Potential Energy Profile

A **potential-energy profile** is a diagram used to describe the mechanism of a reaction. This diagram is used to get a better undertanding of Activation Energy and the Arrhenius Equation, as well as to show the changing potential energy between the reactant and product that occur during a chemical reaction.

Potential energy diagram.bmp

1. The potential energy of the reactant.
2. The difference in potential energy between the reactant and the activated complex (also known as the activation energy of the forward reaction).
3. The potential energy of the activated complex (the transition state).
4. The energy difference between the product and the activated complex.
5. The difference in potential energy between the reactant and the product.
6. The potential energy of the product.

For a chemical reaction to begin, there must be a contact (collision) between the reactants. For further details about the reaction rate, go to Definition of A Reaction Rate. As the reaction proceeds, the potential energy rises to a maximum and the reactants form a cluster of atoms, called the activated complex. The highest point on the diagram is the Activation Energy, E_a, the energy that must be overcome for a reaction to occur. After the maximum, the potential energy starts falling as the atoms rearrange in the cluster, until it reaches a certain state of energy. Finally, colliding reactant molecules form products.

The direction of a reversible reaction is determined by the transition state (also known as activated complex). There is a possibility that a collision between reactant molecules may not form products. The outcome depends on the factors mentioned in the Transition State Theory. If the activated complex can pass the barriers, the product forms. Otherwise, the complex falls apart and reverts to the reactants.

The graph above is an example of an Elementary Reaction, a single step chemical reaction with a single transition state. It does not matter whether there are one or more reactants or products. A combination of multiple elementary reactions is called a stepwise reaction. The potential energy diagram of this type of reaction involves one or more Reaction Intermediates. An intermediate is a chemical molecule that is the product of one step of a reaction and is the reactant for the next step.

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The rate law of a stepwise reaction is rather complex when compared to an elementary reaction. However, there is only one slow step, the Rate-determining Step in the reaction. The Rate-determining Step controls the overall rate of the reaction as the overall rate cannot proceed any faster than this rate-limiting step. In the potential energy profile, the Rate-determining Step is the reaction step with the highest energy of transition state (See: Transition State Theory). The diagram below is an example of a stepwise reaction.

intermediate.bmp

For the diagram above, the Rate-determining Step is the first reaction as the first transition state is higher than the second one. There is one intermediate in this reaction.

For the potential energy profile with the help of catalyst see Activation Energy and Gibbs Free Energy. The important thing to note is that catalysts increase the reaction rate by decreasing the activation energy of the reaction but do not affect the potential energy of the reactants and products.

The concept of potential energy and Gibbs Free Energy are related to each other as Gibbs Free Energy, G^0, is actually a chemical potential energy. Both of them can be used to measure how far the reaction is from equilibrium. Here are two types of potential energy profiles based on the free energy:

