

Structure, Ionization, and Fragmentation of Neutral and Positively Charged Hydrogenated Carbon Clusters: $C_n H_m^{q+}$

($n = 1\text{-}5, m = 1\text{-}4, q = 0\text{-}3$)

Supporting Information

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We here present the results obtained for the studied $C_nH_m^{q+}$ family of compounds ($n = 1 - 5$, $m = 1 - 4$, $q = 0 - 3$). They have been computed at the CCSD(T)//B3LYP level as explained in the main text. This material represents useful information for the reader since it is systematically presented and specific data analysis can be carried out. The information is presented as follows:

- Tables 1 and 2:

Adiabatic and vertical ionization potentials, respectively.

- Figure 1:

Dissociation energy for H, H^+ , C and C^+ loss.

- Figures 2-5:

Dissociation energy windows classified by the number of fragments.

C_nH_m , $C_nH_m^+$, $C_nH_m^{2+}$, $C_nH_m^{3+}$

- Figures 6-25:

Fragmentation channel distribution plots.

CH_n^{q+} , $C_2H_m^{q+}$, $C_3H_m^{q+}$, $C_4H_m^{q+}$, $C_5H_m^{q+}$

- Table 3:

Geometries of all stable isomers.

CH_n^{q+} , $C_2H_m^{q+}$, $C_3H_m^{q+}$, $C_4H_m^{q+}$, $C_5H_m^{q+}$,

- Table 4:

Complete set of energies for all studied structures.

CH_n^{q+} , $C_2H_m^{q+}$, $C_3H_m^{q+}$, $C_4H_m^{q+}$, $C_5H_m^{q+}$,

Ionization Potentials

Adiabatic Ionization Potentials

Table 1: Adiabatic Ionization potentials (IP), in eV, calculated at the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) level of theory including ZPE corrections.

| First IP $C_nH_m \rightarrow C_nH_m^+$ | | | | | |
|--|----------------|--------|--------|-------|--------|
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 11.179 | 10.542 | 10.307 | 9.693 | 12.798 |
| 2 | 11.703 | 11.295 | 11.264 | 8.622 | 10.407 |
| 3 | 11.635 | 9.044 | 9.069 | 7.582 | 9.608 |
| 4 | 10.774 | 10.052 | 10.143 | 7.851 | 9.049 |
| 5 | 11.146 | 8.288 | 8.345 | 7.536 | 9.389 |

| Second IP $C_nH_m^+ \rightarrow C_nH_m^{2+}$ | | | | | |
|--|----------------|--------|--------|--------|--------|
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 24.218 | - | 21.225 | 23.682 | 19.603 |
| 2 | 22.479 | 20.688 | 20.177 | 19.678 | 18.947 |
| 3 | 19.144 | 19.106 | 16.796 | 18.976 | 16.069 |
| 4 | 17.424 | 17.216 | 16.713 | 16.519 | 14.932 |
| 5 | 15.611 | 16.712 | 14.441 | 16.088 | 13.804 |

| Third IP $C_nH_m^{2+} \rightarrow C_nH_m^{3+}$ | | | | | |
|--|----------------|--------|--------|--------|--------|
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 47.795 | - | - | - | 33.554 |
| 2 | 35.196 | - | 30.101 | 28.934 | 29.335 |
| 3 | 30.742 | 28.840 | 27.935 | 26.346 | 26.318 |
| 4 | 26.811 | 24.253 | 24.426 | 23.440 | 24.280 |
| 5 | 25.418 | 23.826 | 23.407 | 22.100 | 23.166 |

Vertical Ionization Potentials

Table 2: Vertical Ionization potentials (IP), in eV, calculated at the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) level of theory. All values have been calculated using the geometry of the neutral system. The values given in the tables correspond to the energies with respect the neutral cluster. ZPE corrections have been included only for the neutral system.

| First vertical IP C_nH_m $C_nH_m \rightarrow C_nH_m^+$ | | | | | |
|--|----------------|--------|--------|--------|--------|
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 11.154 | 10.548 | 10.341 | 9.715 | 14.336 |
| 2 | 12.407 | 13.897 | 11.459 | 9.474 | 10.682 |
| 3 | 11.755 | 9.875 | 9.352 | 8.576 | 10.241 |
| 4 | 11.276 | 10.786 | 10.233 | 7.854 | 9.716 |
| 5 | 10.947 | 8.257 | 9.063 | 8.022 | 9.603 |
| First + Second vertical IP $C_nH_m \rightarrow C_nH_m^{2+}$ | | | | | |
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 35.371 | 34.632 | 32.794 | 35.477 | 39.028 |
| 2 | 36.077 | 35.550 | 33.622 | 29.359 | 31.045 |
| 3 | 30.742 | 29.302 | 28.908 | 26.838 | 29.047 |
| 4 | 30.660 | 27.435 | 27.888 | 24.536 | 26.221 |
| 5 | 25.920 | 25.101 | 25.565 | 23.814 | 26.010 |
| First + Second + Third vertical IP $C_nH_m \rightarrow C_nH_m^{3+}$ | | | | | |
| Carbon Atoms | Hydrogen Atoms | | | | |
| | 0 | 1 | 2 | 3 | 4 |
| 1 | 83.166 | 74.511 | 72.737 | 73.969 | 74.343 |
| 2 | 70.634 | 68.510 | 65.777 | 60.165 | 61.650 |
| 3 | 63.646 | 59.514 | 59.122 | 54.585 | 54.534 |
| 4 | 57.050 | 54.222 | 52.903 | 48.794 | 49.713 |
| 5 | 52.716 | 52.031 | 50.722 | 46.526 | 48.864 |

H , H^+ , C , C^+ loss dissociation energies

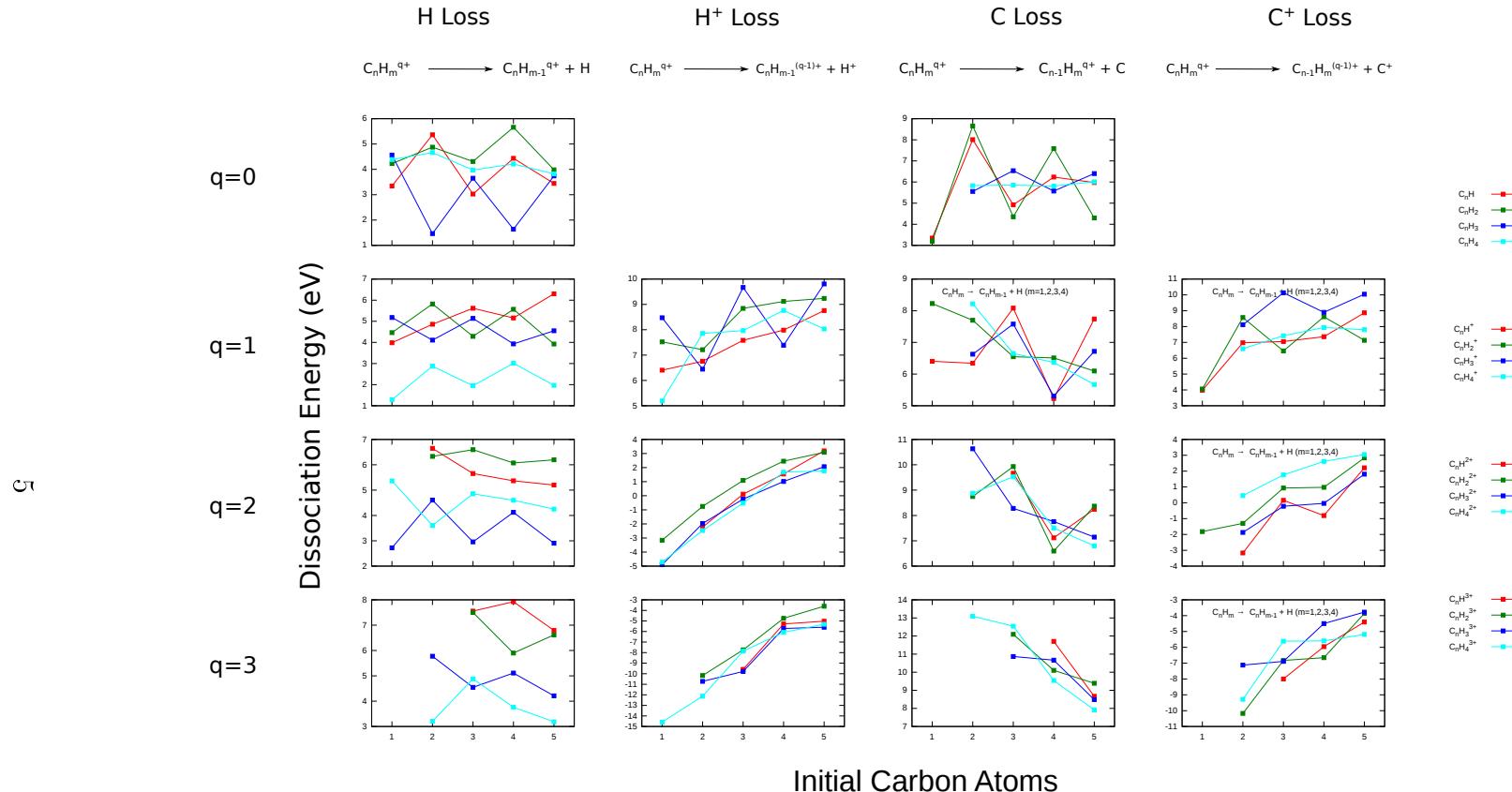


Figure 1: Dissociation energies for the channels corresponding to the loss of H , H^+ , C and C^+ as a function of the initial carbon atoms for the C_nH_m^q+ clusters.

Dissociation Energy Windows by number of fragments

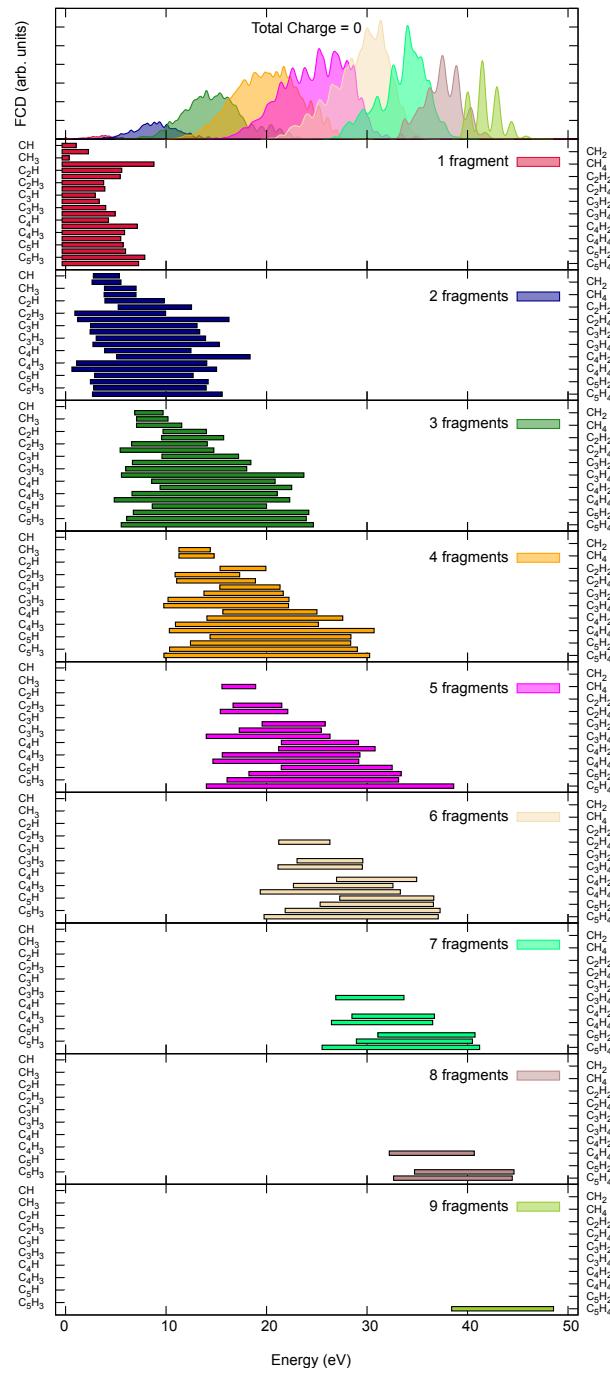


Figure 2: Energetic windows and FCD for neutral C_nH_m by number of fragments.

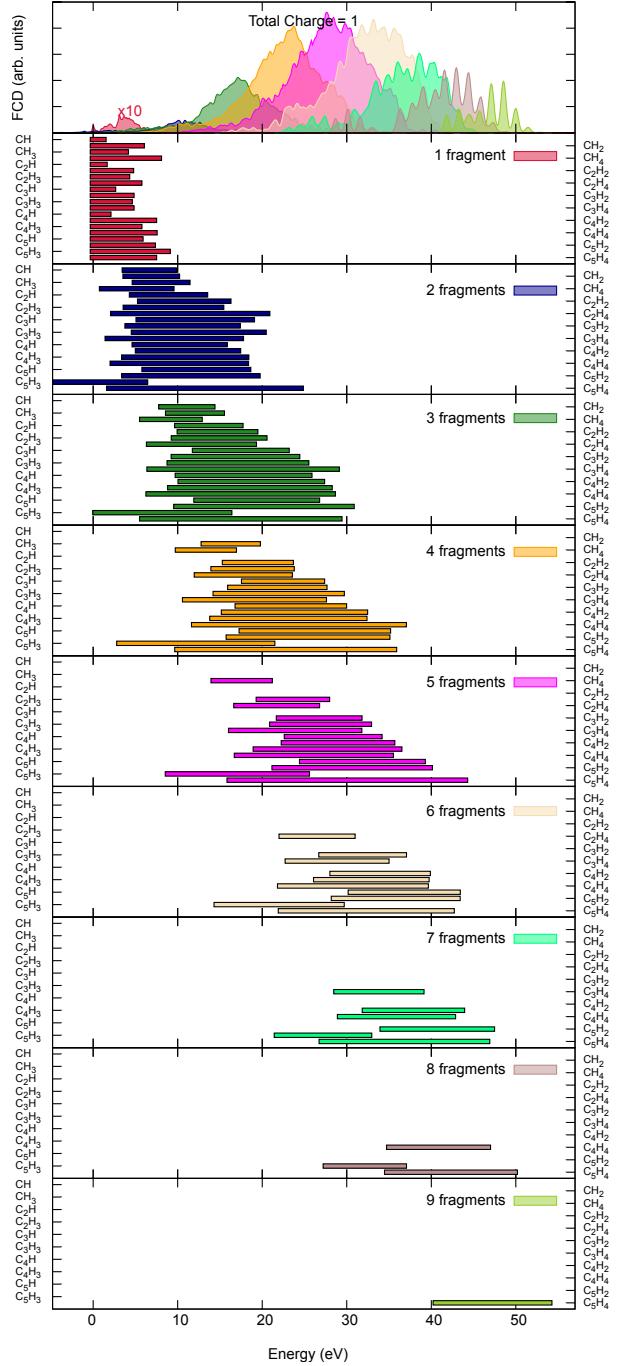


Figure 3: Energetic windows and FCD for $C_nH_m^+$ by number of fragments.

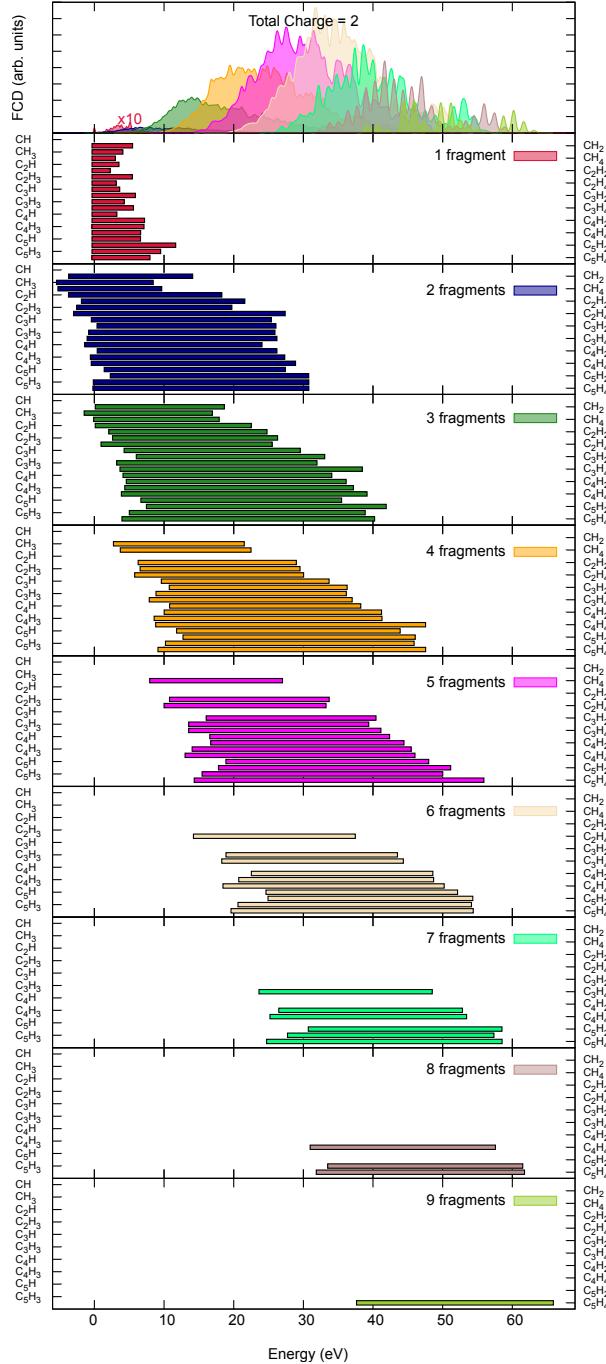


Figure 4: Energetic windows and FCD for $C_nH_m^{2+}$ by number of fragments.

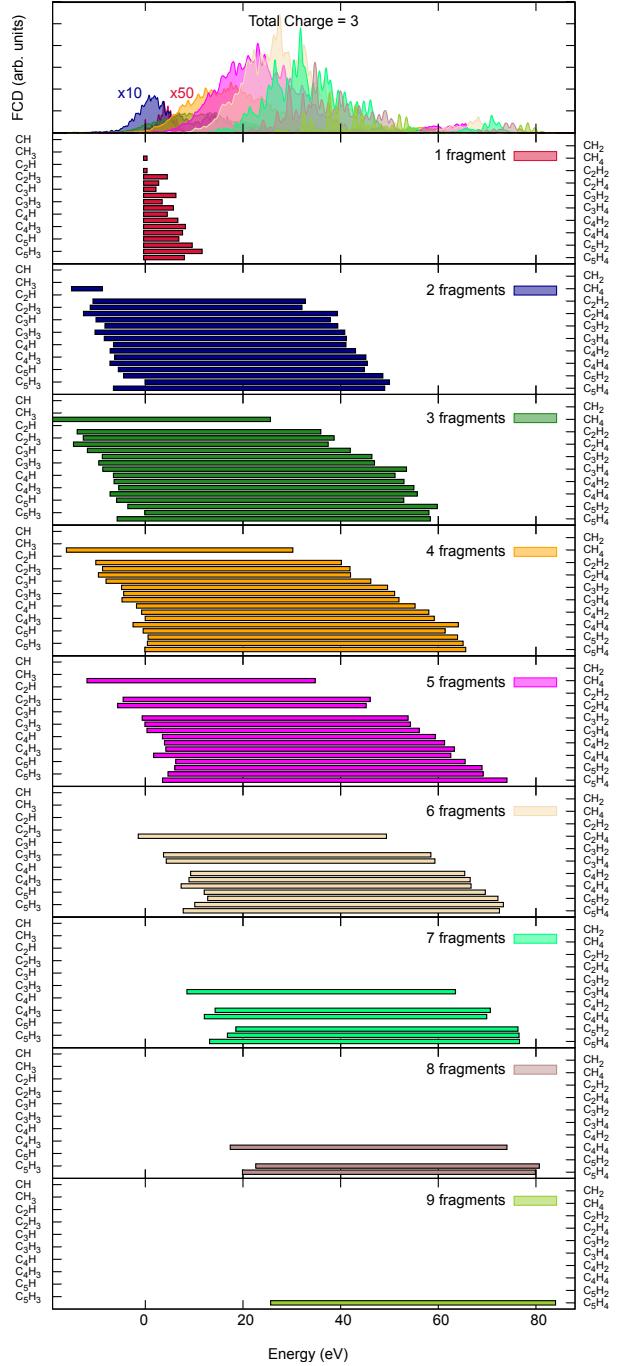


Figure 5: Energetic windows and FCD for $C_nH_m^{3+}$ by number of fragments.

Fragmentation Channel Distribution Plots (FCDs)

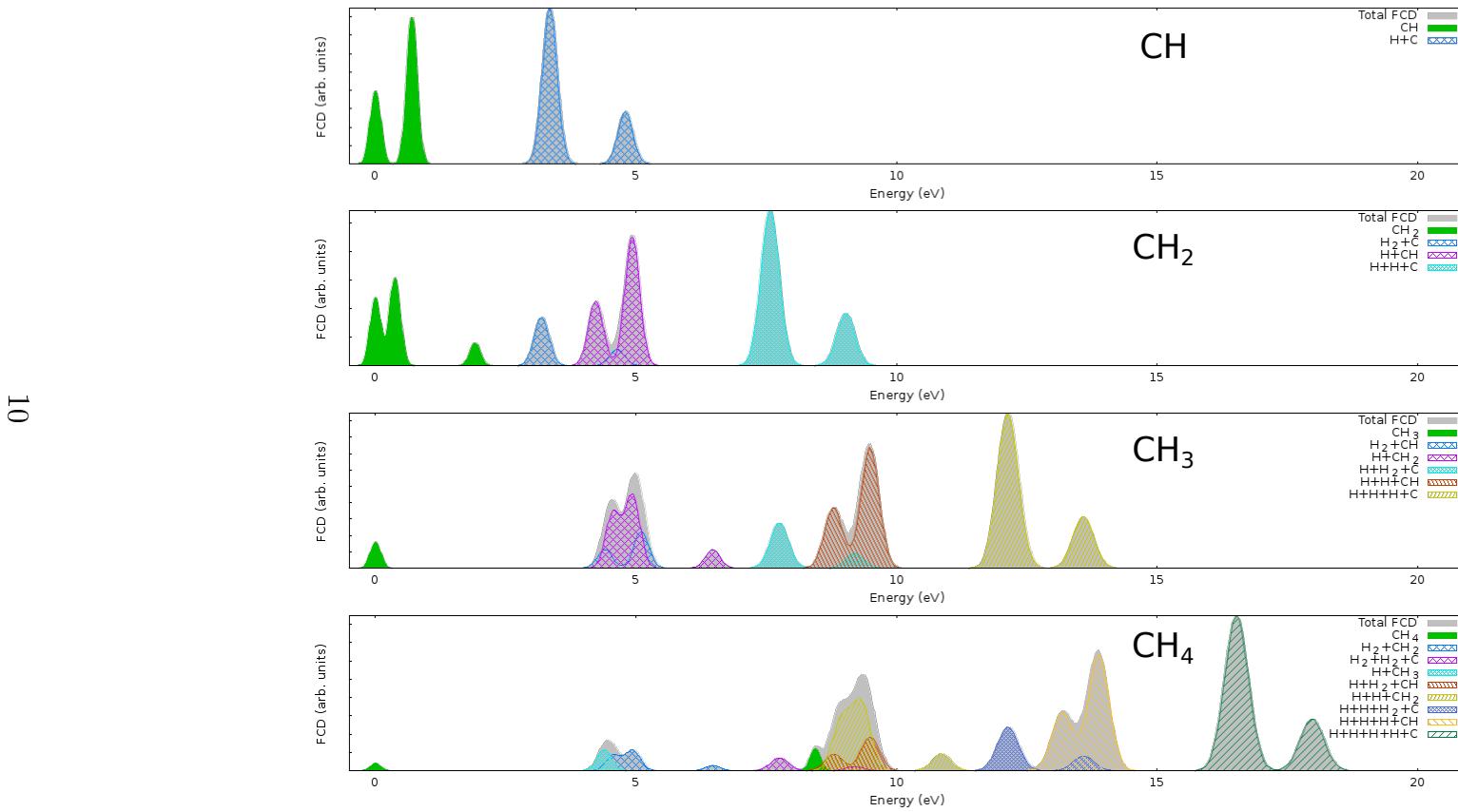


Figure 6: Fragmentation Channel Distribution for CH, CH₂, CH₃ and CH₄. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

