956350 | 0.163042 |
| 23            | 1             | 0           | 1.484833 | 2.370818 | 0.902980 |
| 24            | 13            | 0           | 1.743586 | -0.511819 | 0.041820 |
| 25            | 17            | 0           | 3.630352 | 0.282995 | -0.478075 |
| 26            | 17            | 0           | 1.207664 | -0.191574 | 2.089647 |
| 27            | 17            | 0           | 1.395785 | -2.503501 | -0.592804 |

TS'_{exo-2} (NIMAG=1, 376.9 cm⁻¹)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X     | Y     | Z     |
| 1             | 6             | 0           | -1.910488 | -1.394953 | 0.560987 |
| 2             | 6             | 0           | -3.014376 | -1.519413 | -0.458691 |
| 3             | 6             | 0           | -2.796437 | -0.125886 | 1.243013 |
| 4             | 6             | 0           | -4.080453 | -0.743320 | 0.014913 |
| 5             | 6             | 0           | -3.614367 | 0.136077  | 1.008458 |
| 6             | 1             | 0           | -2.050032 | -2.201980 | 1.296228 |
| 7             | 1             | 0           | -0.889440 | -1.472937 | 0.196388 |
| 8             | 1             | 0           | -3.158755 | -2.413077 | -1.053184 |
| 9             | 1             | 0           | -1.635065 | 0.374068  | 1.955843 |
| 10            | 1             | 0           | -5.082710 | -0.749256 | -0.394330 |
| 11            | 1             | 0           | -4.193805 | 0.923669  | 1.470544 |
| 12            | 6             | 0           | -2.226307 | -0.286755 | -1.839520 |
| 13            | 6             | 0           | -1.767596 | 0.864187  | -1.192384 |
| 14            | 6             | 0           | -0.413833 | 0.978137  | -0.789315 |
| 15            | 8             | 0           | 0.413595  | 0.034989  | -0.955595 |
| 16            | 1             | 0           | -3.092326 | -0.199996 | -2.482120 |
| 17            | 1             | 0           | -1.477580 | -0.998666 | -2.170847 |
| 18            | 1             | 0           | -2.414345 | 1.719798  | -1.076243 |
| 19            | 8             | 0           | 0.078871  | 2.059725  | -0.223363 |
| 20            | 6             | 0           | -0.766651 | 3.153200  | 0.126847 |
| 21            | 1             | 0           | -1.572498 | 2.812200  | 0.780121 |
| 22            | 1             | 0           | -0.125350 | 3.851044  | 0.656239 |
| 23            | 1             | 0           | -1.172199 | 3.624354  | -0.769728 |
| 24            | 13            | 0           | 1.929592  | -0.321945 | 0.032130 |
| 25            | 17            | 0           | 3.467008  | 1.007878  | -0.530367 |
| 26            | 17            | 0           | 1.225047  | -0.067745 | 2.043596 |
| 27            | 17            | 0           | 2.265708  | -2.364209 | -0.421511 |

TS'_{exo-3} (NIMAG=1, 382.5 cm⁻¹)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X     | Y     | Z     |
| 1             | 6             | 0           | 2.809412 | 0.288833 | 1.173534 |
| 2             | 6             | 0           | 3.796923 | -0.077181 | 0.092866 |
| 3             | 6             | 0           | 1.181845 | -0.818650 | 1.052909 |
| 4             | 6             | 0           | 3.636416 | -1.446938 | -0.139951 |
| 5             | 6             | 0           | 2.406631 | -1.875355 | 0.393893 |
| 6             | 1             | 0           | 3.322976 | 0.164518 | 2.137945 |
| Center Number | Atomic Number | Atomic Type | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------------|---------------|-------------|---------------|---------------|---------------|
| 1             | 6             | 0           | -3.942905     | -0.118571     | 0.128691      |
| 2             | 6             | 0           | -3.043549     | -1.230559     | -0.443702     |
| 3             | 6             | 0           | -2.757802     | 0.730541      | 0.620901      |
| 4             | 6             | 0           | -2.121717     | -1.476018     | 0.735883      |
| 5             | 6             | 0           | -1.955765     | -0.315121     | 1.373306      |
| 6             | 1             | 0           | -4.565887     | -0.459676     | 0.955155      |
| 7             | 1             | 0           | -4.552475     | 0.381248      | -0.628582     |
| 8             | 1             | 0           | -3.533378     | -2.105618     | -0.863781     |
| 9             | 1             | 0           | -2.970078     | 1.664059      | 1.137203      |
| 10            | 1             | 0           | -1.608862     | -2.406926     | 0.938126      |
| 11            | 1             | 0           | -1.285304     | -0.113098     | 2.198517      |
| 12            | 6             | 0           | -2.214125     | -0.413599     | -1.484376     |
| 13            | 6             | 0           | -2.026129     | 0.949888      | -0.775601     |
| 14            | 6             | 0           | -0.611678     | 1.344652      | -0.538823     |
| 15            | 8             | 0           | 0.330481      | 0.545673      | -0.578088     |
| 16            | 1             | 0           | -2.777884     | -0.281508     | -2.408810     |
| 17            | 1             | 0           | -1.267907     | -0.898964     | -1.720009     |
| 18            | 1             | 0           | -2.516365     | 1.774249      | -1.295081     |
| 19            | 8             | 0           | -0.426424     | 2.596064      | -0.249026     |
| 20            | 6             | 0           | 0.923869      | 3.023292      | 0.060821      |
| 21            | 1             | 0           | 1.260394      | 2.529046      | 0.971794      |
| 22            | 1             | 0           | 1.585344      | 2.776252      | -0.768385     |
| 23            | 1             | 0           | 0.851536      | 4.096204      | 0.202892      |
| 24            | 13            | 0           | 1.709619      | -0.526214     | 0.014397      |
| 25            | 17            | 0           | 1.175990      | -2.477518     | -0.586339     |
| 26            | 17            | 0           | 1.684756      | -0.182234     | 2.110404      |
| 27            | 17            | 0           | 3.395981      | 0.294140      | -0.956529     |
### PR' endo-3 (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X    | Y    | Z    |
|---------------|---------------|-------------|-------------------------|------|------|------|
| 1             | 6             | 0           |                         | 2.917453 | -1.760029 | -0.267971 |
| 2             | 6             | 0           |                         | 3.751599 | -0.467046 | -0.204498 |
| 3             | 6             | 0           |                         | 1.631432 | -1.082753 | 0.232572  |
| 4             | 6             | 0           |                         | 3.407519 | 0.015058  | 1.194290  |
| 5             | 6             | 0           |                         | 2.153123 | -0.356493 | 1.459280  |
| 6             | 1             | 0           |                         | 3.263964 | -2.525518 | 0.425668  |
| 7             | 1             | 0           |                         | 2.825924 | -2.171810 | -1.275876 |
| 8             | 1             | 0           |                         | 4.810280 | -0.540169 | -0.442898 |
| 9             | 1             | 0           |                         | 0.750460 | -1.705412 | 0.360164  |
| 10            | 1             | 0           |                         | 4.050713 | 0.628402  | 1.811837  |
| 11            | 1             | 0           |                         | 1.555000 | -0.121167 | 2.330814  |
| 12            | 6             | 0           |                         | 2.943228 | 0.428959  | -1.192946 |
| 13            | 6             | 0           |                         | 1.478103 | 0.027338  | -0.88103  |
| 14            | 6             | 0           |                         | 0.578270 | 1.115964  | -0.409236 |
| 15            | 8             | 0           |                         | -0.615550| 0.939783  | -0.111116 |
| 16            | 1             | 0           |                         | 3.192565 | 0.177774  | -2.224704 |
| 17            | 1             | 0           |                         | 3.132946 | 1.489256  | -1.042223 |
| 18            | 1             | 0           |                         | 0.976540 | -0.422115 | -1.749628 |
| 19            | 8             | 0           |                         | 1.083828 | 2.302296  | -0.283497 |
| 20            | 6             | 0           |                         | 0.218195 | 3.342591  | 0.226908  |
| 21            | 1             | 0           |                         | -0.644733| 3.453600  | -0.427057 |
| 22            | 1             | 0           |                         | -0.109252| 3.078082  | 1.230749  |
| 23            | 1             | 0           |                         | 0.830667 | 4.237820  | 0.233438  |
| 24            | 13            | 0           |                         | -1.956915| -0.342941 | 0.016304  |
| 25            | 17            | 0           |                         | -1.555821| -1.706697 | -1.55936  |
| 26            | 17            | 0           |                         | -3.705001| 0.805094  | -0.228294 |
| 27            | 17            | 0           |                         | -1.645939| -1.135966 | 1.954324  |

