

SUPPORTING INFORMATION

**Accurate Density Functional Theory (DFT) Protocol for Screening and Designing Chain Transfer and Branching Agents for Low-Density Polyethylene (LDPE) Systems**

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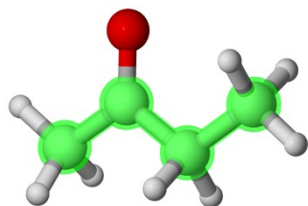
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**1. 1D Potential energy dihedral scans**

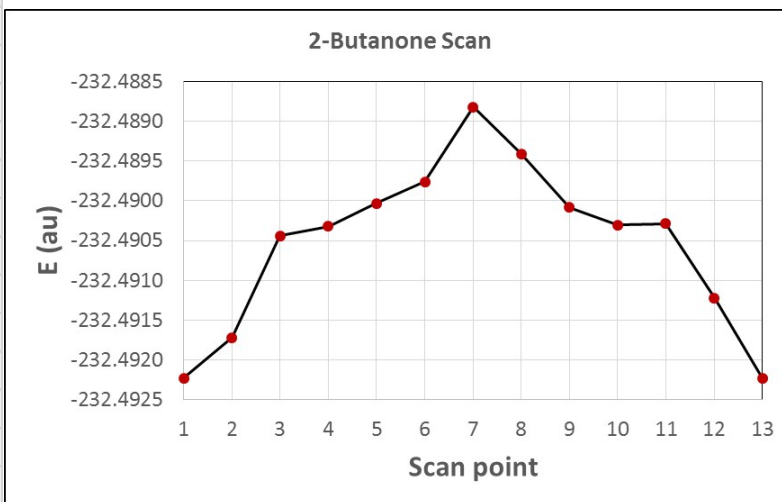
All quantum mechanical (QM) calculations were performed using the density functional theory (DFT) formalism as implemented in the Gaussian09 commercial software package. All relaxed potential energy scans were done at the B3LYP/6-31+G(d,p) level of theory. For reactants, dihedral scans were initiated on an already fully optimized geometry. If the scan revealed another minimum with close or lower electronic energy, that particular scan point geometry was used as an initial guess in a separate full optimization. If the new geometry was lower in electronic energy all dihedrals were again scanned for that structure. The process was repeated until a geometry was found whose dihedral scans did not reveal lower energy rotamers. For TSs, dihedral scans were done on an already optimized TS structure. In this particular case, we were not looking to find the lowest energy TS but rather all possible TSs. Hence, all local minima on the potential energy were used as initial guesses for TS optimization. For the relaxed potential energy scans, the atoms participating in the TS bond formation/breaking were held fixed. Unless explicitly specified, all scan consisted of 12 steps at 30°. All scanned dihedrals are highlighted in the figures below. The structures shown are those corresponding to scan point 1.

## 1.1. Reactants

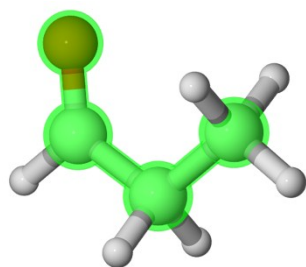
### 1.1.1. 2-Butanone



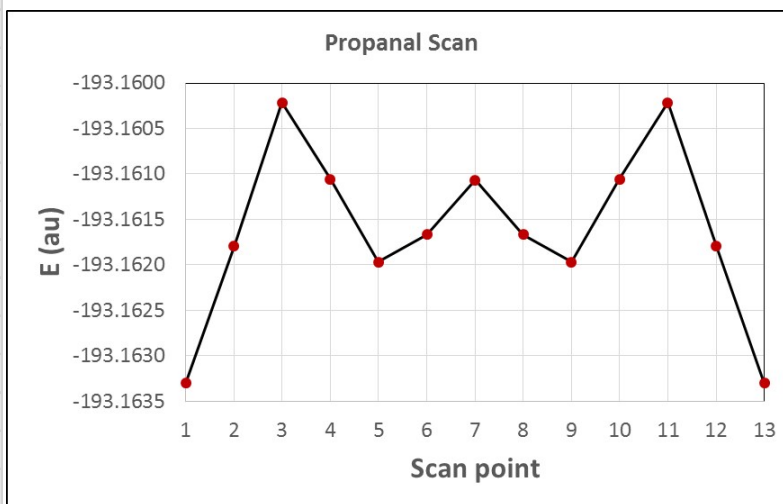
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -232.4922 | Min   |
| 2          | -232.4917 |       |
| 3          | -232.4904 |       |
| 4          | -232.4903 |       |
| 5          | -232.4900 |       |
| 6          | -232.4898 |       |
| 7          | -232.4888 |       |
| 8          | -232.4894 |       |
| 9          | -232.4901 |       |
| 10         | -232.4903 |       |
| 11         | -232.4903 |       |
| 12         | -232.4912 |       |
| 13         | -232.4922 |       |



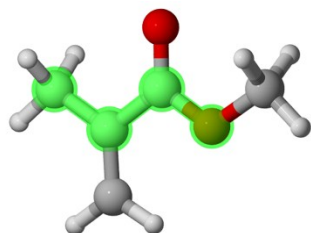
### 1.1.2. Propanal



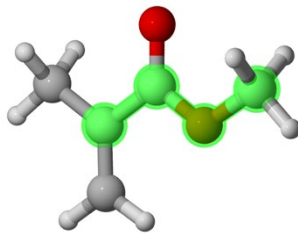
| Scan point | E (au)    |
|------------|-----------|
| 1          | -193.1633 |
| 2          | -193.1618 |
| 3          | -193.1602 |
| 4          | -193.1611 |
| 5          | -193.1620 |
| 6          | -193.1617 |
| 7          | -193.1611 |
| 8          | -193.1617 |
| 9          | -193.1620 |
| 10         | -193.1611 |
| 11         | -193.1602 |
| 12         | -193.1618 |
| 13         | -193.1633 |



### 1.1.3. MMA

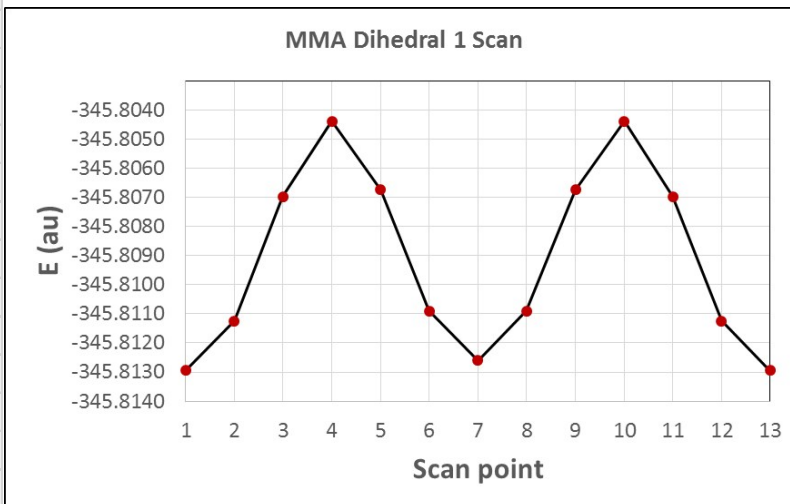


Dihedral 1

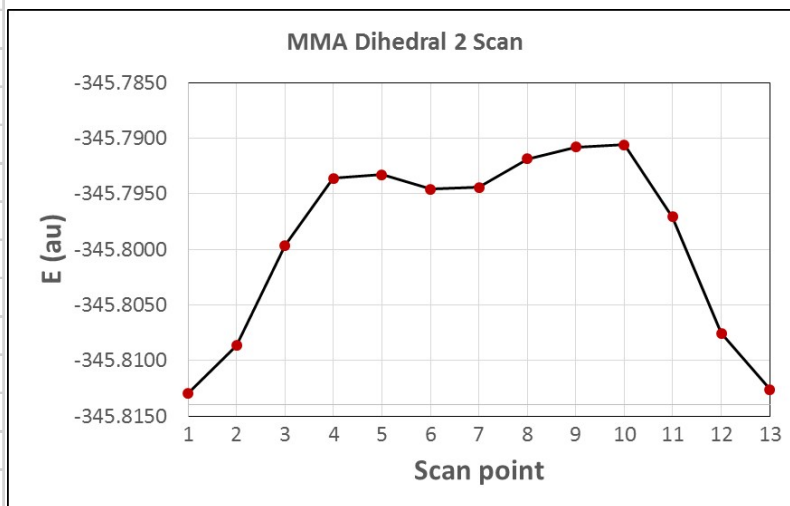


Dihedral 2

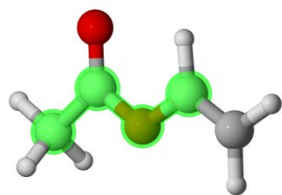
| Scan point | E (au)    | Notes   |
|------------|-----------|---------|
| 1          | -345.8129 | s-trans |
| 2          | -345.8112 |         |
| 3          | -345.8070 |         |
| 4          | -345.8044 |         |
| 5          | -345.8067 |         |
| 6          | -345.8109 |         |
| 7          | -345.8126 | s-cis   |
| 8          | -345.8109 |         |
| 9          | -345.8067 |         |
| 10         | -345.8044 |         |
| 11         | -345.8070 |         |
| 12         | -345.8112 |         |
| 13         | -345.8129 |         |



