Fundamentals of catalysis

Ostwald's interpretation of the phenomenon of catalysis already corresponded to the modern definition in significant aspects:

"A catalyst is a substance which – without itself being consumed to a significant degree in the reaction – increases the rate of formation of reaction products."

The action of a catalyst is based on the fact that it provides a chemical reaction with a new route by which the starting materials can be converted more easily to the end products. In Döbereiner's lighter, such a route is found in the "contact" of hydrogen and oxygen with the platinum catalyst; without catalysts, these gases do not react (or more accurately, react infinitely slowly) to give water. The molecules of the starting materials in the uncatalyzed reaction thus behave like climbers who are crossing a mountain range slowly and laboriously at the highest point. They could get over into the neighboring valley more rapidly by a longer route over a lower pass height. This longer and more complicated but faster route is a representation of the catalyzed reaction.

In an uncatalyzed chemical reaction, the high mountain range corresponds to the high energy barrier that the starting materials have to overcome on their way to the products. This energy barrier is referred to as the activation energy. In the reaction example in Figure 2.6, the product B is lower on the energy scale than the starting material A. In this chemical conversion, heat of reaction is thus released, just as already described by Döbereiner in the combination of hydrogen with oxygen to give water. Such reactions are called exothermic. In industrial processes, this energy can frequently be utilized and the overall energy balance can be improved in this way.

Without catalyst, the high energy barrier E_A has to be overcome in the conversion of A to B; the reaction will thus proceed comparatively slowly. The presence of a suitable catalyst results in a chemical interaction between it and the starting material (state X) and later in the reaction between it and the product B (state Y).

$$A \xrightarrow{+cat} X \longrightarrow Y \xrightarrow{-cat} B$$

A characteristic feature of the catalyzed reaction route is the lower energy barrier E_A, cat between the states X and Y compared to E_A. The interactions of starting material A and product B with the catalyst lead us to think of the "strange contact effects" spoken of by Döbereiner. In many cases, we can now describe these interactions very well at the molecular level.

One example is the catalytic decomposition of nitrogen monoxide over a solid surface to give nitrogen and oxygen (Figure 2.7), a reaction which plays a role in the catalytic cleaning of exhaust gases and flue gases. The nitrogen monoxide molecules diffuse to the catalyst surface and are adsorbed there; this corresponds to state X in Figure 2.6.
At the surface, the bond between nitrogen and oxygen

$$2\,NO \xrightarrow{solid} N_2 + O_2$$

is broken, and the nitrogen and oxygen atoms form bonds with

Fig. 2.6 ENERGY PROFILE OF A REACTION WITH AND WITHOUT A CATALYST.

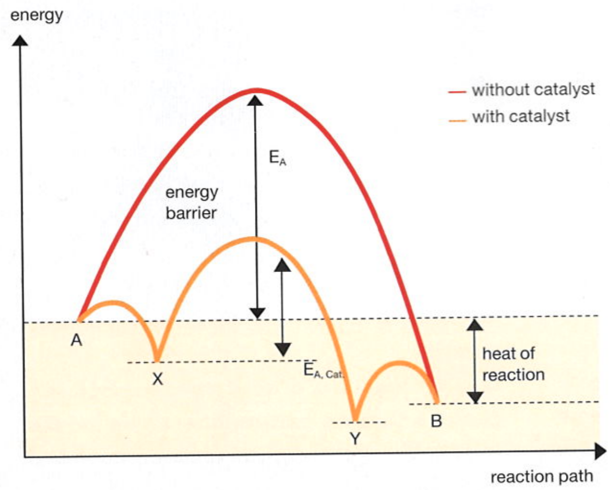

Fig. 2.7 THE DECOMPOSITION OF NITRIC OXIDE ON A CATALYST SURFACE.