### PR' exo-1 (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X    | Y    | Z    |
|---------------|---------------|-------------|-------------------------|------|------|------|
| 1             | 6             | 0           |                         | -2.096833| -1.026550 | 0.781491 |
| 2             | 6             | 0           |                         | -2.965317| -1.275218 | -0.463645 |
| 3             | 6             | 0           |                         | -2.389113| 0.482801  | 0.812528  |
| 4             | 6             | 0           |                         | -4.242810| -0.564049 | -0.056167 |
| 5             | 6             | 0           |                         | -3.902689| 0.479745  | 0.701392  |
| 6             | 1             | 0           |                         | -2.478002| -1.526231 | 1.671282  |
| 7             | 1             | 0           |                         | -1.048098| -1.285474 | 0.634710  |
| 8             | 1             | 0           |                         | -3.066022| -2.303256 | -0.802801 |
| 9             | 1             | 0           |                         | -1.951474| 1.076010  | 1.613489  |
| 10            | 1             | 0           |                         | -5.234026| -0.816534 | -0.409402 |
| 11            | 1             | 0           |                         | -4.547403| 1.258999  | 1.085352  |
| 12            | 6             | 0           |                         | -2.247122| -0.344605 | -1.490953 |
| 13            | 6             | 0           |                         | -1.911820| 0.911748  | -0.647953 |
| 14            | 6             | 0           |                         | -0.465991| 1.255717  | -0.586773 |
| 15            | 8             | 0           |                         | 0.443101 | 0.420392  | -0.723619 |

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| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 16            | 1             | 0           | -2.876485   | -0.096896   | -2.344568   |
| 17            | 1             | 0           | -1.336034   | -0.824970   | -1.851771   |
| 18            | 1             | 0           | -2.445478   | 1.809581    | -0.954448   |
| 19            | 8             | 0           | -0.215825   | 2.503559    | -0.342806   |
| 20            | 6             | 0           | 1.164705    | 2.918803    | -0.198705   |
| 21            | 1             | 0           | 1.734301    | 2.609790    | -1.073472   |
| 22            | 1             | 0           | 1.122369    | 3.999568    | -0.115629   |
| 23            | 1             | 0           | 1.584456    | 2.475962    | 0.703922    |
| 24            | 13            | 0           | 1.809248    | -0.544221   | 0.074931    |
| 25            | 17            | 0           | 3.599272    | 0.287506    | -0.675376   |
| 26            | 17            | 0           | 1.424093    | -0.086440   | 2.117858    |
| 27            | 17            | 0           | 1.420482    | -2.537752   | -0.484050   |

PR'exo-3 (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | 2.907867    | 0.176339    | 1.225648    |
| 2             | 6             | 0           | 3.802435    | 0.012436    | -0.016323   |
| 3             | 6             | 0           | 1.756255    | -0.654900   | 0.635108    |
| 4             | 6             | 0           | 3.718223    | -1.490525   | -0.220376   |
| 5             | 6             | 0           | 2.502360    | -1.885306   | 0.158661    |
| 6             | 1             | 0           | 3.328959    | -0.289494   | 2.115825    |
| 7             | 1             | 0           | 2.642925    | 1.216539    | 1.432277    |
| 8             | 1             | 0           | 4.801171    | 0.441090    | 0.026371    |
| 9             | 1             | 0           | 0.875970    | -0.830098   | 1.251108    |
| 10            | 1             | 0           | 4.481669    | -2.093317   | -0.694296   |
| 11            | 1             | 0           | 2.050178    | -2.862164   | 0.054534    |
| 12            | 6             | 0           | 2.887475    | 0.654378    | -1.106658   |
| 13            | 6             | 0           | 1.475192    | 0.163404    | -0.702094   |
| 14            | 6             | 0           | 0.461547    | 1.212465    | -0.404762   |
| 15            | 8             | 0           | -0.752246   | 0.970079    | -0.287958   |
| 16            | 1             | 0           | 3.147750    | 0.323934    | -2.111144   |
| 17            | 1             | 0           | 2.956865    | 1.741337    | -1.070214   |
| 18            | 1             | 0           | 1.017943    | -0.502111   | -1.433109   |
| 19            | 8             | 0           | 0.878002    | 2.427856    | -0.218232   |
| 20            | 6             | 0           | -0.108520   | 3.416799    | 0.161059    |
| 21            | 1             | 0           | -0.582080   | 3.116138    | 1.094091    |
| 22            | 1             | 0           | -0.856785   | 3.502277    | -0.624575   |
| 23            | 1             | 0           | 0.450706    | 4.338868    | 0.278203    |
| 24            | 13            | 0           | -1.968270   | -0.413198   | 0.001088    |
| 25            | 17            | 0           | -1.994061   | -0.477087   | 2.118164    |
| 26            | 17            | 0           | -1.122017   | -2.149301   | -0.878099   |
| 27            | 17            | 0           | -3.716323   | 0.300186    | -0.926257   |
Cartesian coordinates of stationary points at the MP2/6-311G(p,d) level of theory level of theory are given below:

cyclopentadiene (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 6             | 0           | 0.000000    | 0.000000    | 1.216386    |
| 2             | 6             | 0           | 0.000000    | 1.179416    | 0.286229    |
| 3             | 6             | 0           | 0.000000    | -1.179416   | 0.286229    |
| 4             | 6             | 0           | 0.000000    | 0.733467    | -0.994068   |
| 5             | 6             | 0           | 0.000000    | -0.733467   | -0.994068   |
| 6             | 1             | 0           | -0.882249   | 0.000000    | 1.871298    |
| 7             | 1             | 0           | 0.882249    | 0.000000    | 1.871298    |
| 8             | 1             | 0           | 2.213077    | 0.610874    | 1.871298    |
| 9             | 1             | 0           | -2.213077   | 0.610874    | 1.871298    |

methyl acrylate (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 6             | 0           | 2.362187    | 0.772045    | 0.000000    |
| 2             | 6             | 0           | 1.451022    | -0.208797   | 0.000000    |
| 3             | 6             | 0           | 0.000000    | 0.118787    | 0.000000    |
| 4             | 8             | 0           | -0.475837   | 1.232439    | 0.000000    |
| 5             | 1             | 0           | 2.040449    | 1.808546    | 0.000000    |
| 6             | 1             | 0           | 3.424741    | 0.556682    | 0.000000    |
| 7             | 1             | 0           | 1.724145    | -1.258445   | 0.000000    |
| 8             | 8             | 0           | -0.733990   | -1.015227   | 0.000000    |
| 9             | 6             | 0           | -2.149417   | -0.785519   | 0.000000    |
| 10            | 1             | 0           | -2.602599   | -1.774490   | 0.000000    |
| 11            | 1             | 0           | -2.445436   | -0.224546   | 0.888168    |
| 12            | 1             | 0           | -2.445436   | -0.224546   | -0.888168   |

