❖ Potential Energy Diagrams: Transition States and Intermediates

The potential energy diagrams or the reaction progress curves are nothing but a visual representation of the energy changes that occur during a chemical reaction. The energy of various species participating in the reaction is plotted on the *y*-axis (ordinate) whereas the progress of the reaction on the *x*-axis (abscissa). Now since a reaction can have transition states and intermediates (in addition to the reactants and final product), we must discuss the corresponding potential energy diagrams.

➢ *Potential energy Diagram of Reactions with Reactant, Product and Transition State*

The transition state of an organic reaction is a specific configuration along the reaction coordinate and corresponds to the highest potential energy along with this reaction coordinate. Furthermore, the transition state is not an actual molecule that can be isolated, and therefore it is often marked with the double dagger or star symbol to differentiate. The typical potential energy diagrams of endothermic and exothermic reactions with reactants, products, and transition states are shown below.

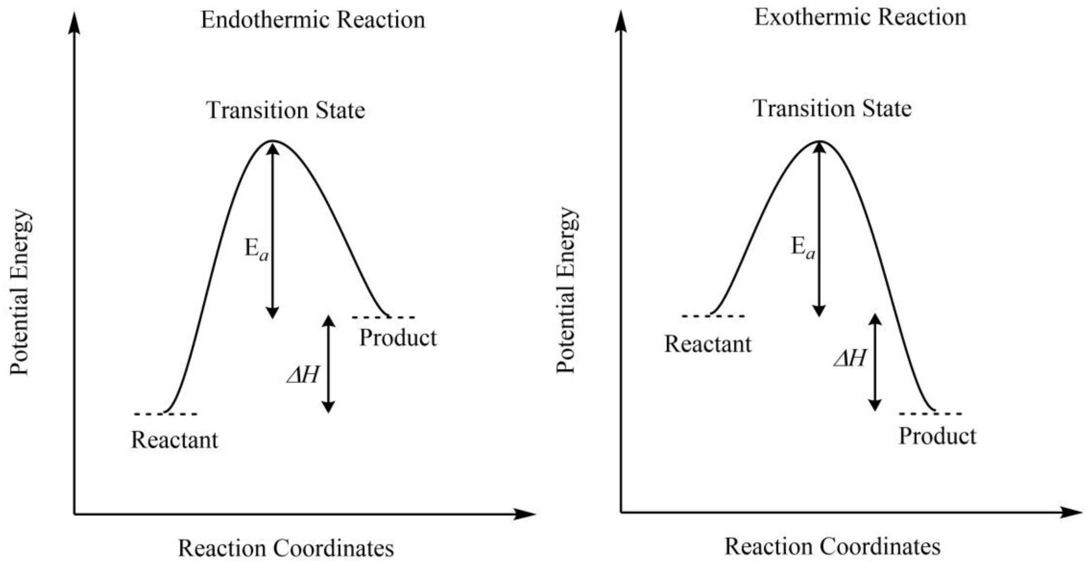

Figure 7. Typical potential energy curves for exothermic and endothermic reactions.

It is obvious from the potential energy diagrams that the enthalpy change is positive for an endothermic reaction (ΔH > 0) and negative for an exothermic reaction (ΔH > 0). For exothermic reactions, the potential energy of the reacting species first increases, attains a maximum at the transition state, and then decreases even more than the reactants. For endothermic reactions, the potential energy of the reacting species first increases, attains a maximum at the transition state, and then decreases less than the reactants.

Furthermore, it should also be noted that the energy gap between the transition state and reactant is the activation energy (E_a) which is responsible for the speed of the reaction. The higher activation energy leads to slow transformation and vice-versa.

➢ ***Potential energy Diagram of Reactions with Reactant, Product, Transition State, and Intermediates***

The chemical species that are formed somewhere during the course of a chemical reaction are called as reaction intermediates. Unlike transition states, these are actual molecules that are short-lived and unstable. Sometimes they are called temporary reactants or products because they are neither present in actual reactants nor the actual products. The typical potential energy diagram of a typical exothermic reaction with a reactant, product, intermediate, and transition state is shown below.

