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Algebraic Interpolating Polynomials of Theobromine Using Numerical Techniques

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Abstract--- *Here applying the known numerical techniques, algebraic interpolating polynomials are derived for Theobromine which is oxidized by potassium permanganate in alkaline medium. The kinetics was measured using uv-visible spectrophotometer. The ionic strength was maintained at 0.05 mol/dm3. For the study, it was observed to be a 1st order reaction with respect to concentration of substrate and oxidant. A complex formed in the intermediate step decomposes slowly to form free radicals. The free radicals which are generated reacts further to form final product which is identified by spot test and spectral studies.*

Keywords--- *Theobromine, Spectroscopy, Oxidation, Interpolatio, Polynomials.*

I. INTRODUCTION

The very basic reactions like oxidation and reduction reactions are very vital reactions in environment and said to be the key transformers in the synthesis of many organic compounds. Many alkaloids added as well as present in our food items gets oxidizes and add to body defensive power. Theobromine, **(**3,7-Dimethylxanthine**)**, also known as xantheose, having a chemical formula $C_7H_8N_4O_2$, is an alkaloid of the cacao plant. Naturally occurring in chocolate, and in many other foods, which includes tea plant leaves and the kola (or cola) nut. It has similarity with caffeine in physiological effects. Xanthine alkaloid is a classification of theobromine, which also includes the similar compounds theophylline and caffeine. Regardless of its name, the compound does not contain any bromine—*theobromine* is derived from *Theobroma*, the name of the genus of the cacao tree. Fig. 1. gives its structure. This has been utilized to treat the common conditions like cough, which affects the vast majority of people lives [1].

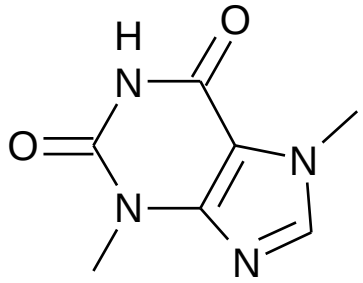

Fig. 1: Chemical Structure of Theobromine MW: 180.17, Formula: $C_7H_8N_4O_2$

This alkaloid has a diuretic, stimulant and relaxing effect. It can dilate the blood vessels and thus can lower the blood pressure [2]. The heart workload can be reduced by smoothening of muscle tissue, thereby reducing adverse effect on cardiac function. Occurrence: Theobromine commonly found in chocolate bar. Chocolate is made from the cocoa bean, which is a natural source of theobromine. A variety of plants like tea and guarana contains theobromine.

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A simple and an effective method in confirming the complex formation and structure is absorption spectral studies [3]. Potassium permanganate is the oxidant preferred in the present study, which is eco-friendly and multi-electron, commonly used oxidizing agent [4-11].The pH of the medium governs the mechanisms [12].

In this current paper, Numerical technique like interpolation was used for the experimental data obtained from the variation studies of substrate, oxidant and temperature. A technique of estimating the value of an unknown function for any intermediate value of the independent variable is called Interpolation. Applying interpolation formulae for equal intervals and unequal intervals [14], we derived algebraic interpolating polynomials.

II. EXPERIMENTAL PART

A. Materials and Reagents

Theobromine-Accurate amount was weighed, recrystallized, dissolved in required volume of sodium hydroxide for stock solution. Oxidant- weighed amount of potassium permanganate dissolved in distilled water, standardized [13]. Sodium hydroxide solution was used to provide the required alkalinity.

Instrument used: A double beam UV/VIS spectrophotometer with PC compatibility was used to study the absorbance study, processing and data interpretation. Water bath used to sustain the temperature to an accuracy of $\pm 0.5^{o}C$.

B. Kinetic Measurements

The absorbance variation was monitored using spectrophotometer with fully thermostatted cell compartment for the kinetic measurements. Stoppered glass boiling tubes covered with black paper are used to prevent photochemical effects which are applied for all kinetic measurements. A known excess of theobromine over permanganate concentration was maintained (called Pseudo first order conditions) at the normal room temperature.