TS\(_{endo-1}\) (NIMAG=1, 360.3 i cm\(^{-1}\))

| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 6             | 0           | 2.207858    | -0.305447   | -1.051816   |
| 2             | 6             | 0           | 2.430651    | 0.233829    | 0.339668    |
| 3             | 6             | 0           | 0.946673    | -1.099866   | -0.857147   |
| 4             | 6             | 0           | 1.781061    | -0.634065   | 1.220211    |
| 5             | 6             | 0           | 0.869028    | -1.432098   | 0.489241    |
| 6             | 1             | 0           | 3.023412    | -1.019855   | -1.255004   |
| 7             | 1             | 0           | 2.186575    | 0.435178    | -1.852372   |
| 8             | 1             | 0           | 3.279600    | 0.854517    | 0.610574    |
| 9             | 1             | 0           | 0.401223    | -1.591353   | -1.656270   |

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| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y          | Z          |
| 1      | 6             | 0           | 1.870496   | 1.321597   | 0.275284   |
| 2      | 6             | 0           | 2.313642   | -0.117029  | 0.387449   |
| 3      | 6             | 0           | 1.88943    | 1.214645   | -0.762738  |
| 4      | 6             | 0           | 1.959947   | -0.747541  | -0.807757  |
| 5      | 6             | 0           | 1.019630   | 0.059077   | -1.493605  |
| 6      | 1             | 0           | 2.707950   | 0.275284   | -0.117029  |
| 7      | 1             | 0           | 1.588106   | 1.805890   | 1.211458   |
| 8      | 1             | 0           | 3.130163   | -0.440267  | 1.026352   |
| 9      | 1             | 0           | 0.166271   | 2.043330   | -1.085100  |
| 10     | 1             | 0           | 2.247389   | -1.751502  | -1.099352  |
| 11     | 1             | 0           | 0.479259   | -0.240344  | -2.384496  |
| 12     | 6             | 0           | 0.605202   | -0.621287  | 1.647989   |
| 13     | 6             | 0           | -0.448664  | 0.038958   | 1.044035   |
| 14     | 6             | 0           | -1.250197  | -0.718055  | 0.063961   |
| 15     | 8             | 0           | -0.919966  | -1.810352  | -0.345853  |
| 16     | 1             | 0           | 1.060030   | -0.200015  | 2.539697   |
| 17     | 1             | 0           | 0.692379   | -1.691731  | 1.500661   |
| 18     | 1             | 0           | -0.760743  | 1.010998   | 1.401710   |
| 19     | 8             | 0           | -2.382268  | -0.149048  | -0.446859  |
| 20     | 6             | 0           | -2.846805  | 1.081145   | 0.100378   |
| 21     | 1             | 0           | -3.775364  | 1.298181   | -0.426234  |
| 22     | 1             | 0           | -3.053250  | 0.992659   | 1.171099   |
| 23     | 1             | 0           | -3.808832  | 0.179851   | 0.579281   |

TSendo-2 (NIMAG=1, 343.7i cm⁻¹)

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y          | Z          |
| 1      | 6             | 0           | -2.385514  | -0.528228  | -0.461965  |
| 2      | 6             | 0           | -2.206954  | 0.477253   | 0.648414   |
| 3      | 6             | 0           | -1.177111  | -0.240555  | -1.308668  |
| 4      | 6             | 0           | -1.433589  | 1.518346   | 0.129861   |

TSendo-3 (NIMAG=1, 370.4i cm⁻¹)
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 5             | 6             | 0           | 0.795732   | 1.071170  | -1.051035  |
| 6             | 1             | 0           | 3.274485   | -0.218198 | -1.036947  |
| 7             | 1             | 0           | 2.515272   | -1.565687 | -0.151475  |
| 8             | 1             | 0           | 2.906454   | 0.588807  | 1.471630   |
| 9             | 1             | 0           | 0.886338   | -0.815223 | -2.182271  |
| 10            | 1             | 0           | 1.238020   | 2.462610  | 0.626790   |
| 11            | 1             | 0           | 0.042221   | 1.624278  | -1.601521  |
| 12            | 6             | 0           | 0.626936   | -0.779509 | 1.550443   |
| 13            | 6             | 0           | 0.054705   | -1.259800 | 0.445461   |
| 14            | 6             | 0           | 1.339159   | -0.705060 | -0.013510  |
| 15            | 8             | 0           | 2.060553   | -1.210314 | -0.848896  |
| 16            | 1             | 0           | -1.357801  | -1.415943 | 2.040855   |
| 17            | 1             | 0           | -0.182407  | 0.006475  | 2.148556   |
| 18            | 1             | 0           | -0.176678  | -2.231442 | 0.021288   |
| 19            | 8             | 0           | 1.628533   | 0.470832  | 0.605865   |
| 20            | 6             | 0           | 2.840765   | 1.075543  | 0.143711   |
| 21            | 1             | 0           | 2.947043   | 1.990980  | 0.723222   |
| 22            | 1             | 0           | 3.691571   | 0.412815  | 0.310924   |
| 23            | 1             | 0           | 2.775609   | 1.301431  | -0.923070  |

**TS_{exo-1} (NIMAG=1, 369.4i cm⁻¹)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 1.264961   | 0.029638  | 1.323853   |
| 2             | 6             | 0           | 2.309151   | 0.660916  | 0.442680   |
| 3             | 6             | 0           | 0.874876   | -1.164318 | 0.503268   |
| 4             | 6             | 0           | 2.828024   | -0.354253 | -0.368738  |
| 5             | 6             | 0           | 1.938958   | -1.452943 | 0.347304   |
| 6             | 1             | 0           | 1.792438   | -0.346890 | 2.217150   |
| 7             | 1             | 0           | 0.449053   | 0.677450  | 1.643640   |
| 8             | 1             | 0           | 2.848389   | 1.564365  | 0.711643   |
| 9             | 1             | 0           | 0.080106   | -1.855446 | 0.766472   |
| 10            | 1             | 0           | 3.690636   | -0.258344 | -1.020236  |
| 11            | 1             | 0           | 2.018180   | -2.335788 | -0.973382  |
| 12            | 6             | 0           | 0.737502   | 1.453864  | -0.887491  |
| 13            | 6             | 0           | -0.161090  | 0.406078  | -0.984235  |
| 14            | 6             | 0           | -1.386117  | 0.400053  | -0.167440  |
| 15            | 8             | 0           | -1.632849  | 1.145397  | 0.761702   |
| 16            | 1             | 0           | 0.495812   | 2.281145  | -0.225899  |
| 17            | 1             | 0           | 1.411916   | 1.660795  | -1.710117  |
| 18            | 1             | 0           | -0.135212  | -0.286712 | -1.816738  |
| 19            | 8             | 0           | -2.241065  | -0.566935 | -0.588191  |
| 20            | 6             | 0           | -3.464460  | -0.615189 | 0.155994   |
| 21            | 1             | 0           | -4.044324  | -1.418506 | -0.294466  |
| 22            | 1             | 0           | -3.267773  | -0.826570 | 1.208979   |
| 23            | 1             | 0           | -3.998735  | 0.333725  | 0.081341   |

