# Problem 12

What I did in this problem I used my local machine to optimize the geometrey for all of my molecules, then I imported them to WebMO to do 'Molecular Energy" Calculations.

| | | | | | | |
|---|---|---|---|---|---|---|
| 20 | C2H2F2 | Geometry Optimization - Mopac | 3/28/2022 14:09 | Complete | 0.0 sec | |
| 19 | C4H8 | Geometry Optimization - Mopac | 3/28/2022 14:08 | Complete | 0.1 sec | |
| 18 | C4H8 | Geometry Optimization - Mopac | 3/28/2022 14:05 | Complete | 0.1 sec | |
| 17 | C2H2F2 | Geometry Optimization - Mopac | 3/28/2022 13:44 | Complete | 0.0 sec | |

**Figure 1:** Jobs from local WebMO, all were imported to Online WebMO.

After doing so, I got these results for the energies. All units are in Hartree. I averaged all of the methods for each basis set, and I will compare the average between basis sets:

| Cis CH3 | HF | MP2 | B3LYP | Average |
|---|---|---|---|---|
| cc-pVDZ | -156.117 | -156.69 | -157.226075 | -156.6775534 |
| aug-cc-pVDZ | -156.121 | -156.717 | -157.23718 | -156.691977 |
| | | | Average | -156.6847652 |
| Trans CH3 | HF | MP2 | B3LYP | Average |
| cc-pVDZ | -156.122 | -156.693 | -157.229402 | -156.6814304 |
| aug-cc-pVDZ | -156.127 | 720678371 | -157.24083 | -156.6836684 |
| | | | | -156.6825494 |
| Cis F | HF | MP2 | B3LYP | Average |
| cc-pVDZ | -275.738 | -276.378 | -277.060502 | -276.39205 |
| aug-cc-pVDZ | -275.761 | -276.446 | -277.089792 | -276.4320097 |
| | | | Average | -276.4120298 |
| Trans F | HF | MP2 | B3LYP | Average |
| cc-pVDZ | -275.738 | -276.378 | -277.060418 | -276.3920147 |
| aug-cc-pVDZ | -275.759 | -276.444 | -277.088062 | -276.4302484 |
| | | | Average | -276.4111316 |

**Figure 2:** Results from WebMO, all units are in Hartree.

# Conclusion

I am by no means a chemist, but I will conclude based on the minimum average energies of the basis sets. The favorable isomer for CH3 is **Cis**, and the favorable isomer for F is **Cis**, although it is very close to Trans.