Applications of Factorial Function $(\alpha)_{n=1}$ in determination of Specific Reaction Rate and Half Life Period

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Abstract: In this research paper, specific reaction rates of first order, second order; third order and m^{th} order reactions are represented in terms of factorial function. These results would be further applied to obtain half life period as a particular case in application section.

Keywords: Factorial function, Order of reaction, Specific Reaction Rate (or velocity constant or rate constant), half life period.

I. Introduction

The factorial function is defined by Earl D. Rainville [4] (P.22) in following manner

$$(\alpha)_n = \prod_{k=1}^{n}(\alpha + k - 1)$$
$$= \alpha(\alpha + 1)(\alpha + 2)........(\alpha + n - 1), \quad n \geq 1 \qquad \text{... (1.1)}$$

So that,
$$(\alpha)_0 = 1$$
And
$$(\alpha)_1 = \alpha$$

II. Specific Reaction Rate

In this section we shall give specific reaction rate of first order, second order, third order and m^{th} order reactions in terms of Arrhenius hypothesis.

Specific reaction rate for first order reaction
Here rate of reaction is determined by change of one concentration term only.

$$A \longrightarrow Products$$

Let a be the concentration of A at the start and after time t, the concentration becomes (a-x),
i.e., x has been changed into products. The rate of reaction after time t is given by the expression,

$$\frac{dx}{dt} \propto (a - x)$$

Or

$$\frac{dx}{a - x} = k_1 dt \qquad \text{... (2.1)}$$

Where, k_1 = First order velocity constant (unit being s^{-1})

Specific reaction rate for second order reaction
Here rate of reaction is determined by variation of two concentration terms.

$$A + B \longrightarrow Products$$

Let a be the concentration of A and b be the concentration of B at the start and after time t, the concentration becomes (a-x) for A and (b-x) for B,
i.e., x of both reactants has been changed into products. The rate of reaction after time t is given by the expression,

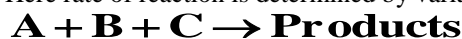$$\frac{dx}{dt} \propto (a-x)(b-x)$$

Or

$$\frac{dx}{(a-x)(b-x)} = k_2 dt \qquad \qquad \dots (2.2)$$

Where, k_2 = Second order velocity constant (unit being $\left[\frac{lt}{mol}\right](s)^{-1}$)

Specific reaction rate for third order reaction
Here rate of reaction is determined by variation of three concentration terms.

$$A + B + C \rightarrow Products$$

Let a be the concentration of A, b be the concentration of B and c be the concentration of C at the start and after time t, the concentration becomes (a-x) for A, (b-x) for B and (c-x) for C
i.e., x of all three reactants has been changed into products. The rate of reaction after time t is given by the expression,
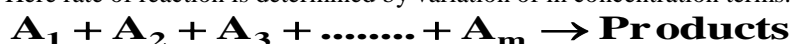
$$\frac{dx}{dt} \propto (a-x)(b-x)(c-x)$$

Or

$$\frac{dx}{(a-x)(b-x)(c-x)} = k_3 dt \qquad \qquad \dots (2.3)$$

Where, k_3 = Third order velocity constant (unit being $\left[\frac{lt}{mol}\right]^2 (s)^{-1}$)

Specific reaction rate for reaction of order m
Here rate of reaction is determined by variation of m concentration terms.

$$A_1 + A_2 + A_3 + \dots\dots + A_m \rightarrow Products$$

Let a_1 be the concentration of A_1, a_2 be the concentration of A_2, a_3 be the concentration of A_3 and a_m be the concentration of A_m at the start and after time t, the concentration becomes (a_1 -x) for A_1, (a_2 -x) for A_2 (a_3 -x) for A_3 and (a_m -x) for A_m.
i.e., x of all m reactants has been changed into products. The rate of reaction after time t is given by the expression,

$$\frac{dx}{dt} \propto (a_1-x)(a_2-x)(a_3-x)\dots\dots(a_m-x)$$

Or

$$\frac{dx}{(a_1-x)(a_2-x)(a_3-x)\dots\dots(a_m-x)} = k_m dt \qquad \qquad \dots (2.4)$$

Where, k_m = m^{th} order velocity constant (unit being $\left[\frac{lt}{mol}\right]^{m-1}(s)^{-1}$)

