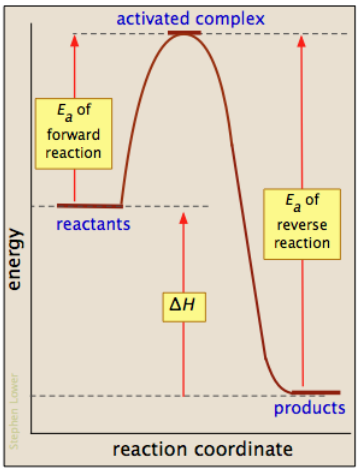
9.17: Basics of Reaction Profiles

Most reactions involving neutral molecules cannot take place at all until they have acquired the energy needed to stretch, bend, or otherwise distort one or more bonds. This critical energy is known as the *activation energy* of the reaction. *Activation energy diagrams* of the kind shown below plot the total energy input to a reaction system as it proceeds from reactants to products.



In examining such diagrams, take special note of the following:

- The "*reaction coordinate*" plotted along the abscissa represents the changes in atomic coordinates as the system progresses from reactants to products. In the very simplest elementary reactions it might correspond to the stretching or twisting of a particular bond, and be shown to a scale. In general, however, the reaction coordinate is a rather abstract concept that cannot be tied to any single measurable and scalable quantity.
- The *activated complex* (also known as the *transition state*) represents the structure of the system as it exists at the peak of the activation energy curve. It does *not* correspond to an identifiable intermediate structure (which would more properly be considered the product of a separate elementary process), but rather to whatever configuration of atoms exists during the collision, which lasts for only about 0.1 picosecond.
- Activation energy diagrams always incorporate the energetics (ΔG or ΔH) of the net reaction, but it is important to understand that the latter quantities depend solely on the thermodynamics of the process which are always independent of the reaction pathway. This means that the same reaction can exhibit different activation energies if it can follow alternative pathways.
- With a few exceptions for very simple processes, activation energy diagrams are largely conceptual constructs based on the standard *collision model* for chemical reactions. It is unwise to read too much into them.

Contributors and Attributions

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