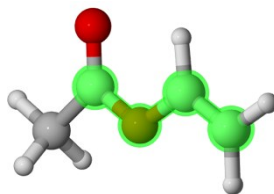
| Scan point | E (au)    | Notes   |
|------------|-----------|---------|
| 1          | -345.8129 | s-trans |
| 2          | -345.8087 |         |
| 3          | -345.7996 |         |
| 4          | -345.7936 |         |
| 5          | -345.7933 |         |
| 6          | -345.7946 |         |
| 7          | -345.7944 |         |
| 8          | -345.7918 |         |
| 9          | -345.7908 |         |
| 10         | -345.7906 |         |
| 11         | -345.7971 |         |
| 12         | -345.8075 |         |
| 13         | -345.8126 |         |



#### 1.1.4. Vinyl acetate

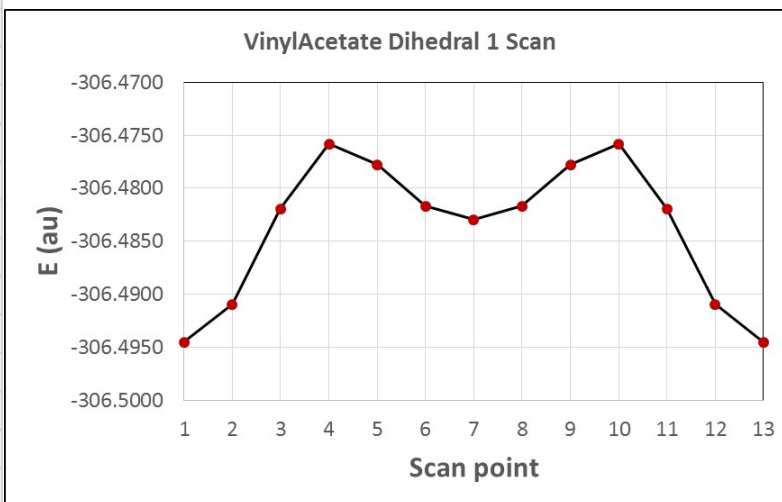


Dihedral 1

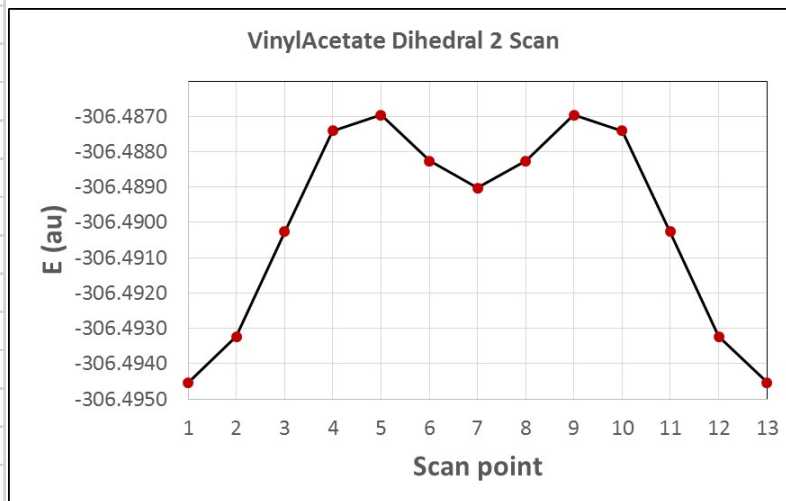


Dihedral 2

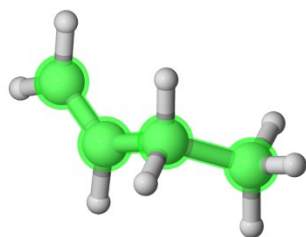
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -306.4945 | Min   |
| 2          | -306.4910 |       |
| 3          | -306.4819 |       |
| 4          | -306.4758 |       |
| 5          | -306.4778 |       |
| 6          | -306.4817 |       |
| 7          | -306.4830 |       |
| 8          | -306.4817 |       |
| 9          | -306.4778 |       |
| 10         | -306.4758 |       |
| 11         | -306.4819 |       |
| 12         | -306.4910 |       |
| 13         | -306.4945 |       |



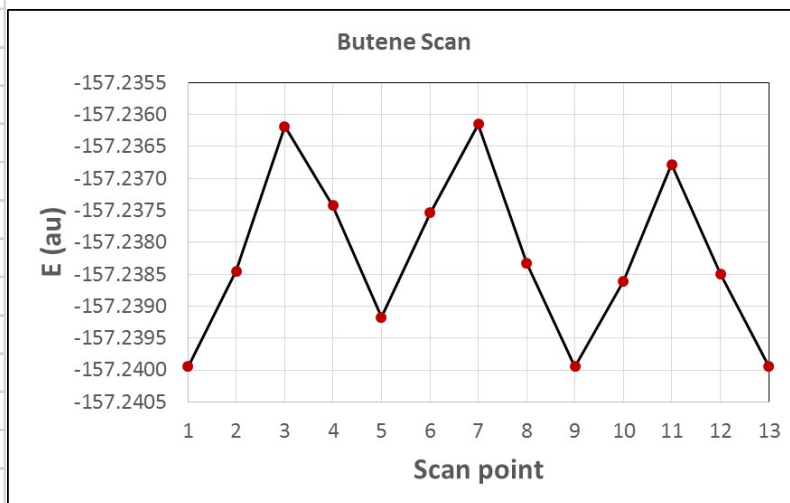
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -306.4945 | Min   |
| 2          | -306.4932 |       |
| 3          | -306.4903 |       |
| 4          | -306.4874 |       |
| 5          | -306.4870 |       |
| 6          | -306.4883 |       |
| 7          | -306.4890 |       |
| 8          | -306.4883 |       |
| 9          | -306.4870 |       |
| 10         | -306.4874 |       |
| 11         | -306.4903 |       |
| 12         | -306.4932 |       |
| 13         | -306.4945 |       |



### 1.1.5. 1-Butene

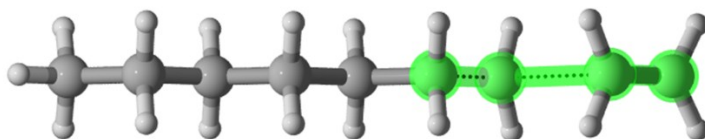


| Scan point | E (au)    | Notes      |
|------------|-----------|------------|
| 1          | -157.2399 | gauche min |
| 2          | -157.2384 |            |
| 3          | -157.2362 |            |
| 4          | -157.2374 |            |
| 5          | -157.2392 | anti min   |
| 6          | -157.2375 |            |
| 7          | -157.2361 |            |
| 8          | -157.2383 |            |
| 9          | -157.2399 | gauche min |
| 10         | -157.2386 |            |
| 11         | -157.2368 |            |
| 12         | -157.2385 |            |
| 13         | -157.2399 |            |

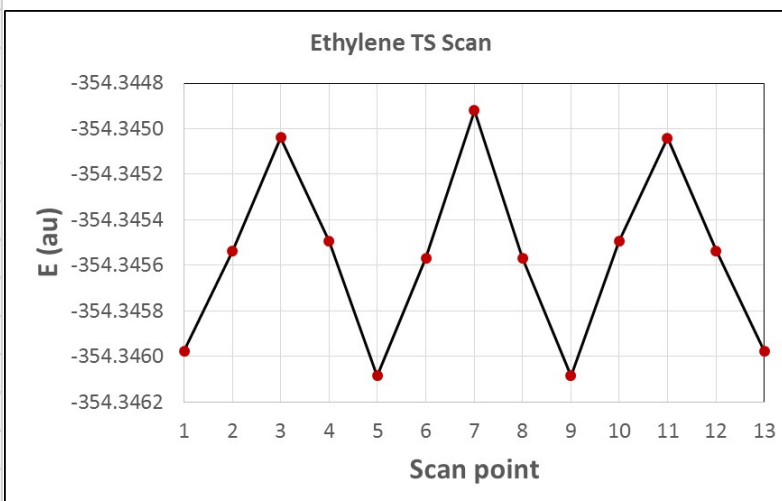


## 1.2. Transition states

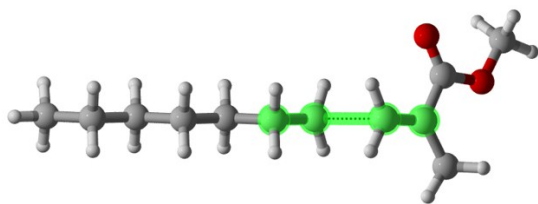
### 1.2.1. Ethylene addition



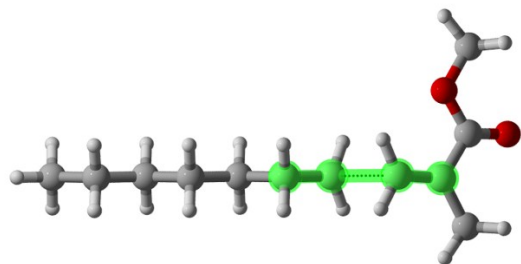
| Scan point | E (au)    | Notes  |
|------------|-----------|--------|
| 1          | -354.3460 | Anti   |
| 2          | -354.3455 |        |
| 3          | -354.3450 |        |
| 4          | -354.3455 |        |
| 5          | -354.3461 | Gauche |
| 6          | -354.3456 |        |
| 7          | -354.3449 |        |
| 8          | -354.3456 |        |
| 9          | -354.3461 | Gauche |
| 10         | -354.3455 |        |
| 11         | -354.3450 |        |
| 12         | -354.3455 |        |
| 13         | -354.3460 |        |