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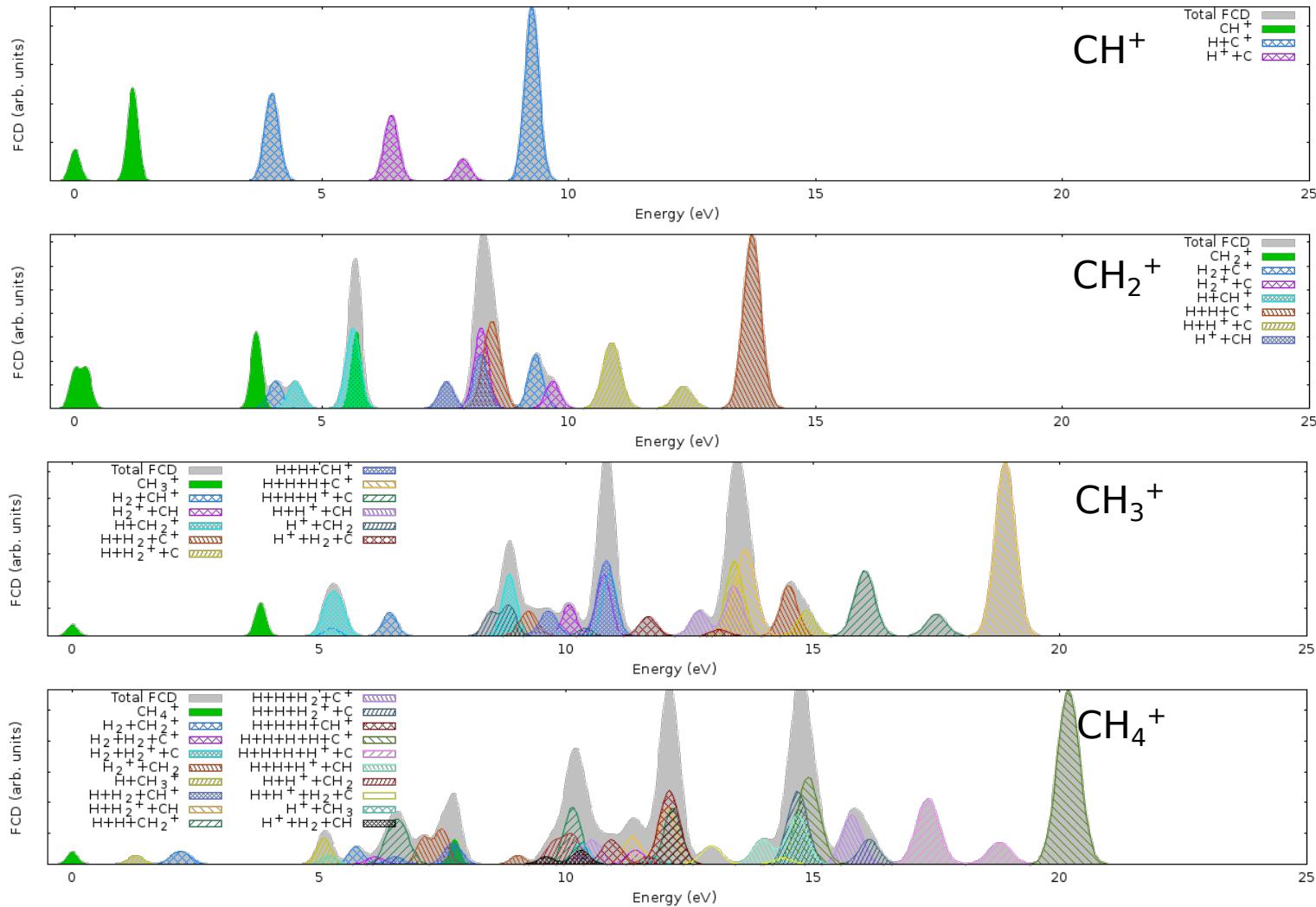


Figure 7: Fragmentation Channel Distribution for CH^+ , CH_2^+ , CH_3^+ and CH_4^+ . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment)..

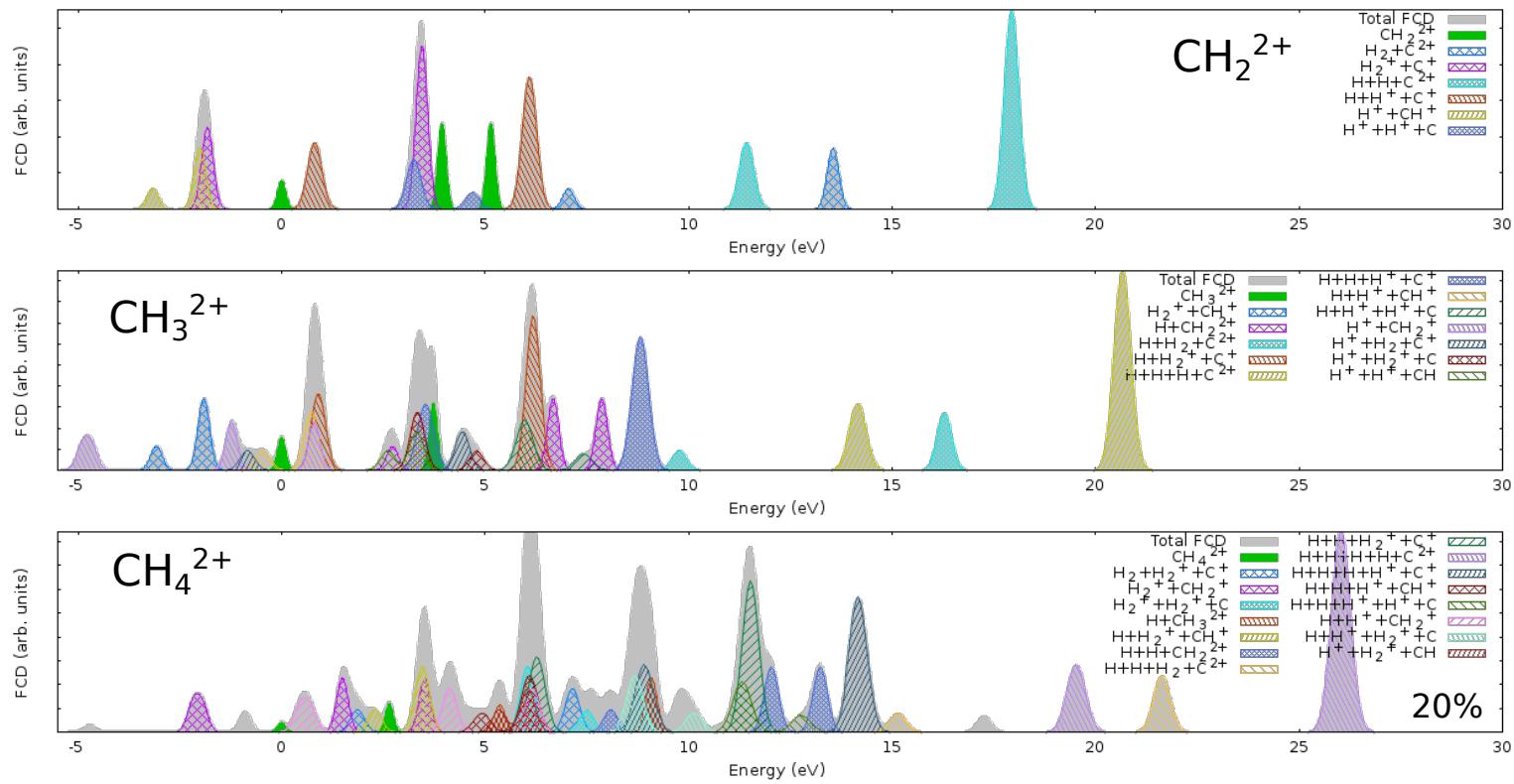


Figure 8: Fragmentation Channel Distribution for CH_2^{2+} , CH_3^{2+} and CH_4^{2+} . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment)..

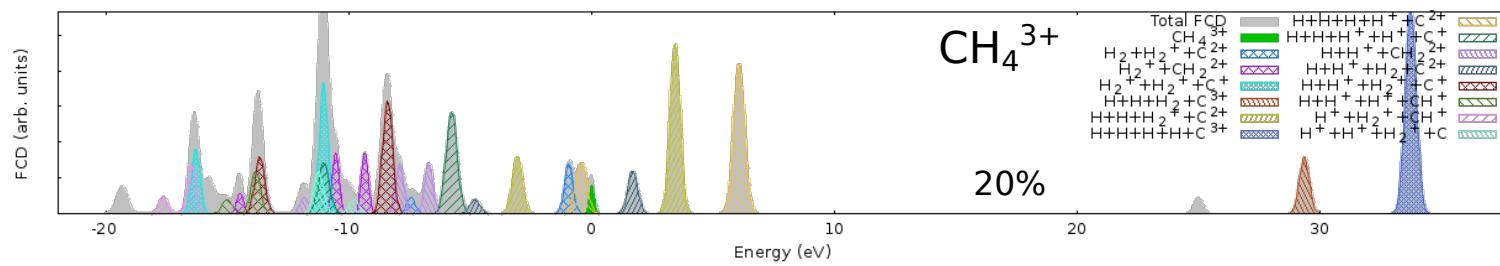


Figure 9: Fragmentation Channel Distribution for CH_4^{3+} . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment)..

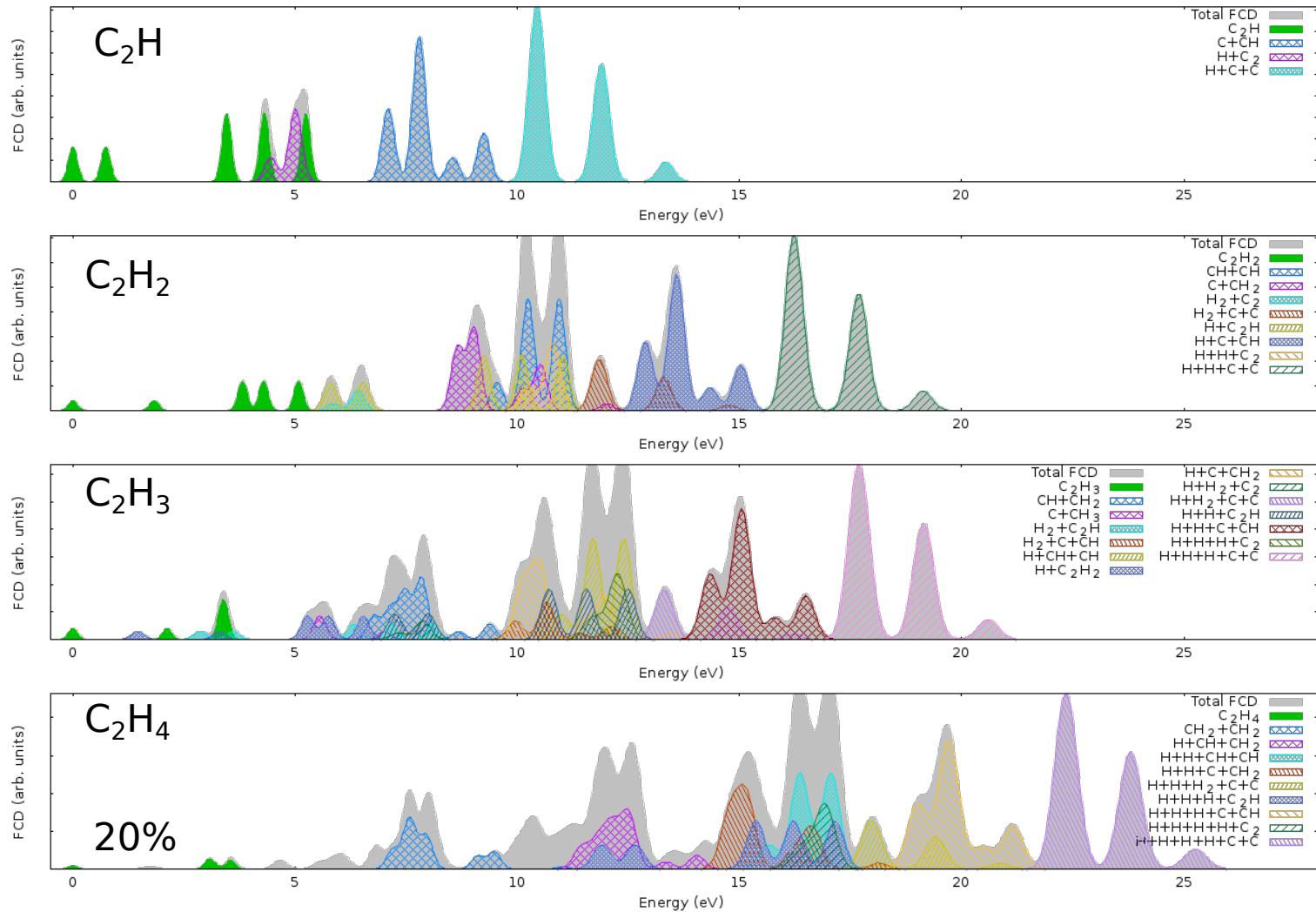


Figure 10: Fragmentation Channel Distribution for C₂H, C₂H₂, C₂H₃ and C₂H₄. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

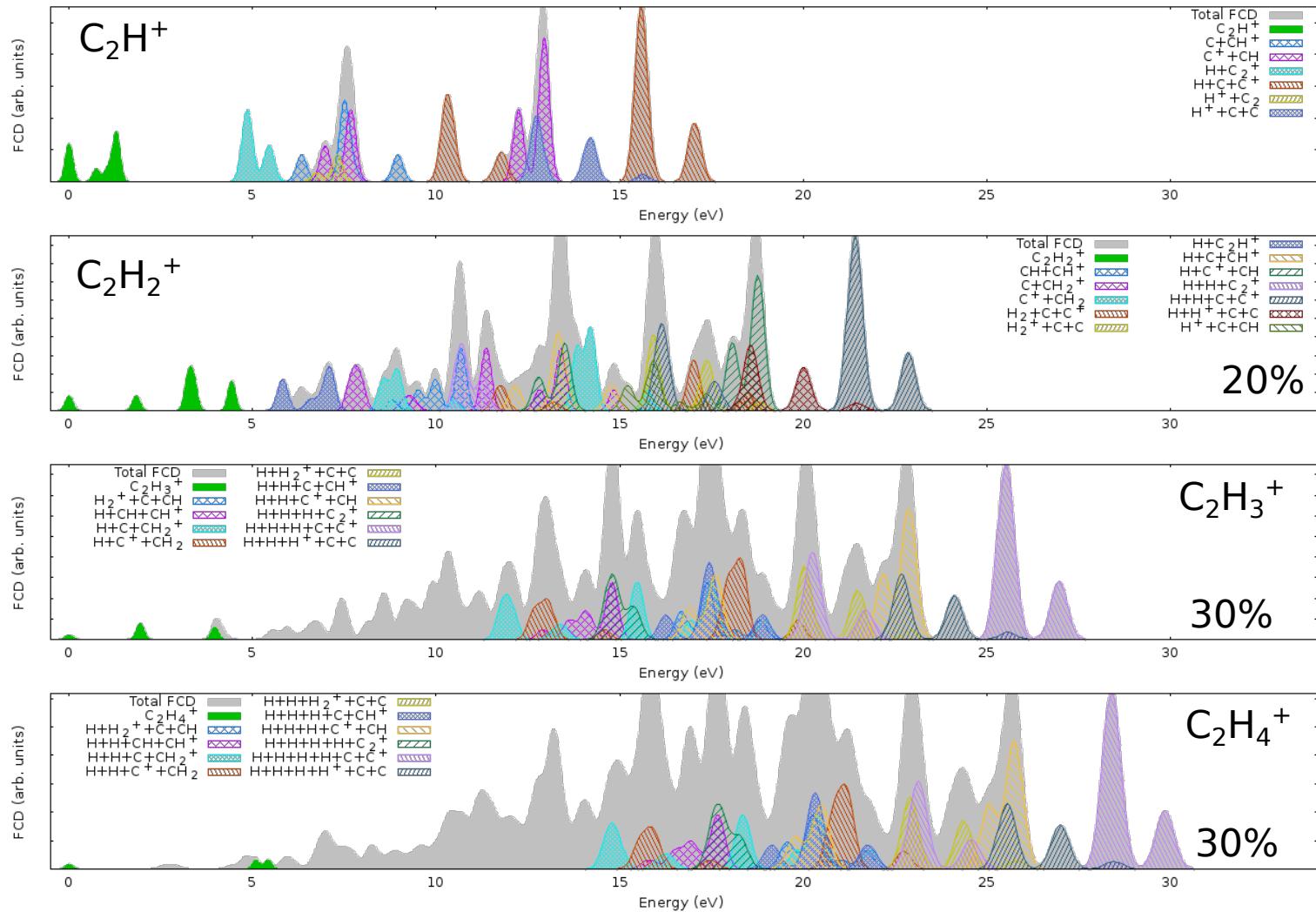


Figure 11: Fragmentation Channel Distribution for C_2H^+ , C_2H_2^+ , C_2H_3^+ and C_2H_4^+ . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

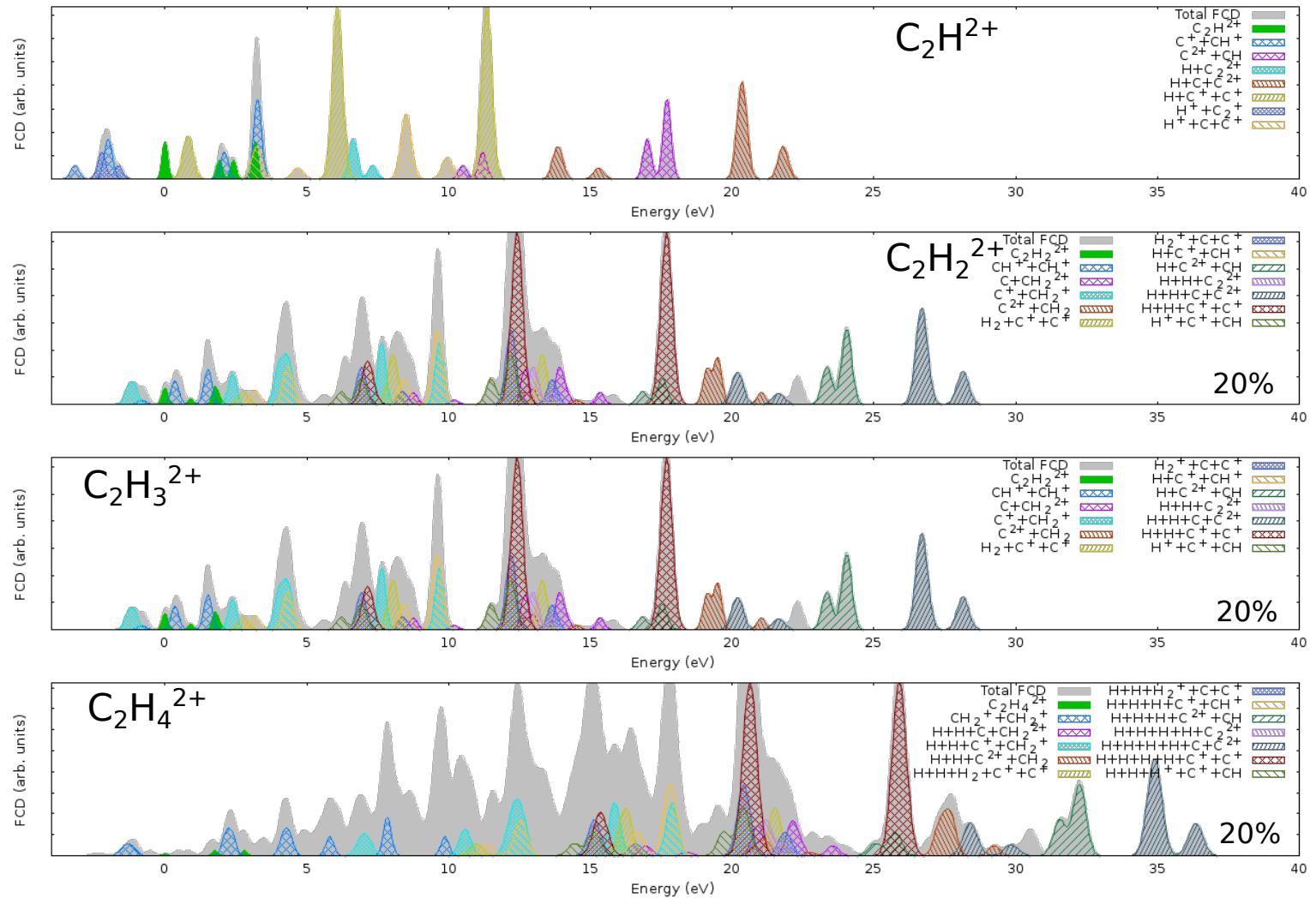


Figure 12: Fragmentation Channel Distribution for C_2H^{2+} , $\text{C}_2\text{H}_2^{2+}$, $\text{C}_2\text{H}_3^{2+}$ an $\text{C}_2\text{H}_4^{2+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

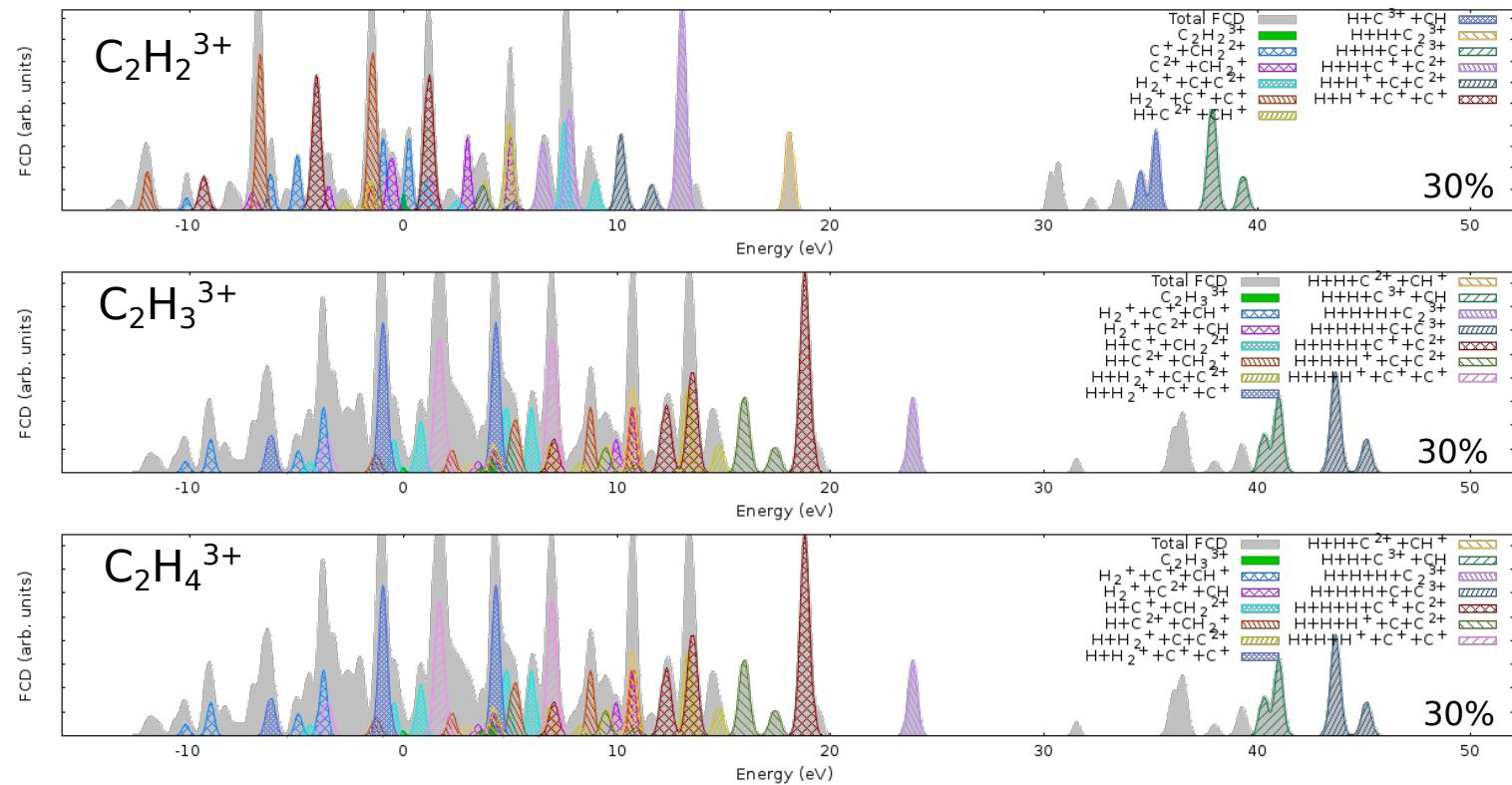


Figure 13: Fragmentation Channel Distribution for $\text{C}_2\text{H}_3^{3+}$ and $\text{C}_2\text{H}_4^{3+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