**TS_{exo-2} (NIMAG=1, 359.7i cm⁻¹)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |

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### TS\textsubscript{exo-3} (NIMAG=1, 376.6 i cm\(^{-1}\))

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               | X           | Y           | Z           |
| 1             | 6             | 0           | 1.037282    | -0.718405   | -1.137871    |
| 2             | 6             | 0           | 2.011001    | -1.121243   | -0.062485    |
| 3             | 6             | 0           | 1.043577    | 0.775773    | -0.990195    |
| 4             | 6             | 0           | 2.858126    | -0.027274   | 0.147150     |
| 5             | 6             | 0           | 2.254518    | 1.128147    | -0.399289    |
| 6             | 1             | 0           | 1.520007    | -0.952283   | -2.102419    |
| 7             | 1             | 0           | 0.061158    | -1.198958   | -1.102981    |
| 8             | 1             | 0           | 2.285617    | -2.152856   | 0.137171     |
| 9             | 1             | 0           | 0.398484    | 1.450399    | -1.544587    |
| 10            | 1             | 0           | 3.757333    | -0.037166   | 0.754691     |
| 11            | 1             | 0           | 2.620371    | 2.142812    | -0.280369    |
| 12            | 6             | 0           | 0.487722    | -0.737758   | 1.491839     |
| 13            | 6             | 0           | -0.110860   | 0.436628    | 1.064730     |
| 14            | 6             | 0           | -1.425837   | 0.505218    | 0.401982     |
| 15            | 8             | 0           | -2.046703   | 1.528664    | 0.200285     |
| 16            | 1             | 0           | -0.025631   | -1.681021   | 1.335188     |
| 17            | 1             | 0           | 1.207021    | -0.701562   | 2.302028     |
| 18            | 1             | 0           | 0.213631    | 1.395408    | 1.453083     |
| 19            | 8             | 0           | -1.891212   | -0.723392   | 0.038311     |
| 20            | 6             | 0           | -3.169287   | -0.682623   | -0.608424    |
| 21            | 1             | 0           | -3.415098   | -1.720347   | -0.826766    |
| 22            | 1             | 0           | -3.918506   | -0.240280   | 0.050172     |
| 23            | 1             | 0           | -3.118528   | -0.097103   | -1.528601    |
## PR<sub>endo-1</sub> (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               | 1             | 6           | 0                       | 2.226992   -0.752064  -0.791136 |
|               | 2             | 6           | 0                       | 2.296218   0.487781   0.122662 |
|               | 3             | 6           | 0                       | 0.765589   -1.070426  -0.429457 |
|               | 4             | 6           | 0                       | 1.754910   -0.092941  1.412189 |
|               | 5             | 6           | 0                       | 0.840009   -1.030487  1.083044 |
|               | 6             | 1           | 0                       | 2.912433   -1.545188  -0.478000 |
|               | 7             | 1           | 0                       | 2.367948   -0.514296  -1.852317 |
|               | 8             | 1           | 0                       | 3.254125   1.007380  0.190724 |
|               | 9             | 1           | 0                       | 0.301278   -1.951397  -0.873853 |
|               | 10            | 1           | 0                       | 1.972604   0.282932   2.406586 |
|               | 11            | 1           | 0                       | 0.175870   -1.561812  1.756775 |
|               | 12            | 6           | 0                       | 1.140801   1.346756  -0.483689 |
|               | 13            | 6           | 0                       | 0.082380   0.280861  -0.856785 |
|               | 14            | 6           | 0                       | -1.246818  0.468115  -0.166052 |
|               | 15            | 8           | 0                       | -1.552987  1.366648  0.583700 |
|               | 16            | 1           | 0                       | 1.487681   1.878963  -1.375231 |
|               | 17            | 1           | 0                       | 0.743128   2.072385  0.228431 |
|               | 18            | 1           | 0                       | -0.102980  0.253093  -1.936855 |
|               | 19            | 8           | 0                       | -2.079531  -0.552112  -0.487085 |
|               | 20            | 6           | 0                       | -3.362208  -0.476379  0.151515 |
|               | 21            | 1           | 0                       | -3.251328  -0.506667  1.237019 |
|               | 22            | 1           | 0                       | -3.874904  0.446101  -0.126483 |
|               | 23            | 1           | 0                       | -3.912958  -1.345070  -0.203460 |

## PR<sub>exo-1</sub> (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               | 1             | 6           | 0                       | -1.315453  -0.362165  1.305742 |
|               | 2             | 6           | 0                       | -2.108350  -0.867072  0.085341 |
|               | 3             | 6           | 0                       | -0.743631  0.857838  0.559791 |
|               | 4             | 6           | 0                       | -2.826177  0.402691  -0.323362 |
|               | 5             | 6           | 0                       | -2.005862  1.437536  -0.041563 |
|               | 6             | 1           | 0                       | -1.967254  -0.066808  2.132921 |
|               | 7             | 1           | 0                       | -0.548944  -1.066917  1.642272 |
|               | 8             | 1           | 0                       | -2.730504  -1.753220  0.225888 |
|               | 9             | 1           | 0                       | -0.104111  1.547640  1.114698 |
|               | 10            | 1           | 0                       | -3.766593  0.444981  -0.863458 |
|               | 11            | 1           | 0                       | -2.144808  2.479661  -0.310128 |
|               | 12            | 6           | 0                       | -0.943900  -1.059646  -0.938897 |
|               | 13            | 6           | 0                       | -0.007971  0.137567  -0.638025 |
|               | 14            | 6           | 0                       | 1.368763   -0.280800  -0.183460 |
|               | 15            | 8           | 0                       | 1.667675   -1.340754  0.323154 |
|               | 16            | 1           | 0                       | -0.422237  -2.000973  -0.745361 |
|               | 17            | 1           | 0                       | -1.301420  -1.052940  -1.971587 |
|               | 18            | 1           | 0                       | 0.099204   0.829836  -1.476111 |
|               | 19            | 8           | 0                       | 2.246339   0.734759  -0.355407 |
|               | 20            | 6           | 0                       | 3.565665   0.451578  0.134191 |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X  | Y  | Z   |
|--------|---------------|-------------|-------------------------|----|----|-----|
| 21     | 1             | 0           |                         | 4.151416 | 1.341555 | -0.086113 |
| 22     | 1             | 0           |                         | 3.542408 | 0.260602 | 1.208613  |
| 23     | 1             | 0           |                         | 3.982222 | -0.420621 | -0.372159 |

**PR_{exo-3} (NIMAG=0)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X  | Y  | Z   |
|--------|---------------|-------------|-------------------------|----|----|-----|
| 1      | 6             | 0           |                         | 1.104806 | -0.931692 | -1.033361 |
| 2      | 6             | 0           |                         | 1.819902 | -1.073560 | 0.323161  |
| 3      | 6             | 0           |                         | 0.877413 | 0.582632 | -0.871941 |
| 4      | 6             | 0           |                         | 2.839780 | 0.041108 | 0.215004  |
| 5      | 6             | 0           |                         | 2.275398 | 1.034676 | -0.504724 |
| 6      | 1             | 0           |                         | 1.765546 | -1.154427 | -1.876201 |
| 7      | 1             | 0           |                         | 0.177935 | -1.506954 | -1.688678 |
| 8      | 1             | 0           |                         | 2.206028 | -2.061056 | 0.584276  |
| 9      | 1             | 0           |                         | 0.389676 | 1.119742 | -1.688678 |
| 10     | 1             | 0           |                         | 3.791719 | 0.072629 | 0.735175  |
| 11     | 1             | 0           |                         | 2.671939 | 2.030039 | -0.676517 |
| 12     | 6             | 0           |                         | 0.700021 | -0.553369 | 1.281199  |
| 13     | 6             | 0           |                         | 0.078818 | 0.631165 | 0.490199  |
| 14     | 6             | 0           |                         | -1.409394 | 0.566391 | 0.245457  |
| 15     | 8             | 0           |                         | -2.142294 | 1.530751 | 0.235592  |
| 16     | 1             | 0           |                         | 1.101855 | -0.230994 | 2.245292  |
| 17     | 1             | 0           |                         | -0.041347 | -1.338018 | 1.451027  |
| 18     | 1             | 0           |                         | 0.251331 | 1.594318 | 0.975683  |
| 19     | 8             | 0           |                         | -1.840193 | -0.691347 | -0.021614 |
| 20     | 6             | 0           |                         | -3.239317 | -0.769973 | -0.333648 |
| 21     | 1             | 0           |                         | -3.466211 | -0.180176 | -1.223436 |
| 22     | 1             | 0           |                         | -3.837355 | -0.399001 | 0.500077  |
| 23     | 1             | 0           |                         | -3.435781 | -1.825593 | -0.509958 |

