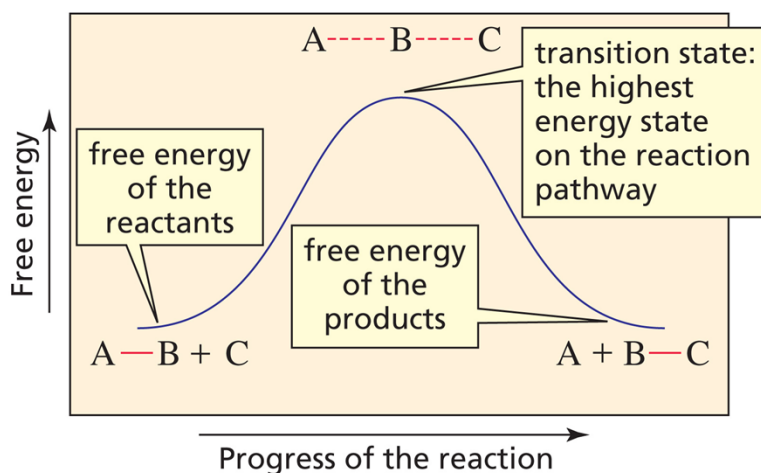


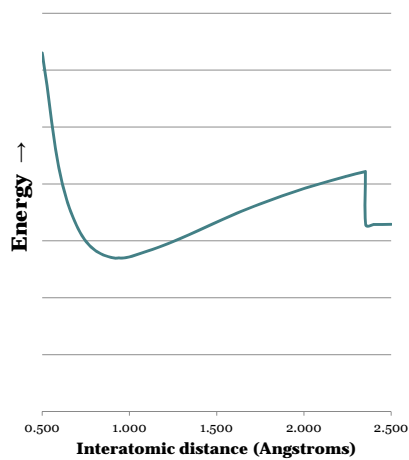
Outline

- Thermodynamics
 - Equilibrium and equilibrium constants
 - Equilibrium expressions
 - Relative energies and absolute energies
- Kinetics
 - Rates and rate constants
 - Rate expressions
 - Reversible and irreversible reactions
 - Transition state energies and reaction coordinates
- Reaction coordinate diagrams (3.8)
 - Transition states: diagrams and structures
- The Hammond Postulate (4.3)
 - Transition state structure, vs reactants & products
- Thermodynamic and kinetic control of reactions (7.11)
 - Used when two possible pathways compete
 - Th. control is by stability of products
 - Equilibrium conditions
 - K. control is by stability of transition states
 - Speed of reaction controls the product

Reaction coordinate diagrams

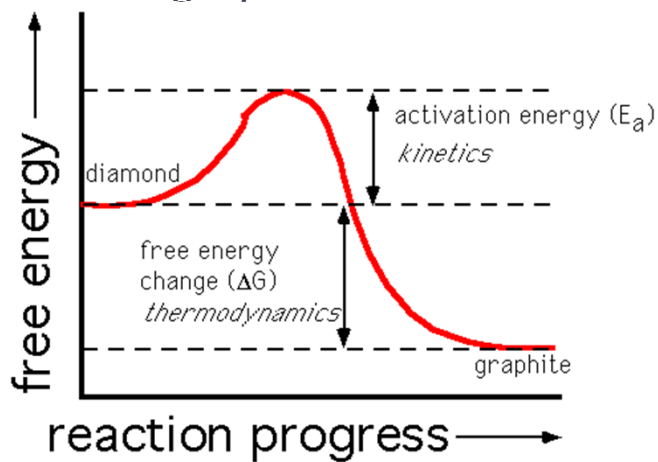


Bond energy diagram: $\text{HF} \rightarrow \text{H} + \text{F}$

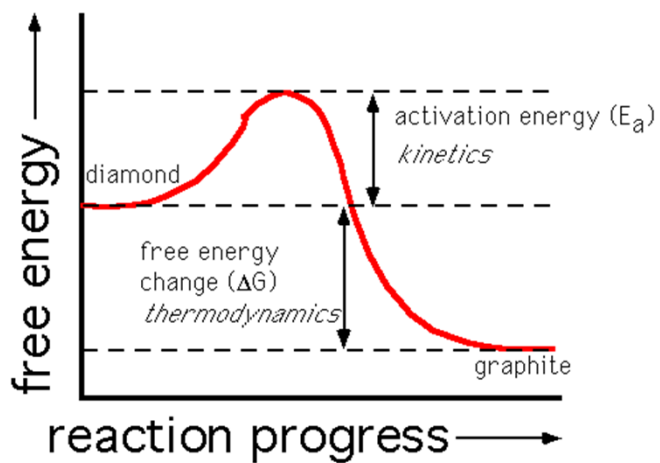


- Along the reaction coordinate:
 - There is a specific point at which energy is at a minimum: the **equilibrium bond distance**
 - There is a specific point at which energy is at a maximum: **transition state for bond breaking**

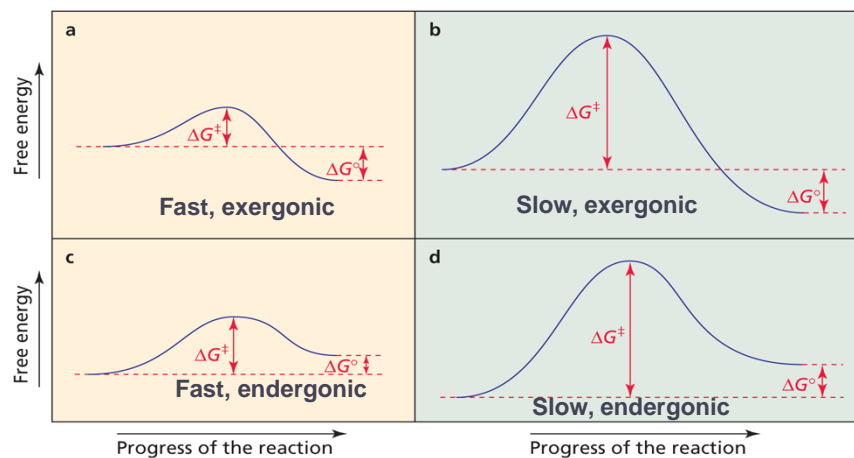
Reaction energy diagram: diamond \rightarrow graphite



The Hammond Postulate



Rates and Equilibrium are independent



Potential Energy Surface

$A \leftarrow \text{Reactant} \rightarrow B$

