ME 5329 Homework 2

Combustion Reactions

September 11, 2025

Dr. Aquino Fall 2025

Due: September 18, 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.

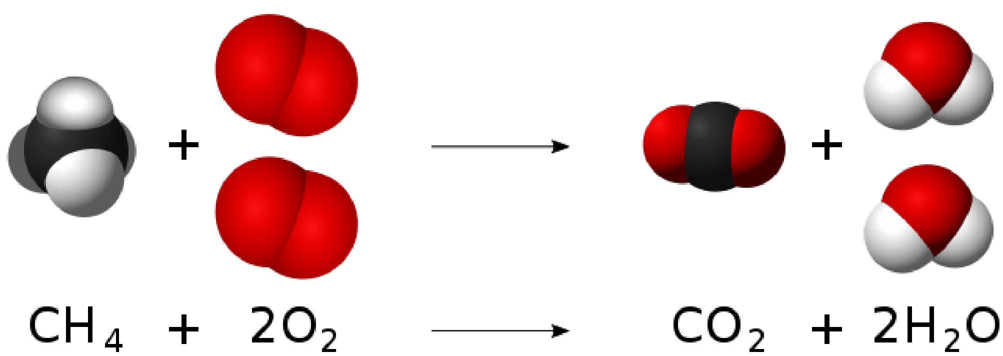

Figure 1: Combustion Reaction of Methane (CH_4) Visualized

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), Napthalene ($C_{10}H_8$), Methane (CH_4) and Propane (C_3H_8). It should follow the form below where A, B, C and D are coefficients:
   - $\mathrm{A} \cdot \mathrm{Fuel} + \mathrm{B} \cdot \mathrm{O_2} \longrightarrow \mathrm{C} \cdot \mathrm{CO_2} + \mathrm{D} \cdot \mathrm{H_2O}$
   - 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, perform a geometry optimization in ORCA using the KS-DFT functional PBE and the DEF2-TZVP basis set. After the optimization, calculate the vibrational frequencies of the structure. Include Grimme's D3 dispersion correction in all calculations. Each system has a charge of 0 and a multiplicity of 1.
   - Ensure there are the correct number of near-zero frequencies for each structure and that no large imaginary frequencies (reported as a negative frequency) are present.
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 at a constant pressure of 1.0 atm.
   - 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
```

   - The generic reaction energy equation is listed below:

$$\Delta Z = \sum_i \nu_i \, Z_{\text{products},i} - \sum_j \nu_j \, Z_{\text{reactants},j}$$

     Where ν are stoichiometric coefficients and Z can be E, H or G.
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).

Submission Requirements:

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 format for the report is a Microsoft Word document.

Please submit it under the **'Homework 2'** assignment in Canvas.