### 1.2.2. MMA addition

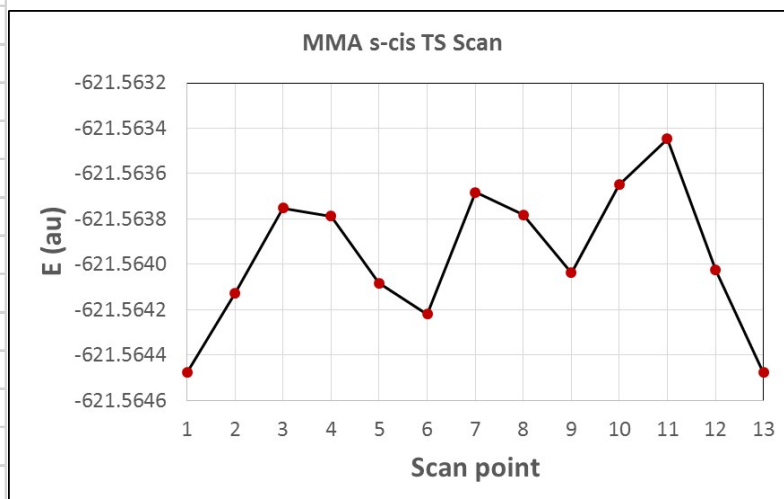


s-cis TS scan

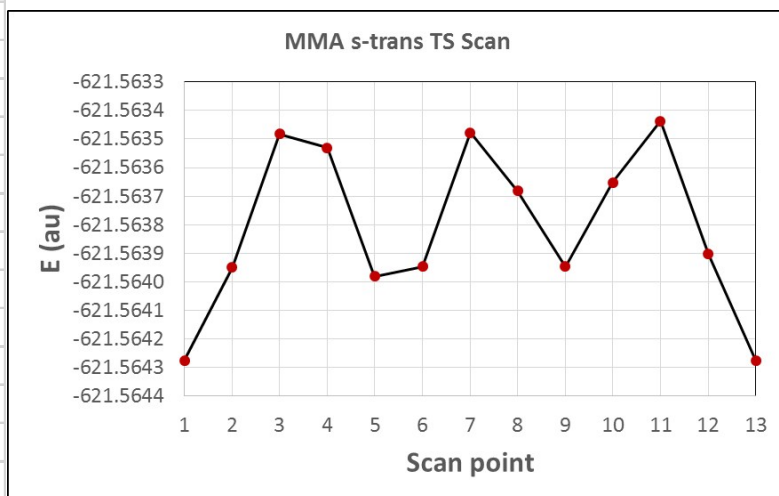


s-trans TS scan

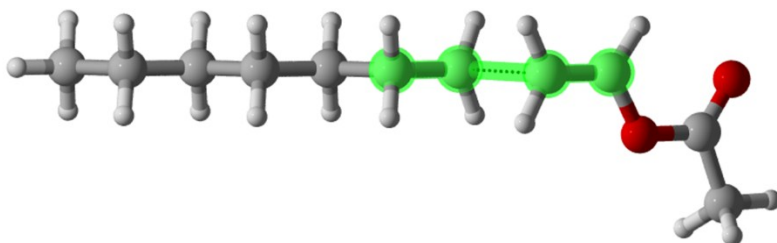
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -621.5645 | TS1   |
| 2          | -621.5641 |       |
| 3          | -621.5638 |       |
| 4          | -621.5638 |       |
| 5          | -621.5641 |       |
| 6          | -621.5642 | TS3   |
| 7          | -621.5637 |       |
| 8          | -621.5638 |       |
| 9          | -621.5640 | TS2   |
| 10         | -621.5636 |       |
| 11         | -621.5634 |       |
| 12         | -621.5640 |       |
| 13         | -621.5645 |       |



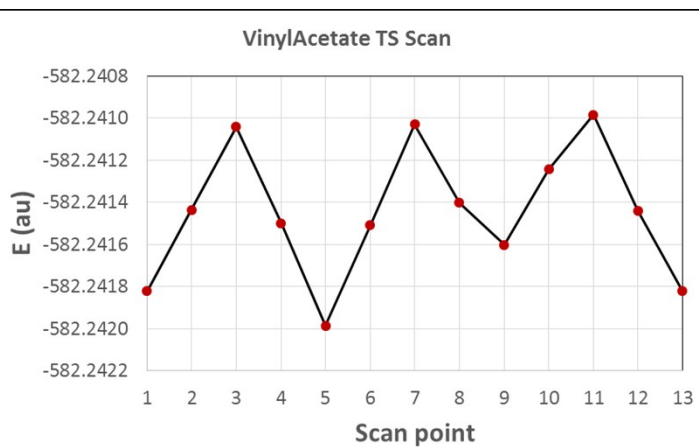
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -621.5643 | TS4   |
| 2          | -621.5639 |       |
| 3          | -621.5635 |       |
| 4          | -621.5635 |       |
| 5          | -621.5640 | TS5   |
| 6          | -621.5639 |       |
| 7          | -621.5635 |       |
| 8          | -621.5637 |       |
| 9          | -621.5639 | TS6   |
| 10         | -621.5637 |       |
| 11         | -621.5634 |       |
| 12         | -621.5639 |       |
| 13         | -621.5643 |       |



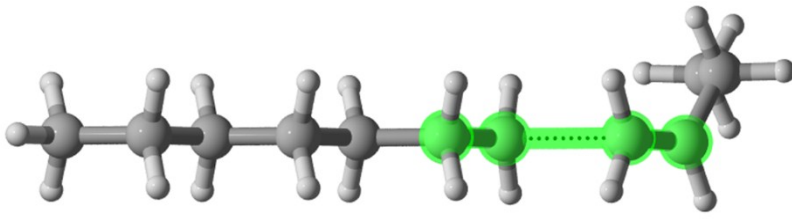
### 1.2.3. Vinyl acetate addition



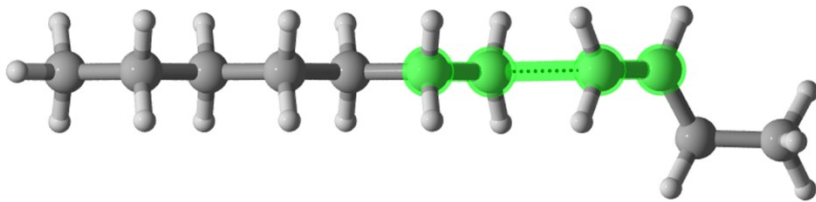
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -582.2418 | TS1   |
| 2          | -582.2414 |       |
| 3          | -582.2410 |       |
| 4          | -582.2415 |       |
| 5          | -582.2420 | TS3   |
| 6          | -582.2415 |       |
| 7          | -582.2410 |       |
| 8          | -582.2414 |       |
| 9          | -582.2416 | TS2   |
| 10         | -582.2412 |       |
| 11         | -582.2410 |       |
| 12         | -582.2414 |       |
| 13         | -582.2418 |       |



#### 1.2.4. 1-Butene addition

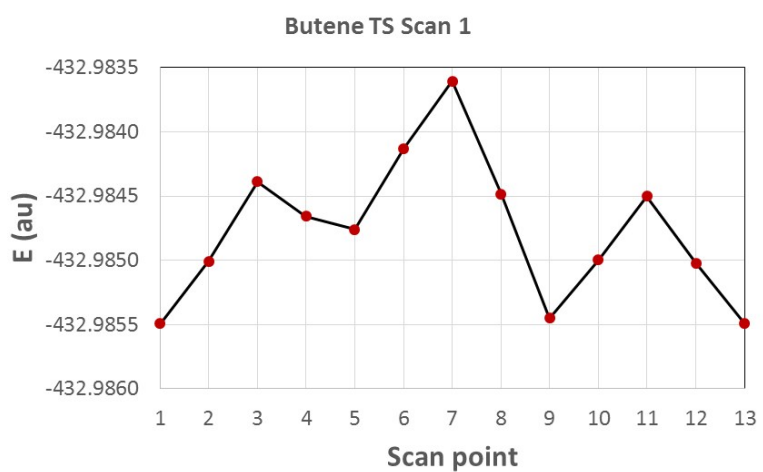


1-butene tail towards radical (scan 1)

