This page examines simple energy profiles for reactions, and shows how they are slightly different for reactions involving an intermediate, as opposed to just a transition state.

Energy Profiles

Any work involving activation energy or catalysis involves diagram such as the one shown below:

This diagram shows the following:

- Overall, the reaction is exothermic. The products have a lower energy than the reactants, so energy is released when the reaction happens.
- Reactants must possess the right amount of energy (called the activation energy) to overcome the so-called "activation energy barrier."
- In this reaction profile, a catalyst offers a reaction route that requires less activation energy. This causes the reaction to proceed faster.

Graphs like this are known as energy profiles. The diagram above shows that an input of energy is required to initiate the reaction. Once the activation energy barrier is overcome, more energy is released, and thus the reaction is overall exothermic.

For an endothermic reaction, a simple energy profile for a non-catalyzed reaction looks like the figure below:

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This diagram shows the following:

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For an endothermic reaction, a simple energy profile for a non-catalyzed reaction looks like the figure below:
Unfortunately, for many reactions, the real shapes of the energy profiles are slightly different from these, and the rest of this page explores some simple differences. These differences depend on whether the reaction proceeds via a single transition state or an intermediate.

### Energy profiles for reactions with a single transition state

The equation below shows an organic reaction in which a bromine atom is replaced with an OH group in an organic compound. The starting compound is bromoethane, and the product is ethanol.

\[
\text{CH}_3\text{CH}_2\text{Br} + \text{OH}^- \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{Br}^-
\]

During the reaction, one of the lone pairs of electrons on the negatively-charged oxygen atom in the -OH group is attracted to the carbon atom attached to bromine. This is because the bromine is more electronegative than carbon, and so the electron pair in the C-Br bond is slightly closer to the bromine. The carbon atom is consequently partially positively-charged and the bromine partially negative.

As the hydroxide ion approaches the partially-positive carbon, a new bond starts to form between oxygen and carbon. At the same time, the bond between carbon and bromine starts to break as the electrons in the bond are repelled towards the bromine. At some point, the process is exactly half complete. The carbon atom is now half-attached to oxygen and to bromine.
The process completes as the carbon-oxygen bond is fully formed, and the carbon-bromine bond fully broken:

The second species, in which the bonds are half-made and half-broken, is called the transition state, and it is at this point that the energy of the system is at its maximum. This is what is at the top of the activation energy barrier.

The transition state is extremely unstable. Any miniscule change in either direction sends it either forward to the products or back to the reactants. Neither is there anything special about a transition state except that it is the highest-energy complex. It cannot be isolated, even for a very short time. The situation is entirely different if the reaction goes through an intermediate, as discussed in the next section.

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Energy profiles for reactions with intermediates

Consider an alternate reaction between a bromine-containing organic compound and a hydroxide ion. In this case, the organic compound ionizes slightly in a slow reaction to produce an intermediate carbocation. This ion proceeds to react very
rapidly with hydroxide ions.

The difference in this case is that the positively charged organic ion can actually be detected in the mixture. It is very unstable, and soon reacts with a hydroxide ion (or picks up its bromide ion again). But, for however short a time, it is noticeably present in the system. This is shown in the energy profile for the reaction:

The stability (however temporary and fragile) of the intermediate is indicated by the fact that there are small activation barriers to its conversion either into the products or back into the reactants again.

Notice that the barrier on the product side of the intermediate is lower than that on the reactant side. That means that there is a greater chance of it converting into products. A greater amount of energy is required to convert it back to the reactants.

The peaks labeled "ts1" and "ts2" represent transition states between the intermediate and either the reactants or the products. During either conversion, there is some arrangement of the atoms that causes an energy maximum.

It is perfectly possible to get reactions which take several steps, passing through a number of different intermediates and transition states. In cases like this, a whole "mountain range" of peaks is observed, some of which might be simple transition states, and others with the little dips representing intermediates.

Contributors

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