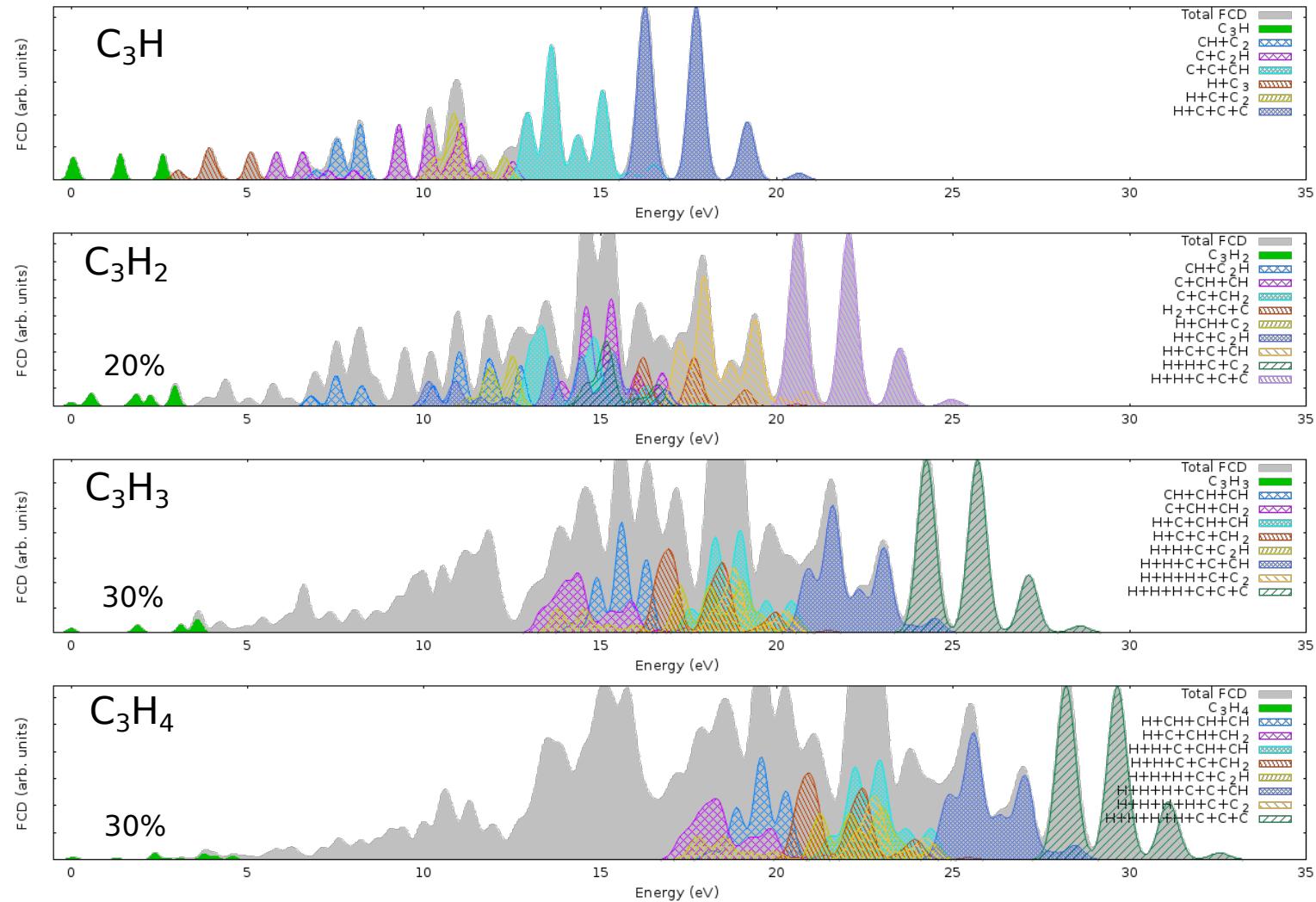


Figure 14: Fragmentation Channel Distribution for C₃H, C₃H₂, C₃H₃ and C₃H₄. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

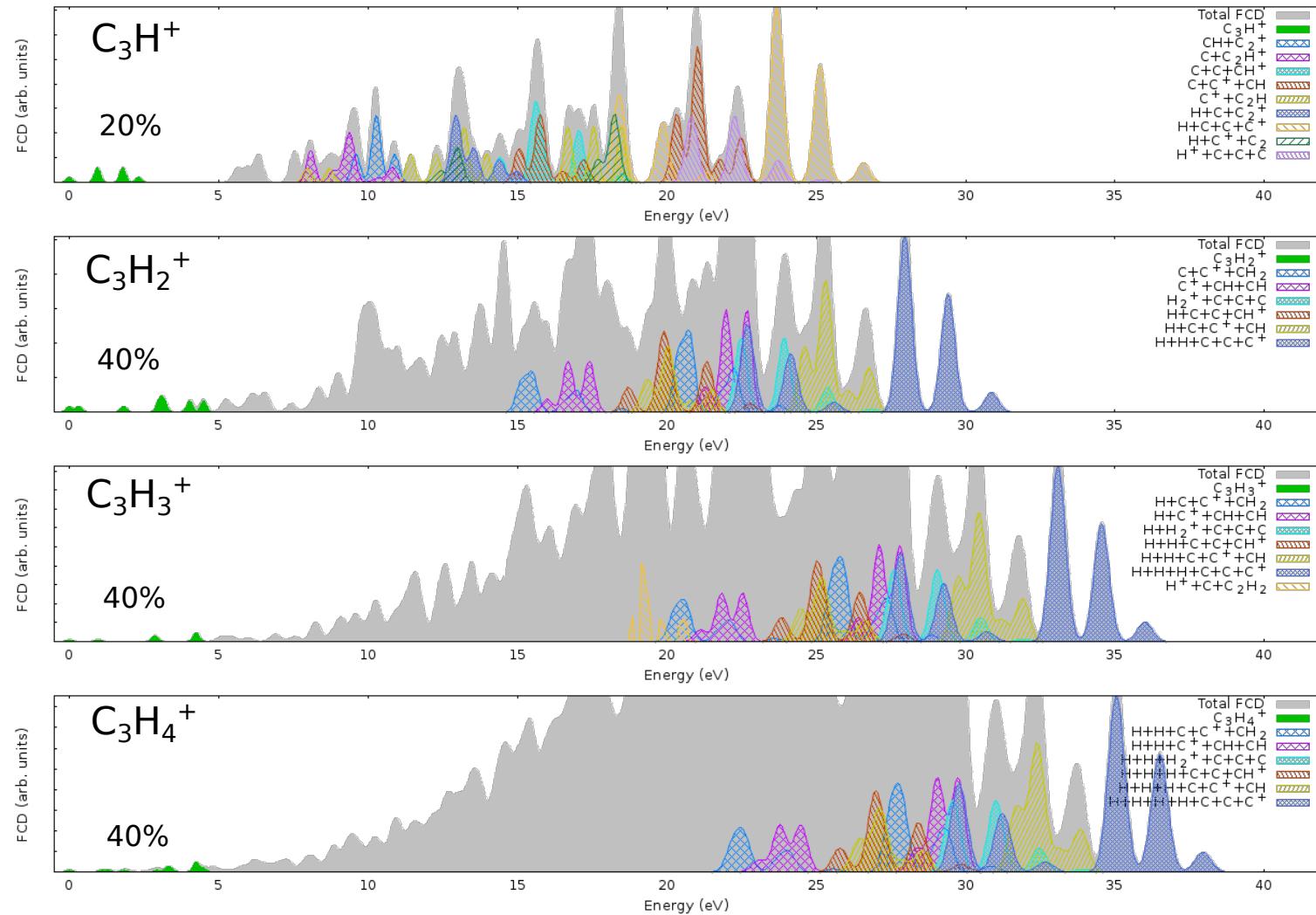


Figure 15: Fragmentation Channel Distribution for C_3H^+ , C_3H_2^+ , C_3H_3^+ and C_3H_4^+ . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

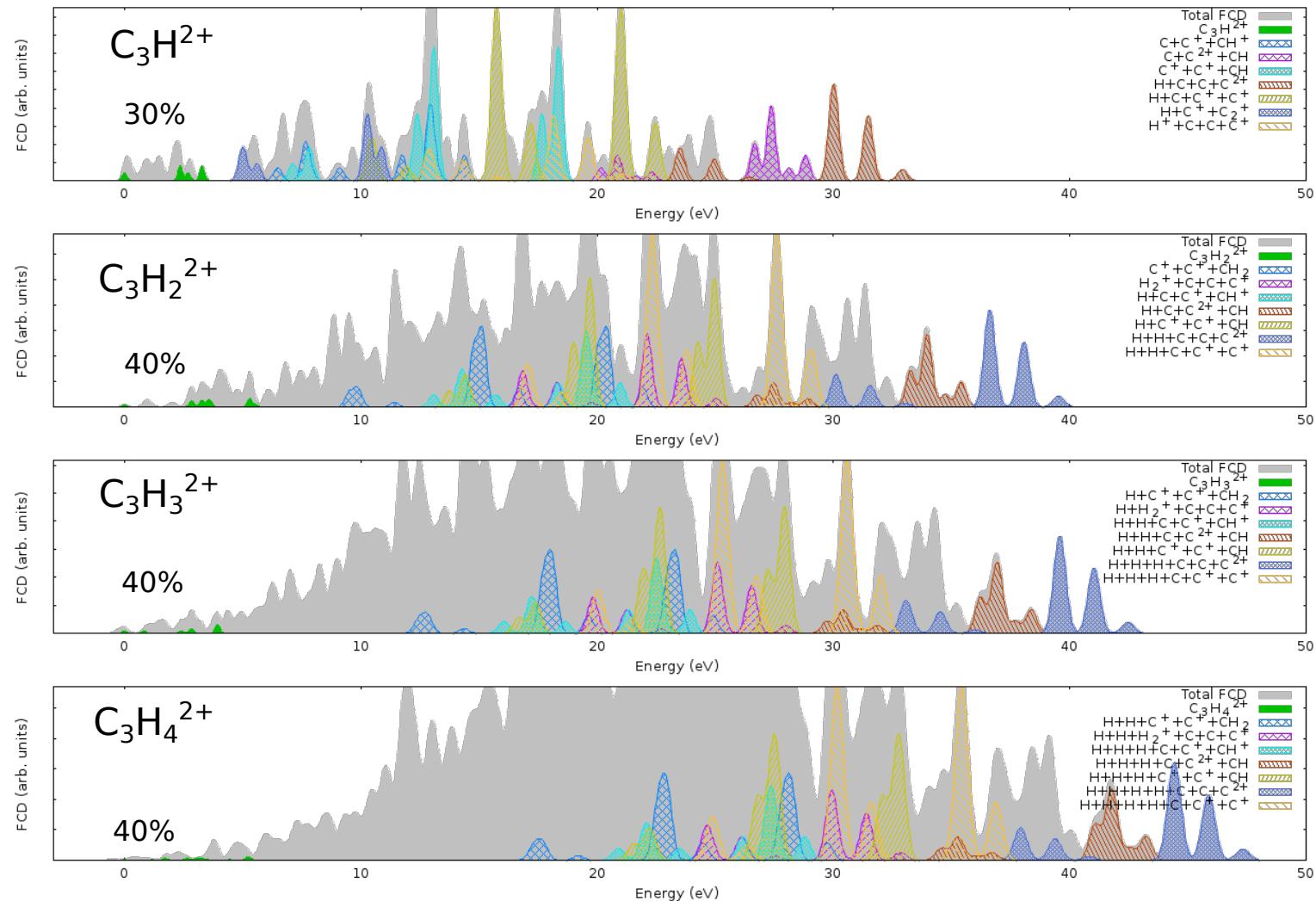


Figure 16: Fragmentation Channel Distribution for C_3H^{2+} , $\text{C}_3\text{H}_2^{2+}$, $\text{C}_3\text{H}_3^{2+}$ and $\text{C}_3\text{H}_4^{2+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

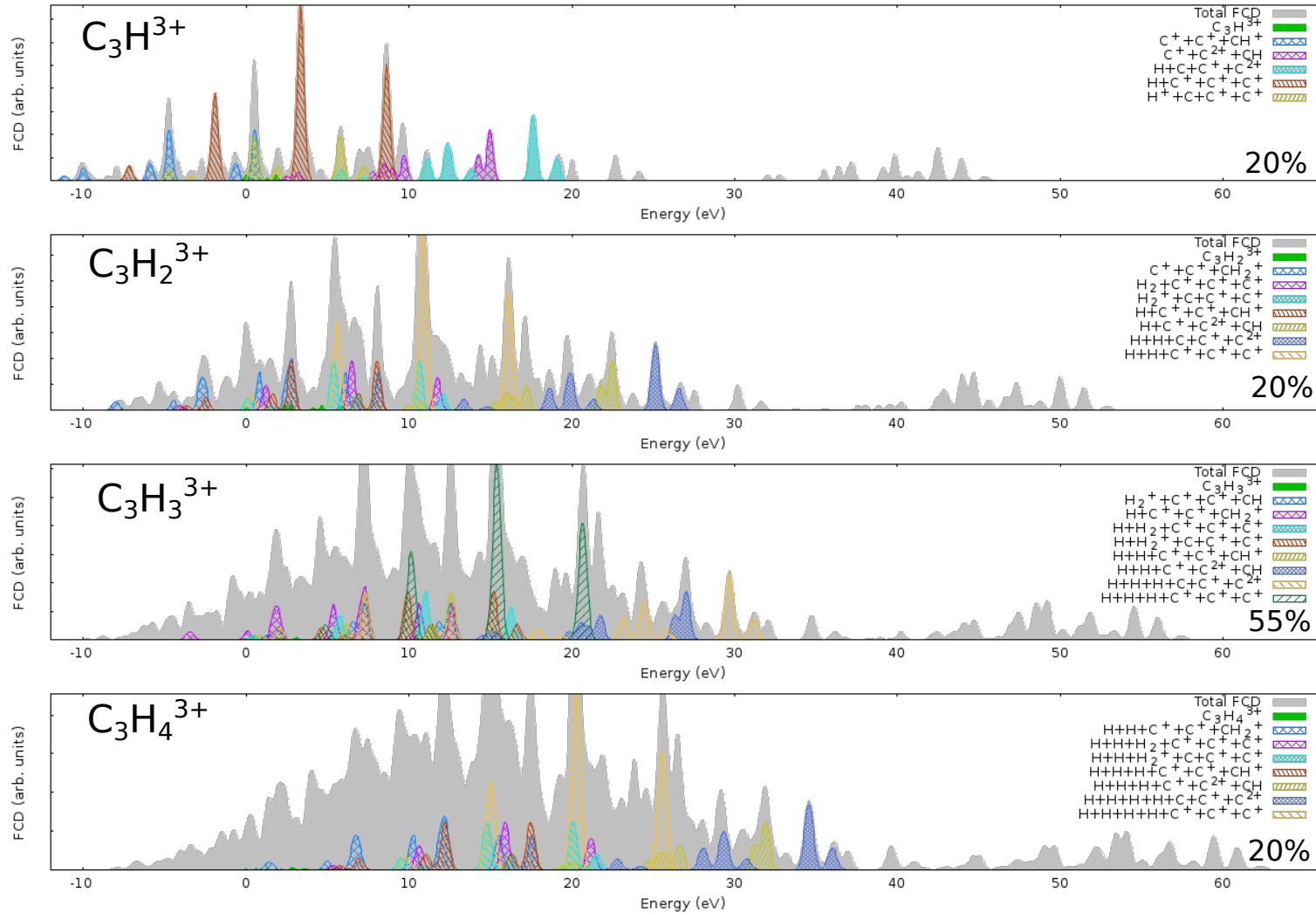


Figure 17: Fragmentation Channel Distribution for C_3H^{3+} , $\text{C}_3\text{H}_2^{3+}$, $\text{C}_3\text{H}_3^{3+}$ and $\text{C}_3\text{H}_4^{3+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

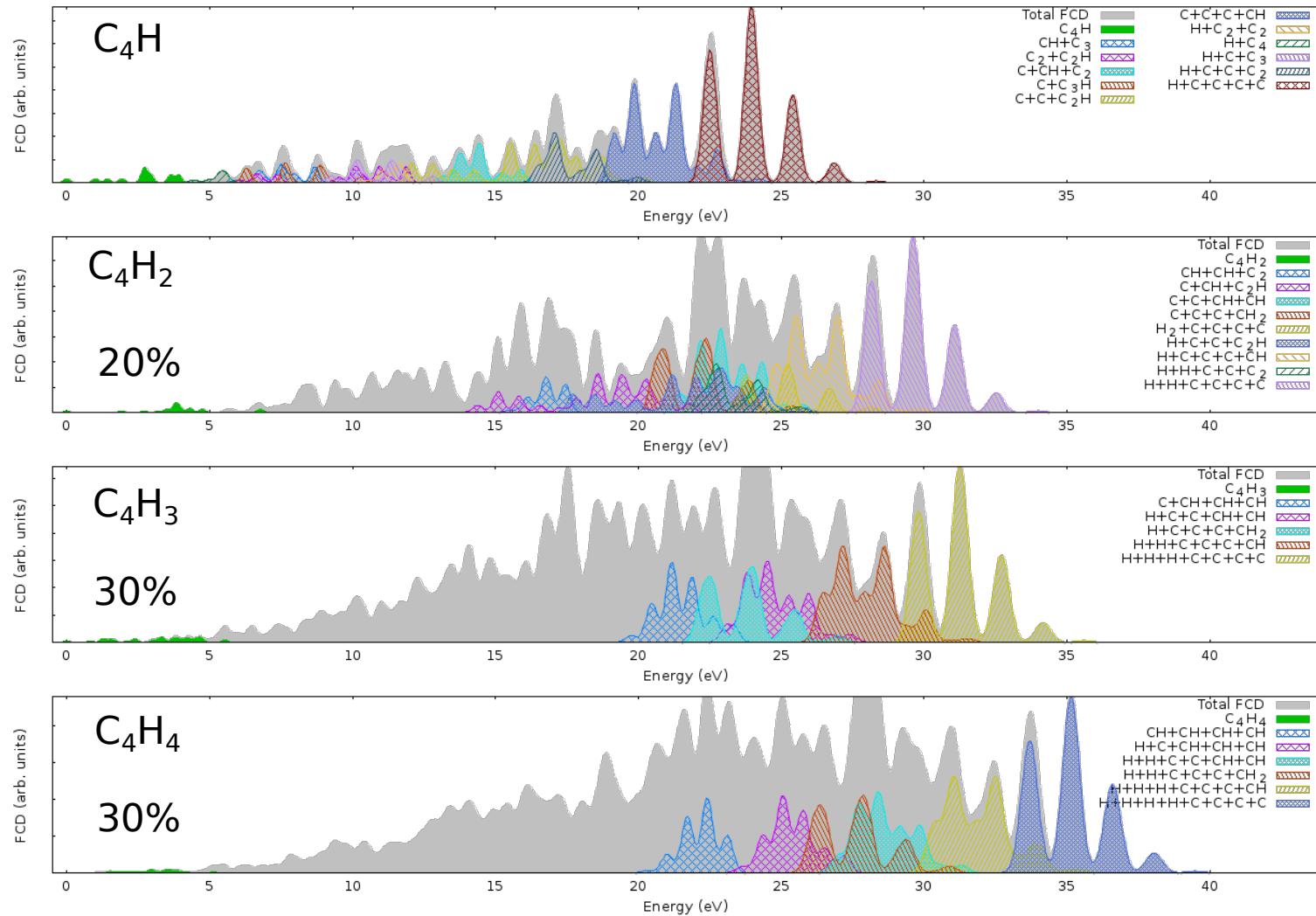


Figure 18: Fragmentation Channel Distribution for C₄H, C₄H₂, C₄H₃ and C₄H₄. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

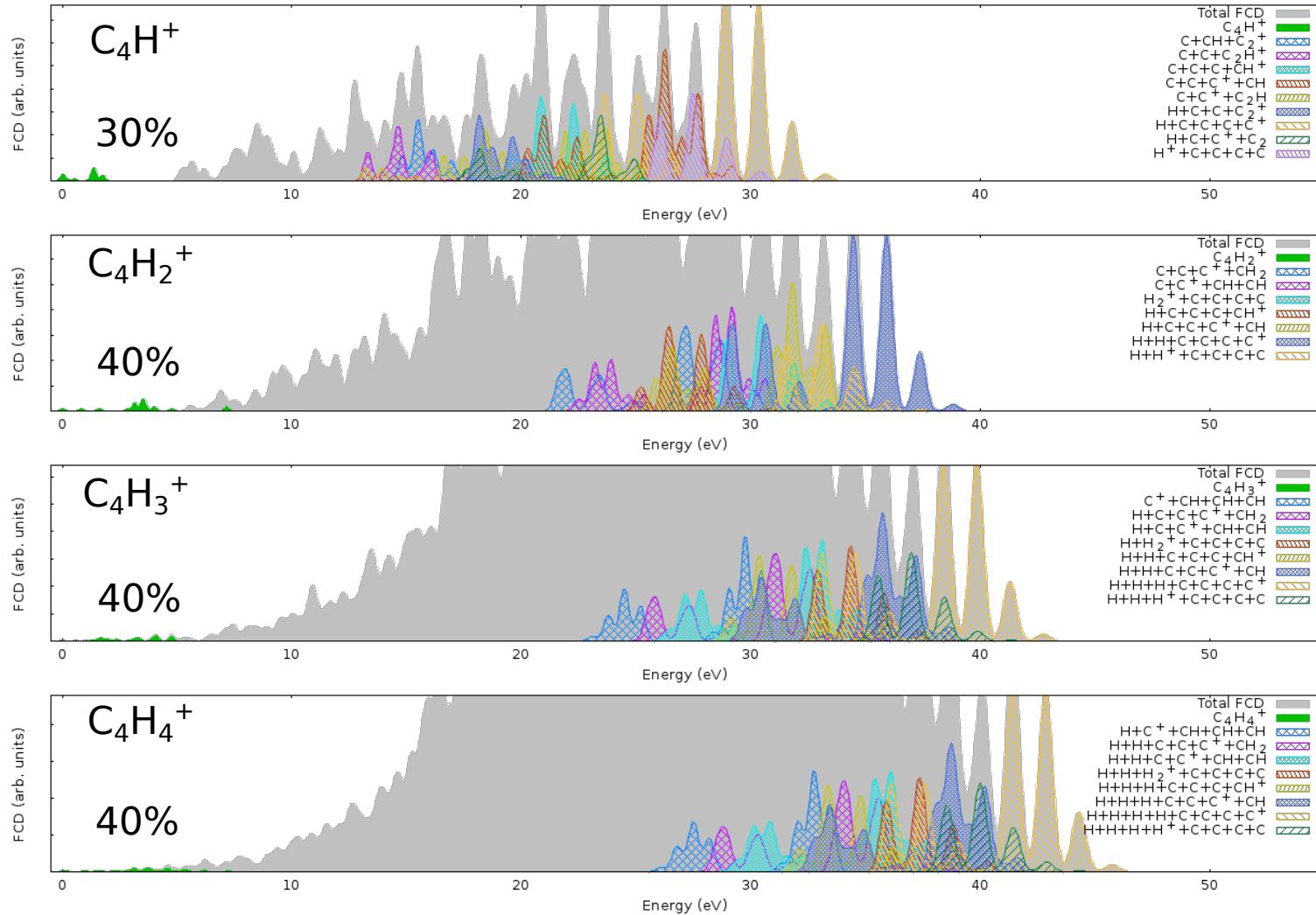


Figure 19: Fragmentation Channel Distribution for C_4H^+ , C_4H_2^+ , C_4H_3^+ and C_4H_4^+ . Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