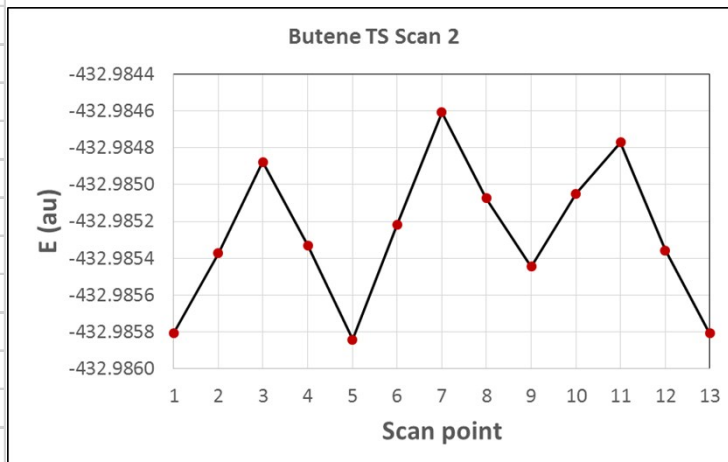


1-butene tail away from radical (scan 2)

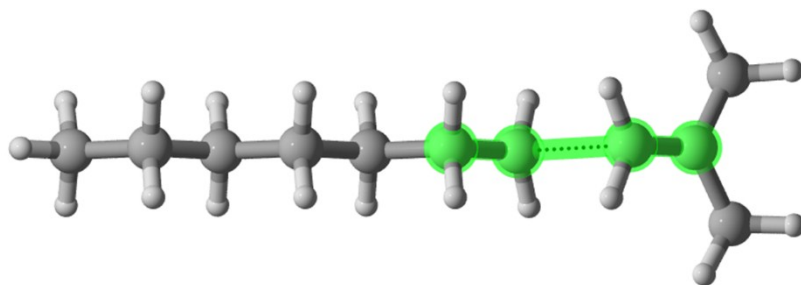
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -432.9855 | TS1   |
| 2          | -432.9850 |       |
| 3          | -432.9844 |       |
| 4          | -432.9847 |       |
| 5          | -432.9848 | TS3   |
| 6          | -432.9841 |       |
| 7          | -432.9836 |       |
| 8          | -432.9845 |       |
| 9          | -432.9855 | TS2   |
| 10         | -432.9850 |       |
| 11         | -432.9845 |       |
| 12         | -432.9850 |       |
| 13         | -432.9855 |       |



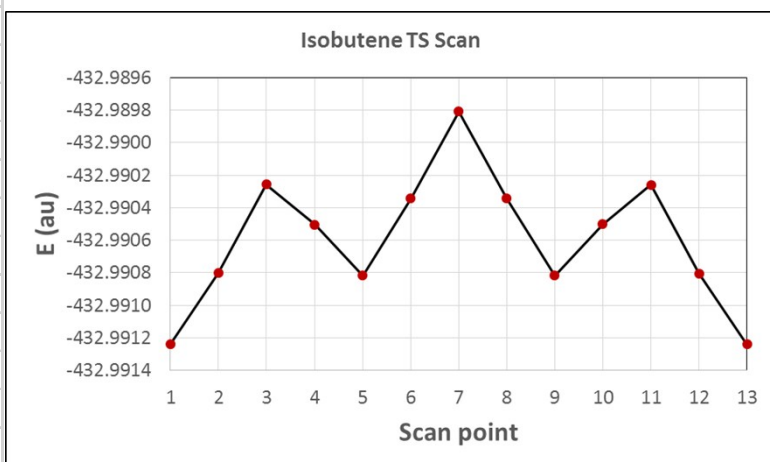
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -432.9858 | TS4   |
| 2          | -432.9854 |       |
| 3          | -432.9849 |       |
| 4          | -432.9853 | TS5   |
| 5          | -432.9858 |       |
| 6          | -432.9852 |       |
| 7          | -432.9846 | TS6   |
| 8          | -432.9851 |       |
| 9          | -432.9854 |       |
| 10         | -432.9850 |       |
| 11         | -432.9848 |       |
| 12         | -432.9854 |       |
| 13         | -432.9858 |       |



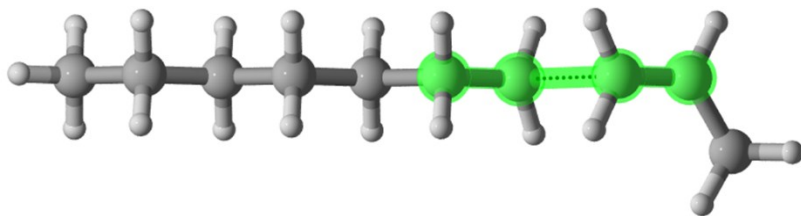
### 1.2.5. Isobutene addition



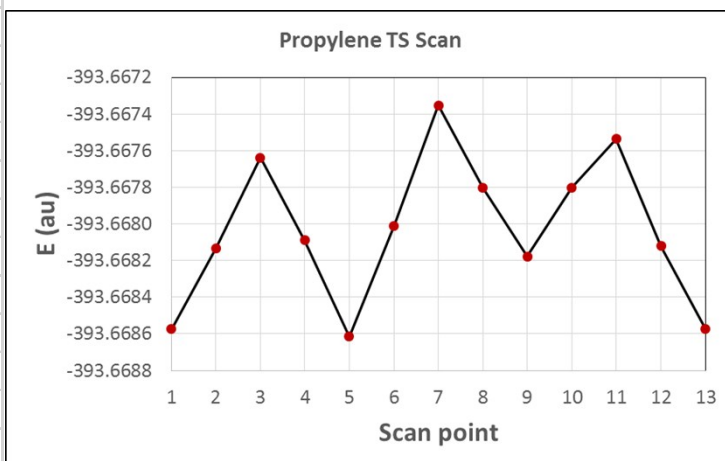
| Scan point | E (au)    | Notes      |
|------------|-----------|------------|
| 1          | -432.9912 | TS1        |
| 2          | -432.9908 |            |
| 3          | -432.9903 |            |
| 4          | -432.9905 |            |
| 5          | -432.9908 | gauche TS2 |
| 6          | -432.9903 |            |
| 7          | -432.9898 |            |
| 8          | -432.9903 |            |
| 9          | -432.9908 | gauche TS2 |
| 10         | -432.9905 |            |
| 11         | -432.9903 |            |
| 12         | -432.9908 |            |
| 13         | -432.9912 |            |



### 1.2.6. Propylene addition

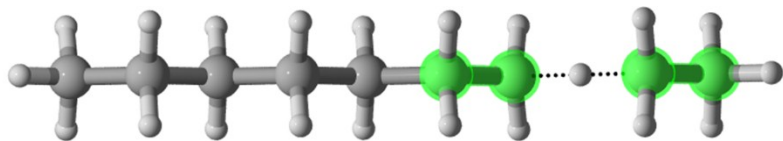


| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -393.6686 | TS1   |
| 2          | -393.6681 |       |
| 3          | -393.6676 |       |
| 4          | -393.6681 |       |
| 5          | -393.6686 | TS3   |
| 6          | -393.6680 |       |
| 7          | -393.6674 |       |
| 8          | -393.6678 |       |
| 9          | -393.6682 | TS2   |
| 10         | -393.6678 |       |
| 11         | -393.6675 |       |
| 12         | -393.6681 |       |
| 13         | -393.6686 |       |