**AlCl₃ (NIMAG=0)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X  | Y  | Z   |
|--------|---------------|-------------|-------------------------|----|----|-----|
| 1      | 13            | 0           |                         | 0.000000 | 0.000000 | 0.000000 |
| 2      | 17            | 0           |                         | 0.000000 | 2.064511 | 0.000000 |
| 3      | 17            | 0           |                         | 1.787919 | -1.032256 | 0.000000 |
| 4      | 17            | 0           |                         | -1.787919 | -1.032256 | 0.000000 |

**AlCl₃-attached methyl acrylate (NIMAG=0)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) | X  | Y  | Z   |
|--------|---------------|-------------|-------------------------|----|----|-----|
| 1      | 6             | 0           |                         | 1.485569 | -2.496937 | -0.181017 |
| 2      | 6             | 0           |                         | 2.330896 | -1.482775 | 0.055218  |
| 3      | 6             | 0           |                         | 1.919629 | -0.086153 | -0.113514 |
### RC'_{endo-1} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | X       | Y       | Z       |
|---------------|---------------|-------------|---------|---------|---------|
| 1             | 6             | 0           | -3.992656 | -0.418179 | 0.156299 |
| 2             | 6             | 0           | -3.090823 | -1.613625 | 0.035163 |
| 3             | 6             | 0           | -3.204720 | 0.523392  | 1.020221 |
| 4             | 6             | 0           | -1.992958 | -1.424822 | 0.817955 |
| 5             | 6             | 0           | -2.067640 | -0.102907 | 1.431729 |
| 6             | 1             | 0           | -4.919401 | -0.703863 | 0.677018 |
| 7             | 1             | 0           | -4.290022 | 0.010067  | -0.807495 |
| 8             | 1             | 0           | -3.333807 | -2.510163 | -0.523664 |
| 9             | 1             | 0           | -3.546789 | 1.504734  | 1.329558 |
| 10            | 1             | 0           | -1.184577 | -2.130983 | 0.968084 |
| 11            | 1             | 0           | -1.327878 | 0.291536  | 2.119351 |
| 12            | 6             | 0           | -1.770491 | -0.191635 | -2.230085 |
| 13            | 6             | 0           | -1.712033 | 1.024197  | -1.657045 |
| 14            | 6             | 0           | -0.594856 | 1.352362  | -0.776610 |
| 15            | 8             | 0           | 0.307761  | 0.543444  | -0.511357 |
| 16            | 1             | 0           | -2.582143 | -0.451008 | -2.901080 |
| 17            | 1             | 0           | -0.994202 | -0.927828 | -2.052311 |
| 18            | 1             | 0           | -2.450069 | 1.800280  | -1.819921 |
| 19            | 8             | 0           | -0.606900 | 2.574194  | -0.310519 |
| 20            | 6             | 0           | 0.488244  | 2.930393  | 0.574940 |
| 21            | 1             | 0           | 0.475035  | 2.281737  | 1.450309 |
| 22            | 1             | 0           | 1.435995  | 2.833463  | 0.046629 |
| 23            | 1             | 0           | 0.294182  | 3.963454  | 0.848092 |
| 24            | 13            | 0           | 1.765494  | -0.469506 | 0.045486 |
| 25            | 17            | 0           | 1.460814  | -2.341023 | -0.878664 |
| 26            | 17            | 0           | 1.561207  | -0.487616 | 2.151836 |
| 27            | 17            | 0           | 3.418711  | 0.636050  | -0.660601 |

### RC'_{endo-3} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | X       | Y       | Z       |
|---------------|---------------|-------------|---------|---------|---------|
| 1             | 6             | 0           | 2.918292 | -1.870605 | -0.054592 |
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|-------------------------|
|        |               |             | X          | Y          | Z          |
| 1      | 6             | 0           | -2.062308  | -1.273803  | 0.798181   |
| 2      | 6             | 0           | -3.321229  | -1.538309  | 0.027999   |
| 3      | 6             | 0           | -2.248389  | 0.123620   | 1.305091   |
| 4      | 6             | 0           | -4.148290  | -0.464093  | 0.145688   |
| 5      | 6             | 0           | -3.483598  | 0.566332   | 0.937250   |
| 6      | 1             | 0           | -1.968207  | -1.970018  | 1.644869   |
| 7      | 1             | 0           | -1.154816  | -1.411122  | 0.200593   |
| 8      | 1             | 0           | -3.538555  | -2.467826  | -0.485488  |
| 9      | 1             | 0           | -1.535713  | 0.635825   | 1.940842   |
| 10     | 1             | 0           | -5.143031  | -0.376279  | -0.277776  |
| 11     | 1             | 0           | -3.917561  | 1.526074   | 1.198272   |
| 12     | 6             | 0           | -1.744309  | -0.147461  | -2.263906  |
| 13     | 6             | 0           | -1.661236  | 1.030902   | -1.622374  |
| 14     | 6             | 0           | -0.477128  | 1.363911   | -0.835164  |
| 15     | 8             | 0           | 0.481426   | 0.584538   | -0.693038  |
| 16     | 1             | 0           | -2.614713  | -0.389107  | -2.862030  |
| 17     | 1             | 0           | -0.938454  | -0.872875  | -2.205203  |
| 18     | 1             | 0           | -2.441346  | 1.781029   | -1.659027  |
| 19     | 8             | 0           | -0.478842  | 2.574584   | -0.342678  |
| 20     | 6             | 0           | 0.692656   | 2.960132   | 0.425887   |
| 21     | 1             | 0           | 1.586568   | 2.858640   | -0.188558  |
| 22     | 1             | 0           | 0.513707   | 3.997419   | 0.693201   |
| 23     | 1             | 0           | 0.768751   | 2.333351   | 1.313489   |

**RC'_{exo-1} (NIMAG=0)**
| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y           | Z          |
| 24     | 13            | 0           | 1.790369   | -0.501653  | 0.070621   |
| 25     | 17            | 0           | 3.598095   | 0.442405   | -0.454596  |
| 26     | 17            | 0           | 1.322695   | -0.425949  | 2.134957   |
| 27     | 17            | 0           | 1.421028   | -2.376690  | -0.824916  |