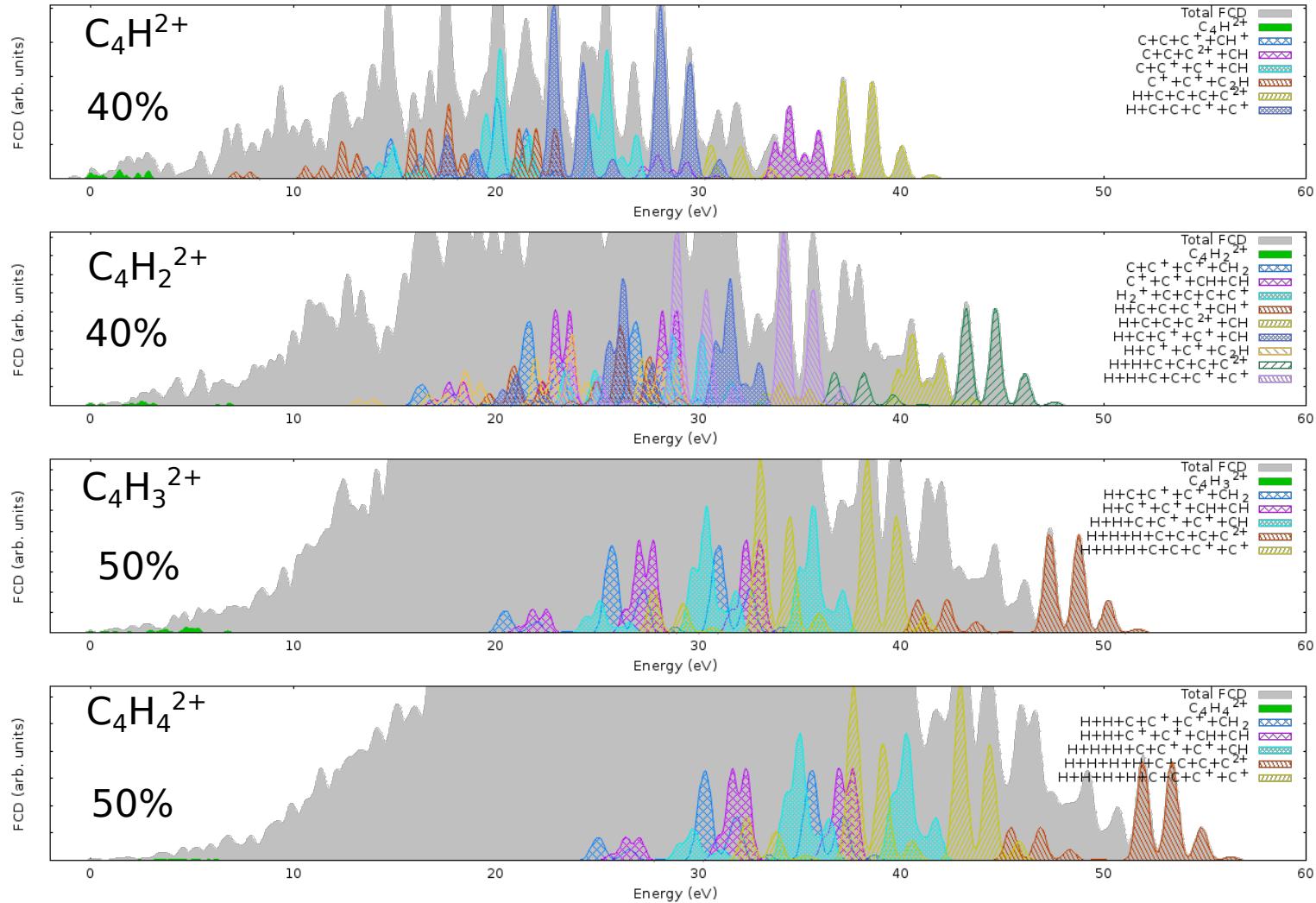


Figure 20: Fragmentation Channel Distribution for C_4H^{2+} , $\text{C}_4\text{H}_2^{2+}$, $\text{C}_4\text{H}_3^{2+}$ and $\text{C}_4\text{H}_4^{2+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

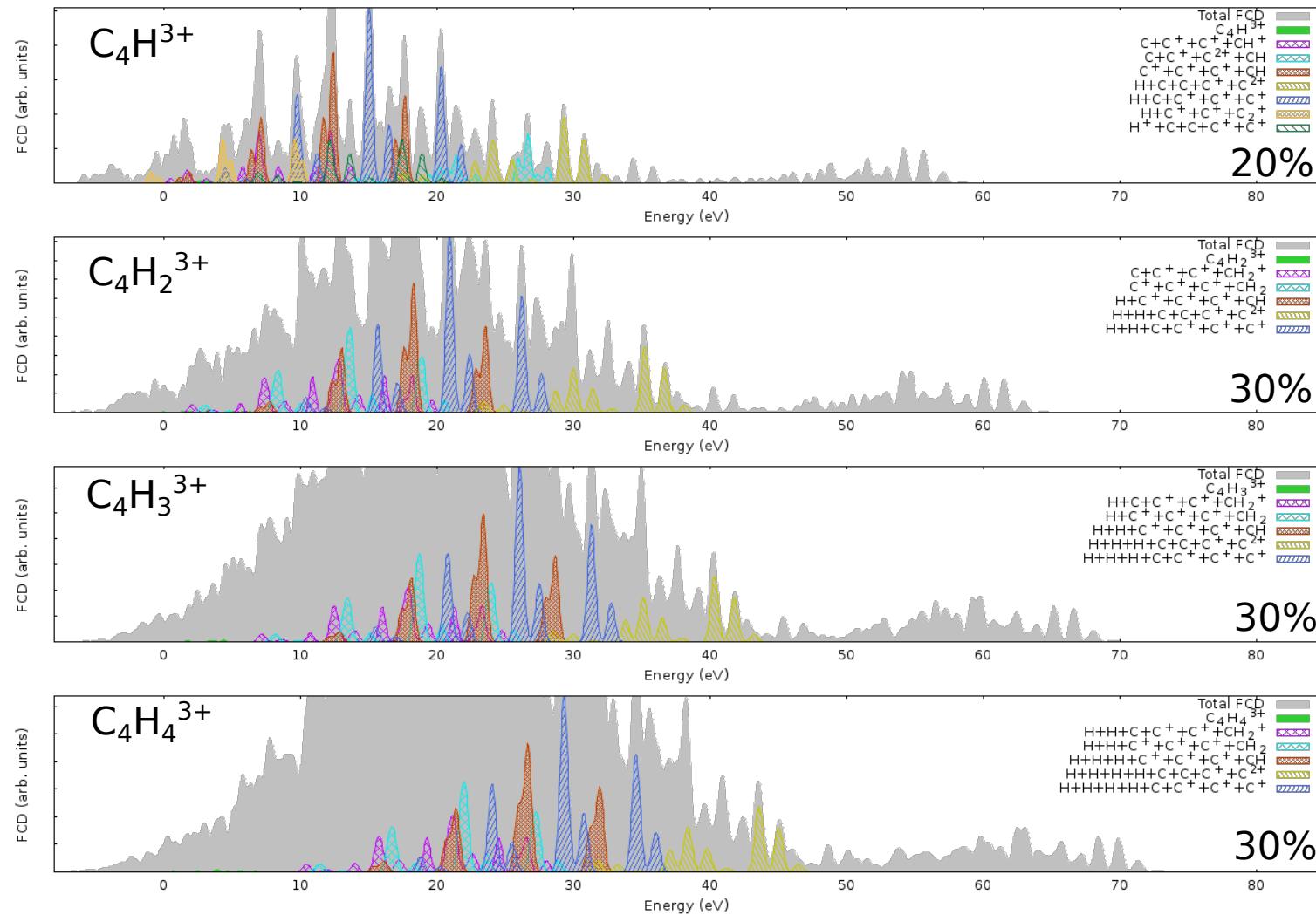


Figure 21: Fragmentation Channel Distribution for C_4H^{3+} , $\text{C}_4\text{H}_2^{3+}$, $\text{C}_4\text{H}_3^{3+}$ and $\text{C}_4\text{H}_4^{3+}$. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

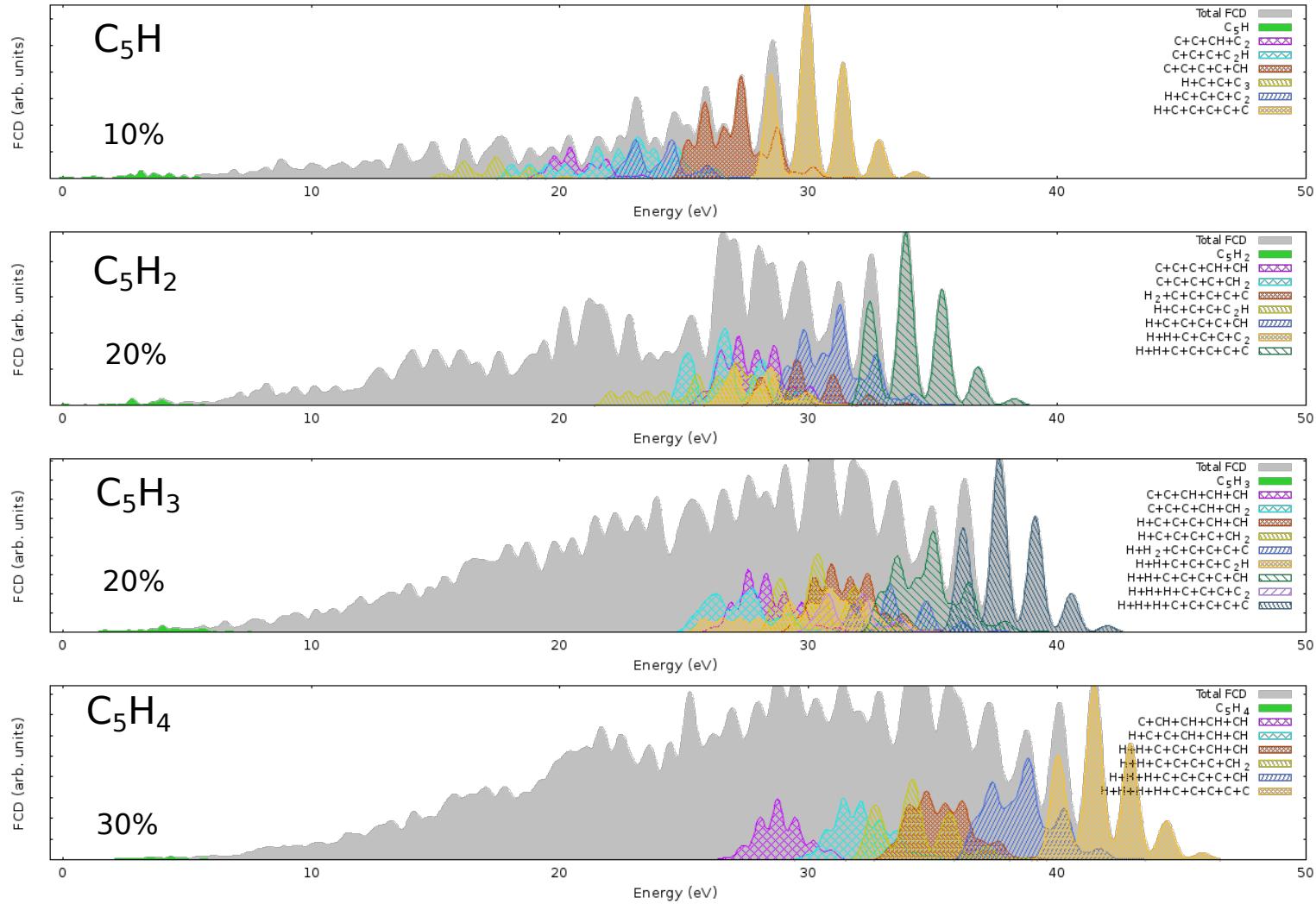


Figure 22: Fragmentation Channel Distribution for C₅H, C₅H₂, C₅H₃ and C₅H₄. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

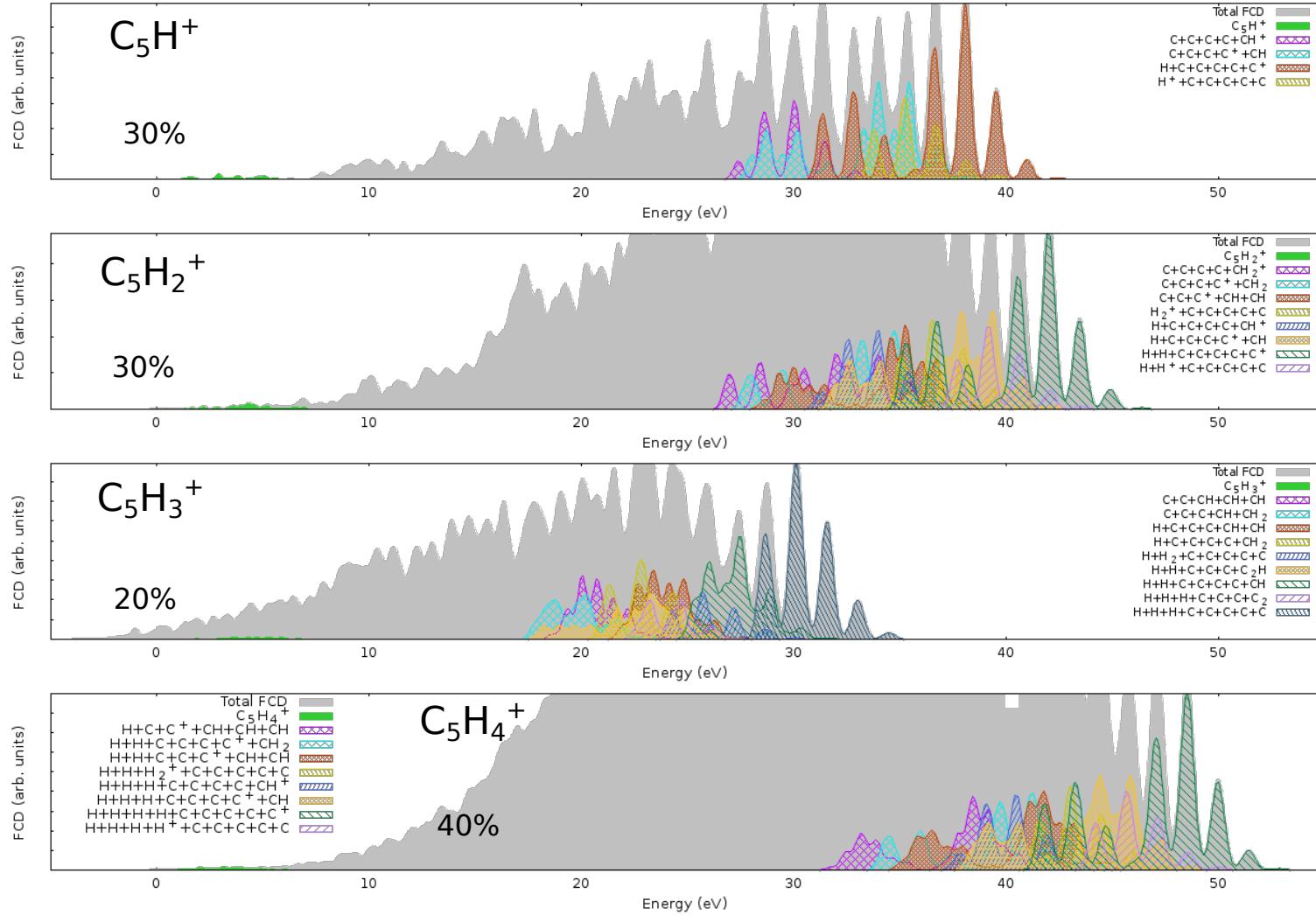


Figure 23: Fragmentation Channel Distribution for C₅H⁺, C₅H₂⁺, C₅H₃⁺ and C₅H₄⁺. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

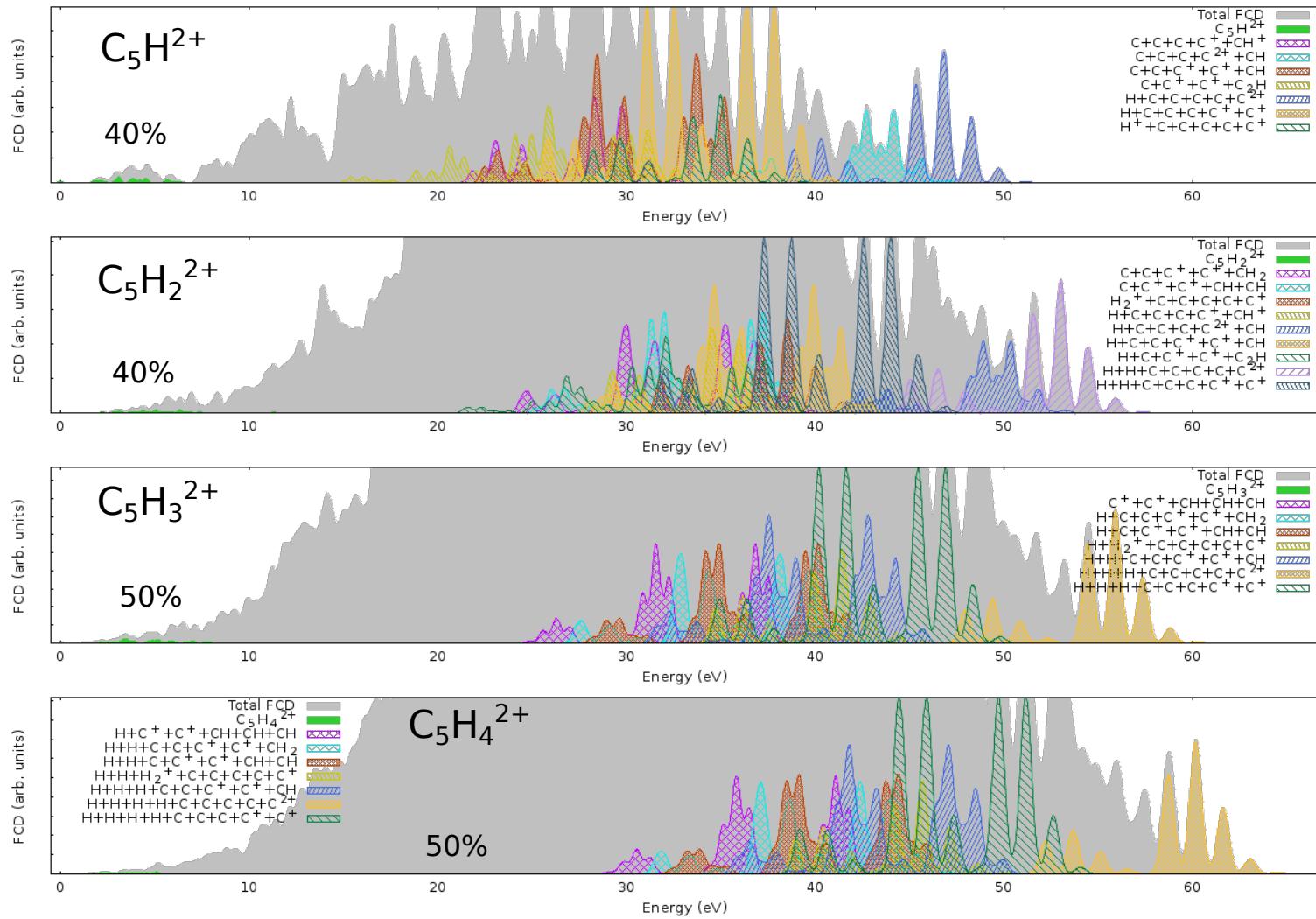


Figure 24: Fragmentation Channel Distribution for C₅H²⁺, C₅H₂²⁺, C₅H₃²⁺ and C₅H₄²⁺. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

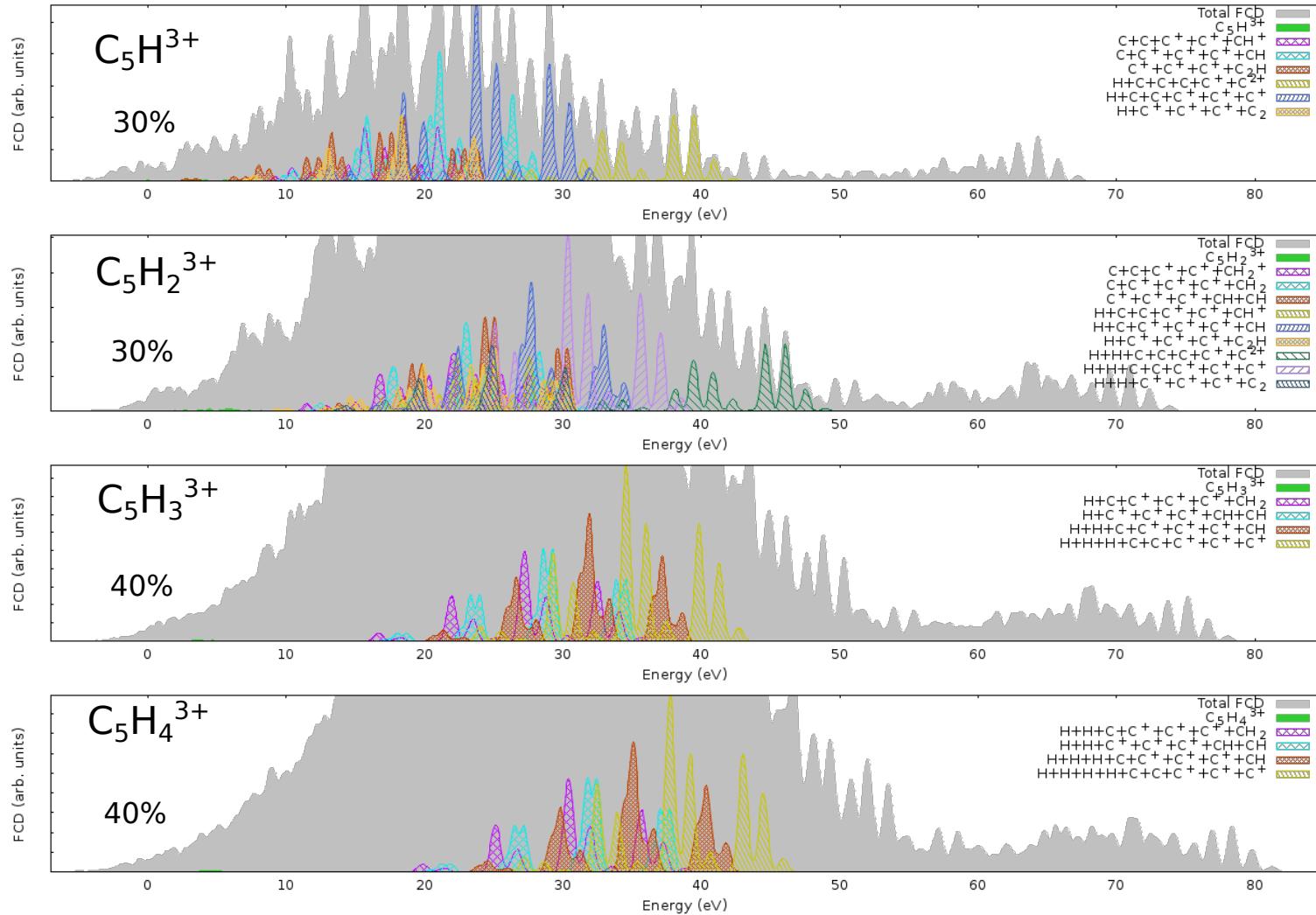


Figure 25: Fragmentation Channel Distribution for C₅H³⁺, C₅H₂³⁺, C₅H₃³⁺ and C₅H₄³⁺. Those channels with a maximum value of the curve below the given percentage of the highest maximum were not included for simplicity (except the channel with 1 fragment).