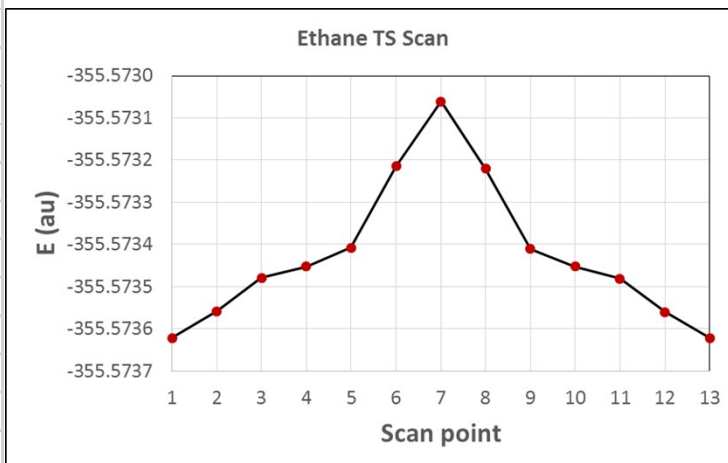


### 1.3. Hydrogen abstraction

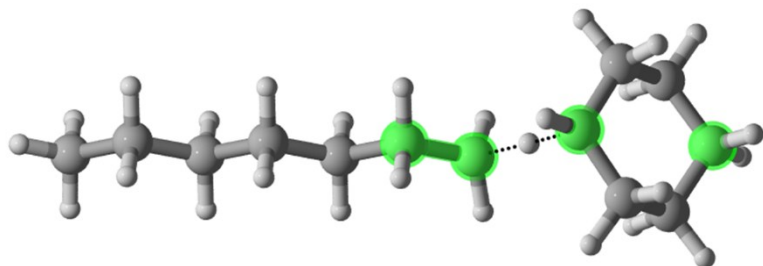
#### 1.3.1. Ethane H abstraction



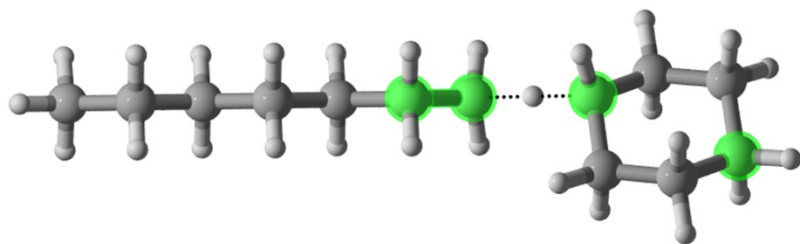
| Scan point | E (au)    | Notes        |
|------------|-----------|--------------|
| 1          | -355.5736 | anti TS      |
| 2          | -355.5736 |              |
| 3          | -355.5735 |              |
| 4          | -355.5735 | No gauche TS |
| 5          | -355.5734 |              |
| 6          | -355.5732 |              |
| 7          | -355.5731 |              |
| 8          | -355.5732 |              |
| 9          | -355.5734 |              |
| 10         | -355.5735 | No gauche TS |
| 11         | -355.5735 |              |
| 12         | -355.5736 |              |
| 13         | -355.5736 |              |



**1.3.2. Cyclohexane H abstraction (36 steps of 10°)**

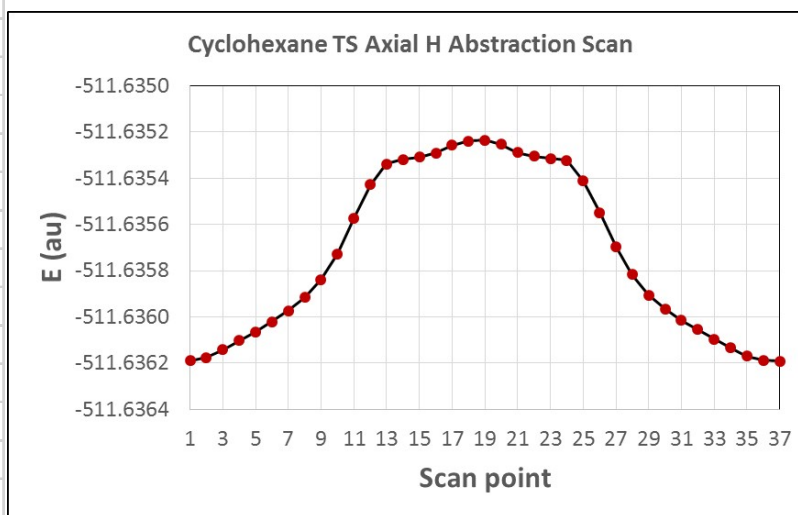


TS axial H abstraction

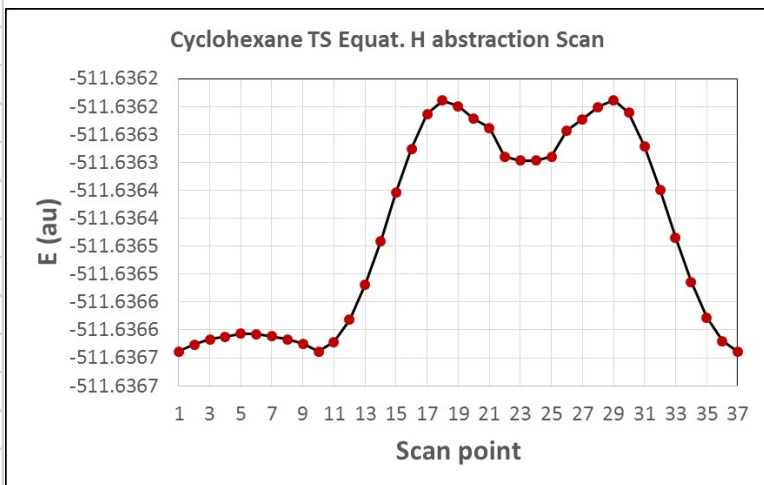


TS equatorial H abstraction

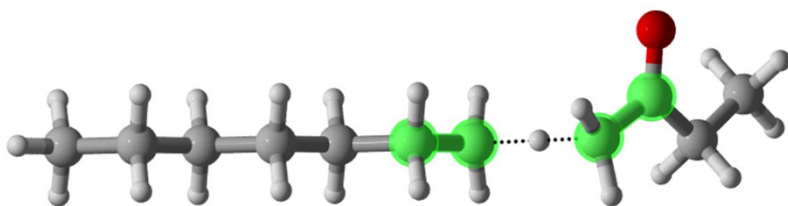
| Scan point | E (au)    | Notes      |
|------------|-----------|------------|
| 1          | -511.6362 | TS1        |
| 2          | -511.6362 |            |
| 3          | -511.6361 |            |
| 4          | -511.6361 |            |
| 5          | -511.6361 |            |
| 6          | -511.6360 |            |
| 7          | -511.6360 |            |
| 8          | -511.6359 |            |
| 9          | -511.6358 |            |
| 10         | -511.6357 |            |
| 11         | -511.6356 |            |
| 12         | -511.6354 |            |
| 13         | -511.6353 |            |
| 14         | -511.6353 |            |
| 15         | -511.6353 | gauche TS2 |
| 16         | -511.6353 |            |
| 17         | -511.6353 |            |
| 18         | -511.6352 |            |
| 19         | -511.6352 | TS3        |
| 20         | -511.6353 |            |
| 21         | -511.6353 |            |
| 22         | -511.6353 | gauche TS2 |
| 23         | -511.6353 |            |
| 24         | -511.6353 |            |
| 25         | -511.6354 |            |
| 26         | -511.6355 |            |
| 27         | -511.6357 |            |
| 28         | -511.6358 |            |
| 29         | -511.6359 |            |
| 30         | -511.6360 |            |
| 31         | -511.6360 |            |
| 32         | -511.6361 |            |
| 33         | -511.6361 |            |
| 34         | -511.6361 |            |
| 35         | -511.6362 |            |
| 36         | -511.6362 |            |
| 37         | -511.6362 |            |



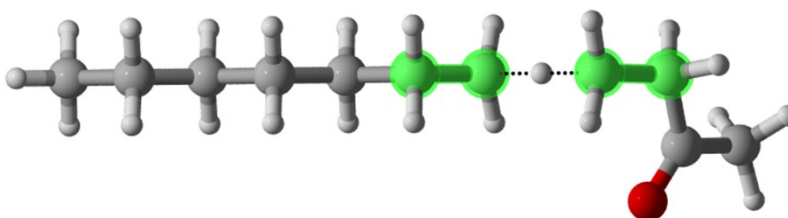
| Scan point | E (au)    | Notes      |
|------------|-----------|------------|
| 1          | -511.6366 | TS4 gauche |
| 2          | -511.6366 |            |
| 3          | -511.6366 |            |
| 4          | -511.6366 |            |
| 5          | -511.6366 |            |
| 6          | -511.6366 |            |
| 7          | -511.6366 |            |
| 8          | -511.6366 |            |
| 9          | -511.6366 |            |
| 10         | -511.6366 | TS4 gauche |
| 11         | -511.6366 |            |
| 12         | -511.6366 |            |
| 13         | -511.6365 |            |
| 14         | -511.6364 |            |
| 15         | -511.6364 |            |
| 16         | -511.6363 |            |
| 17         | -511.6362 |            |
| 18         | -511.6362 |            |
| 19         | -511.6362 |            |
| 20         | -511.6362 |            |
| 21         | -511.6362 |            |
| 22         | -511.6363 |            |
| 23         | -511.6363 | TS5        |
| 24         | -511.6363 |            |
| 25         | -511.6363 |            |
| 26         | -511.6362 |            |
| 27         | -511.6362 |            |
| 28         | -511.6362 |            |
| 29         | -511.6362 |            |
| 30         | -511.6362 |            |
| 31         | -511.6363 |            |
| 32         | -511.6363 |            |
| 33         | -511.6364 |            |
| 34         | -511.6365 |            |
| 35         | -511.6366 |            |
| 36         | -511.6366 |            |
| 37         | -511.6366 |            |



