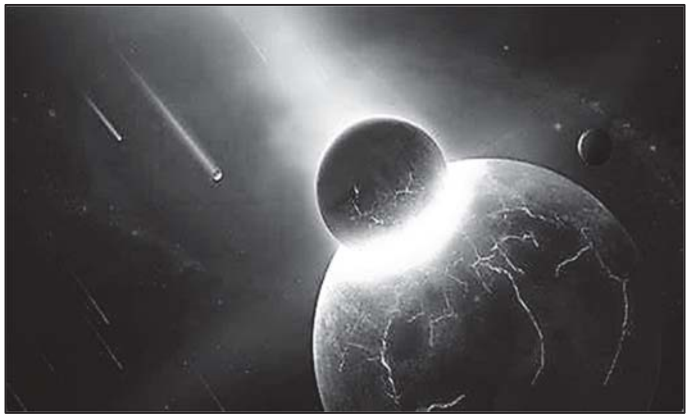
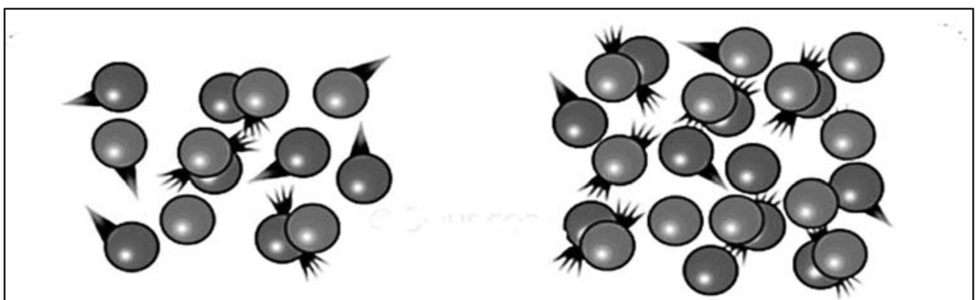
COLLISION THEORY (part I)



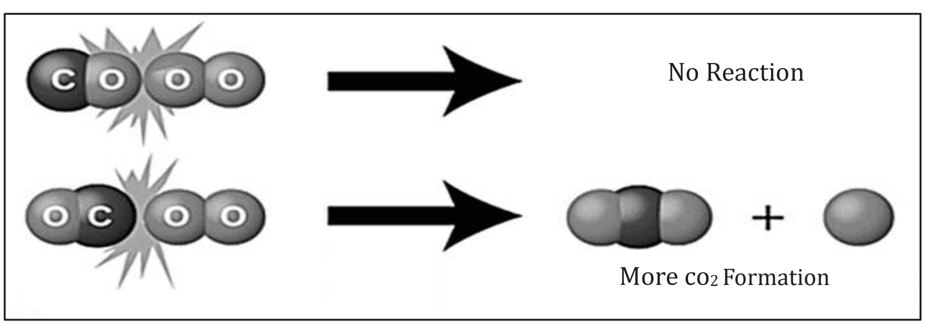
The collision theory asserts that a chemical reaction occurs only when particles collide, meaning they come into contact with each other. However, it is crucial to note that the collision between reactant particles is a necessary condition but not sufficient for a reaction to occur; the collisions must also be effective. Understanding the precise characteristics of an effective collision is vital because it dictates whether particles will react with each other and produce new products.

Molecular Collisions

The higher the number of molecules present, the greater the frequency of collisions. For a reaction to commence, molecules must first collide. To ensure an effective initiation of a reaction, these collisions need to possess adequate energy, specifically kinetic energy, to facilitate bond disruption. With an increase in temperature, molecules exhibit faster movement and engage in more forceful collisions, significantly enhancing the probability of bond cleavages and rearrangements. In the case of reactions involving neutral molecules, they are often unable to occur until they acquire the activation energy required to stretch, bend, or otherwise distort one or more bonds.



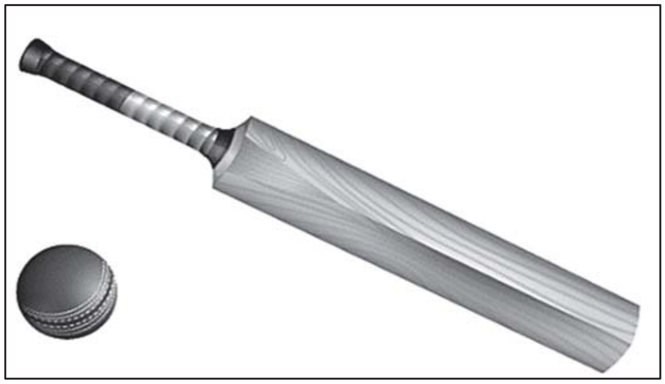
Low concentration = Few collisions High concentration = More collisions



Model

Collision theory

In the image provided, Reactant A is symbolized by the cricket bat, while Reactant B is represented by the cricket ball. The success of the reaction hinges on the batter hitting a boundary. If the batter fails to achieve this, the reaction is deemed unsuccessful.



Scenario 1: The bowler delivers a fastball down the middle of the pitch, and the batsman takes a powerful swing but completely misses the ball.

Scenario 2: The bowler opts for an off-speed delivery, and the batsman cautiously checks his swing. The batsman manages to make slight contact with the ball, causing it to dribble in front of his feet and into foul territory.

Scenario 3: The bowler throws a curveball that seems poised to catch the outside corner of the pitch. The batsman swings forcefully, but the bat grazes the underside of the ball, sending it skewing to the right and flying into the crowd. The umpire declares, "Foul ball, still two strikes!"