Suitable amount of all the reactants that is theobromine, KOH and water added to keep the total volume constant were equilibrated at constant temperature ($\pm 0.1^{o}C$). Accurate amount of permanganate solution also pre-equilibrated at the same temperature was rapidly added to the reactants. The absorbance of unreacted permanganate in the reaction mixture helped the study of progress of the reaction followed by measured values kept in 1 cm cell in a thermostatted compartment of a Systronics UV-Vis spectrophotometer at its maximum absorbance of 510 nm as a function of time.

III. RESULTS AND DISCUSSION

A. Variation of Theobromine

Various sets of concentrations of substrate (Theobromine) in 0.5 mol dm^{-3}NaOH were kept in a closed container under nitrogen atmosphere at $25^{o}C$, to each set $2.5x10^{-4}$ M potassium permanganate was added. $KMnO_4$ concentration was assayed by measuring the absorbance at 510 nm.

Table 1: Shows the Variation in Absorbance for various Concentration of Theobromine.

x	0.0025	0.0050	0.01	0.02	0.03
y	0.314	0.342	0.238	0.198	0.184

Where x denotes Theobromine Concentration in Molar and y denotes Absorbance. It was noted that when

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$C_7H_8N_4O_2$ concentration increases, absorbance also increases.

Interpolation formula for unequal intervals: By using the Newton's divided difference formula or Newton's general interpolation formula

$$y = f(x) = f(x_0) + (x - x_0)f(x_0, x_1) + (x - x_0)(x - x_1)f(x_0, x_1, x_2) + \ldots$$

We get the interpolating polynomial as

$$f(x) = 12633080.5\,x^4 - 165930.779\,x^3 - 4126.3675\,x^2 + 46.4464\,x + 0.2258$$

B. Variation of time

The effect of time on the reaction was monitored with the help of instrument spectrophotometer. At theobromine concentration of 0.01 N and potassium permanganate concentration 2.5×10^{-4} M and 0.5 mol dm^{-3} NaOH, the Table 2: shows the absorbance monitored for various time as given.

Table 2: Shows the Absorbance Monitored for various Time as given

x	0	5	10	15	20	25	30	35	40
y	0.420	0.342	0.300	0.266	0.238	0.222	0.201	0.183	0.168

Where x denotes the time in minutes and y denotes Absorbance. It was observed that when time increases, absorbance decreases.

Interpolation formula for equal intervals: By using the Forward difference interpolation formula or Newton's forward interpolation formula $y_r = y_0 + r\,\Delta y_0 + \frac{r(r-1)}{2!}\Delta^2 y_0 + \ldots$

where $x = x_0 + rh$, r is any real number and h is the step length.

We get the interpolating polynomial as

$$f(x) = -0.00000006\,x^5 + 0.000005\,x^4 - 0.000153\,x^3 + 0.002204\,x^2 - 0.02348\,x + 0.420$$

C. Variation of Potassium Permanganate

For a fixed concentration of theobromine 0.01 N and 0.5 $moldm^{-3}$ NaOH , potassium permanganate concentration was varied and the absorbance change was monitored using spectrophotometer and noted as given in Table. 3.

Table 3

x	0.00005	0.00015	0.00025	0.0005	0.00075
y	0.159	0.199	0.238	0.576	0.806

Where x denotes the concentration of potassium permanganate and y denotes Absorbance. As the concentration of potassium permanganate increases, the absorbance increases steadily.

Applying the Newton's general interpolation formula, we get the interpolating polynomial as

$$f(x) = -17487142900000\,x^4 + 22831833400\,x^3 - 7788690\,x^2 + 1303.139\,x + 0.1105701$$

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IV. CONCLUSION

Applying the Numerical Techniques like Newton's forward and divided difference interpolation formulae, cross verified and satisfied the experimental datas of theobromine by using potassium permanganate in the variational studies of theobromine. Work can be extended further using the available experimental data.

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