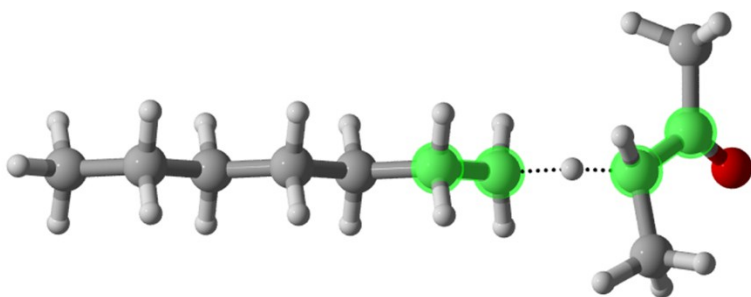
**1.3.3. 2-Butanone H abstraction (36 steps of 10°)**



TS H abstraction Scan 1

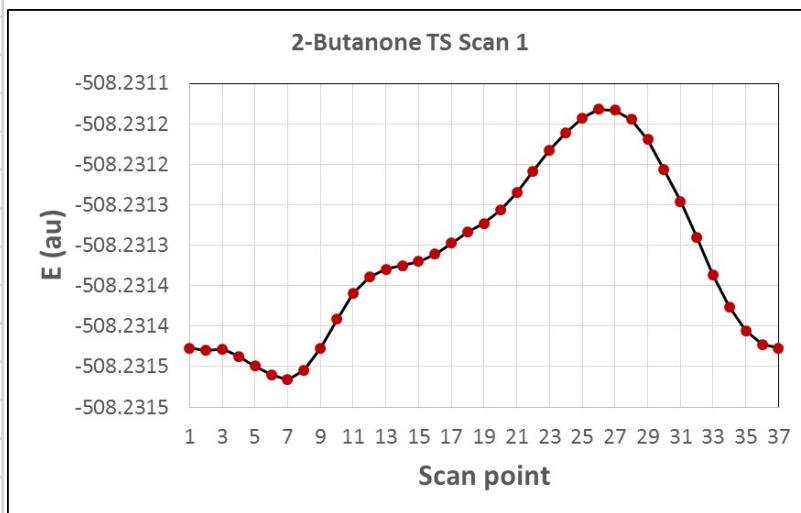


TS H abstraction Scan 2

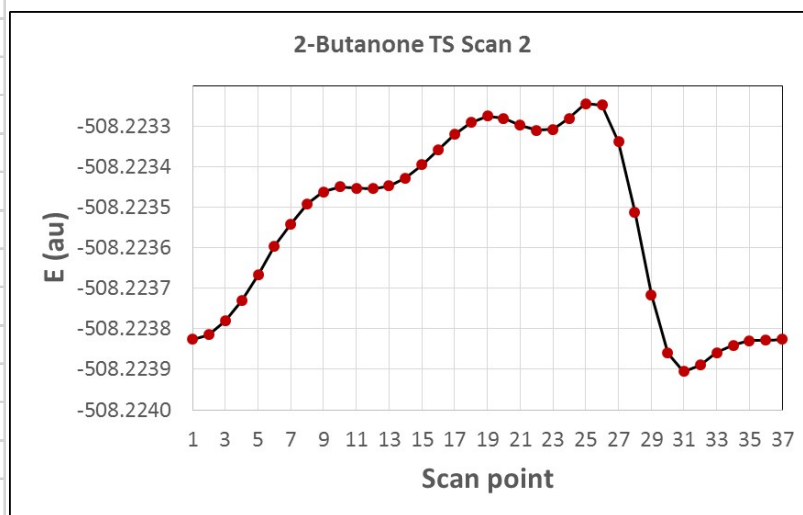


TS H abstraction Scan 3

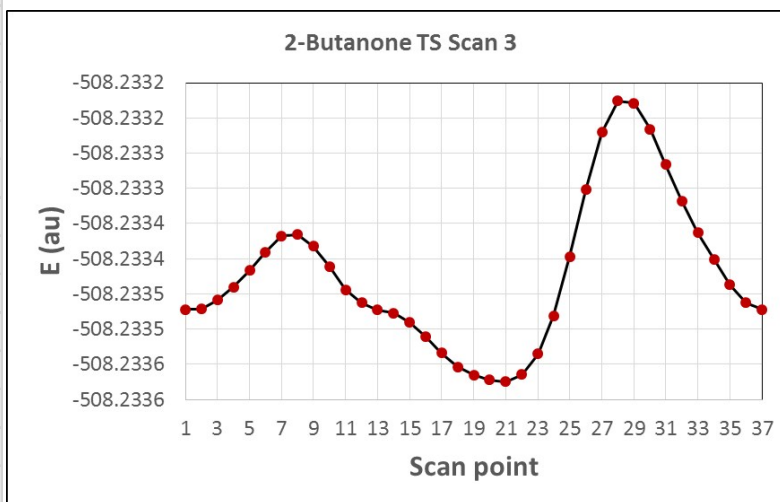
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -508.2314 | TS1   |
| 2          | -508.2314 |       |
| 3          | -508.2314 |       |
| 4          | -508.2314 |       |
| 5          | -508.2314 |       |
| 6          | -508.2315 | TS2   |
| 7          | -508.2315 |       |
| 8          | -508.2315 |       |
| 9          | -508.2314 |       |
| 10         | -508.2314 |       |
| 11         | -508.2314 |       |
| 12         | -508.2313 |       |
| 13         | -508.2313 |       |
| 14         | -508.2313 |       |
| 15         | -508.2313 | TS3   |
| 16         | -508.2313 |       |
| 17         | -508.2313 |       |
| 18         | -508.2313 |       |
| 19         | -508.2313 |       |
| 20         | -508.2313 |       |
| 21         | -508.2312 |       |
| 22         | -508.2312 |       |
| 23         | -508.2312 |       |
| 24         | -508.2312 |       |
| 25         | -508.2311 |       |
| 26         | -508.2311 |       |
| 27         | -508.2311 |       |
| 28         | -508.2311 |       |
| 29         | -508.2312 |       |
| 30         | -508.2312 |       |
| 31         | -508.2312 |       |
| 32         | -508.2313 |       |
| 33         | -508.2313 |       |
| 34         | -508.2314 |       |
| 35         | -508.2314 |       |
| 36         | -508.2314 |       |
| 37         | -508.2314 |       |



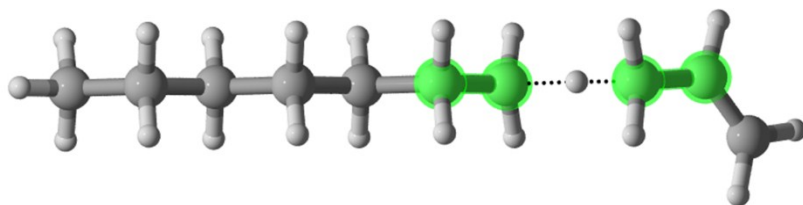
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -508.2238 | TS4   |
| 2          | -508.2238 |       |
| 3          | -508.2238 |       |
| 4          | -508.2237 |       |
| 5          | -508.2237 |       |
| 6          | -508.2236 |       |
| 7          | -508.2235 |       |
| 8          | -508.2235 |       |
| 9          | -508.2235 |       |
| 10         | -508.2234 |       |
| 11         | -508.2235 | TS6   |
| 12         | -508.2235 |       |
| 13         | -508.2234 |       |
| 14         | -508.2234 |       |
| 15         | -508.2234 |       |
| 16         | -508.2234 |       |
| 17         | -508.2233 |       |
| 18         | -508.2233 |       |
| 19         | -508.2233 |       |
| 20         | -508.2233 |       |
| 21         | -508.2233 | TS5   |
| 22         | -508.2233 |       |
| 23         | -508.2233 |       |
| 24         | -508.2233 |       |
| 25         | -508.2232 |       |
| 26         | -508.2232 |       |
| 27         | -508.2233 |       |
| 28         | -508.2235 |       |
| 29         | -508.2237 |       |
| 30         | -508.2239 | No TS |
| 31         | -508.2239 |       |
| 32         | -508.2239 |       |
| 33         | -508.2239 |       |
| 34         | -508.2238 |       |
| 35         | -508.2238 |       |
| 36         | -508.2238 |       |
| 37         | -508.2238 |       |



