Types of Composite Reactions

(1) Simultaneous Reactions

$$A \rightarrow Y$$
$$A \rightarrow Z$$

Two products can be obtained from same set of reactants

or
$$A + Y \rightarrow B$$
$$A + Y \rightarrow C$$

Sometimes there may be reactant competition.

$$A + B \rightarrow Y$$
$$A + C \rightarrow Z$$

where B and C compete with A for reaction

(2) Opposing reactions

$$A + B \rightleftharpoons Z$$

when the reaction takes place in both forward and backward directions

(3) Consecutive reactions:

$$A \rightarrow X \rightarrow Y \rightarrow Z$$

When the reaction proceeds with multisteps before final product formation

Rate equation for composite reaction:

For composite reaction

$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} X \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} Z$$

There can be four elementary reactions and their rate is given as

$$V_1 = k_1 [A]$$
$$V_{-1} = k_{-1} [X]$$
$$V_2 = k_2 [X]$$
$$V_{-2} = k_{-2} [Z]$$

for intermediate X total rate of formation

$$V_X = V_1 + V_{-2}$$

$$= k_1 [A] + k_{-2} [Z]$$

and total rate of X consumption is

$$V_{-X} = V_{-1} + V_2$$
$$= k_{-1}[X] + k_2 [X]$$

$$= [(k_{-1}) + k_2] [X]$$
$$= (k_{-1} + k_2) [X]$$

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Now for consecutive reaction we have

$$A \xrightarrow{k_1} X \xrightarrow{k_2} Z$$

for if initial concentration of [A] is $[A]_0$. The rate of reaction for A is

$$V_1 = \frac{d[A]}{dt} = k_1 [A]$$

Integration of this term in boundary condition $[A] = [A]_0$ for $t = 0$

$$[A] = [A]_0 \, e^{-k_1 t}$$

For the rate of formation of [X]

$$\frac{d[X]}{dt} = k_1 [A] - k_2 [X]$$

$$= k_1 [A]_0 \, e^{-k_1 t} - k_2 [X]$$

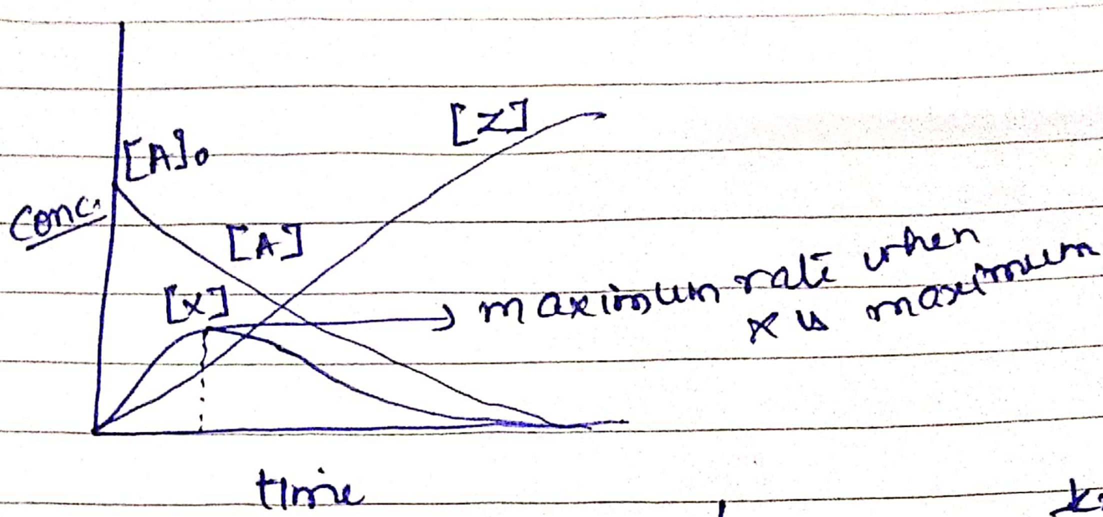
On integrating we get

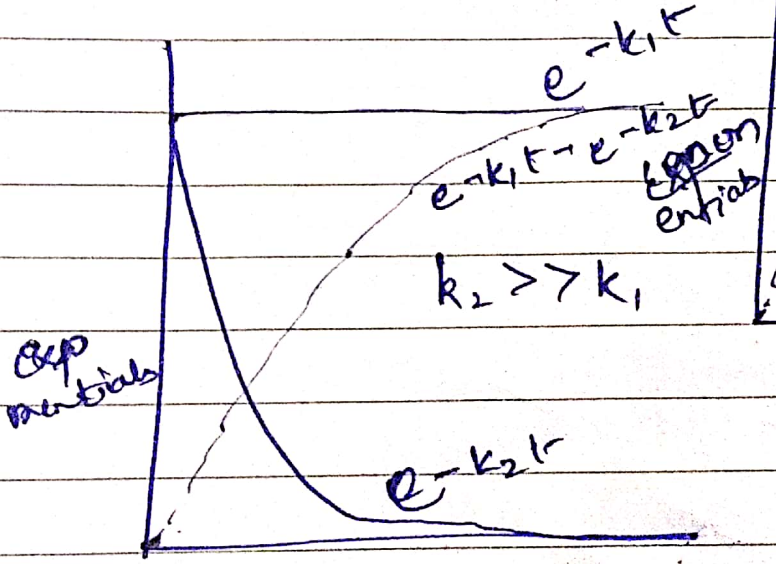
$$[X] = [A]_0 \frac{k_1}{k_2 - k_1} \left(e^{-k_1 t} - e^{-k_2 t} \right)$$

$$[A] + [X] + [Z] = [A]_0$$

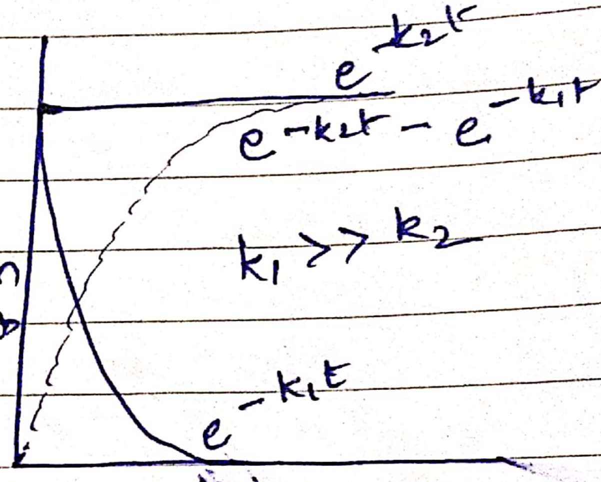
so $[Z] = [A]_0 - [A] - [X]$

$$[Z] = \frac{[A]_0}{k_2 - k_1} \left[k_2 (1 - e^{-k_1 t}) - k_1 (1 - e^{-k_2 t}) \right]$$





(1)



(2)

The graph shows that formation of [Z] is proportional to the concentration of X. The rate is zero when [X] = 0 and reaches maximum for maximum value of [X].

Graph (1) and (2) shows two limiting conditions.