Reaction Energetics Lab Report

$CO + H_2 \rightarrow H_2CO$

Due at the end of lab

Name: _____ **Student ID:** _____

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

Molecule	E(SCF) (kJ/mol)	ZPE (kJ/mol)	E(total) (kJ/mol)
CO			
H_2			
H_2CO			

Conversion: 1 Hartree = 2625.5 kJ/mol. Set E(CO + H_2) = 0 kJ/mol as your reference.

2. Reaction Coordinate Diagram

Instructions: Sketch your reaction coordinate diagram showing:

- Reactants (CO + H_2) at 0 kJ/mol; Product (H_2CO) at calculated energy
- Transition state at +440.7 kJ/mol above H_2CO
- Label: ΔE_{rxn}, E_a^f, E_a^r

3. Analysis Questions

3.1 Why does Hartree-Fock overestimate activation barriers?

3.2 What is ΔE_{rxn}? Exothermic or endothermic? $E_a^f =$ _____ $E_a^r =$ _____