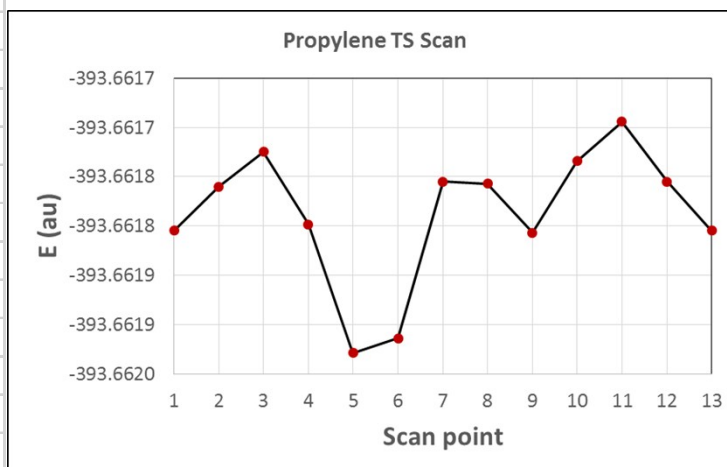
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -508.2335 | TS7   |
| 2          | -508.2335 |       |
| 3          | -508.2335 |       |
| 4          | -508.2334 |       |
| 5          | -508.2334 |       |
| 6          | -508.2334 |       |
| 7          | -508.2334 |       |
| 8          | -508.2334 |       |
| 9          | -508.2334 |       |
| 10         | -508.2334 |       |
| 11         | -508.2334 |       |
| 12         | -508.2335 |       |
| 13         | -508.2335 | No TS |
| 14         | -508.2335 |       |
| 15         | -508.2335 |       |
| 16         | -508.2335 |       |
| 17         | -508.2335 |       |
| 18         | -508.2336 |       |
| 19         | -508.2336 |       |
| 20         | -508.2336 |       |
| 21         | -508.2336 |       |
| 22         | -508.2336 | TS8   |
| 23         | -508.2335 |       |
| 24         | -508.2335 |       |
| 25         | -508.2334 |       |
| 26         | -508.2333 |       |
| 27         | -508.2332 |       |
| 28         | -508.2332 |       |
| 29         | -508.2332 |       |
| 30         | -508.2332 |       |
| 31         | -508.2333 |       |
| 32         | -508.2333 |       |
| 33         | -508.2334 |       |
| 34         | -508.2334 |       |
| 35         | -508.2334 |       |
| 36         | -508.2335 |       |
| 37         | -508.2335 |       |



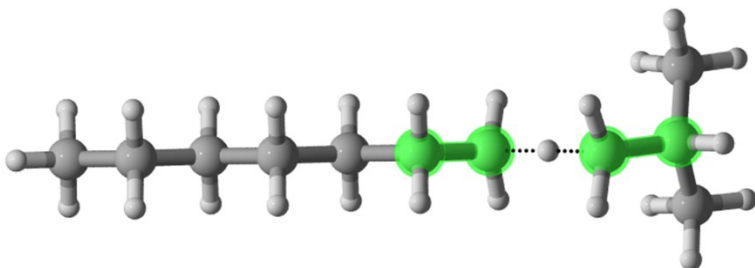
### 1.3.4. Propylene H abstraction



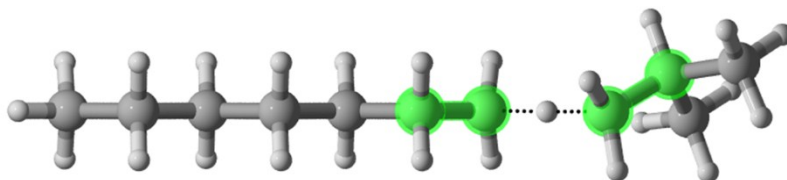
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -393.6618 | TS1   |
| 2          | -393.6618 |       |
| 3          | -393.6617 |       |
| 4          | -393.6618 |       |
| 5          | -393.6619 | TS3   |
| 6          | -393.6619 |       |
| 7          | -393.6618 |       |
| 8          | -393.6618 |       |
| 9          | -393.6618 | TS2   |
| 10         | -393.6617 |       |
| 11         | -393.6617 |       |
| 12         | -393.6618 |       |
| 13         | -393.6618 |       |



### 1.3.5. Isobutane H abstraction

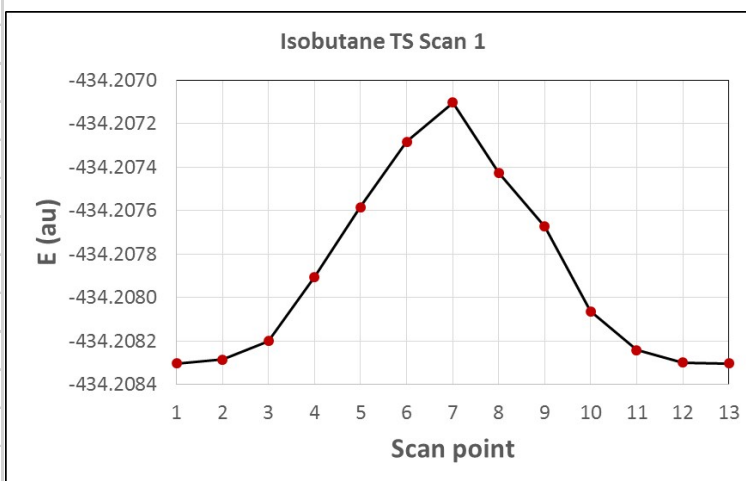


Isobutane TS H abstraction Scan 1

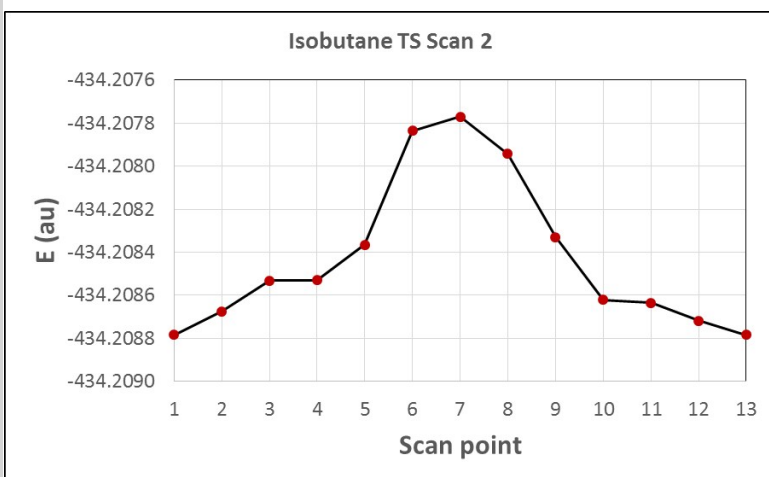


Isobutane TS H abstraction Scan 2

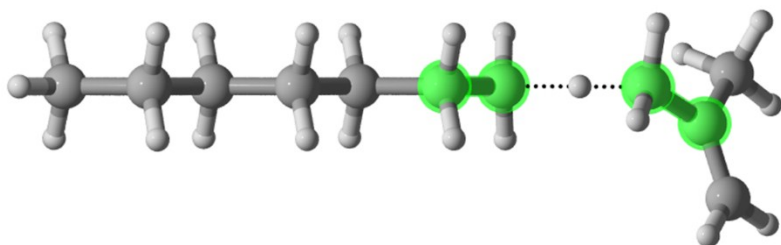
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -434.2083 | TS2   |
| 2          | -434.2083 |       |
| 3          | -434.2082 |       |
| 4          | -434.2079 |       |
| 5          | -434.2076 |       |
| 6          | -434.2073 |       |
| 7          | -434.2071 |       |
| 8          | -434.2074 |       |
| 9          | -434.2077 |       |
| 10         | -434.2081 |       |
| 11         | -434.2082 |       |
| 12         | -434.2083 |       |
| 13         | -434.2083 |       |



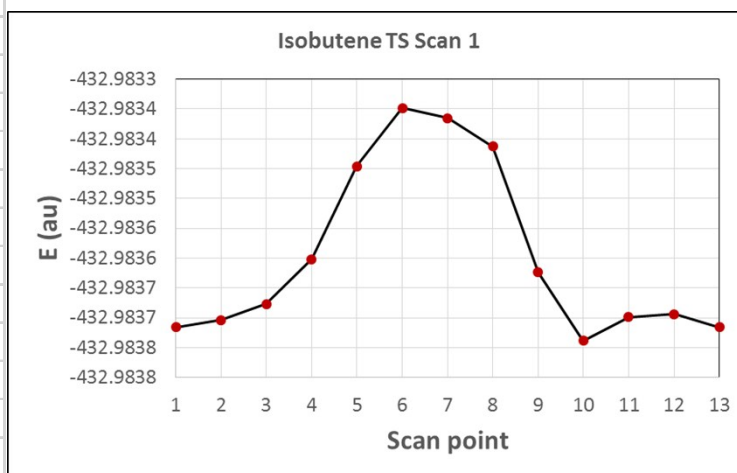
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -434.2088 | TS3   |
| 2          | -434.2087 |       |
| 3          | -434.2085 |       |
| 4          | -434.2085 | TS4   |
| 5          | -434.2084 |       |
| 6          | -434.2078 |       |
| 7          | -434.2078 |       |
| 8          | -434.2079 |       |
| 9          | -434.2083 |       |
| 10         | -434.2086 | No TS |
| 11         | -434.2086 |       |
| 12         | -434.2087 |       |
| 13         | -434.2088 |       |