**RC'_{exo-3} (NIMAG=0)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y           | Z          |
| 1      | 6             | 0           | -2.062801   | -1.273745  | 0.798281   |
| 2      | 6             | 0           | -3.321810   | -1.538057  | 0.028241   |
| 3      | 6             | 0           | -2.248500   | 0.123760   | 1.305049   |
| 4      | 6             | 0           | -4.148558   | -0.463575  | 0.145755   |
| 5      | 6             | 0           | -3.483585   | 0.566776   | 0.937079   |
| 6      | 1             | 0           | -1.968634   | -1.970009  | 1.644915   |
| 7      | 1             | 0           | -1.155327   | -1.411134  | 0.200642   |
| 8      | 1             | 0           | -3.539518   | -2.467642  | -0.484941  |
| 9      | 1             | 0           | -1.535690   | 0.636029   | 1.940578   |
| 10     | 1             | 0           | -5.143302   | -0.375665  | -0.277668  |
| 11     | 1             | 0           | -3.917200   | 1.526732   | 1.197902   |
| 12     | 6             | 0           | -1.743775   | -0.147227  | -2.264581  |
| 13     | 6             | 0           | -1.660976   | 1.030788   | -1.622352  |
| 14     | 6             | 0           | -0.476822   | 1.363819   | -0.835225  |
| 15     | 8             | 0           | 0.481962    | 0.584565   | -0.693634  |
| 16     | 1             | 0           | -2.614284   | -0.388741  | -2.862593  |
| 17     | 1             | 0           | -0.937643   | -0.872371  | -2.206343  |
| 18     | 1             | 0           | -2.441314   | 1.780688   | -1.658483  |
| 19     | 8             | 0           | -0.478633   | 2.574292   | -0.342364  |
| 20     | 6             | 0           | 0.693235    | 2.959953   | 0.425914   |
| 21     | 1             | 0           | 1.586966    | 2.857646   | -0.188617  |
| 22     | 1             | 0           | 0.514592    | 3.997476   | 0.692477   |
| 23     | 1             | 0           | 0.768996    | 2.333679   | 1.313887   |
| 24     | 13            | 0           | 1.790203    | -0.501695  | 0.070453   |
| 25     | 17            | 0           | 3.598243    | 0.442296   | -0.454102  |
| 26     | 17            | 0           | 1.322405    | -0.426032  | 2.134788   |
| 27     | 17            | 0           | 1.420802    | -2.376879  | -0.824723  |

**TS'_{endo-1} (NIMAG=1, 264.1i cm⁻¹)**

| Center | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|--------|---------------|-------------|------------------------|
|        |               |             | X          | Y           | Z          |
| 1      | 6             | 0           | -3.868879   | -0.318693  | 0.157954   |
| 2      | 6             | 0           | -2.947225   | -1.465142  | -0.177231  |
| 3      | 6             | 0           | -2.974158   | 0.558113   | 0.983097   |
| 4      | 6             | 0           | -1.924051   | -1.462709  | 0.771989   |
| 5      | 6             | 0           | -1.932886   | -0.219125  | 1.458969   |
| 6      | 1             | 0           | -4.641274   | -0.724162  | 0.832816   |
| 7      | 1             | 0           | -4.371061   | 0.160499   | -0.683631  |
| 8      | 1             | 0           | -3.261522   | -2.348143  | -0.725020  |
| 9      | 1             | 0           | -3.243774   | 1.544853   | 1.345748   |
| 10     | 1             | 0           | -1.177097   | -2.238718  | 0.894876   |
| Center Number | Atomic Number | Atomic Type | X     | Y     | Z     |
|---------------|---------------|-------------|-------|-------|-------|
| 11            | 1             | 0           | -1.187400 | 0.085945 | 2.184430 |
| 12            | 6             | 0           | -1.988618 | -0.357935 | -1.805054 |
| 13            | 6             | 0           | -1.896131 | 0.933327  | -1.322645 |
| 14            | 6             | 0           | -0.690769 | 1.350833  | -0.660545 |
| 15            | 8             | 0           | 0.239527  | 0.554924  | -0.406781 |
| 16            | 1             | 0           | -2.781583 | -0.603463 | -2.504826 |
| 17            | 1             | 0           | -1.104177 | 0.085945  | -1.826030 |
| 18            | 1             | 0           | -2.639636 | 1.696152  | -1.516967 |
| 19            | 8             | 0           | -0.619975 | 2.623756  | -0.333336 |
| 20            | 6             | 0           | 0.586409  | 3.033883  | 0.357316  |
| 21            | 1             | 0           | 0.683989  | -2.482734 | 1.293250  |
| 22            | 1             | 0           | 1.457168  | 2.858528  | -0.273204 |
| 23            | 1             | 0           | 0.447375  | 4.095123  | 0.544254  |
| 24            | 13            | 0           | 1.716330  | -0.456915 | 0.015045  |
| 25            | 17            | 0           | 1.337207  | -2.344555 | -0.863121 |
| 26            | 17            | 0           | 1.694504  | -0.475880 | 2.135108  |
| 27            | 17            | 0           | 3.342886  | 0.595184  | -0.826307 |

**TS′_{endo-2} (NIMAG=1, 226.1i cm⁻¹)**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
| 1             | 6             | 0           | -3.857844, -0.506069, 0.292616 |
| 2             | 6             | 0           | -3.091489, -1.552791, -0.476348 |
| 3             | 6             | 0           | -2.806397, 0.030605, 1.217987 |
| 4             | 6             | 0           | -1.948371, -1.858719, 0.256792 |
| 5             | 6             | 0           | -1.770404, -0.879682, 1.276092 |
| 6             | 1             | 0           | -4.598225, -1.041638, 0.909495 |
| 7             | 1             | 0           | -4.394089, 0.232935, -0.305684 |
| 8             | 1             | 0           | -3.546766, -2.218738, -1.202577 |
| 9             | 1             | 0           | -2.956171, 0.856897, 1.905675 |
| 10            | 1             | 0           | -1.245916, -2.655469, 0.036161 |
| 11            | 1             | 0           | -0.915005, -0.822868, 1.939357 |
| 12            | 6             | 0           | -2.247606, -0.073958, -1.904312 |
| 13            | 6             | 0           | -1.920239, 1.007534, -1.114581 |
| 14            | 6             | 0           | -0.596704, 1.061173, -0.549963 |
| 15            | 8             | 0           | 0.169592, 0.073034, -0.675934 |
| 16            | 1             | 0           | -3.163075, -0.046793, -2.487379 |
| 17            | 1             | 0           | -1.463038, -0.742695, -2.237917 |
| 18            | 1             | 0           | -2.601801, 1.835574, -0.980942 |
| 19            | 8             | 0           | -0.126758, 2.102368, 0.105518 |
| 20            | 6             | 0           | -0.958609, 3.259795, 0.280847 |
| 21            | 1             | 0           | -1.215597, 3.693231, -0.687425 |
| 22            | 1             | 0           | -1.857299, 2.996429, 0.842011 |
| 23            | 1             | 0           | -0.348659, 3.954190, 0.852693 |
| 24            | 13            | 0           | 1.877002, -0.299562, 0.005555 |
| 25            | 17            | 0           | 2.043023, -2.353343, -0.476377 |
| 26            | 17            | 0           | 1.746552, 0.042396, 2.097122 |
| 27            | 17            | 0           | 3.195597, 0.988754, -1.018813 |

