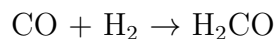


Reaction Energetics Lab Report



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 ₂ CO			

Conversion: 1 Hartree = 2625.5 kJ/mol. Set $E(\text{CO} + \text{H}_2) = 0$ kJ/mol as your reference.

2. Reaction Coordinate Diagram

Instructions: Sketch your reaction coordinate diagram showing:

- Reactants ($\text{CO} + \text{H}_2$) 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? $E_a^f =$ _____ $E_a^r =$ _____