ME 5329 Assignment 4

Combustion Reactions

September X, 2025

Dr. Aquino Fall 2025

Objectives:

- Create and chemically balance combustion reactions.
- Learn how to model combustion reactions using DFT.
- Understand how to calculate ΔE, ΔH and ΔG theoretically for a combustion reaction.
- Understand how total electronic energy (E), enthalpy (H), and Gibbs free energy (G) change due to temperature.

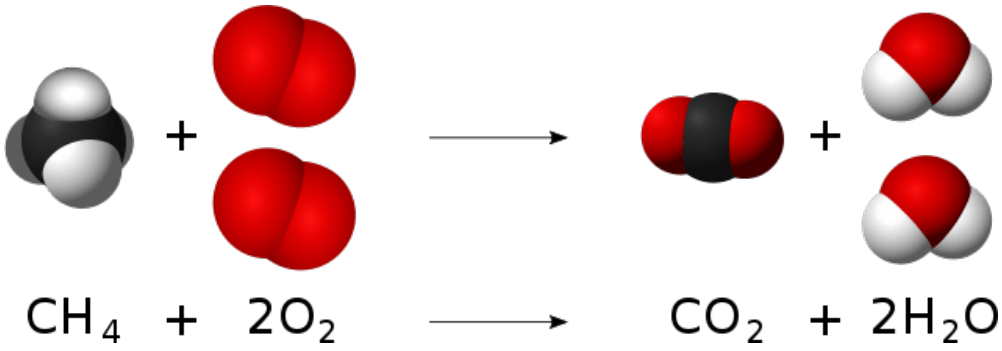

Figure 1: Combustion Reaction of Methane (CH_4) Visualized

Tasks to Model Combustion Reactions:

1. Create the combustion reaction (and chemically balance it) for the fuels Acetone (C_3H_6O), Ethanol (C_2H_5OH), and Propane (C_3H_8). It should follow the form below where A, B, C and D are coefficients:
   - $A \cdot \text{Fuel} + B \cdot O_2 \longrightarrow C \cdot CO_2 + D \cdot H_2O$
   - Note: If A is not equal to 1, divide all of the coefficients until A is equal to 1.
2. Create each structure found in the combustion reactions we are calculating.
3. For each structure, do an ORCA geometry optimization using KS-DFT functional PBE and basis set DEF2-TZVP and calculate the vibrational frequencies of the optimized structure using ORCA. Please include Grimme's D3 dispersion correction. The charge of each system is 0 and the multiplicity of this system is 1.
   - Ensure there are the correct number of near zero frequencies for each structure and no large negative frequencies reported.
4. Calculate ΔE, ΔH and ΔG for each reaction in kJ/mol. For ΔH and ΔG, calculate at a range of temperatures from 300 to 2,500 K with a step of 200 K.
   - To have ORCA print out multiple temperatures, add the block below in the ORCA input. Where each number in the temperature line is the temperature at you want ORCA to print out thermochemistry data (H and G) for at a given pressure of 1.0 atm.

```
%freq
  Temp 77, 298, 330, 450
  Pressure 1.0
end
```

5. In one table, report ΔE in kJ/mol for each reaction.
6. For each reaction, create a graph with temperature in Kelvin on the x-axis and with ΔE, ΔH and ΔG in kJ/mol on the y-axis. Make sure to include a legend.
7. Report how increasing temperature affects H and G.
8. For each reaction, include the visualized structures for each reactant and product (similar to Figure 1).

Grading Rubric

Please include the scripts you used to generate the structures or information on where the structures were found, paths to where the calculations were ran on the HPC (a parent directory for this specific project works also) and your post processing scripts that generated the graphs and results in the Canvas Assignment submission. Including this information is the student's way of showing work in this class. If the information requested above is not provided, the instructor will assume plagaraism or collusion occured and respond accordingly.

The only accepted submission for the report is a MS Word document.

Criteria	**Points**
Calculation of Reactions	45
Analysis of Reactions	45
Formatting and Submission of Word Document	5
Incusion of scripts and paths to calculations on HPC	5
Total	**100**