Isomer's Geometries

Table 3: Geometries of all stable isomers considered in this study and their geometry identifiers

| CH | CH ₂ | CH ₃ | CH ₄ | | |
|-------------------------------|-----------------|-------------------------------|-----------------|---|---|
| | | | | | |
| 1 | 1 | 2 | 1 | 1 | 2 |
| <hr/> | | | | | |
| C ₂ H | | C ₂ H ₂ | | | |
| | | | | | |
| 1 | 2 | 3 | 1 | 2 | 3 |
| C ₂ H ₃ | | C ₂ H ₄ | | | |
| | | | | | |
| 1 | 2 | 1 | 2 | | |
| <hr/> | | | | | |

C₃H



1



2



3

C₃H₂



1



2



3



4



5

C₃H₃



1



2



3



4

C₃H₄



1



2



3



4



5



6

C₄H



1



2



3



4



5



6

C₄H₂



1



2



3



4



5



6



7



8



9

C₄H₃



1



2



3



4



5



6



7



8



9



10



11



12



13



14



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1



2



3



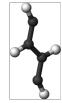
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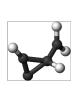
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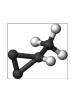
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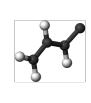
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C₅H



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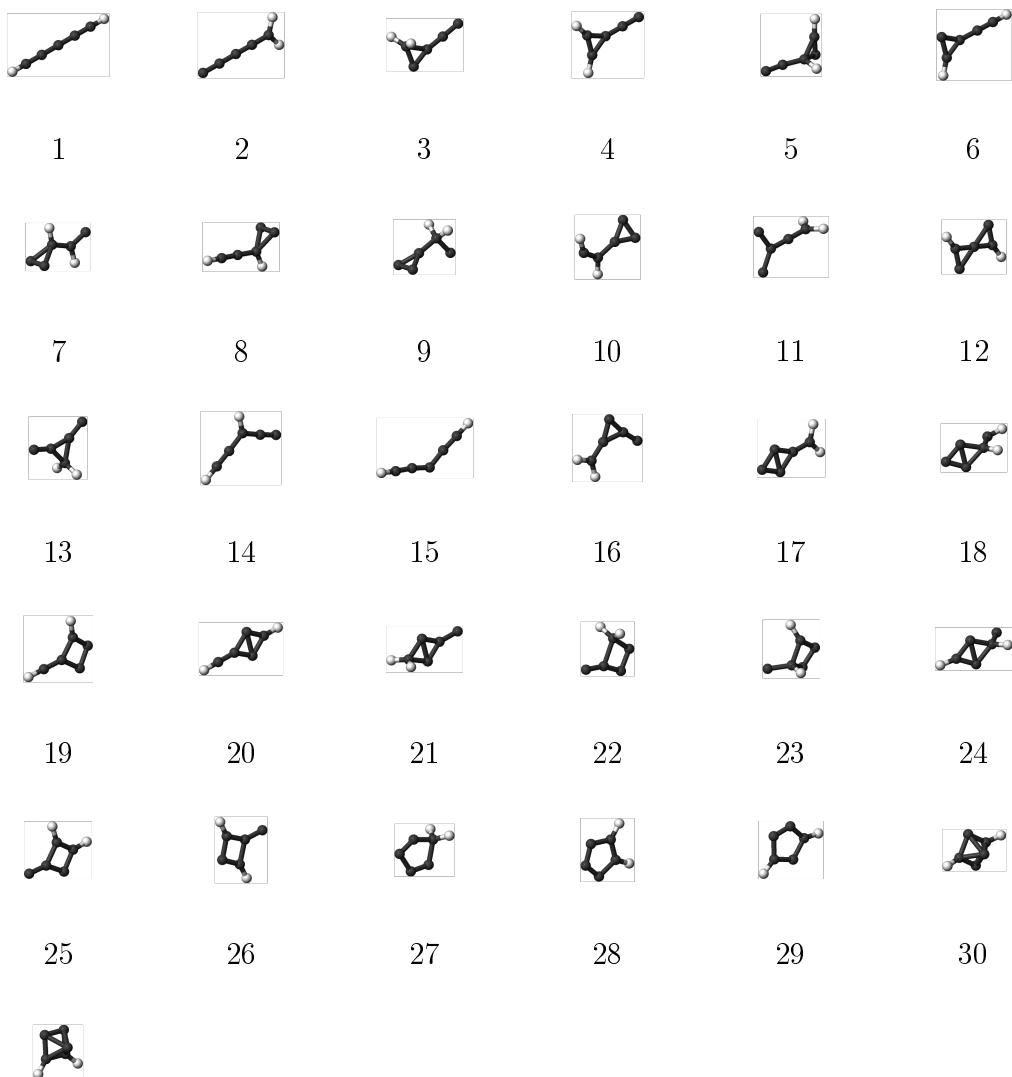
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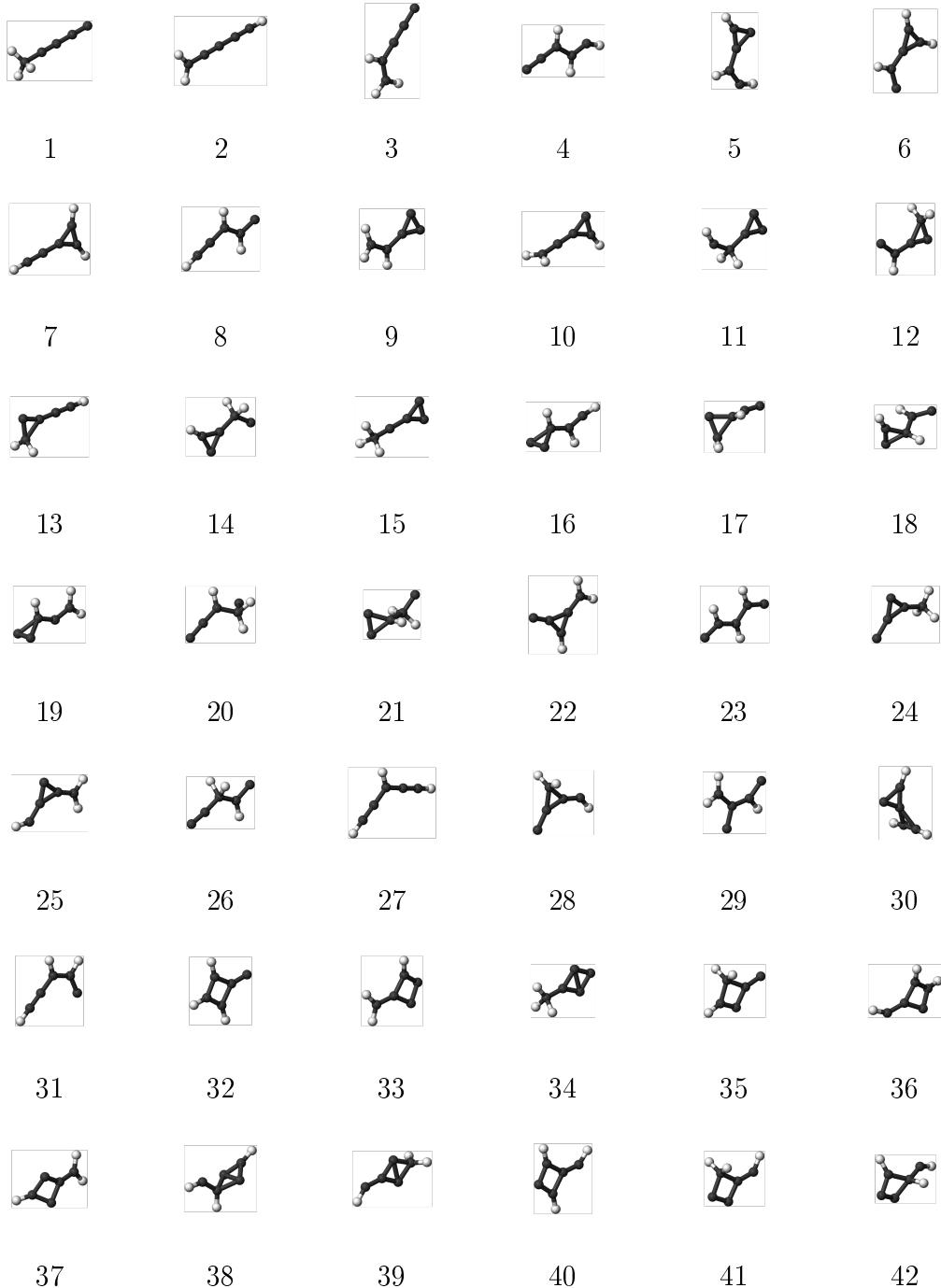
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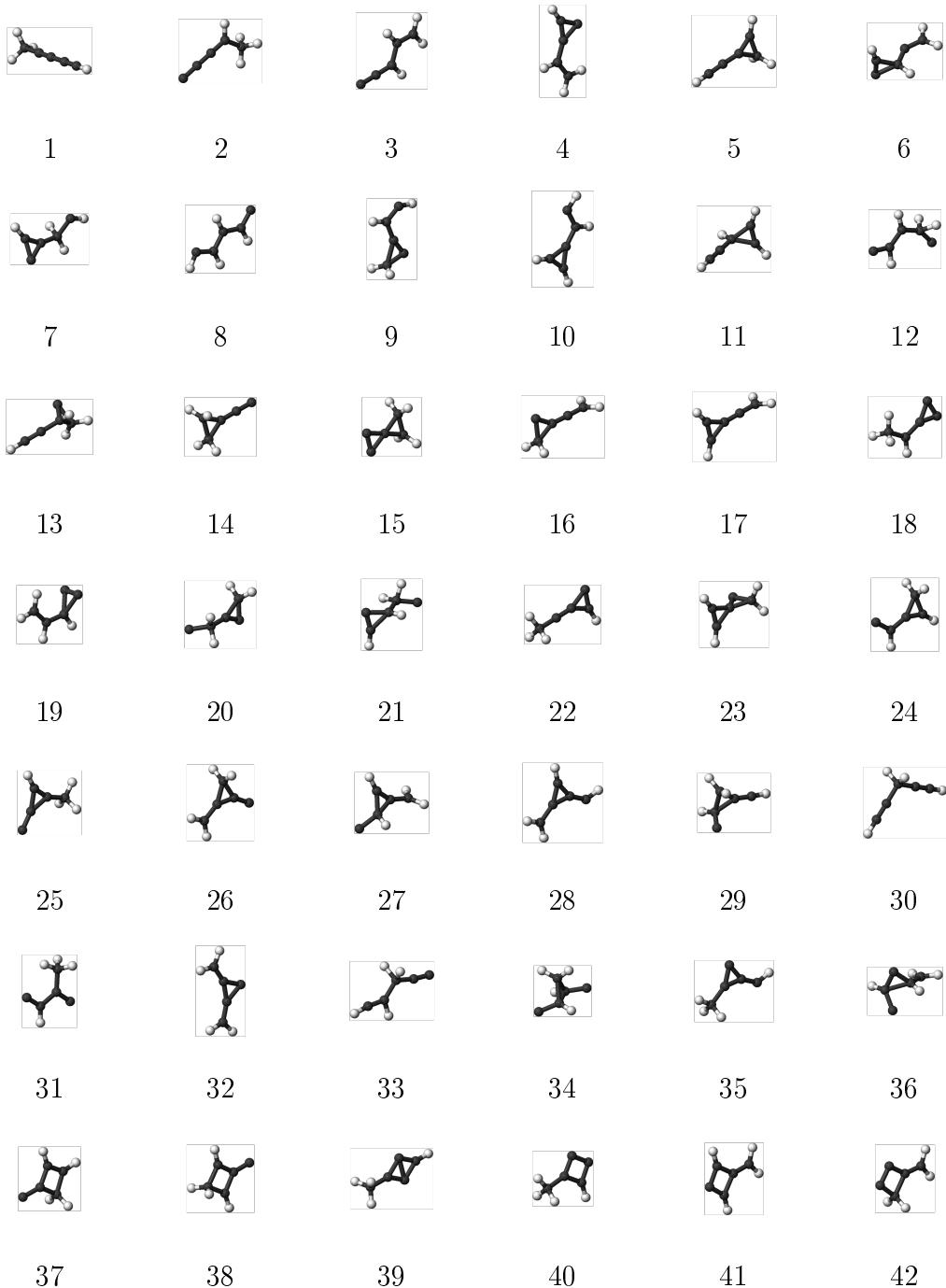
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70



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Total energies

Table 4: Data of energies, ZPE corrections, DFT Stability and T₁ Coefficients for all the structures calculated. The data is in order of increasing energy for each combination of n , m and q available

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|-------------------------------|-------------------|-----------------------|------------|----------|-------------------------|---------------|-------------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| CH | 1 | 2 | 0.000 | -1047.53 | 0.185 | 0.000 | Stable | -1045.154 | 0.000 | 0.760 | 0.012 |
| | 1 | 4 | 0.694 | -1046.61 | 0.194 | 0.918 | Stable | -1044.468 | 0.686 | 3.754 | 0.020 |
| CH ¹⁺ | 1 | 1 | 0.000 | -1036.51 | 0.181 | 0.000 | RHF->UHF | -1034.608 | 0.000 | 0.000 | 0.011 |
| | 1 | 3 | 1.168 | -1035.59 | 0.179 | 0.911 | Stable | -1033.438 | 1.170 | 2.003 | 0.017 |
| CH ²⁺ | Coulomb Explosion | | | | | | | | | | |
| | Coulomb Explosion | | | | | | | | | | |
| CH ³⁺ | Coulomb Explosion | | | | | | | | | | |
| | Coulomb Explosion | | | | | | | | | | |
| CH ₂ | 2 | 3 | 0.000 | -1065.82 | 0.492 | 0.000 | Internal | -1063.289 | 0.000 | 2.017 | 0.012 |
| | 1 | 3 | 0.357 | -1065.61 | 0.598 | 0.203 | Internal | -1063.038 | 0.251 | 2.036 | 0.014 |
| CH ₂ ¹⁺ | 2 | 1 | 0.414 | -1065.33 | 0.467 | 0.488 | RHF->UHF/Internal | -1062.850 | 0.439 | 0.000 | 0.010 |
| | 1 | 1 | 1.903 | -1063.96 | 0.599 | 1.851 | RHF->UHF/Internal | -1061.492 | 1.797 | 0.000 | 0.006 |
| | 2 | 2 | 0.000 | -1055.39 | 0.478 | 0.000 | Stable | -1052.968 | 0.000 | 0.756 | 0.008 |
| | 1 | 2 | 0.233 | -1055.28 | 0.577 | 0.110 | Stable | -1052.834 | 0.134 | 0.763 | 0.009 |
| | 2 | 4 | 3.668 | -1051.52 | 0.408 | 3.874 | Stable | -1049.230 | 3.738 | 3.753 | 0.014 |

| | Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|-------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | | |
| CH ₂ ²⁺ | 1 | 4 | 5.699 | -1049.66 | 0.486 | 5.728 | Stable | -1047.277 | 5.691 | 3.756 | 0.007 | |
| | 1 | 1 | 0.000 | -1033.78 | 0.431 | 0.000 | Stable | -1031.696 | 0.000 | 0.000 | 0.006 | |
| | 2 | 3 | 3.941 | -1030.64 | 0.918 | 3.134 | Stable | -1028.241 | 3.455 | 2.014 | 0.016 | |
| | 1 | 3 | 5.147 | -1029.76 | 1.205 | 4.019 | Stable | -1027.322 | 4.374 | 2.006 | 0.008 | |
| CH ₂ ³⁺ | Coulomb Explosion | | | | | | | | | | | |
| | CH ₃ | 1 | 2 | 0.000 | -1084.59 | 0.888 | 0.000 | Stable | -1081.851 | 0.000 | 0.762 | 0.009 |
| CH ₃ ¹⁺ | 1 | 1 | 0.000 | -1074.68 | 0.873 | 0.000 | Stable | -1072.143 | 0.000 | 0.000 | 0.005 | |
| | 1 | 3 | 3.811 | -1070.96 | 0.815 | 3.722 | Stable | -1068.274 | 3.869 | 2.019 | 0.010 | |
| | CH ₃ ²⁺ | 1 | 2 | 0.000 | -1050.90 | 0.723 | 0.000 | Stable | -1048.311 | 0.000 | 0.759 | 0.008 |
| | 1 | 4 | 3.724 | -1047.09 | 0.606 | 3.810 | Stable | -1044.470 | 3.841 | 3.752 | 0.009 | |
| CH ₃ ³⁺ | Coulomb Explosion | | | | | | | | | | | |
| | CH ₄ | 1 | 1 | 0.000 | -1103.06 | 1.286 | 0.000 | Stable | -1100.238 | 0.000 | 0.000 | 0.008 |
| CH ₄ ¹⁺ | 1 | 3 | 8.442 | -1094.72 | 1.200 | 8.343 | Internal | -1091.710 | 8.528 | 2.017 | 0.014 | |
| | 1 | 2 | 0.000 | -1090.36 | 1.242 | 0.000 | Stable | -1087.396 | 0.000 | 0.758 | 0.009 | |
| | 1 | 4 | 7.743 | -1083.64 | 2.388 | 6.719 | Stable | -1080.799 | 6.597 | 3.760 | 0.020 | |
| | CH ₄ ²⁺ | 2 | 1 | 0.000 | -1070.37 | 1.151 | 0.000 | Stable | -1067.702 | 0.000 | 0.000 | 0.006 |
| <i>(Continues on next page)</i> | | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|--|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 1 | 3 | 0.588 | -3139.71 | 1.007 | 0.373 | Stable | -3132.274 | 0.680 | 2.344 | 0.039 |
| 1 | 1 | 1.686 | -3138.61 | 1.009 | 1.470 | RHF->UHF | -3131.177 | 1.776 | 0.000 | 0.024 |
| 2 | 3 | 1.851 | -3138.27 | 0.972 | 1.811 | Stable | -3130.976 | 1.978 | 2.187 | 0.096 |
| 5 | 3 | 2.245 | -3137.85 | 1.025 | 2.231 | Stable | -3130.634 | 2.319 | 2.052 | 0.023 |
| 4 | 3 | 2.894 | -3136.97 | 0.982 | 3.109 | Stable | -3129.942 | 3.011 | 2.028 | 0.023 |
| 3 | 3 | 2.969 | -3137.06 | 0.896 | 3.021 | Stable | -3129.781 | 3.173 | 2.463 | 0.056 |
| <i>C₃H₂¹⁺</i> | | | | | | | | | | |
| 5 | 2 | 0.000 | -3130.96 | 1.097 | 0.000 | Stable | -3123.883 | 0.000 | 0.767 | 0.019 |
| 1 | 2 | 0.311 | -3130.76 | 0.998 | 0.197 | Stable | -3123.473 | 0.410 | 0.901 | 0.035 |
| 2 | 2 | 1.815 | -3129.19 | 0.953 | 1.768 | Stable | -3121.924 | 1.959 | 1.036 | 0.057 |
| 1 | 4 | 3.007 | -3128.16 | 0.974 | 2.798 | Stable | -3120.753 | 3.130 | 3.954 | 0.033 |
| 2 | 4 | 3.164 | -3127.76 | 0.916 | 3.205 | Stable | -3120.538 | 3.345 | 3.922 | 0.037 |
| 4 | 4 | 4.022 | -3126.80 | 0.969 | 4.161 | Stable | -3119.734 | 4.149 | 3.767 | 0.031 |
| 3 | 4 | 4.501 | -3126.65 | 1.285 | 4.308 | Stable | -3119.570 | 4.313 | 3.995 | 0.042 |
| <i>C₃H₂²⁺</i> | | | | | | | | | | |
| 1 | 1 | 0.000 | -3113.84 | 0.925 | 0.000 | Stable | -3106.915 | 0.000 | 0.000 | 0.025 |
| 1 | 3 | 2.838 | -3111.38 | 0.941 | 2.459 | Stable | -3104.092 | 2.823 | 2.017 | 0.028 |
| 2 | 3 | 3.277 | -3110.79 | 0.889 | 3.056 | Stable | -3103.602 | 3.313 | 2.353 | 0.051 |
| 5 | 3 | 3.563 | -3110.57 | 1.214 | 3.272 | Stable | -3103.641 | 3.274 | 2.082 | 0.030 |
| 2 | 1 | 3.669 | -3110.10 | 0.851 | 3.742 | RHF->UHF | -3103.171 | 3.744 | 0.000 | 0.039 |
| 4 | 3 | 5.294 | -3108.70 | 0.976 | 5.139 | Stable | -3101.671 | 5.244 | 2.090 | 0.032 |
| 4 | 1 | 5.297 | -3108.14 | 0.844 | 5.702 | RHF->UHF | -3101.537 | 5.378 | 0.000 | 0.031 |
| 3 | 1 | 5.538 | -3110.91 | 3.620 | 2.932 | Stable | -3104.071 | 2.844 | 0.000 | 0.039 |
| <i>C₃H₂³⁺</i> | | | | | | | | | | |
| 1 | 2 | 0.000 | -3085.88 | 0.812 | 0.000 | Stable | -3078.867 | 0.000 | 0.757 | 0.025 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|--|-------------------------------|-----------------------|------------|---------|-------------------------|-------------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| | 2 | 0.819 | -3130.57 | 1.654 | 0.638 | Stable | -3123.382 | 0.387 | 0.771 | 0.017 |
| | 3 | 2.398 | -3128.54 | 1.214 | 2.666 | Stable | -3121.364 | 2.405 | 1.178 | 0.061 |
| | 1 | 2.828 | -3128.49 | 1.196 | 2.714 | Stable | -3120.915 | 2.854 | 3.773 | 0.030 |
| | 4 | 3.704 | -3127.47 | 1.228 | 3.735 | Internal | -3120.072 | 3.697 | 3.764 | 0.032 |
| | 3 | 3.933 | -3127.06 | 1.194 | 4.148 | Stable | -3119.808 | 3.961 | 3.760 | 0.039 |
| | 2 | 3.943 | -3127.30 | 1.198 | 3.906 | Stable | -3119.803 | 3.966 | 3.776 | 0.061 |
| | 4 | 4.266 | -3126.80 | 1.275 | 4.410 | Internal | -3119.556 | 4.213 | 1.292 | 0.074 |
| ⁴⁷ C ₃ H ₃ ³⁺ | 1 | 0.000 | -3104.50 | 1.104 | 0.801 | Stable | -3097.306 | 0.896 | 0.000 | 0.059 |
| | 2 | 0.205 | -3105.30 | 2.204 | 0.000 | Stable | -3098.202 | 0.000 | 0.000 | 0.026 |
| | 1 | 0.433 | -3104.17 | 1.122 | 1.131 | Stable | -3096.892 | 1.310 | 2.016 | 0.025 |
| | 3 | 1.523 | -3102.60 | 1.114 | 2.699 | RHF->UHF | -3095.793 | 2.409 | 0.000 | 0.029 |
| | 3 | 2.176 | -3102.34 | 1.110 | 2.956 | Stable | -3095.136 | 3.066 | 2.005 | 0.036 |
| | 4 | 2.520 | -3101.40 | 1.097 | 3.897 | Stable | -3094.779 | 3.422 | 0.000 | 0.031 |
| | 2 | 3.107 | -3102.79 | 2.462 | 2.508 | Stable | -3095.558 | 2.644 | 2.010 | 0.029 |
| | C ₃ H ₄ | | | | | | | | | |
| | 2 | 0.000 | -3175.68 | 1.494 | 0.000 | Internal | -3168.174 | 0.057 | 0.000 | 0.012 |
| | 1 | 0.103 | -3175.60 | 1.655 | 0.082 | Stable | -3168.231 | 0.000 | 0.000 | 0.012 |
| ⁸⁰ | 6 | 1.282 | -3174.57 | 1.825 | 1.112 | Internal | -3167.222 | 1.009 | 0.000 | 0.010 |
| | 2 | 2.371 | -3173.53 | 1.585 | 2.149 | Internal | -3165.894 | 2.338 | 2.121 | 0.027 |
| | 4 | 2.389 | -3173.42 | 1.592 | 2.263 | Internal | -3165.882 | 2.349 | 2.230 | 0.030 |
| | 4 | 2.711 | -3172.96 | 1.557 | 2.714 | RHF->UHF/Internal | -3165.525 | 2.706 | 0.000 | 0.020 |
| | 5 | 3.095 | -3172.63 | 1.718 | 3.050 | RHF->UHF/Internal | -3165.302 | 2.929 | 0.000 | 0.013 |
| | 5 | 3.721 | -3172.06 | 1.703 | 3.621 | Internal | -3164.661 | 3.570 | 2.015 | 0.019 |
| | 6 | 3.833 | -3171.98 | 1.676 | 3.700 | Internal | -3164.522 | 3.709 | 2.015 | 0.018 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---|---|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| C ₃ H ₄ ¹⁺ | 3 | 4.084 | -3171.47 | 1.590 | 4.207 | Internal | -3164.185 | 4.046 | 2.327 | 0.042 | |
| | 1 | 3 | 4.580 | -3171.59 | 1.561 | 4.092 | Internal | -3163.660 | 4.571 | 2.024 | 0.017 |
| | 2 | 2 | 0.000 | -3166.15 | 1.425 | 0.000 | Stable | -3158.497 | 0.000 | 0.852 | 0.031 |
| | 4 | 2 | 1.080 | -3165.10 | 1.593 | 1.055 | Stable | -3157.585 | 0.912 | 1.053 | 0.044 |
| | 6 | 2 | 1.324 | -3165.07 | 1.816 | 1.086 | Stable | -3157.565 | 0.932 | 0.768 | 0.022 |
| | 1 | 2 | 1.831 | -3165.43 | 2.644 | 0.720 | Stable | -3157.885 | 0.612 | 0.762 | 0.019 |
| | 3 | 2 | 2.947 | -3163.16 | 1.589 | 2.998 | Stable | -3155.715 | 2.782 | 0.756 | 0.022 |
| | 2 | 4 | 3.271 | -3162.94 | 1.537 | 3.211 | Stable | -3155.338 | 3.158 | 3.763 | 0.014 |
| | 4 | 4 | 3.404 | -3162.81 | 1.542 | 3.344 | Stable | -3155.209 | 3.287 | 3.772 | 0.022 |
| | 1 | 4 | 4.224 | -3161.95 | 1.536 | 4.207 | Stable | -3154.384 | 4.113 | 3.764 | 0.020 |
| 6 ⁺ | 6 | 4 | 4.230 | -3161.91 | 1.654 | 4.243 | Stable | -3154.496 | 4.000 | 3.796 | 0.018 |
| | 3 | 4 | 4.289 | -3161.70 | 1.596 | 4.454 | Stable | -3154.379 | 4.118 | 3.754 | 0.027 |
| | 5 | 4 | 4.505 | -3161.39 | 1.695 | 4.760 | Stable | -3154.262 | 4.235 | 3.757 | 0.019 |
| | C ₃ H ₄ ²⁺ | | | | | | | | | | |
| | 2 | 1 | 0.000 | -3149.95 | 1.351 | 0.000 | Stable | -3142.354 | 0.000 | 0.000 | 0.027 |
| 7 ⁺ | 6 | 1 | 1.194 | -3148.97 | 1.973 | 0.979 | Internal | -3141.781 | 0.573 | 0.000 | 0.011 |
| | 2 | 3 | 1.727 | -3148.32 | 1.349 | 1.633 | Stable | -3140.625 | 1.730 | 2.012 | 0.030 |
| | 1 | 3 | 2.634 | -3147.68 | 1.562 | 2.274 | Stable | -3139.930 | 2.424 | 2.022 | 0.029 |
| | 1 | 1 | 2.860 | -3147.37 | 1.921 | 2.585 | Stable | -3140.063 | 2.291 | 0.000 | 0.024 |
| | 4 | 3 | 3.101 | -3147.00 | 1.518 | 2.950 | Stable | -3139.420 | 2.935 | 2.011 | 0.025 |
| | 6 | 3 | 3.287 | -3147.06 | 1.732 | 2.889 | Internal | -3139.448 | 2.906 | 2.028 | 0.038 |
| | 5 | 1 | 3.490 | -3146.20 | 1.532 | 3.747 | Stable | -3139.044 | 3.310 | 0.000 | 0.025 |
| | 3 | 1 | 4.454 | -3145.15 | 1.543 | 4.799 | RHF->UHF | -3138.091 | 4.263 | 0.000 | 0.018 |
| | 3 | 3 | 5.239 | -3144.86 | 1.564 | 5.092 | Stable | -3137.328 | 5.026 | 2.123 | 0.038 |
| | <i>(Continues on next page)</i> | | | | | | | | | | |

| | | | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| Geometry | Multiplicity | ΔE_{ZPE} (eV) | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| $C_3H_4^{3+}$ | 5 | 3 | 5.253 | -3144.85 | 1.535 | 5.102 | Internal | -3137.285 | 5.069 | 2.005 | 0.025 |
| | 2 | 2 | 0.000 | -3123.32 | 1.162 | 0.038 | Stable | -3115.847 | 0.070 | 0.760 | 0.028 |
| | 4 | 2 | 0.619 | -3123.36 | 1.851 | 0.000 | Stable | -3115.917 | 0.000 | 0.757 | 0.028 |
| | 1 | 2 | 1.262 | -3122.46 | 1.488 | 0.905 | Stable | -3114.912 | 1.005 | 1.121 | 0.055 |
| | 6 | 2 | 2.171 | -3121.83 | 1.887 | 1.535 | Stable | -3114.401 | 1.516 | 0.786 | 0.028 |
| | 2 | 4 | 2.758 | -3120.65 | 1.017 | 2.714 | Stable | -3112.943 | 2.973 | 3.767 | 0.033 |
| | 1 | 4 | 2.867 | -3120.86 | 1.531 | 2.497 | Stable | -3113.348 | 2.569 | 3.769 | 0.017 |
| | 5 | 2 | 2.938 | -3120.32 | 1.409 | 3.038 | Stable | -3113.156 | 2.761 | 0.778 | 0.027 |
| | 3 | 2 | 3.484 | -3119.96 | 1.487 | 3.398 | Stable | -3112.687 | 3.229 | 0.908 | 0.061 |
| | 4 | 4 | 3.667 | -3120.22 | 1.600 | 3.145 | Stable | -3112.618 | 3.299 | 3.773 | 0.023 |
| C_5H | 3 | 4 | 4.666 | -3118.95 | 1.424 | 4.411 | Stable | -3111.443 | 4.474 | 3.768 | 0.037 |
| | 5 | 4 | 5.382 | -3117.98 | 1.360 | 5.384 | Stable | -3110.663 | 5.254 | 3.758 | 0.031 |
| C_4H | | | | | | | | | | | |
| C_4H | 1 | 2 | 0.000 | -4158.61 | 0.801 | 0.000 | Stable | -4149.003 | 0.000 | 1.248 | 0.059 |
| | 6 | 2 | 1.003 | -4157.22 | 0.865 | 1.388 | Stable | -4148.064 | 0.938 | 0.816 | 0.022 |
| | 3 | 2 | 1.408 | -4157.08 | 0.865 | 1.530 | Stable | -4147.659 | 1.343 | 0.791 | 0.032 |
| | 5 | 2 | 1.938 | -4156.30 | 0.861 | 2.315 | Stable | -4147.126 | 1.877 | 0.826 | 0.037 |
| | 6 | 4 | 2.699 | -4155.57 | 0.842 | 3.041 | Stable | -4146.345 | 2.658 | 3.870 | 0.044 |
| | 1 | 4 | 2.713 | -4155.96 | 0.797 | 2.650 | Stable | -4146.286 | 2.717 | 4.036 | 0.042 |
| | 4 | 4 | 2.932 | -4155.46 | 0.785 | 3.151 | Stable | -4146.055 | 2.947 | 3.836 | 0.034 |
| | 3 | 4 | 3.644 | -4154.93 | 0.856 | 3.683 | Stable | -4145.414 | 3.589 | 3.787 | 0.035 |
| | 2 | 4 | 3.912 | -4154.83 | 1.029 | 3.781 | Stable | -4145.318 | 3.684 | 3.917 | 0.059 |
| C_4H^{1+} | | | | | | | | | | | |
| | 1 | 3 | 0.000 | -4148.57 | 0.784 | 0.000 | Stable | -4138.934 | 0.000 | 2.442 | 0.050 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|-------------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 6 | 1 | 0.139 | -4147.70 | 0.846 | 0.873 | RHF->UHF/Internal | -4138.857 | 0.077 | 0.000 | 0.016 |
| 1 | 1 | 0.524 | -4147.71 | 0.782 | 0.863 | RHF->UHF | -4138.408 | 0.526 | 0.000 | 0.027 |
| 5 | 1 | 1.240 | -4146.68 | 0.869 | 1.893 | RHF->UHF/Internal | -4137.779 | 1.155 | 0.000 | 0.016 |
| 3 | 1 | 1.327 | -4146.74 | 0.861 | 1.836 | RHF->UHF | -4137.684 | 1.250 | 0.000 | 0.038 |
| 5 | 3 | 1.366 | -4146.84 | 0.918 | 1.734 | Internal | -4137.703 | 1.231 | 2.095 | 0.033 |
| 3 | 3 | 1.405 | -4146.97 | 0.886 | 1.600 | Stable | -4137.631 | 1.303 | 2.051 | 0.038 |
| 4 | 3 | 1.757 | -4146.60 | 0.821 | 1.968 | Internal | -4137.214 | 1.720 | 2.157 | 0.034 |
| C₄H²⁺ | | | | | | | | | | |
| 1 | 4 | 0.000 | -4131.30 | 0.818 | 0.000 | Internal | -4121.752 | 0.000 | 4.241 | 0.048 |
| 1 | 2 | 0.296 | -4130.60 | 0.734 | 0.699 | Internal | -4121.372 | 0.380 | 0.950 | 0.042 |
| 6 | 2 | 0.594 | -4130.10 | 0.842 | 1.203 | Internal | -4121.182 | 0.570 | 0.794 | 0.028 |
| 3 | 2 | 1.268 | -4129.50 | 0.846 | 1.807 | Internal | -4120.512 | 1.240 | 0.796 | 0.036 |
| 5 | 2 | 1.436 | -4128.75 | 0.905 | 2.557 | Internal | -4120.403 | 1.349 | 0.767 | 0.027 |
| 4 | 4 | 1.452 | -4129.61 | 0.794 | 1.693 | Internal | -4120.276 | 1.476 | 3.897 | 0.037 |
| 4 | 2 | 1.763 | -4128.96 | 0.771 | 2.340 | Internal | -4119.942 | 1.810 | 1.085 | 0.088 |
| 5 | 4 | 2.337 | -4128.50 | 0.815 | 2.804 | Internal | -4119.412 | 2.340 | 3.784 | 0.027 |
| 2 | 2 | 2.780 | -4127.90 | 0.720 | 3.400 | Internal | -4118.874 | 2.878 | 1.036 | 0.057 |
| 2 | 4 | 2.874 | -4128.21 | 0.728 | 3.094 | Internal | -4118.787 | 2.965 | 3.962 | 0.048 |
| C₄H³⁺ | | | | | | | | | | |
| 1 | 1 | 0.000 | -4105.94 | 0.709 | 0.000 | RHF->UHF | -4097.390 | 0.000 | 0.000 | 0.026 |
| 1 | 3 | 0.981 | -4105.73 | 0.735 | 0.213 | Stable | -4096.435 | 0.955 | 2.402 | 0.060 |
| 5 | 1 | 2.568 | -4103.22 | 0.816 | 2.717 | RHF->UHF/Internal | -4094.929 | 2.461 | 0.000 | 0.018 |
| 4 | 3 | 2.699 | -4103.85 | 0.740 | 2.088 | Internal | -4094.722 | 2.668 | 2.430 | 0.054 |
| 6 | 3 | 3.037 | -4103.31 | 0.777 | 2.635 | Internal | -4094.421 | 2.969 | 2.109 | 0.027 |
| 2 | 1 | 3.172 | -4102.85 | 0.898 | 3.095 | RHF->UHF/Internal | -4094.407 | 2.984 | 0.000 | 0.049 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|--|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 2 | 1 | 3.242 | -4209.70 | 2.541 | 2.474 | RHF->UHF | -4199.812 | 2.691 | 0.000 | 0.020 | |
| 5 | 3 | 3.286 | -4208.94 | 1.901 | 3.231 | Stable | -4199.129 | 3.374 | 2.204 | 0.031 | |
| 14 | 3 | 3.297 | -4209.25 | 2.413 | 2.920 | Stable | -4199.629 | 2.873 | 2.233 | 0.031 | |
| 1 | 3 | 3.515 | -4208.55 | 1.816 | 3.621 | Stable | -4198.814 | 3.688 | 2.169 | 0.044 | |
| 3 | 3 | 3.722 | -4208.38 | 1.858 | 3.799 | Stable | -4198.649 | 3.853 | 2.037 | 0.018 | |
| 16 | 3 | 3.791 | -4208.09 | 1.821 | 4.087 | Stable | -4198.543 | 3.960 | 2.011 | 0.017 | |
| 12 | 3 | 3.812 | -4208.34 | 1.747 | 3.833 | Stable | -4198.449 | 4.054 | 2.283 | 0.037 | |
| 7 | 1 | 3.914 | -4208.19 | 1.961 | 3.980 | RHF->UHF | -4198.560 | 3.943 | 0.000 | 0.015 | |
| 18 | 3 | 3.962 | -4208.18 | 1.963 | 3.992 | Stable | -4198.514 | 3.988 | 2.022 | 0.018 | |
| 11 | 3 | 3.979 | -4208.06 | 1.736 | 4.111 | Stable | -4198.271 | 4.232 | 2.180 | 0.024 | |
| 8 | 3 | 4.155 | -4207.93 | 1.878 | 4.242 | Stable | -4198.236 | 4.266 | 2.142 | 0.030 | |
| C₄H₄¹⁺ | 17 | 3 | 4.228 | -4207.77 | 1.884 | 4.401 | Stable | -4198.170 | 4.333 | 2.026 | 0.020 |
| | 9 | 3 | 4.508 | -4207.33 | 1.816 | 4.841 | Stable | -4197.821 | 4.682 | 2.038 | 0.041 |
| | 10 | 3 | 5.459 | -4206.52 | 1.719 | 5.652 | Stable | -4196.773 | 5.729 | 2.181 | 0.033 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 7 | 2 | 2.422 | -4200.84 | 2.149 | 2.370 | Internal | -4191.191 | 2.266 | 0.844 | 0.023 |
| 1 | 2 | 2.822 | -4200.27 | 1.804 | 2.941 | Stable | -4190.446 | 3.011 | 0.917 | 0.059 |
| 17 | 2 | 2.865 | -4200.09 | 1.927 | 3.122 | Internal | -4190.526 | 2.931 | 0.763 | 0.019 |
| 19 | 4 | 2.961 | -4200.09 | 1.465 | 3.120 | Internal | -4189.968 | 3.489 | 3.796 | 0.026 |
| 7 | 4 | 3.118 | -4200.02 | 1.716 | 3.193 | Internal | -4190.062 | 3.395 | 3.974 | 0.029 |
| 5 | 2 | 3.157 | -4199.86 | 1.887 | 3.350 | Internal | -4190.194 | 3.262 | 0.853 | 0.026 |
| 4 | 4 | 3.161 | -4200.04 | 1.709 | 3.174 | Internal | -4190.012 | 3.444 | 3.950 | 0.032 |
| 11 | 2 | 3.163 | -4199.77 | 1.904 | 3.435 | Stable | -4190.205 | 3.252 | 0.869 | 0.063 |
| 6 | 4 | 3.510 | -4199.58 | 1.697 | 3.631 | Internal | -4189.650 | 3.806 | 3.912 | 0.028 |
| 12 | 4 | 3.708 | -4199.22 | 1.751 | 3.985 | Stable | -4189.508 | 3.949 | 3.978 | 0.033 |
| 13 | 4 | 3.744 | -4199.43 | 1.919 | 3.779 | Stable | -4189.639 | 3.817 | 3.776 | 0.031 |
| 15 | 4 | 3.752 | -4199.29 | 1.813 | 3.919 | Stable | -4189.525 | 3.931 | 3.773 | 0.022 |
| 14 | 4 | 3.900 | -4199.10 | 1.796 | 4.109 | Stable | -4189.360 | 4.097 | 3.771 | 0.026 |
| 16 | 4 | 4.214 | -4198.71 | 1.806 | 4.496 | Internal | -4189.056 | 4.401 | 3.762 | 0.021 |
| 1 | 4 | 4.548 | -4198.44 | 1.770 | 4.768 | Stable | -4188.686 | 4.771 | 3.906 | 0.032 |
| 17 | 4 | 4.579 | -4198.30 | 1.885 | 4.913 | Internal | -4188.770 | 4.687 | 3.829 | 0.022 |
| 2 | 4 | 4.620 | -4199.46 | 2.556 | 3.751 | Internal | -4189.400 | 4.057 | 3.925 | 0.030 |
| 10 | 2 | 4.673 | -4198.62 | 2.000 | 4.586 | Stable | -4188.791 | 4.665 | 0.978 | 0.049 |
| 8 | 4 | 4.913 | -4198.14 | 1.818 | 5.067 | Internal | -4188.369 | 5.087 | 3.779 | 0.024 |
| 9 | 4 | 5.300 | -4197.52 | 1.785 | 5.691 | Internal | -4187.949 | 5.507 | 3.768 | 0.029 |
| 3 | 4 | 5.325 | -4197.55 | 1.818 | 5.656 | Internal | -4187.956 | 5.500 | 4.029 | 0.038 |
| 11 | 4 | 5.530 | -4197.52 | 1.756 | 5.685 | Stable | -4187.690 | 5.767 | 3.911 | 0.054 |
| 16 | 2 | 6.182 | -4196.71 | 1.761 | 6.500 | Internal | -4187.043 | 6.414 | 0.869 | 0.030 |
| 10 | 4 | 6.203 | -4196.89 | 1.719 | 6.315 | Stable | -4186.981 | 6.476 | 3.960 | 0.040 |
| 5 | 4 | 7.238 | -4197.34 | 3.796 | 5.868 | Internal | -4188.022 | 5.435 | 3.809 | 0.256 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|--|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 13 | 3 | 4.103 | -5208.52 | 1.319 | 4.735 | Stable | -5197.001 | 4.207 | 2.149 | 0.047 |
| 31 | 3 | 4.231 | -5208.44 | 1.510 | 4.809 | Stable | -5197.064 | 4.144 | 2.028 | 0.032 |
| 18 | 1 | 4.256 | -5208.27 | 1.285 | 4.985 | RHF->UHF | -5196.814 | 4.394 | 0.000 | 0.019 |
| 22 | 3 | 4.365 | -5208.33 | 1.320 | 4.925 | Stable | -5196.739 | 4.469 | 2.115 | 0.031 |
| 24 | 3 | 4.789 | -5207.89 | 1.322 | 5.361 | Stable | -5196.318 | 4.890 | 2.147 | 0.032 |
| 7 | 3 | 4.944 | -5207.73 | 1.277 | 5.522 | Stable | -5196.118 | 5.090 | 2.313 | 0.066 |
| 9 | 3 | 5.129 | -5207.72 | 1.294 | 5.531 | Stable | -5195.950 | 5.258 | 2.063 | 0.024 |
| 23 | 3 | 5.620 | -5207.17 | 1.343 | 6.082 | Stable | -5195.507 | 5.700 | 2.140 | 0.034 |
| C₅H₂¹⁺ | | | | | | | | | | |
| 1 | 2 | 0.000 | -5204.96 | 1.354 | 0.000 | Stable | -5192.794 | 0.000 | 1.095 | 0.042 |
| 6 | 2 | 0.446 | -5204.23 | 1.425 | 0.725 | Internal | -5192.419 | 0.375 | 0.830 | 0.028 |
| 4 | 2 | 1.307 | -5203.35 | 1.527 | 1.604 | Internal | -5191.660 | 1.134 | 1.224 | 0.046 |
| 2 | 2 | 1.596 | -5203.36 | 1.278 | 1.593 | Stable | -5191.122 | 1.672 | 1.456 | 0.056 |
| 20 | 2 | 1.702 | -5202.83 | 1.483 | 2.122 | Stable | -5191.221 | 1.573 | 1.042 | 0.039 |
| 29 | 2 | 2.056 | -5202.42 | 1.553 | 2.541 | Internal | -5190.938 | 1.856 | 0.876 | 0.033 |
| 28 | 2 | 2.198 | -5202.11 | 1.419 | 2.844 | Internal | -5190.662 | 2.132 | 0.783 | 0.021 |
| 17 | 2 | 2.215 | -5202.25 | 1.406 | 2.703 | Stable | -5190.631 | 2.163 | 1.087 | 0.046 |
| 1 | 4 | 2.222 | -5202.91 | 1.332 | 2.050 | Stable | -5190.550 | 2.244 | 4.146 | 0.042 |
| 12 | 2 | 2.625 | -5201.88 | 1.385 | 3.076 | Stable | -5190.200 | 2.594 | 0.777 | 0.021 |
| 14 | 2 | 2.840 | -5202.63 | 2.103 | 2.331 | Stable | -5190.704 | 2.090 | 1.656 | 0.060 |
| 2 | 4 | 2.859 | -5202.06 | 1.290 | 2.898 | Stable | -5189.871 | 2.923 | 4.342 | 0.047 |
| 25 | 2 | 3.332 | -5201.15 | 1.435 | 3.809 | Internal | -5189.543 | 3.251 | 1.072 | 0.047 |
| 29 | 4 | 3.429 | -5201.06 | 1.301 | 3.898 | Internal | -5189.312 | 3.482 | 4.632 | 0.051 |
| 30 | 2 | 3.538 | -5200.54 | 1.568 | 4.414 | Internal | -5189.470 | 3.324 | 0.894 | 0.037 |
| 28 | 4 | 3.598 | -5200.93 | 1.305 | 4.028 | Internal | -5189.147 | 3.647 | 4.669 | 0.050 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 26 | 2 | 3.628 | -5200.85 | 1.430 | 4.107 | Internal | -5189.241 | 3.552 | 1.039 | 0.043 |
| 27 | 2 | 3.660 | -5200.69 | 1.457 | 4.267 | Internal | -5189.238 | 3.556 | 0.843 | 0.036 |
| 21 | 2 | 3.782 | -5200.48 | 1.383 | 4.474 | Internal | -5189.041 | 3.753 | 0.780 | 0.021 |
| 31 | 2 | 3.865 | -5200.21 | 1.600 | 4.742 | Internal | -5189.175 | 3.619 | 0.795 | 0.036 |
| 24 | 2 | 3.947 | -5200.30 | 1.367 | 4.657 | Internal | -5188.860 | 3.934 | 0.771 | 0.021 |
| 10 | 4 | 3.965 | -5200.52 | 1.308 | 4.434 | Stable | -5188.783 | 4.011 | 3.912 | 0.033 |
| 20 | 4 | 4.007 | -5200.43 | 1.332 | 4.529 | Stable | -5188.766 | 4.028 | 3.883 | 0.035 |
| 4 | 4 | 4.138 | -5200.69 | 1.528 | 4.269 | Internal | -5188.830 | 3.964 | 3.865 | 0.032 |
| 12 | 4 | 4.216 | -5200.24 | 1.378 | 4.716 | Stable | -5188.602 | 4.192 | 4.125 | 0.040 |
| 17 | 4 | 4.286 | -5200.23 | 1.333 | 4.724 | Stable | -5188.487 | 4.307 | 3.871 | 0.035 |
| 14 | 4 | 4.342 | -5200.96 | 1.793 | 3.999 | Stable | -5188.891 | 3.903 | 4.297 | 0.054 |
| 19 | 4 | 4.343 | -5200.28 | 1.377 | 4.672 | Stable | -5188.475 | 4.319 | 4.194 | 0.047 |
| 27 | 4 | 4.369 | -5200.07 | 1.428 | 4.889 | Internal | -5188.499 | 4.295 | 3.986 | 0.042 |
| 6 | 4 | 4.452 | -5200.73 | 1.745 | 4.224 | Internal | -5188.733 | 4.061 | 4.398 | 0.054 |
| 21 | 4 | 4.577 | -5199.58 | 1.389 | 5.375 | Internal | -5188.253 | 4.541 | 3.791 | 0.022 |
| 26 | 4 | 4.606 | -5199.94 | 1.382 | 5.012 | Internal | -5188.216 | 4.578 | 3.840 | 0.035 |
| 25 | 4 | 4.628 | -5199.80 | 1.279 | 5.153 | Internal | -5188.092 | 4.702 | 3.822 | 0.032 |
| 5 | 2 | 4.812 | -5200.41 | 1.414 | 4.546 | Internal | -5188.042 | 4.752 | 1.119 | 0.185 |
| 18 | 4 | 4.988 | -5199.37 | 1.332 | 5.584 | Stable | -5187.784 | 5.010 | 3.815 | 0.029 |
| 13 | 2 | 5.002 | -5199.56 | 1.359 | 5.400 | Stable | -5187.797 | 4.997 | 0.906 | 0.033 |
| 3 | 4 | 5.189 | -5199.95 | 1.778 | 5.008 | Internal | -5188.029 | 4.765 | 4.255 | 0.044 |
| 16 | 4 | 5.200 | -5199.48 | 1.397 | 5.476 | Stable | -5187.637 | 5.157 | 4.093 | 0.050 |
| 31 | 4 | 5.257 | -5199.10 | 1.516 | 5.856 | Internal | -5187.699 | 5.094 | 3.781 | 0.019 |
| 22 | 4 | 5.600 | -5198.86 | 1.290 | 6.096 | Internal | -5187.131 | 5.663 | 4.150 | 0.048 |
| 5 | 4 | 5.831 | -5198.94 | 1.424 | 6.019 | Internal | -5187.033 | 5.761 | 4.260 | 0.064 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 48 | 4 | 3.771 | -5226.96 | 1.630 | 4.055 | Internal | -5214.987 | 3.786 | 3.977 | 0.048 |
| 32 | 4 | 3.963 | -5226.76 | 1.672 | 4.247 | Internal | -5214.837 | 3.937 | 3.864 | 0.042 |
| 18 | 2 | 3.963 | -5226.69 | 1.714 | 4.319 | Internal | -5214.878 | 3.896 | 0.945 | 0.033 |
| 47 | 4 | 3.976 | -5226.83 | 1.631 | 4.179 | Internal | -5214.783 | 3.991 | 4.434 | 0.093 |
| 4 | 4 | 3.980 | -5226.76 | 1.628 | 4.253 | Internal | -5214.776 | 3.998 | 4.490 | 0.051 |
| 12 | 2 | 3.997 | -5226.69 | 1.691 | 4.325 | Internal | -5214.822 | 3.952 | 1.234 | 0.053 |
| 22 | 4 | 4.015 | -5226.81 | 1.601 | 4.201 | Internal | -5214.714 | 4.060 | 4.401 | 0.054 |
| 37 | 4 | 4.018 | -5226.53 | 1.620 | 4.478 | Internal | -5214.730 | 4.044 | 4.306 | 0.046 |
| 39 | 2 | 4.022 | -5227.08 | 2.167 | 3.932 | Internal | -5215.273 | 3.501 | 0.911 | 0.028 |
| 46 | 2 | 4.028 | -5226.61 | 1.752 | 4.398 | Internal | -5214.852 | 3.922 | 1.032 | 0.041 |
| 3 | 4 | 4.038 | -5227.58 | 2.431 | 3.436 | Internal | -5215.520 | 3.253 | 4.396 | 0.043 |
| 25 | 4 | 4.061 | -5226.88 | 1.710 | 4.134 | Internal | -5214.776 | 3.997 | 4.081 | 0.036 |
| 27 | 4 | 4.087 | -5226.97 | 1.764 | 4.046 | Internal | -5214.805 | 3.969 | 4.121 | 0.036 |
| 23 | 2 | 4.090 | -5226.58 | 1.561 | 4.431 | Internal | -5214.599 | 4.175 | 1.309 | 0.054 |