1. Endergonic reaction

- The potential energy of the product is greater than that of the reactant

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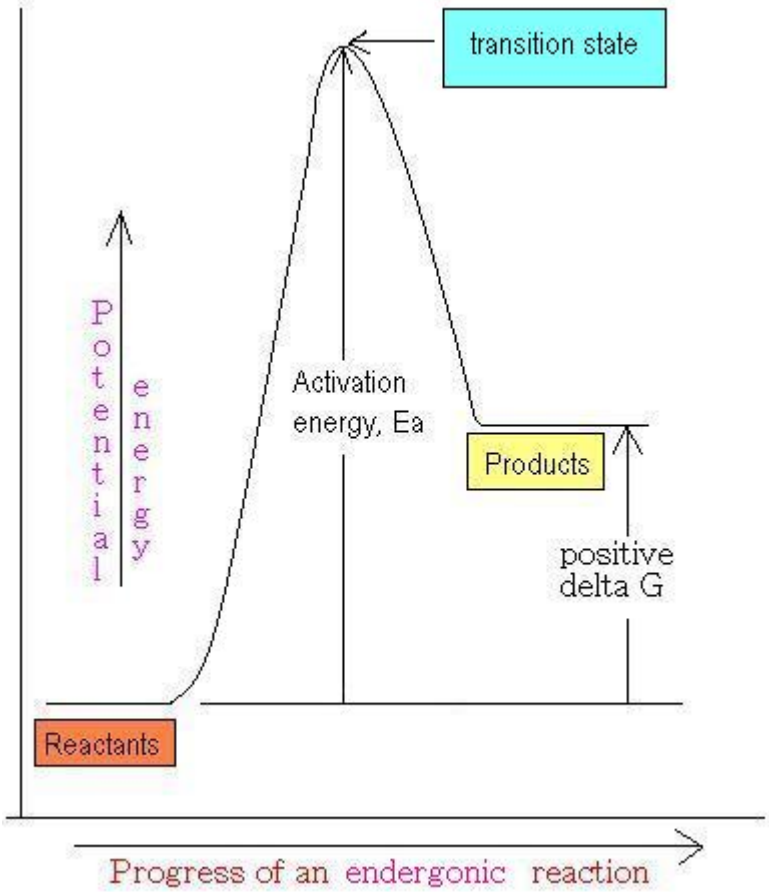
- Since $\Delta G^0 > 0$, the reaction absorbs energy from the environment (energy *put into* the system)



2. Exergonic reaction

- The potential energy of the product is less than that of the reactant
- Since $\Delta G^0 < 0$, the reaction releases energy into the environment (energy *out of* the system)

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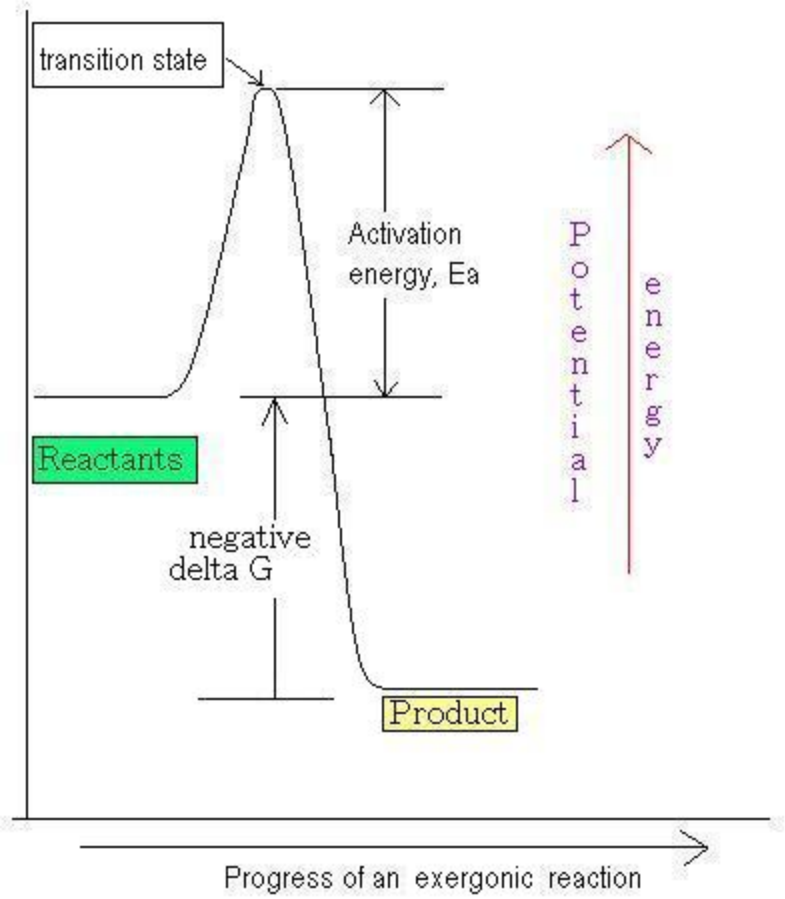

References

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