III. Representing specific reaction rate in terms of factorial function for n=1

(i)First Order Reaction
From (2.1)

$$\int \frac{dx}{(a-x)_{n=1}} = k_1(t)_{n=1} + c_1 \qquad \text{... (3.1)}$$

Where, k_1 = First order velocity constant

(ii)Second Order Reaction
From (2.2)

$$\int \frac{dx}{(a-x)_{n=1}(b-x)_{n=1}} = k_2(t)_{n=1} + c_2 \qquad \text{... (3.2)}$$

Where, k_2 = Second order velocity constant

(III) Third Order Reaction
From (2.3)

$$\int \frac{dx}{(a-x)_{n=1}(b-x)_{n=1}(c-x)_{n=1}} = k_3(t)_{n=1} + c_3 \qquad \text{... (3.3)}$$

Where, k_3 = Third order velocity constant

(iv) m^{th} Order Reaction
From (2.4)

$$\int \frac{dx}{(a_1-x)_{n=1}(a_2-x)_{n=1}(a_3-x)_{n=1}......(a_m-x)_{n=1}} = k_m(t)_{n=1} + c_m$$
$$\text{... (3.4)}$$

Where, k_m = m^{th} order velocity constant

IV. Half Life Period of Reactions

In this Section we will discuss some particular cases of section 3 in form of determination of half life period of reactions of various orders by using factorial function $(\alpha)_{n=1}$ only.

(i) Half Life Period for first order reaction
In eqn (3.1) put t=T and (a-x) = $\frac{a}{2}$, where T is half life period, Thus we obtain.

$$(T)_{n=1} = \frac{1}{k_1} \int \frac{dx}{\left(\frac{a}{2}\right)_{n=1}}$$

$$= \frac{1}{\left(\frac{a}{2}\right)_{n=1}} \frac{x}{k_1} \qquad \text{... (4.1)}$$

Where, k_1 = First order velocity constant

(ii) Half Life Period For second order reaction

In eqn (3.2) put t=T, b=a and (a-x) = $\dfrac{a}{2}$, where T is half life period, Thus we obtain.

$$(T)_{n=1} = \frac{1}{k_2} \int \frac{dx}{\left(\dfrac{a}{2}\right)_{n=1}\left(\dfrac{a}{2}\right)_{n=1}}$$

$$= \frac{1}{\left[\left(\dfrac{a}{2}\right)_{n=1}\right]^2} \frac{x}{k_2} \qquad \dots (4.2)$$

Where, k_2 = Second order velocity constant

(iii) Half Life Period For third order reaction

In eqn (3.3) put t=T, b=a=c and (a-x) = $\dfrac{a}{2}$, where T is half life period, Thus we obtain.

$$(T)_{n=1} = \frac{1}{k_3} \int \frac{dx}{\left(\dfrac{a}{2}\right)_{n=1}\left(\dfrac{a}{2}\right)_{n=1}\left(\dfrac{a}{2}\right)_{n=1}}$$

$$= \frac{1}{\left[\left(\dfrac{a}{2}\right)_{n=1}\right]^3} \frac{x}{k_3} \qquad \dots (4.3)$$

Where, k_3 = Third order velocity constant

(iv) Half Life Period For m^{th} order reaction

In eqn (3.4) put t=T, $a_1 = a_2 = a_3 = \dots\dots = a_m$ and $\left(a_1 - x\right) = \dfrac{a_1}{2}$ where T is half life period, Thus we obtain.

$$(T)_{n=1} = \frac{1}{k_m} \int \frac{dx}{\left(\dfrac{a_1}{2}\right)_{n=1}\left(\dfrac{a_1}{2}\right)_{n=1}\overset{m-times}{\dots\dots}\left(\dfrac{a_1}{2}\right)_{n=1}}$$

$$= \frac{1}{\left[\left(\dfrac{a_1}{2}\right)_{n=1}\right]^m} \frac{x}{k_m} \qquad \dots (4.4)$$

Where, k_m = m^{th} order velocity constant

V. Proof

Equations (2.1), (2.2), (2.3) and (2.4) may be established by using factorial function of (1.1).

VI. Summary

In this research article we have obtained the values of velocity constants and half life period of a reaction by using factorial function which is true for fractional part of reactant and minute fraction of time. This serves as a new technique to obtain values of velocity constants and half life period of a reaction against the previously used integration method or logarithmic method to obtain the values of velocity constants and half life period of a reaction.

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