**TS′_{endo-3} (NIMAG=1, 261.8i cm⁻¹)**
| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 6             | 0           | 2.812884    | -1.802407   | 0.139469    |
| 2             | 6             | 0           | 3.771534    | -0.651153   | -0.029907   |
| 3             | 6             | 0           | 1.681941    | -1.158049   | 0.880420    |
| 4             | 6             | 0           | 3.442820    | 0.301010    | 0.935247    |
| 5             | 6             | 0           | 2.158148    | 0.003377    | 1.463231    |
| 6             | 1             | 0           | 3.291239    | -2.509471   | 0.838380    |
| 7             | 1             | 0           | 2.541757    | -2.351557   | -0.762979   |
| 8             | 1             | 0           | 4.756535    | -0.749276   | -0.475912   |
| 9             | 1             | 0           | 0.746836    | -1.648107   | 1.122226    |
| 10            | 1             | 0           | 4.029014    | 1.183284    | 1.170557    |
| 11            | 1             | 0           | 1.603527    | 0.613314    | 2.168343    |
| 12            | 6             | 0           | 2.661663    | 0.139631    | -1.761896   |
| 13            | 6             | 0           | 1.339160    | -0.056482   | -1.416200   |
| 14            | 6             | 0           | 0.563838    | 0.989378    | -0.805483   |
| 15            | 8             | 0           | -0.672910   | 0.938546    | -0.579102   |
| 16            | 1             | 0           | 3.133628    | -0.564511   | -2.440236   |
| 17            | 1             | 0           | 3.089802    | 1.133547    | -1.713105   |
| 18            | 8             | 0           | 0.787744    | -0.944100   | -1.696958   |
| 19            | 8             | 0           | 1.220964    | 2.093119    | -0.512281   |
| 20            | 6             | 0           | 0.456548    | 3.118752    | 0.165639    |
| 21            | 1             | 0           | -0.365297   | 3.450132    | -0.468022   |
| 22            | 1             | 0           | 0.066281    | 2.729727    | 1.106333    |
| 23            | 1             | 0           | 1.168743    | 3.921717    | 0.337206    |
| 24            | 13            | 0           | -1.957949   | -0.261954   | 0.024238    |
| 25            | 17            | 0           | -1.525945   | -2.141785   | -0.861750   |
| 26            | 17            | 0           | -3.783241   | 0.599382    | 0.559383    |
| 27            | 17            | 0           | -1.579763   | -0.246829   | 2.115663    |

**TS'_{exo-1} (NIMAG=1, 273.8i cm⁻¹)**

| Center Number | Atomic Number | Atomic Type | X           | Y           | Z           |
|---------------|---------------|-------------|-------------|-------------|-------------|
| 1             | 6             | 0           | -1.959377   | -1.089471   | 0.668074    |
| 2             | 6             | 0           | -3.087985   | -1.365122   | -0.284263   |
| 3             | 6             | 0           | -2.311313   | 0.268134    | 1.184193    |
| 4             | 6             | 0           | -4.153620   | -0.540973   | 0.092530    |
| 5             | 6             | 0           | -3.667317   | 0.470281    | 0.956819    |
| 6             | 1             | 0           | -2.074186   | -1.792834   | 1.510522    |
| 7             | 1             | 0           | -0.958380   | -1.227186   | 0.271088    |
| 8             | 1             | 0           | -3.196774   | -2.301134   | -0.823330   |
| 9             | 1             | 0           | -1.683578   | 0.846375    | 1.854251    |
| 10            | 1             | 0           | -5.163243   | -0.597825   | -0.301441   |
| 11            | 1             | 0           | -4.247783   | 1.307691    | 1.329691    |
| 12            | 6             | 0           | -2.159073   | -0.143007   | -1.839725   |
| 13            | 6             | 0           | -1.817948   | 1.029189    | -1.188998   |
| 14            | 6             | 0           | -0.478168   | 1.299227    | -0.741314   |
| 15            | 8             | 0           | 0.458148    | 0.462263    | -0.823352   |
| 16            | 1             | 0           | -3.034447   | -0.149360   | -2.478721   |
| 17            | 1             | 0           | -1.381710   | -0.869941   | -2.060619   |
| 18            | 1             | 0           | -2.497953   | 1.870665    | -1.137987   |
| 19            | 8             | 0           | -0.284944   | 2.529035    | -0.314925   |
### TS'_{exo-2} (NIMAG=1, 250.2\text{ cm}^{-1})

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -1.905202   | -1.406367   | 0.548938    |
| 2             | 6             | 0           | -3.069965   | -1.599017   | -0.380970   |
| 3             | 6             | 0           | -2.226090   | -0.094876   | 1.187588    |
| 4             | 6             | 0           | -4.110034   | -0.787864   | 0.084794    |
| 5             | 6             | 0           | -3.583232   | 0.146539    | 1.009831    |
| 6             | 1             | 0           | -2.007263   | -2.171611   | 1.337946    |
| 7             | 1             | 0           | -0.910299   | -1.514235   | 0.121024    |
| 8             | 1             | 0           | -3.213546   | -2.492270   | -0.981033   |
| 9             | 1             | 0           | -1.566385   | 0.409781    | 1.886197    |
| 10            | 1             | 0           | -5.131405   | -0.802396   | -0.281712   |
| 11            | 1             | 0           | -4.143956   | 0.953738    | 1.470342    |
| 12            | 6             | 0           | -2.206181   | -0.291406   | -1.908146   |
| 13            | 6             | 0           | -1.799303   | 0.828648    | -1.206744   |
| 14            | 6             | 0           | -0.442792   | 0.968215    | -0.749470   |
| 15            | 8             | 0           | 0.395598    | 0.042851    | -0.913168   |
| 16            | 1             | 0           | -3.112493   | -0.235875   | -2.500437   |
| 17            | 1             | 0           | -1.462901   | -1.025300   | -2.205770   |
| 18            | 1             | 0           | -2.473452   | 1.665249    | -1.087123   |
| 19            | 8             | 0           | 0.005121    | 2.066458    | -0.173848   |
| 20            | 6             | 0           | -0.895039   | 3.149968    | 0.104405    |
| 21            | 1             | 0           | -1.720720   | 2.803033    | 0.729012    |
| 22            | 1             | 0           | -0.292777   | 3.876225    | 0.644088    |
| 23            | 1             | 0           | -1.265097   | 3.584928    | -0.825946   |
| 24            | 13            | 0           | 1.965812    | -0.313468   | 0.051091    |
| 25            | 17            | 0           | 3.457502    | 1.022683    | -0.598127   |
| 26            | 17            | 0           | 1.328088    | -0.048190   | 2.066553    |
| 27            | 17            | 0           | 2.271234    | -2.347063   | -0.434072   |

### TS'_{exo-3} (NIMAG=1, 267.9\text{ cm}^{-1})

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 6             | 0           | -3.202014   | 0.370716    | -0.982914   |
| 2             | 6             | 0           | -3.918361   | -0.293169   | 0.161995    |
| 3             | 6             | 0           | -2.070266   | -0.577079   | -1.231482   |
| 4             | 6             | 0           | -3.552838   | -1.640554   | 0.147643    |
| 5             | 6             | 0           | -2.406430   | -1.801221   | -0.670426   |
| 6             | 1             | 0           | -3.877848   | 0.301171    | -1.852071   |
7  1  0  -2.935387  1.417637  -0.842378
8  1  0  -4.835151  0.090217   0.599182
9  1  0  -1.268481   0.842378  -2.935387
10  1  0  -4.000005 -2.417903   0.758660
11  6  0  -2.436816   0.480783  -1.945458
12  6  0  -2.436816   0.480783  -1.945458
13  6  0  -1.222101   0.209080   1.031952
14  6  0  -0.451734   1.189198  -0.312614
15  8  0  -0.722326  1.016049   0.768944
16  1  0  -2.779600   0.168720   2.427585
17  1  0  -2.833979  1.490975   1.614474
18  1  0  -0.704187  1.025792   1.598795
19  8  0  -1.024733  2.362018   0.618934
20  6  0  -0.225557  3.344081  -0.590456
21  6  0  -0.225557  3.344081  -0.590456
22  6  0  -0.225557  3.344081  -0.590456
23  1  0  -0.859923  4.225221  -0.641885
24  13 0  1.995216   0.358430   0.010728
25  17 0  3.718701  0.528009  -0.806295
26  17 0  1.169160  1.931569  -1.149393
27  17 0  2.089299  0.812167   2.074372

