Mechanisms, Catalysts & Coordinate Diagrams



Outcomes:

- Draw potential energy diagrams for endothermic & exothermic reactions.
- Explain the concept of a reaction mechanism.

Reaction Coordinate Diagrams From Mechanisms:

We can draw a coordinate diagram from a mechanism with more than one step, if we know the **<u>RATES</u>** of each step, and the **<u>ENTHALPY</u>** of the reaction...

The LARGER the \underline{E}_A , the SLOWER the reaction, so the RATE DETERMINING STEP should have the HIGHEST \underline{E}_A .

FASTER steps should have **LOWER** $E_A^{'s}$, with the **FASTEST** having the **LOWEST**. If **EXOTHERMIC**, $H_{reacts} > H_{prods}$

If <u>ENDOTHERMIC</u>, $H_{reacts} < H_{prods}$

Example 1:

Given the following mechanism for an exothermic reaction:

Step 1: $NO_2 + NO_2 \rightarrow NO_3 + NO (slow) - High End$ $Step 2: <math>NO_3 + CO \rightarrow NO_2 + CO_2 (fast) - Low End$

The coordinate diagram may look like:



- AH

Notice: \rightarrow STEP 1 has a much higher \underline{E}_A

 $\rightarrow \Delta H$ is **NEGATIVE** for the reaction.

Example 2:

Draw the coordinate diagram, given the following mechanism:

Step 1: $A + B \rightarrow I_1 + C$ (moderate, exothermic)Step 2: $I_1 + B \rightarrow I_2 + D$ (slow, endothermic)Step 3: $I_2 + A \rightarrow C + E$ (fast, exothermic)

Net Rxn: $2A + 2B \rightarrow 2C + D + E$ (slow, exo)

Reaction Coordinate Diagram:



Catalysts:

- **<u>SPEED</u>** up a reaction without being <u>USED</u> <u>UP</u> in the reaction.
- **ENZYMES** are **BIOLOGICAL** catalysts.
- **HOMOGENOUS** Catalysts are in the **SAME PHASE** as the reactants.
- <u>HETEROGENEOUS</u> Catalysts are in a <u>DIFFERENT</u> <u>PHASE</u> as the reactants.

How Catalysts Work:

- Catalysts allow reactions to proceed by a <u>DIFFERENT MECHANISM</u> a new <u>PATHWAY</u>.
- New <u>PATHWAY</u> has a <u>LOWER ACTIVATION ENERGY</u>:



How Catalysts Work:

MORE MOLECULES will have the required Ea:



• Catalysts do not change ΔH , since ΔH is determined by the **BONDS BROKEN** and **FORMED**.

Examples of Catalysts:

- **<u>ENZYMES</u>** in your body
- **CATALYTIC CONVERTERS** in cars
- <u>CFC'S</u> catalyze the reaction of <u>OZONE</u> into <u>OXYGEN</u> gas

Notes:

- They can be <u>INVOLVED</u> in the reaction as a <u>REACTANT</u>, but are NOT <u>USED</u> UP like a reactant.
- After the reaction is <u>OVER</u>, the catalyst is left behind <u>UNCONSUMED</u>.