| 38 | 2 | 4.209 | -5226.27 | 1.694 | 4.745 | Internal | -5214.613 | 4.160 | 0.786 | 0.042 |
| 39 | 4 | 4.218 | -5226.39 | 1.681 | 4.621 | Internal | -5214.591 | 4.182 | 3.943 | 0.026 |
| 25 | 2 | 4.351 | -5228.24 | 3.549 | 2.772 | Internal | -5216.326 | 2.448 | 1.141 | 0.043 |
| 5 | 4 | 4.381 | -5226.50 | 1.713 | 4.515 | Internal | -5214.460 | 4.313 | 3.983 | 0.028 |
| 1 | 4 | 4.417 | -5226.60 | 1.656 | 4.410 | Stable | -5214.367 | 4.406 | 4.020 | 0.036 |
| 10 | 4 | 4.490 | -5226.48 | 1.698 | 4.530 | Stable | -5214.336 | 4.438 | 3.861 | 0.025 |
| 9 | 4 | 4.493 | -5226.22 | 1.655 | 4.791 | Internal | -5214.290 | 4.483 | 4.063 | 0.042 |
| 34 | 4 | 4.493 | -5226.04 | 1.675 | 4.972 | Internal | -5214.309 | 4.464 | 3.866 | 0.038 |
| 31 | 4 | 4.578 | -5226.97 | 2.593 | 4.040 | Internal | -5215.143 | 3.630 | 4.203 | 0.040 |
| 14 | 2 | 4.599 | -5226.04 | 1.700 | 4.970 | Internal | -5214.228 | 4.545 | 0.860 | 0.030 |
| 38 | 4 | 4.673 | -5225.79 | 1.673 | 5.222 | Internal | -5214.127 | 4.646 | 3.893 | 0.028 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|-------------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 34 | 1 | 3.693 | -5219.08 | 1.707 | 4.251 | RHF->UHF/Internal | -5207.605 | 3.856 | 0.000 | 0.016 |
| 6 | 3 | 3.708 | -5219.45 | 1.821 | 3.879 | Internal | -5207.704 | 3.757 | 2.365 | 0.037 |
| 37 | 3 | 3.715 | -5219.38 | 1.696 | 3.957 | Internal | -5207.572 | 3.889 | 2.117 | 0.031 |
| 36 | 3 | 3.740 | -5219.56 | 1.825 | 3.770 | Internal | -5207.675 | 3.786 | 2.526 | 0.047 |
| 52 | 1 | 3.874 | -5219.01 | 1.950 | 4.319 | Internal | -5207.667 | 3.794 | 0.000 | 0.024 |
| 39 | 3 | 3.886 | -5219.14 | 1.736 | 4.197 | Internal | -5207.441 | 4.020 | 2.059 | 0.021 |
| 33 | 3 | 4.040 | -5219.19 | 1.738 | 4.143 | Internal | -5207.289 | 4.171 | 2.378 | 0.045 |
| 40 | 3 | 4.044 | -5219.20 | 1.778 | 4.128 | Internal | -5207.325 | 4.135 | 2.377 | 0.039 |
| 32 | 3 | 4.197 | -5218.93 | 1.675 | 4.398 | Internal | -5207.069 | 4.392 | 2.069 | 0.028 |
| 43 | 1 | 4.237 | -5218.75 | 1.887 | 4.580 | Internal | -5207.241 | 4.220 | 0.000 | 0.021 |
| 38 | 3 | 4.251 | -5218.63 | 1.699 | 4.700 | Internal | -5207.038 | 4.423 | 2.030 | 0.019 |
| 48 | 3 | 4.266 | -5218.60 | 1.653 | 4.734 | Internal | -5206.978 | 4.483 | 2.112 | 0.031 |
| 35 | 1 | 4.393 | -5218.89 | 2.090 | 4.440 | RHF->UHF/Internal | -5207.287 | 4.173 | 0.000 | 0.015 |
| 39 | 1 | 4.396 | -5218.55 | 1.717 | 4.784 | RHF->UHF/Internal | -5206.912 | 4.549 | 0.000 | 0.020 |
| 34 | 3 | 4.455 | -5218.55 | 1.731 | 4.783 | Internal | -5206.867 | 4.594 | 2.087 | 0.027 |
| 47 | 3 | 4.475 | -5218.38 | 1.645 | 4.949 | Internal | -5206.762 | 4.699 | 2.073 | 0.031 |
| 23 | 1 | 4.622 | -5218.34 | 1.559 | 4.993 | Stable | -5206.528 | 4.932 | 0.000 | 0.019 |
| 1 | 1 | 4.639 | -5219.27 | 2.312 | 4.058 | RHF->UHF | -5207.264 | 4.197 | 0.000 | 0.023 |
| 13 | 3 | 4.692 | -5219.80 | 2.773 | 3.528 | Stable | -5207.673 | 3.788 | 2.279 | 0.038 |
| 51 | 3 | 4.715 | -5218.24 | 1.911 | 5.089 | Internal | -5206.786 | 4.674 | 2.029 | 0.019 |
| 27 | 3 | 4.718 | -5220.72 | 3.517 | 2.609 | Internal | -5208.391 | 3.070 | 2.486 | 0.043 |
| 3 | 3 | 4.739 | -5219.08 | 2.060 | 4.256 | Internal | -5206.912 | 4.549 | 2.809 | 0.055 |
| 24 | 1 | 4.970 | -5217.98 | 1.707 | 5.349 | RHF->UHF/Internal | -5206.328 | 5.133 | 0.000 | 0.033 |
| 30 | 1 | 4.983 | -5218.86 | 2.588 | 4.476 | Internal | -5207.195 | 4.266 | 0.000 | 0.015 |
| 46 | 1 | 5.084 | -5217.80 | 1.736 | 5.532 | Internal | -5206.243 | 5.218 | 0.000 | 0.034 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 7 | 2 | 0.041 | -5207.30 | 1.839 | 0.233 | Internal | -5195.301 | 0.000 | 0.801 | 0.026 | |
| 10 | 2 | 1.238 | -5205.98 | 1.674 | 1.549 | Internal | -5193.939 | 1.362 | 0.792 | 0.029 | |
| 37 | 2 | 1.526 | -5205.30 | 1.692 | 2.234 | Internal | -5193.668 | 1.632 | 0.804 | 0.021 | |
| 5 | 2 | 1.742 | -5205.45 | 1.941 | 2.079 | Internal | -5193.701 | 1.600 | 0.790 | 0.024 | |
| 2 | 4 | 2.103 | -5205.51 | 1.593 | 2.018 | Internal | -5192.992 | 2.308 | 4.052 | 0.047 | |
| 6 | 2 | 2.282 | -5204.74 | 1.800 | 2.787 | Internal | -5193.021 | 2.279 | 1.040 | 0.041 | |
| 50 | 2 | 2.357 | -5204.60 | 1.865 | 2.932 | Internal | -5193.010 | 2.290 | 1.033 | 0.044 | |
| 40 | 2 | 2.541 | -5204.42 | 1.754 | 3.110 | Internal | -5192.715 | 2.585 | 0.822 | 0.029 | |
| 32 | 2 | 2.640 | -5204.31 | 1.803 | 3.224 | Internal | -5192.665 | 2.635 | 0.805 | 0.021 | |
| 49 | 2 | 2.743 | -5204.13 | 1.630 | 3.403 | Internal | -5192.389 | 2.912 | 1.382 | 0.053 | |
| 48 | 2 | 2.757 | -5204.20 | 1.859 | 3.335 | Internal | -5192.604 | 2.696 | 1.069 | 0.044 | |
| 81 | 50 | 4 | 2.860 | -5204.19 | 1.738 | 3.346 | Internal | -5192.380 | 2.921 | 3.838 | 0.030 |
| | 27 | 2 | 2.865 | -5206.17 | 3.271 | 1.363 | Internal | -5193.909 | 1.392 | 0.913 | 0.039 |
| | 10 | 4 | 3.049 | -5204.21 | 1.644 | 3.325 | Internal | -5192.098 | 3.203 | 3.834 | 0.027 |
| | 27 | 4 | 3.058 | -5204.75 | 2.067 | 2.781 | Internal | -5192.511 | 2.789 | 4.079 | 0.038 |
| | 47 | 2 | 3.229 | -5203.56 | 1.737 | 3.971 | Internal | -5192.010 | 3.291 | 0.814 | 0.028 |
| | 8 | 2 | 3.247 | -5203.93 | 1.877 | 3.601 | Internal | -5192.133 | 3.168 | 1.246 | 0.174 |
| | 36 | 4 | 3.297 | -5203.79 | 1.729 | 3.738 | Internal | -5191.935 | 3.365 | 3.793 | 0.023 |
| | 39 | 2 | 3.350 | -5203.54 | 1.693 | 3.996 | Internal | -5191.846 | 3.455 | 0.771 | 0.023 |
| | 40 | 4 | 3.357 | -5203.58 | 1.602 | 3.948 | Internal | -5191.748 | 3.553 | 3.850 | 0.023 |
| | 49 | 4 | 3.375 | -5203.58 | 1.617 | 3.949 | Internal | -5191.745 | 3.556 | 3.807 | 0.042 |
| | 1 | 4 | 3.422 | -5204.06 | 1.626 | 3.471 | Internal | -5191.707 | 3.594 | 4.156 | 0.040 |
| | 30 | 2 | 3.445 | -5204.28 | 2.578 | 3.248 | Internal | -5192.635 | 2.665 | 0.770 | 0.018 |
| | 38 | 2 | 3.457 | -5203.28 | 1.695 | 4.249 | Internal | -5191.741 | 3.560 | 0.799 | 0.025 |
| | 5 | 4 | 3.469 | -5203.58 | 1.664 | 3.948 | Internal | -5191.698 | 3.603 | 3.782 | 0.018 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|-------------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 68 | 70 | 1 | 3.638 | -5244.38 | 2.106 | 4.220 | Internal | -5233.017 | 3.548 | 0.000 | 0.014 |
| | 10 | 3 | 3.649 | -5245.15 | 2.116 | 3.452 | Internal | -5233.016 | 3.549 | 2.188 | 0.025 |
| | 42 | 3 | 3.706 | -5244.68 | 1.987 | 3.917 | Internal | -5232.830 | 3.734 | 2.053 | 0.025 |
| | 2 | 3 | 3.715 | -5245.26 | 2.098 | 3.339 | Internal | -5232.932 | 3.632 | 2.255 | 0.031 |
| | 1 | 3 | 3.745 | -5245.19 | 2.146 | 3.410 | Internal | -5232.951 | 3.614 | 2.530 | 0.059 |
| | 13 | 1 | 3.756 | -5245.22 | 2.601 | 3.381 | RHF->UHF/Internal | -5233.393 | 3.171 | 0.000 | 0.014 |
| | 18 | 3 | 3.832 | -5244.82 | 2.004 | 3.783 | Internal | -5232.721 | 3.843 | 2.070 | 0.026 |
| | 35 | 3 | 3.901 | -5244.76 | 2.022 | 3.841 | Internal | -5232.670 | 3.895 | 2.067 | 0.024 |
| | 44 | 3 | 3.950 | -5244.46 | 2.040 | 4.140 | Internal | -5232.639 | 3.926 | 2.138 | 0.026 |
| | 22 | 3 | 3.951 | -5244.77 | 2.041 | 3.834 | Internal | -5232.639 | 3.926 | 2.060 | 0.023 |
| | 71 | 1 | 3.995 | -5244.34 | 2.248 | 4.262 | Internal | -5232.802 | 3.762 | 0.000 | 0.013 |
| | 37 | 3 | 4.024 | -5244.54 | 2.009 | 4.056 | Internal | -5232.535 | 4.030 | 2.245 | 0.033 |
| | 30 | 3 | 4.098 | -5244.64 | 2.070 | 3.958 | Internal | -5232.521 | 4.044 | 2.189 | 0.032 |
| | 69 | 1 | 4.109 | -5244.04 | 2.133 | 4.557 | Internal | -5232.573 | 3.992 | 0.000 | 0.014 |
| | 31 | 1 | 4.242 | -5244.03 | 1.887 | 4.575 | Internal | -5232.193 | 4.371 | 0.000 | 0.017 |
| | 8 | 3 | 4.252 | -5244.32 | 1.899 | 4.279 | Internal | -5232.197 | 4.368 | 2.592 | 0.048 |
| | 54 | 3 | 4.270 | -5244.29 | 2.074 | 4.307 | Internal | -5232.354 | 4.211 | 2.409 | 0.044 |
| | 6 | 3 | 4.279 | -5244.39 | 2.055 | 4.210 | Internal | -5232.325 | 4.240 | 2.128 | 0.028 |
| | 29 | 3 | 4.302 | -5243.97 | 1.944 | 4.634 | Internal | -5232.191 | 4.373 | 2.326 | 0.035 |
| | 61 | 3 | 4.327 | -5244.21 | 1.974 | 4.392 | Internal | -5232.196 | 4.368 | 2.043 | 0.023 |
| | 19 | 3 | 4.346 | -5244.02 | 1.984 | 4.576 | Internal | -5232.187 | 4.377 | 2.242 | 0.033 |
| | 15 | 3 | 4.349 | -5244.19 | 1.975 | 4.414 | Internal | -5232.176 | 4.389 | 2.046 | 0.016 |
| | 23 | 1 | 4.351 | -5244.30 | 2.230 | 4.300 | Internal | -5232.429 | 4.136 | 0.000 | 0.015 |
| | 34 | 1 | 4.362 | -5243.89 | 1.874 | 4.713 | Internal | -5232.061 | 4.503 | 0.000 | 0.017 |
| | 25 | 3 | 4.367 | -5244.29 | 2.004 | 4.306 | Internal | -5232.185 | 4.379 | 2.296 | 0.033 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|--|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 58 | 3 | 5.738 | -5242.63 | 1.954 | 5.966 | Internal | -5230.765 | 5.799 | 2.311 | 0.040 |
| 49 | 3 | 5.738 | -5242.81 | 2.085 | 5.792 | Internal | -5230.896 | 5.669 | 2.058 | 0.025 |
| 27 | 3 | 5.832 | -5244.54 | 3.546 | 4.059 | Internal | -5232.264 | 4.301 | 2.251 | 0.035 |
| 31 | 3 | 6.075 | -5242.51 | 1.870 | 6.092 | Internal | -5230.343 | 6.221 | 2.234 | 0.041 |
| 34 | 3 | 6.281 | -5241.91 | 1.864 | 6.692 | Internal | -5230.133 | 6.432 | 2.466 | 0.048 |
| 23 | 3 | 6.317 | -5242.31 | 2.045 | 6.290 | Internal | -5230.278 | 6.287 | 2.109 | 0.028 |
| 21 | 3 | 6.614 | -5241.87 | 2.010 | 6.729 | Internal | -5229.945 | 6.619 | 2.184 | 0.033 |
| 20 | 3 | 6.902 | -5241.59 | 1.868 | 7.012 | Internal | -5229.515 | 7.049 | 2.409 | 0.047 |
| C₅H₄¹⁺ | | | | | | | | | | |
| 17 | 2 | 0.000 | -5239.50 | 2.122 | 0.000 | Stable | -5227.282 | 0.000 | 0.883 | 0.031 |
| 60 | 4 | 0.195 | -5238.95 | 2.022 | 0.555 | Internal | -5226.987 | 0.295 | 3.769 | 0.014 |
| 10 | 2 | 0.228 | -5239.13 | 2.164 | 0.374 | Stable | -5227.097 | 0.186 | 0.948 | 0.030 |
| 4 | 2 | 0.423 | -5238.82 | 2.092 | 0.682 | Internal | -5226.830 | 0.453 | 0.795 | 0.022 |
| 60 | 2 | 0.520 | -5238.63 | 2.144 | 0.874 | Internal | -5226.784 | 0.498 | 0.853 | 0.030 |
| 46 | 2 | 0.795 | -5238.44 | 2.145 | 1.066 | Internal | -5226.510 | 0.772 | 1.136 | 0.045 |
| 53 | 2 | 0.942 | -5238.35 | 2.196 | 1.156 | Internal | -5226.415 | 0.868 | 1.126 | 0.040 |
| 5 | 2 | 0.970 | -5239.00 | 2.441 | 0.501 | Internal | -5226.632 | 0.650 | 1.213 | 0.045 |
| 47 | 2 | 1.055 | -5238.01 | 2.086 | 1.496 | Internal | -5226.192 | 1.091 | 0.782 | 0.018 |
| 39 | 2 | 1.124 | -5237.93 | 2.097 | 1.569 | Internal | -5226.133 | 1.150 | 0.821 | 0.019 |
| 41 | 2 | 1.211 | -5238.05 | 2.137 | 1.455 | Internal | -5226.087 | 1.196 | 1.075 | 0.039 |
| 11 | 2 | 1.225 | -5238.29 | 2.278 | 1.210 | Stable | -5226.214 | 1.069 | 0.873 | 0.026 |
| 63 | 2 | 1.373 | -5237.68 | 2.118 | 1.820 | Internal | -5225.906 | 1.377 | 0.860 | 0.034 |
| 65 | 2 | 1.401 | -5237.53 | 2.018 | 1.970 | Internal | -5225.777 | 1.505 | 0.861 | 0.050 |
| 67 | 2 | 1.433 | -5237.61 | 2.354 | 1.896 | Internal | -5226.081 | 1.201 | 0.763 | 0.015 |
| 44 | 2 | 1.496 | -5237.48 | 2.067 | 2.024 | Internal | -5225.732 | 1.550 | 0.772 | 0.018 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 62 | 2 | 1.496 | -5237.40 | 2.006 | 2.106 | Internal | -5225.671 | 1.611 | 0.886 | 0.039 | |
| 1 | 2 | 1.581 | -5239.46 | 3.508 | 0.040 | Stable | -5227.088 | 0.195 | 1.101 | 0.044 | |
| 66 | 2 | 1.617 | -5237.34 | 2.128 | 2.161 | Internal | -5225.672 | 1.611 | 0.845 | 0.028 | |
| 59 | 2 | 1.645 | -5237.35 | 1.993 | 2.147 | Internal | -5225.509 | 1.773 | 0.889 | 0.027 | |
| 32 | 2 | 1.762 | -5237.61 | 2.075 | 1.890 | Internal | -5225.474 | 1.809 | 0.764 | 0.022 | |
| 65 | 4 | 1.842 | -5237.29 | 1.995 | 2.211 | Internal | -5225.314 | 1.968 | 3.920 | 0.028 | |
| 63 | 4 | 1.941 | -5237.21 | 1.982 | 2.288 | Internal | -5225.202 | 2.081 | 3.897 | 0.031 | |
| 22 | 2 | 1.986 | -5237.40 | 2.032 | 2.097 | Stable | -5225.206 | 2.076 | 1.242 | 0.046 | |
| 53 | 4 | 1.994 | -5237.20 | 1.959 | 2.304 | Internal | -5225.125 | 2.158 | 3.843 | 0.025 | |
| 2 | 2 | 1.997 | -5237.39 | 1.962 | 2.110 | Stable | -5225.125 | 2.157 | 1.000 | 0.037 | |
| 62 | 4 | 2.018 | -5237.11 | 1.996 | 2.388 | Internal | -5225.138 | 2.145 | 3.870 | 0.026 | |
| 92 | 17 | 4 | 2.034 | -5237.26 | 1.639 | 2.245 | Stable | -5224.766 | 2.517 | 4.061 | 0.035 |
| | 3 | 2 | 2.051 | -5237.33 | 2.119 | 2.167 | Stable | -5225.228 | 2.054 | 1.617 | 0.056 |
| | 25 | 2 | 2.089 | -5237.23 | 2.144 | 2.273 | Stable | -5225.216 | 2.067 | 0.770 | 0.020 |
| | 37 | 2 | 2.140 | -5236.98 | 2.003 | 2.525 | Internal | -5225.023 | 2.259 | 0.874 | 0.026 |
| | 59 | 4 | 2.142 | -5237.01 | 1.982 | 2.488 | Internal | -5225.001 | 2.282 | 3.807 | 0.022 |
| | 28 | 4 | 2.237 | -5237.17 | 2.101 | 2.331 | Stable | -5225.024 | 2.258 | 3.812 | 0.018 |
| | 41 | 4 | 2.240 | -5237.03 | 2.053 | 2.472 | Internal | -5224.973 | 2.309 | 3.840 | 0.024 |
| | 46 | 4 | 2.247 | -5236.91 | 1.968 | 2.587 | Internal | -5224.882 | 2.401 | 3.828 | 0.026 |
| | 64 | 2 | 2.405 | -5236.52 | 2.159 | 2.978 | Internal | -5224.915 | 2.367 | 0.762 | 0.015 |
| | 28 | 2 | 2.420 | -5239.44 | 4.376 | 0.064 | Stable | -5227.117 | 0.165 | 0.928 | 0.031 |
| | 32 | 4 | 2.458 | -5236.89 | 2.040 | 2.607 | Internal | -5224.742 | 2.541 | 3.827 | 0.023 |
| | 40 | 2 | 2.467 | -5236.65 | 2.089 | 2.855 | Internal | -5224.783 | 2.500 | 0.984 | 0.052 |
| | 45 | 2 | 2.526 | -5236.39 | 2.058 | 3.110 | Internal | -5224.692 | 2.590 | 0.780 | 0.026 |
| | 68 | 2 | 2.538 | -5236.51 | 2.316 | 2.989 | Internal | -5224.938 | 2.345 | 0.801 | 0.020 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 1 | 4 | 2.551 | -5236.71 | 1.653 | 2.792 | Stable | -5224.263 | 3.020 | 3.991 | 0.035 |
| 71 | 2 | 2.584 | -5236.44 | 2.186 | 3.064 | Internal | -5224.763 | 2.519 | 0.817 | 0.025 |
| 42 | 2 | 2.589 | -5236.66 | 2.043 | 2.845 | Internal | -5224.615 | 2.668 | 0.947 | 0.030 |
| 38 | 2 | 2.650 | -5236.47 | 2.149 | 3.029 | Internal | -5224.659 | 2.623 | 0.850 | 0.024 |
| 14 | 2 | 2.695 | -5236.64 | 2.083 | 2.858 | Stable | -5224.548 | 2.734 | 0.826 | 0.031 |
| 11 | 4 | 2.738 | -5236.66 | 1.933 | 2.845 | Stable | -5224.355 | 2.927 | 3.898 | 0.035 |
| 8 | 2 | 2.770 | -5236.40 | 1.896 | 3.102 | Internal | -5224.286 | 2.996 | 1.137 | 0.041 |
| 23 | 2 | 2.813 | -5236.42 | 2.144 | 3.084 | Stable | -5224.491 | 2.791 | 0.762 | 0.017 |
| 24 | 2 | 3.016 | -5236.35 | 2.089 | 3.156 | Stable | -5224.234 | 3.048 | 0.854 | 0.025 |
| 4 | 4 | 3.036 | -5236.30 | 2.038 | 3.201 | Internal | -5224.162 | 3.120 | 3.790 | 0.021 |
| 5 | 4 | 3.047 | -5237.23 | 2.598 | 2.273 | Internal | -5224.711 | 2.572 | 4.063 | 0.045 |
| 52 | 4 | 3.057 | -5236.19 | 2.067 | 3.310 | Internal | -5224.170 | 3.112 | 3.923 | 0.026 |