PR' endo-1 (NIMAG=0)

Center  Atomic  Atomic  Coordinates (Angstroms)
        Number  Number  Type          X       Y       Z

1       6        0       -3.974647 -0.113650  0.156583
2       6        0       -3.107417 -1.216943 -0.478666
3       6        0       -2.767179  0.694231  0.664953
4       6        0       -2.176710 -1.534401  0.670835
5       6        0       -1.972617 -0.389546  1.359085
6       1        0       -4.589040  0.432228 -0.569226
7       1        0       -4.589040  0.432228 -0.569226
8       1        0       -3.624614 -2.063871 -0.932350
9       1        0       -2.956682  1.612214  1.224554
10      1       13       1.748775 -0.522895  0.015745
11      16       0       1.250315  2.510234   0.975878
12      16       0       1.557874  2.767338  -0.769440
13      16       0       0.846250  4.085737   0.222580
14      16       0       1.754846 -0.175921  2.104779
15      16       0       3.382794  0.340158 -1.003177
### PR′ \text{endo-3} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | 2.877734  | -1.804191 | -0.154689 |
| 2             | 6             | 0           | 3.747619  | -0.538491 | -0.273780 |
| 3             | 6             | 0           | 1.643992  | -1.044266 | 0.359407  |
| 4             | 6             | 0           | 3.518539  | 0.083458  | 1.087994  |
| 5             | 6             | 0           | 2.258618  | -0.221410 | 1.469898  |
| 6             | 1             | 0           | 3.254749  | -2.507050 | 0.593072  |
| 7             | 1             | 0           | 2.706406  | -2.30935  | -1.11171  |
| 8             | 1             | 0           | 4.787810  | -0.66945  | -0.577466 |
| 9             | 1             | 0           | 0.753447  | -1.619899 | 0.604039  |
| 10            | 1             | 0           | 4.212742  | 0.743331  | 1.598101  |
| 11            | 1             | 0           | 1.726781  | 0.129572  | 2.348337  |
| 12            | 6             | 0           | 2.892328  | -0.288313 | -1.286472 |
| 13            | 6             | 0           | 1.441675  | -0.049661 | -0.861201 |
| 14            | 6             | 0           | 0.578618  | 1.088347  | 0.438252  |
| 15            | 8             | 0           | -0.632124 | 0.976039  | -0.160156 |
| 16            | 6             | 0           | 3.068414  | -0.058509 | -2.309212 |
| 17            | 8             | 0           | -0.632124 | 0.976039  | -0.160156 |
| 18            | 1             | 0           | 3.113021  | 1.354973  | -1.236921 |
| 19            | 1             | 0           | 0.893085  | -0.586586 | -1.640438 |
| 20            | 1             | 0           | 1.545784  | 2.252792  | -0.327669 |
| 21            | 6             | 0           | 0.317882  | 3.336365  | 0.159704  |
| 22            | 6             | 0           | -0.528238 | 3.477123  | 0.511355  |
| 23            | 1             | 0           | -0.034733 | 3.099130  | 1.162732  |
| 24            | 1             | 0           | 0.972433  | 4.203097  | 0.163835  |
| 25            | 13            | 0           | -1.991213 | -0.328932 | 0.023423  |
| 26            | 17            | 0           | -1.559394 | -1.794018 | -1.440795 |
| 27            | 17            | 0           | -3.732863 | 0.792892  | -0.327929 |

### PR′ \text{exo-1} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 6             | 0           | -2.091942  | -1.122186 | 0.657550  |
| 2             | 6             | 0           | -3.016983  | -1.227858 | -0.567230 |
| 3             | 6             | 0           | -2.350708  | 0.380182  | 0.859739  |
| 4             | 6             | 0           | -4.261359  | -0.547863 | -0.037319 |
| 5             | 6             | 0           | -3.863147  | 0.416476  | 0.820587  |
| 6             | 1             | 0           | -2.453499  | -1.705281 | 1.508400  |
| 7             | 1             | 0           | -1.054710  | -1.378900 | 0.437062  |
| 8             | 1             | 0           | -3.150209  | -2.217101 | -1.007884 |
| 9             | 1             | 0           | -1.862280  | 0.878092  | 1.700010  |
| 10            | 1             | 0           | -5.273648  | -0.736661 | -0.379148 |
| 11            | 1             | 0           | -4.478196  | 1.170050  | 1.300842  |
| 12            | 6             | 0           | -2.319478  | -0.205467 | -1.521690 |
| 13            | 6             | 0           | -1.929809  | 0.953465  | -0.567348 |
| 14            | 6             | 0           | -0.477463  | 1.275628  | -0.544142 |
| 15            | 8             | 0           | 0.413709   | 0.422722  | -0.716186 |
### PR'_{exo-3} (NIMAG=0)

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------|-------------------------|-------|-------|-------|
| 1             | 6             | 0           | 2.912738                | 0.165516 | 1.221050 |
| 2             | 6             | 0           | 3.796466                | -0.019132 | -0.026107 |
| 3             | 6             | 0           | 1.743746                | -0.654701 | 0.649356 |
| 4             | 6             | 0           | 3.698409                | -1.519306 | -0.213288 |
| 5             | 6             | 0           | 2.464982                | -1.899063 | 0.183321 |
| 6             | 1             | 0           | 3.339088                | -0.306375 | 2.109987 |
| 7             | 1             | 0           | 2.664177                | 1.213253  | 1.423789 |
| 8             | 1             | 0           | 4.802702                | 0.402679  | 0.005864 |
| 9             | 1             | 0           | 0.862656                | -0.807090 | 1.273494 |
| 10            | 1             | 0           | 4.446741                | -2.137828 | -0.697506 |
| 11            | 1             | 0           | 1.998990                | -2.872276 | 0.079945 |
| 12            | 6             | 0           | 2.877754                | 0.619861  | -1.117583 |
| 13            | 6             | 0           | 1.462100                | 0.156371  | -0.692019 |
| 14            | 6             | 0           | 0.469969                | 1.225286  | -0.388576 |
| 15            | 8             | 0           | -0.751424               | 1.011462  | -0.255582 |
| 16            | 1             | 0           | 3.123900                | 0.265302  | -2.121002 |
| 17            | 1             | 0           | 2.963705                | 1.708696  | -1.098996 |
| 18            | 1             | 0           | 0.989175                | -0.512206 | -1.412112 |
| 19            | 8             | 0           | 0.930435                | 2.435242  | -0.210117 |
| 20            | 6             | 0           | -0.046593               | 3.440204  | 0.177468 |
| 21            | 1             | 0           | -0.499055               | 3.160406  | 1.128070 |
| 22            | 1             | 0           | -0.812029               | 3.521528  | -0.592843 |
| 23            | 1             | 0           | 0.528886                | 4.357183  | 0.265351 |
| 24            | 13            | 0           | -1.978060               | -0.412344 | 0.000185 |
| 25            | 17            | 0           | -1.918447               | -0.610406 | 2.103214 |
| 26            | 17            | 0           | -1.177505               | -2.076829 | -1.029869 |
| 27            | 17            | 0           | -3.751322               | 0.375666  | -0.802907 |