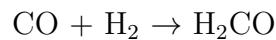


## Reaction Energetics Lab Report



**Due at the end of lab**

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Name: \_\_\_\_\_ Student ID: \_\_\_\_\_

### 1. Calculated Energies (RHF/STO-3G)

Molecule	E(SCF) (kJ/mol)	ZPE (kJ/mol)	E(total) (kJ/mol)
CO			
H <sub>2</sub>			
H <sub>2</sub> CO			

Conversion: 1 Hartree = 2625.5 kJ/mol. Set E(CO + H<sub>2</sub>) = 0 kJ/mol as your reference.

### 2. Reaction Coordinate Diagram

**Instructions:** Sketch your reaction coordinate diagram showing:

- Reactants (CO + H<sub>2</sub>) at 0 kJ/mol; Product (H<sub>2</sub>CO) at calculated energy
- Transition state at +440.7 kJ/mol above H<sub>2</sub>CO
- Label:  $\Delta E_{\text{rxn}}$ ,  $E_a^f$ ,  $E_a^r$

### 3. Analysis Questions

**3.1** Why does Hartree-Fock overestimate activation barriers?

**3.2** What is  $\Delta E_{\text{rxn}}$ ? Exothermic or endothermic?  $E_a^f = \underline{\hspace{2cm}}$      $E_a^r = \underline{\hspace{2cm}}$