| 30 | 2 | 3.058 | -5238.26 | 3.965 | 1.238 | Stable | -5226.067 | 1.215 | 0.924 | 0.029 |
| 61 | 2 | 3.062 | -5236.08 | 1.997 | 3.422 | Internal | -5224.096 | 3.186 | 1.581 | 0.045 |
| 6 | 2 | 3.093 | -5237.19 | 2.887 | 2.316 | Internal | -5224.954 | 2.328 | 0.886 | 0.029 |
| 54 | 2 | 3.094 | -5236.10 | 2.091 | 3.401 | Internal | -5224.158 | 3.125 | 0.956 | 0.074 |
| 54 | 4 | 3.100 | -5236.09 | 2.082 | 3.413 | Internal | -5224.143 | 3.140 | 3.946 | 0.027 |
| 10 | 4 | 3.115 | -5236.19 | 2.095 | 3.314 | Stable | -5224.141 | 3.142 | 3.774 | 0.017 |
| 50 | 4 | 3.155 | -5236.04 | 1.966 | 3.459 | Internal | -5223.972 | 3.310 | 3.935 | 0.030 |
| 6 | 4 | 3.186 | -5235.78 | 1.715 | 3.717 | Internal | -5223.690 | 3.593 | 3.955 | 0.032 |
| 35 | 4 | 3.209 | -5236.03 | 2.036 | 3.473 | Internal | -5223.988 | 3.295 | 3.816 | 0.022 |
| 42 | 4 | 3.301 | -5235.84 | 1.967 | 3.662 | Internal | -5223.827 | 3.456 | 3.904 | 0.027 |
| 22 | 4 | 3.308 | -5236.03 | 2.048 | 3.470 | Stable | -5223.901 | 3.382 | 3.799 | 0.022 |
| 25 | 4 | 3.340 | -5235.75 | 2.132 | 3.748 | Stable | -5223.952 | 3.330 | 3.780 | 0.019 |
| 37 | 4 | 3.384 | -5235.59 | 1.996 | 3.912 | Internal | -5223.773 | 3.510 | 3.918 | 0.029 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 16 | 2 | 3.482 | -5235.73 | 2.039 | 3.774 | Stable | -5223.717 | 3.565 | 1.050 | 0.040 | |
| 40 | 4 | 3.528 | -5235.53 | 1.969 | 3.975 | Internal | -5223.602 | 3.680 | 3.812 | 0.036 | |
| 47 | 4 | 3.550 | -5235.59 | 2.052 | 3.914 | Internal | -5223.663 | 3.620 | 3.977 | 0.026 | |
| 18 | 4 | 3.608 | -5235.54 | 1.987 | 3.965 | Stable | -5223.540 | 3.742 | 3.795 | 0.024 | |
| 55 | 2 | 3.613 | -5235.53 | 2.083 | 3.975 | Internal | -5223.631 | 3.652 | 0.859 | 0.107 | |
| 14 | 4 | 3.630 | -5235.60 | 1.919 | 3.897 | Stable | -5223.450 | 3.832 | 4.186 | 0.038 | |
| 55 | 4 | 3.638 | -5235.45 | 2.078 | 4.050 | Internal | -5223.601 | 3.682 | 3.904 | 0.027 | |
| 38 | 4 | 3.694 | -5235.26 | 2.143 | 4.236 | Internal | -5223.610 | 3.673 | 3.899 | 0.026 | |
| 15 | 2 | 3.707 | -5235.55 | 2.232 | 3.953 | Stable | -5223.686 | 3.596 | 0.899 | 0.026 | |
| 70 | 2 | 3.741 | -5235.05 | 2.095 | 4.448 | Internal | -5223.515 | 3.768 | 0.778 | 0.018 | |
| 7 | 2 | 3.785 | -5235.41 | 2.020 | 4.091 | Internal | -5223.396 | 3.886 | 0.760 | 0.124 | |
| 46 | 49 | 2 | 3.808 | -5235.27 | 2.133 | 4.233 | Internal | -5223.486 | 3.796 | 0.862 | 0.026 |
| | 9 | 4 | 3.827 | -5235.56 | 2.005 | 3.938 | Internal | -5223.339 | 3.944 | 3.971 | 0.032 |
| | 7 | 4 | 3.886 | -5235.22 | 2.017 | 4.281 | Internal | -5223.291 | 3.991 | 3.788 | 0.021 |
| | 39 | 4 | 3.912 | -5235.18 | 2.057 | 4.318 | Internal | -5223.305 | 3.977 | 3.791 | 0.027 |
| | 61 | 4 | 3.936 | -5235.16 | 1.974 | 4.337 | Internal | -5223.198 | 4.084 | 3.764 | 0.023 |
| | 2 | 4 | 3.943 | -5235.92 | 2.455 | 3.586 | Stable | -5223.672 | 3.611 | 4.147 | 0.038 |
| | 23 | 4 | 3.998 | -5234.96 | 2.145 | 4.542 | Stable | -5223.307 | 3.976 | 3.758 | 0.016 |
| | 3 | 4 | 4.013 | -5235.65 | 2.321 | 3.851 | Stable | -5223.469 | 3.814 | 4.135 | 0.046 |
| | 29 | 2 | 4.087 | -5236.10 | 2.941 | 3.398 | Stable | -5224.014 | 3.269 | 0.898 | 0.029 |
| | 56 | 4 | 4.126 | -5234.72 | 2.142 | 4.783 | Internal | -5223.176 | 4.106 | 3.769 | 0.020 |
| | 44 | 4 | 4.152 | -5234.95 | 2.053 | 4.556 | Internal | -5223.061 | 4.221 | 4.042 | 0.031 |
| | 43 | 4 | 4.277 | -5234.80 | 2.037 | 4.706 | Internal | -5222.920 | 4.363 | 3.805 | 0.025 |
| | 15 | 4 | 4.350 | -5234.68 | 1.968 | 4.821 | Stable | -5222.778 | 4.504 | 3.791 | 0.024 |
| | 8 | 4 | 4.457 | -5234.71 | 1.987 | 4.788 | Internal | -5222.691 | 4.592 | 3.962 | 0.040 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 28 | 1 | 1.631 | -5224.51 | 2.534 | 1.121 | Stable | -5212.260 | 1.214 | 0.000 | 0.026 |
| 5 | 1 | 1.694 | -5224.97 | 3.121 | 0.659 | Stable | -5212.783 | 0.691 | 0.000 | 0.025 |
| 60 | 1 | 1.721 | -5223.34 | 1.984 | 2.287 | Internal | -5211.620 | 1.855 | 0.000 | 0.029 |
| 17 | 3 | 1.758 | -5223.98 | 2.094 | 1.643 | Stable | -5211.692 | 1.783 | 2.054 | 0.026 |
| 1 | 3 | 1.807 | -5224.14 | 1.963 | 1.489 | Stable | -5211.513 | 1.962 | 2.325 | 0.037 |
| 60 | 3 | 2.092 | -5223.21 | 1.990 | 2.413 | Internal | -5211.255 | 2.220 | 2.123 | 0.033 |
| 1 | 1 | 2.097 | -5223.50 | 1.960 | 2.127 | RHF->UHF | -5211.219 | 2.255 | 0.000 | 0.027 |
| 10 | 3 | 2.104 | -5223.41 | 2.108 | 2.213 | Stable | -5211.360 | 2.114 | 2.010 | 0.016 |
| 53 | 3 | 2.247 | -5223.20 | 2.139 | 2.429 | Internal | -5211.249 | 2.225 | 2.043 | 0.017 |
| 47 | 1 | 2.300 | -5222.83 | 2.033 | 2.792 | Stable | -5211.089 | 2.385 | 0.000 | 0.019 |
| 63 | 1 | 2.315 | -5222.83 | 2.204 | 2.794 | Internal | -5211.245 | 2.229 | 0.000 | 0.017 |
| 67 | 1 | 2.365 | -5222.86 | 2.462 | 2.765 | Internal | -5211.453 | 2.021 | 0.000 | 0.016 |
| 39 | 1 | 2.371 | -5222.75 | 2.060 | 2.880 | Stable | -5211.046 | 2.428 | 0.000 | 0.020 |
| 41 | 1 | 2.393 | -5222.81 | 2.205 | 2.819 | RHF->UHF | -5211.168 | 2.306 | 0.000 | 0.041 |
| 46 | 3 | 2.470 | -5222.94 | 2.083 | 2.683 | Stable | -5210.970 | 2.505 | 2.034 | 0.021 |
| 44 | 1 | 2.479 | -5222.51 | 2.037 | 3.115 | Stable | -5210.914 | 2.560 | 0.000 | 0.017 |
| 65 | 1 | 2.491 | -5222.58 | 2.093 | 3.044 | Internal | -5210.958 | 2.516 | 0.000 | 0.020 |
| 41 | 3 | 2.588 | -5222.67 | 1.950 | 2.955 | Stable | -5210.719 | 2.756 | 2.085 | 0.022 |
| 4 | 3 | 2.620 | -5222.72 | 2.004 | 2.904 | Stable | -5210.741 | 2.734 | 2.047 | 0.020 |
| 23 | 1 | 2.667 | -5222.51 | 2.113 | 3.119 | Stable | -5210.802 | 2.672 | 0.000 | 0.016 |
| 28 | 3 | 2.838 | -5223.42 | 2.543 | 2.204 | Stable | -5211.061 | 2.413 | 2.236 | 0.034 |
| 5 | 3 | 2.854 | -5223.12 | 2.205 | 2.504 | Internal | -5210.707 | 2.768 | 2.268 | 0.043 |
| 64 | 1 | 2.952 | -5222.14 | 2.181 | 3.487 | Internal | -5210.586 | 2.889 | 0.000 | 0.015 |
| 32 | 1 | 2.958 | -5222.45 | 2.016 | 3.175 | Stable | -5210.415 | 3.059 | 0.000 | 0.042 |
| 62 | 1 | 3.166 | -5221.91 | 2.175 | 3.712 | Internal | -5210.366 | 3.109 | 0.000 | 0.024 |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|-------------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 59 | 1 | 3.176 | -5221.83 | 1.957 | 3.796 | Internal | -5210.138 | 3.337 | 0.000 | 0.033 |
| 61 | 1 | 3.204 | -5221.90 | 2.120 | 3.727 | Internal | -5210.273 | 3.202 | 0.000 | 0.021 |
| 63 | 3 | 3.227 | -5222.15 | 2.084 | 3.473 | Internal | -5210.214 | 3.260 | 2.120 | 0.032 |
| 11 | 3 | 3.251 | -5222.64 | 2.298 | 2.987 | Stable | -5210.404 | 3.071 | 2.308 | 0.037 |
| 30 | 1 | 3.292 | -5222.09 | 1.910 | 3.536 | RHF->UHF | -5209.975 | 3.500 | 0.000 | 0.021 |
| 65 | 3 | 3.326 | -5222.05 | 2.075 | 3.576 | Internal | -5210.105 | 3.369 | 2.311 | 0.041 |
| 30 | 3 | 3.406 | -5222.47 | 2.433 | 3.156 | RHF->UHF | -5210.384 | 3.091 | 2.012 | 0.017 |
| 6 | 1 | 3.437 | -5222.26 | 2.270 | 3.362 | RHF->UHF/Internal | -5210.190 | 3.285 | 0.000 | 0.026 |
| 24 | 1 | 3.449 | -5222.32 | 2.434 | 3.312 | Stable | -5210.341 | 3.133 | 0.000 | 0.022 |
| 32 | 3 | 3.489 | -5222.10 | 2.002 | 3.531 | Stable | -5209.869 | 3.605 | 2.106 | 0.025 |
| 22 | 3 | 3.495 | -5222.18 | 2.030 | 3.448 | Stable | -5209.891 | 3.583 | 2.080 | 0.030 |
| 22 | 1 | 3.614 | -5221.72 | 1.989 | 3.910 | RHF->UHF | -5209.732 | 3.743 | 0.000 | 0.034 |
| 56 | 1 | 3.688 | -5221.36 | 2.114 | 4.263 | RHF->UHF/Internal | -5209.782 | 3.692 | 0.000 | 0.017 |
| 38 | 1 | 3.708 | -5221.35 | 1.973 | 4.277 | RHF->UHF | -5209.621 | 3.853 | 0.000 | 0.020 |
| 13 | 1 | 3.830 | -5221.46 | 2.111 | 4.167 | Stable | -5209.638 | 3.836 | 0.000 | 0.023 |
| 59 | 3 | 3.834 | -5221.48 | 1.976 | 4.142 | Internal | -5209.498 | 3.976 | 2.122 | 0.033 |
| 4 | 1 | 3.845 | -5221.78 | 2.126 | 3.848 | Stable | -5209.638 | 3.837 | 0.000 | 0.033 |
| 14 | 3 | 3.857 | -5221.38 | 1.903 | 4.247 | Stable | -5209.402 | 4.072 | 2.226 | 0.036 |
| 7 | 3 | 3.866 | -5221.41 | 2.007 | 4.212 | Internal | -5209.497 | 3.977 | 2.025 | 0.019 |
| 62 | 3 | 3.883 | -5221.43 | 1.976 | 4.196 | Internal | -5209.450 | 4.024 | 2.142 | 0.034 |
| 25 | 1 | 3.991 | -5221.31 | 2.105 | 4.321 | RHF->UHF | -5209.470 | 4.004 | 0.000 | 0.021 |
| 37 | 1 | 4.042 | -5221.01 | 2.115 | 4.614 | RHF->UHF | -5209.429 | 4.045 | 0.000 | 0.019 |
| 66 | 3 | 4.144 | -5220.97 | 2.244 | 4.659 | Internal | -5209.457 | 4.017 | 2.062 | 0.019 |
| 14 | 1 | 4.178 | -5221.87 | 2.912 | 3.760 | Stable | -5210.091 | 3.384 | 0.000 | 0.021 |
| 23 | 3 | 4.236 | -5221.05 | 2.118 | 4.580 | Stable | -5209.238 | 4.236 | 2.007 | 0.018 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | | |
|---------------------------------------|--------------|-----------------------|------------|----------|-------------------------|---------------|-------------------|----------------------|-----------------------|----------------------|-------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff | |
| <i>(Continued from previous page)</i> | | | | | | | | | | | |
| 3 | 3 | 4.249 | -5221.36 | 2.147 | 4.270 | Stable | -5209.255 | 4.219 | 2.633 | 0.046 | |
| 37 | 3 | 4.254 | -5221.19 | 1.993 | 4.434 | Stable | -5209.096 | 4.379 | 2.641 | 0.047 | |
| 47 | 3 | 4.258 | -5221.02 | 2.053 | 4.609 | Stable | -5209.152 | 4.323 | 2.126 | 0.023 | |
| 15 | 3 | 4.261 | -5220.86 | 1.964 | 4.762 | Stable | -5209.060 | 4.414 | 2.030 | 0.021 | |
| 44 | 3 | 4.435 | -5220.85 | 2.051 | 4.778 | Stable | -5208.973 | 4.502 | 2.115 | 0.033 | |
| 39 | 3 | 4.546 | -5220.77 | 2.052 | 4.861 | Stable | -5208.863 | 4.611 | 2.073 | 0.023 | |
| 40 | 3 | 4.610 | -5220.70 | 2.054 | 4.923 | Stable | -5208.801 | 4.674 | 2.024 | 0.025 | |
| 18 | 3 | 4.620 | -5220.71 | 1.994 | 4.920 | Stable | -5208.731 | 4.744 | 2.034 | 0.027 | |
| 6 | 3 | 4.689 | -5221.06 | 2.098 | 4.572 | Internal | -5208.766 | 4.708 | 2.223 | 0.035 | |
| 16 | 1 | 4.907 | -5221.78 | 3.347 | 3.845 | Stable | -5209.797 | 3.678 | 0.000 | 0.023 | |
| 8 | 3 | 4.927 | -5220.60 | 2.223 | 5.025 | Internal | -5208.653 | 4.821 | 2.019 | 0.026 | |
| 86 | 3 | 1 | 4.929 | -5220.25 | 1.965 | 5.376 | RHF->UHF | -5208.393 | 5.081 | 0.000 | 0.078 |
| | 38 | 3 | 4.987 | -5220.20 | 1.974 | 5.426 | Stable | -5208.344 | 5.130 | 2.142 | 0.025 |
| | 56 | 3 | 5.018 | -5220.20 | 2.119 | 5.429 | Internal | -5208.457 | 5.017 | 2.010 | 0.024 |
| | 54 | 1 | 5.022 | -5220.98 | 2.935 | 4.645 | RHF->UHF/Internal | -5209.270 | 4.205 | 0.000 | 0.042 |
| | 25 | 3 | 5.083 | -5221.08 | 2.566 | 4.545 | Stable | -5208.840 | 4.635 | 2.389 | 0.043 |
| | 2 | 1 | 5.090 | -5221.56 | 3.378 | 4.066 | RHF->UHF | -5209.645 | 3.830 | 0.000 | 0.029 |
| | 2 | 3 | 5.104 | -5221.18 | 2.586 | 4.452 | Stable | -5208.839 | 4.635 | 2.537 | 0.049 |
| | 29 | 3 | 5.127 | -5220.25 | 2.066 | 5.375 | Stable | -5208.296 | 5.178 | 2.217 | 0.037 |
| | 16 | 3 | 5.129 | -5220.05 | 1.841 | 5.579 | Stable | -5208.069 | 5.405 | 2.034 | 0.024 |
| | 43 | 3 | 5.129 | -5220.03 | 2.023 | 5.600 | Stable | -5208.250 | 5.224 | 2.021 | 0.024 |
| | 26 | 3 | 5.138 | -5220.68 | 2.482 | 4.950 | Stable | -5208.701 | 4.773 | 2.222 | 0.039 |
| | 27 | 3 | 5.243 | -5221.11 | 2.270 | 4.512 | Stable | -5208.383 | 5.091 | 2.649 | 0.079 |
| | 24 | 3 | 5.627 | -5219.93 | 2.076 | 5.699 | Stable | -5207.806 | 5.669 | 2.286 | 0.042 |
| | 20 | 1 | 5.915 | -5219.02 | 1.995 | 6.603 | Stable | -5207.437 | 6.038 | 0.000 | 0.020 |
| <i>(Continues on next page)</i> | | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 60 | 2 | 1.434 | -5200.50 | 1.896 | 2.138 | Internal | -5188.652 | 1.754 | 0.908 | 0.033 |
| 17 | 4 | 1.937 | -5200.56 | 1.934 | 2.078 | Internal | -5188.187 | 2.219 | 4.003 | 0.041 |
| 1 | 4 | 2.112 | -5200.63 | 2.080 | 2.002 | Stable | -5188.158 | 2.248 | 3.938 | 0.045 |
| 6 | 2 | 2.113 | -5200.29 | 2.022 | 2.344 | Internal | -5188.099 | 2.307 | 1.260 | 0.052 |
| 44 | 2 | 2.200 | -5199.57 | 1.983 | 3.062 | Internal | -5187.974 | 2.432 | 0.850 | 0.022 |
| 8 | 2 | 2.443 | -5199.83 | 2.069 | 2.807 | Internal | -5187.816 | 2.590 | 1.474 | 0.061 |
| 11 | 4 | 2.515 | -5200.26 | 2.161 | 2.378 | Stable | -5187.836 | 2.570 | 3.789 | 0.031 |
| 30 | 4 | 2.598 | -5200.23 | 2.099 | 2.411 | Internal | -5187.691 | 2.715 | 3.897 | 0.028 |
| 4 | 2 | 2.610 | -5199.50 | 1.946 | 3.132 | Internal | -5187.526 | 2.880 | 1.004 | 0.040 |
| 16 | 2 | 2.649 | -5199.71 | 2.097 | 2.930 | Internal | -5187.638 | 2.768 | 0.885 | 0.041 |
| 24 | 2 | 2.700 | -5199.70 | 2.098 | 2.940 | Internal | -5187.588 | 2.818 | 1.334 | 0.057 |
| 5 | 4 | 2.793 | -5200.39 | 2.554 | 2.248 | Internal | -5187.951 | 2.455 | 3.880 | 0.032 |
| 65 | 2 | 2.886 | -5199.08 | 2.003 | 3.560 | Internal | -5187.307 | 3.099 | 0.903 | 0.036 |
| 3 | 4 | 2.900 | -5199.43 | 1.956 | 3.205 | Internal | -5187.246 | 3.160 | 3.976 | 0.034 |
| 3 | 2 | 2.935 | -5199.15 | 1.905 | 3.491 | Internal | -5187.161 | 3.245 | 0.869 | 0.086 |
| 39 | 2 | 3.039 | -5198.95 | 2.018 | 3.687 | Internal | -5187.169 | 3.237 | 0.889 | 0.030 |
| 10 | 4 | 3.162 | -5199.34 | 2.235 | 3.294 | Stable | -5187.263 | 3.143 | 3.822 | 0.025 |
| 14 | 2 | 3.255 | -5199.78 | 2.814 | 2.855 | Internal | -5187.749 | 2.657 | 1.788 | 0.062 |
| 6 | 4 | 3.271 | -5199.17 | 1.960 | 3.463 | Internal | -5186.879 | 3.527 | 4.088 | 0.044 |
| 14 | 4 | 3.340 | -5198.66 | 1.817 | 3.976 | Internal | -5186.667 | 3.738 | 3.902 | 0.032 |
| 23 | 2 | 3.374 | -5198.88 | 2.077 | 3.760 | Internal | -5186.892 | 3.514 | 0.772 | 0.065 |
| 22 | 2 | 3.531 | -5198.98 | 2.169 | 3.658 | Internal | -5186.828 | 3.578 | 0.794 | 0.040 |
| 62 | 2 | 3.679 | -5198.37 | 2.008 | 4.264 | Internal | -5186.520 | 3.886 | 0.791 | 0.038 |
| 59 | 2 | 3.725 | -5198.23 | 1.887 | 4.404 | Internal | -5186.352 | 4.054 | 1.045 | 0.045 |
| 4 | 4 | 3.742 | -5198.46 | 1.960 | 4.172 | Internal | -5186.408 | 3.998 | 3.956 | 0.036 |
| <i>(Continues on next page)</i> | | | | | | | | | | |

| Geometry | Multiplicity | ΔE_{ZPE} (eV) | DFT | | | | CCSD(T) | | | |
|---------------------------------------|--------------|-----------------------|------------|---------|-------------------------|---------------|------------|----------------------|-----------------------|----------------------|
| | | | Energy(eV) | ZPE(eV) | ΔE_{B3LYP} (eV) | DFT Stability | Energy(eV) | $\Delta E_{CCSD(T)}$ | $\langle S^2 \rangle$ | T ₁ Coeff |
| <i>(Continued from previous page)</i> | | | | | | | | | | |
| 34 | 4 | 6.630 | -5195.60 | 1.812 | 7.041 | Internal | -5183.372 | 7.034 | 4.186 | 0.046 |
| 57 | 4 | 6.770 | -5195.08 | 1.857 | 7.556 | Internal | -5183.277 | 7.128 | 3.770 | 0.030 |
| 34 | 2 | 7.651 | -5195.42 | 1.804 | 7.220 | Internal | -5182.343 | 8.063 | 1.754 | 0.040 |