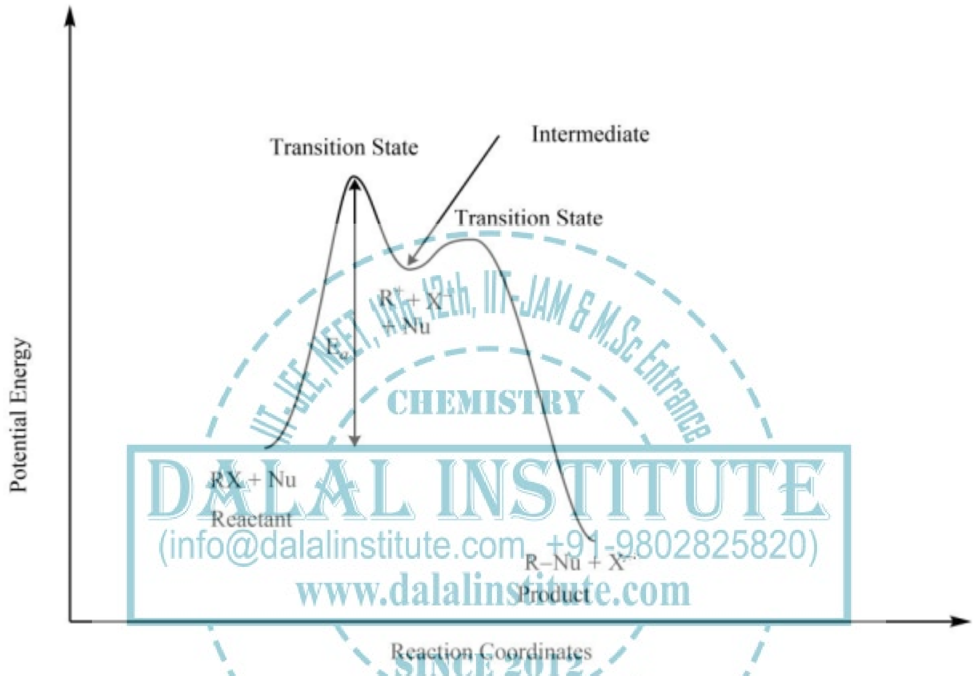

Figure 8. Potential energy diagram for the SN_1 reaction.

It is obvious from the potential energy diagrams that the intermediates are situated at the minima whereas the transition states are shown at the maxima. Also, just like the previous case, the energy gap between the transition state and reactant is the activation energy (E_a) which is responsible for the speed of the reaction i.e. the higher activation energy leads to slow transformation and vice-versa.

Reaction coordinate diagrams also give information about the equilibrium between a reactant or a product and an intermediate. If the barrier energy for going from intermediate to product is much higher than the one for the reactant to intermediate transition, it can be safely concluded that a complete equilibrium is established between the reactant and intermediate. Nevertheless, if the reactant-to-intermediate barrier is almost equal in energy to intermediate-to-product change, then no full equilibrium is set and steady-state approximation becomes activated to dictate the kinetic rate expressions.

International Edition

A TEXTBOOK OF ORGANIC CHEMISTRY

Volume I

MANDEEP DALAL

First Edition

DALAL INSTITUTE

Table of Contents

Mandeep Dalal
(M.Sc, Ph.D, CSIR UGC – NET JRF, IIT-GATE)
Founder & Educator, Dalal Institute
E-Mail: dr.mandeep.dalal@gmail.com
www.mandeepdalal.com

Mandeep Dalal is an Indian research scholar who is primarily working in the field of Science and Philosophy. He received his Ph.D in Chemistry from Maharshi Dayanand University, Rohtak, in 2018. He is also the Founder of "Dalal Institute" (India's best coaching centre for academic and competitive chemistry exams), the organization that is committed to revolutionize the field of school-level and higher education in Chemistry across the globe. He has published more than 40 research papers in various international scientific journals, including mostly from Elsevier (USA), IOP (UK), and Springer (Netherlands).

Other Books by the Author

A TEXTBOOK OF INORGANIC CHEMISTRY – VOLUME I, II, III, IV

A TEXTBOOK OF PHYSICAL CHEMISTRY – VOLUME I, II, III, IV

A TEXTBOOK OF ORGANIC CHEMISTRY – VOLUME I, II, III, IV

ISBN: 978-81-952427-3-3
9 788195 242733
MRP: Rs 800.00

DALAL INSTITUTE
..... Chemical Science Demystified .....
Main Market, Sector 14, Rohtak, Haryana 124001, India
(info@dalalinstitute.com, +91-9802825820)
www.dalalinstitute.com