Scenario 4: The bowler bowls another pace delivery down the middle of the pitch. The batsman swings and smashes the ball high into the air, clearing the center field wall marked at 410 feet. The umpire signals a six.

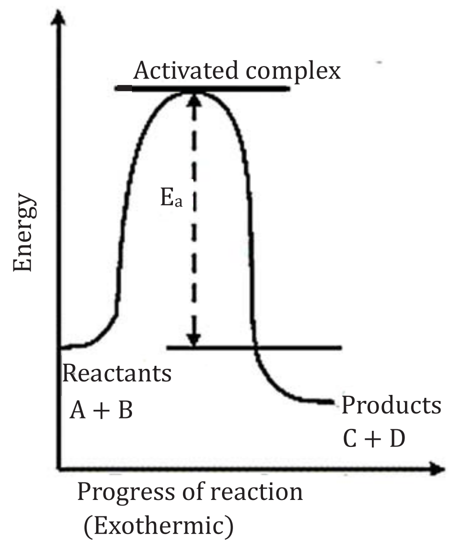
Collision Theory (part II)

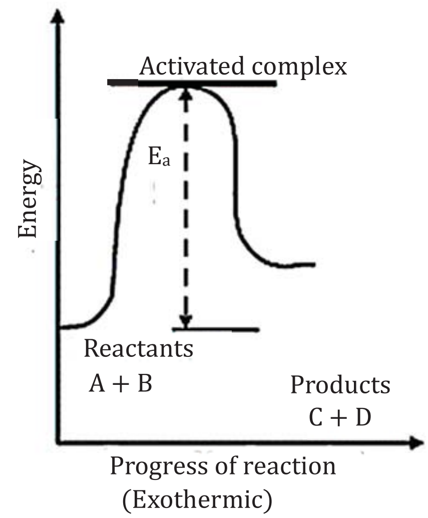
In accordance with collision theory, a reaction occurs due to the collision of molecules. The quantity of collisions per second per unit volume of the reaction mixture is termed collision frequency. At standard temperature and pressure, the collision frequency reaches remarkably high values (approximately 10^{25} to 10^{26} in a gaseous reaction). If all these collisions were effective, the reaction would theoretically be completed in a fraction of a second. However, in practical terms, this is not the case. This discrepancy is elucidated based on two factors.

(i) Energy factor

To ensure the effectiveness of a collision, the colliding molecules must possess energy exceeding a specific threshold. The minimum energy required for colliding molecules to achieve an effective collision is referred to as threshold energy. Therefore, at standard temperature and pressure, the majority of molecules may not have energy equal to or greater than this threshold value.

Collisions involving high-energy molecules can overcome repulsion, leading to the formation of an unstable molecule cluster known as the activated complex.





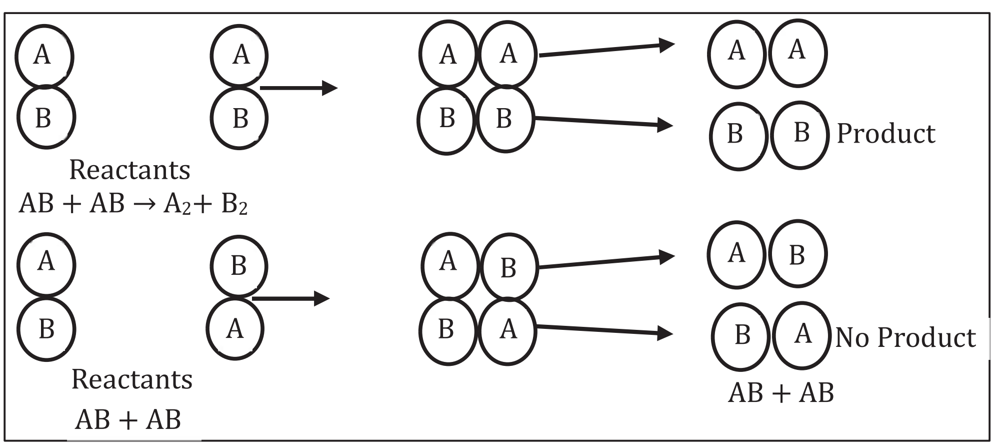
In every chemical reaction, whether exothermic or endothermic, an energy barrier must be surmounted before reactants can undergo transformation into products. Provided that the reactant molecules possess sufficient energy, they can ascend to the peak of the energy barrier following a collision, leading to the conversion into products. When the activation energy for a reaction is low, the proportion of effective collisions is substantial, resulting in a fast reaction. Conversely, with a high activation energy, the fraction of effective collisions is diminished, leading to a slower reaction. Increasing the temperature augments the number of active molecules, thereby elevating the count of effective collisions and consequently accelerating the reaction rate.

Activation energy Ea = E(activated complex) – E(ground state)

ΔH = activation energy of forward reaction − activation energy of backward reaction.

(ii) **Orientation factor**

In certain instances, it is observed that despite a higher number of colliding molecules possessing energy exceeding the threshold value, the reaction remains slow. This is attributed to the improper orientation of the colliding molecules at the moment of collision.



Rate of reaction is directly proportional to the number of effective collisions.

$$\text{Rate} = \frac{dx}{dt} = \text{Collision frequency} \times \text{fraction of effective molecules}$$

$$= z \times f$$

According to kinetic theory of gases, the fraction of molecules having energy more than a particular value, E at temperature T is given by

$$f = e^{-E_a/RT}$$

$$\text{Rate } = Ze^{-E_a/RT}$$

As rate of reaction is directly related to rate constant K, we can also write $K = Ze^{-E_a/RT}$