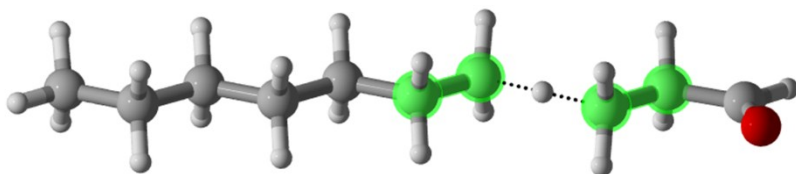
### 1.3.6. Isobutene H abstraction



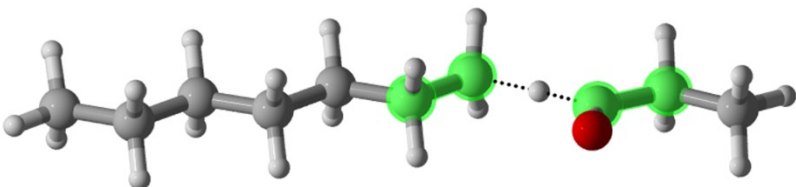
| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -432.9837 | TS1   |
| 2          | -432.9837 |       |
| 3          | -432.9837 |       |
| 4          | -432.9836 |       |
| 5          | -432.9834 |       |
| 6          | -432.9833 |       |
| 7          | -432.9834 |       |
| 8          | -432.9834 |       |
| 9          | -432.9836 |       |
| 10         | -432.9837 | TS2   |
| 11         | -432.9837 |       |
| 12         | -432.9837 |       |
| 13         | -432.9837 |       |



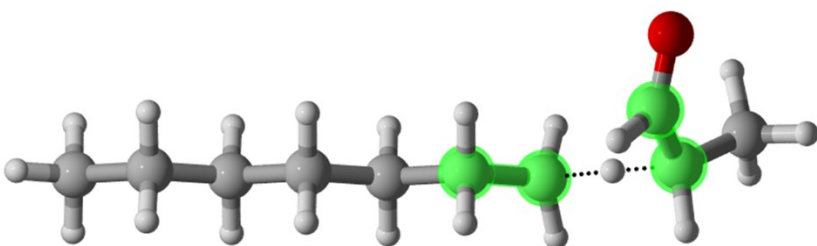
**1.3.7. Propanal H abstraction (36 steps of 10°)**



propanal TS 1 scan

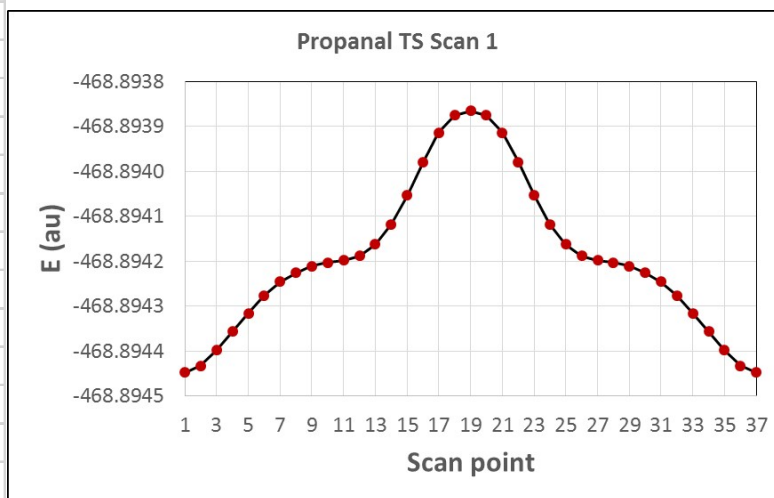


propanal TS 2 scan

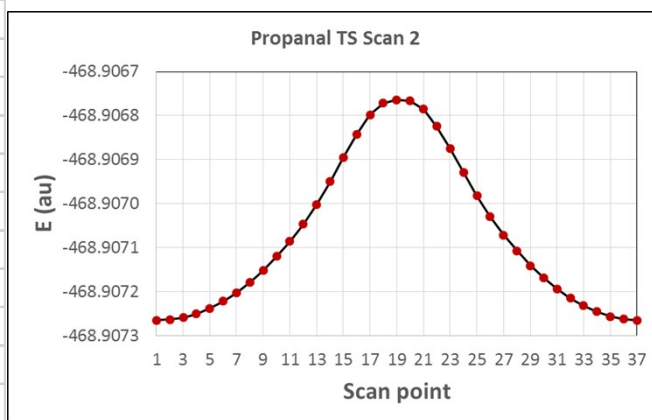


propanal TS 3 scan

| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -468.8944 | TS1   |
| 2          | -468.8944 |       |
| 3          | -468.8944 |       |
| 4          | -468.8944 |       |
| 5          | -468.8943 |       |
| 6          | -468.8943 |       |
| 7          | -468.8942 |       |
| 8          | -468.8942 |       |
| 9          | -468.8942 |       |
| 10         | -468.8942 |       |
| 11         | -468.8942 | No TS |
| 12         | -468.8942 |       |
| 13         | -468.8942 |       |
| 14         | -468.8941 |       |
| 15         | -468.8941 |       |
| 16         | -468.8940 |       |
| 17         | -468.8939 |       |
| 18         | -468.8939 |       |
| 19         | -468.8939 |       |
| 20         | -468.8939 |       |
| 21         | -468.8939 |       |
| 22         | -468.8940 |       |
| 23         | -468.8941 |       |
| 24         | -468.8941 |       |
| 25         | -468.8942 | No TS |
| 26         | -468.8942 |       |
| 27         | -468.8942 |       |
| 28         | -468.8942 |       |
| 29         | -468.8942 |       |
| 30         | -468.8942 |       |
| 31         | -468.8942 |       |
| 32         | -468.8943 |       |
| 33         | -468.8943 |       |
| 34         | -468.8944 |       |
| 35         | -468.8944 |       |
| 36         | -468.8944 |       |
| 37         | -468.8944 |       |



| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -468.9073 | TS2   |
| 2          | -468.9073 |       |
| 3          | -468.9073 |       |
| 4          | -468.9073 |       |
| 5          | -468.9072 |       |
| 6          | -468.9072 |       |
| 7          | -468.9072 |       |
| 8          | -468.9072 |       |
| 9          | -468.9072 |       |
| 10         | -468.9071 |       |
| 11         | -468.9071 |       |
| 12         | -468.9070 |       |
| 13         | -468.9070 |       |
| 14         | -468.9070 |       |
| 15         | -468.9069 |       |
| 16         | -468.9068 |       |
| 17         | -468.9068 |       |
| 18         | -468.9068 |       |
| 19         | -468.9068 |       |
| 20         | -468.9068 |       |
| 21         | -468.9068 |       |
| 22         | -468.9068 |       |
| 23         | -468.9069 |       |
| 24         | -468.9069 |       |
| 25         | -468.9070 |       |
| 26         | -468.9070 |       |
| 27         | -468.9071 |       |
| 28         | -468.9071 |       |
| 29         | -468.9071 |       |
| 30         | -468.9072 |       |
| 31         | -468.9072 |       |
| 32         | -468.9072 |       |
| 33         | -468.9072 |       |
| 34         | -468.9072 |       |
| 35         | -468.9073 |       |
| 36         | -468.9073 |       |
| 37         | -468.9073 |       |



| Scan point | E (au)    | Notes |
|------------|-----------|-------|
| 1          | -468.9059 | TS3   |
| 2          | -468.9059 |       |
| 3          | -468.9058 |       |
| 4          | -468.9058 |       |
| 5          | -468.9057 |       |
| 6          | -468.9057 |       |
| 7          | -468.9056 |       |
| 8          | -468.9056 |       |
| 9          | -468.9056 |       |
| 10         | -468.9056 | No TS |
| 11         | -468.9056 |       |
| 12         | -468.9055 |       |
| 13         | -468.9054 |       |
| 14         | -468.9053 |       |
| 15         | -468.9052 |       |
| 16         | -468.9051 |       |
| 17         | -468.9051 |       |
| 18         | -468.9051 |       |
| 19         | -468.9052 |       |
| 20         | -468.9053 |       |
| 21         | -468.9053 |       |
| 22         | -468.9054 |       |
| 23         | -468.9054 |       |
| 24         | -468.9055 |       |
| 25         | -468.9055 |       |
| 26         | -468.9055 | No TS |
| 27         | -468.9055 |       |
| 28         | -468.9055 |       |
| 29         | -468.9055 |       |
| 30         | -468.9056 |       |
| 31         | -468.9056 |       |
| 32         | -468.9057 |       |
| 33         | -468.9057 |       |
| 34         | -468.9058 |       |
| 35         | -468.9058 |       |
| 36         | -468.9058 |       |
| 37         | -468.9059 |       |

