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Mechanistic Insights into the Oxidation of Aminophylline by Potassium Permanganate in Basic Medium: A Kinetic and Spectrophotometric Approach

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Abstract

The kinetics of oxidation of Aminophylline by potassium permanganate in alkaline medium has been studied spectrophotometrically at 25°C keeping ionic strength constant at 0.1 mole dm^{-3}. The stoichiometric ratio of permanganate to aminophylline in alkaline media was found to be 1:4. The kinetic study of the reaction between Aminophylline and permanganate ion has shown that the reaction obeys first order kinetics. It was observed that the reaction was sub-unit order dependent on both Aminophylline and hydroxide ion [OH^-]. Increasing ionic strength did not have any significant effect on the rate of the reaction. The main products were identified by IR spectral analysis. The ionic strength and the dielectric constant had no effect on the rate of reaction. The introduction of some products did not affect the reaction rate significantly. The rate equation for this oxidation reaction has been established. Reaction constants and mechanism have been calculated. The activation parameters associated with rate determining step of the reaction as well as the thermodynamic values of the equilibrium constants have been estimated and discussed.

1. Introduction

Aminophylline is a compound of the bronchodilator, theophylline with ethylenediamine in 2:1 ratio. Aminophylline is usually a dihydrate and ethylenediamine improves solubility. [1] They increase the flow of air through the bronchial tubes and relieve cough, wheezing, shortness of breath and troubled breathing. It is less potent than theophylline and has a shorter duration of action. Most often it is used for the treatment of airway obstruction from asthma or receptor antagonist and phosphodiesterase inhibitor. [2]

It is used to reverse infusions of regadenoson, dipyridamole or adenosine in nuclear cardiology stress testing. It has also been reported to be useful in preventing

slow heart rates during complex cardiovascular interventions (atherectomy of right coronary artery). [3] It is also used in treatment of heart block due to acute inferior myocardial infarction. It can cause cardiac arrest. Aminophylline has shown some promise as a topical cream body fat reducer. [4] Aminophylline may lead to theophylline toxicity. It has found to reduce the ant seizure action of topiramate and reduce the sedative effects of propofol[5-6].

It is more water-soluble than theophylline. White to slightly yellowish granules or powder, with a slightly ammoniacal odour and a bitter taste. On exposure to air it slowly loses ethylenediamine and absorbs carbon dioxide with liberation of free theophylline. Its solutions are alkaline. Soluble in 25 ml water to give a clear solution (1 g); crystallizes on standing when 1 g is dissolved in 5 ml water, but redissolves on addition of a small amount of ethylenediamine. It is insoluble in alcohol and ether. It is a competitive nonselective phosphodiesterase inhibitor [7], similar to other methylated xanthine derivatives, that increases intracellular cAMP, activates PKA, inhibits TNF-alpha [8][9] and leukotriene [10] synthesis and reduces inflammation and innate immunity [11].

Potassium permanganate is a strong oxidizing agent. It has several other advantages over other oxidizing agents: easier to handle, a readily soluble solid and, as shown for some contaminants, a higher efficiency in water and soil treatment [12]. Permanganate ion is a strong oxidant in acidic, neutral and basic media and has been shown to be a leading, environment friendly and active oxidant in kinetic studies [13,14]. The oxidation by permanganate ion proceeds through different mechanism and hence acts as a multi-equivalent oxidant [15,16].

Potassium permanganate is a common oxidizing agent and is of importance in the kinetics of a number of organic and biologically active compounds [17-21]. Oxidation reactions by Potassium permanganate have great academic and technological importance due to variable oxidation states. Permanganate is one such powerful multi-electron oxidant which can exist in various oxidation states out of which +7 is its highest oxidation state which occurs in the Oxo compounds like MnO4-, Mn_2O_7, MnO_3F. MnO_4^- is the most widely used well known oxidant species for the kinetic studies in acidic, neutral and alkaline media. The permanganate ion has been widely used as an oxidant in organic syntheses [22]. Kinetic studies are essential for the mechanistic information of these reactions. This has been confirmed by result stating to unsaturated acids in aqueous [23,24] and non-aqueous media. It is known that in aqueous alkaline medium permanganate ion oxidizes a number of organic compounds which are not or only very slowly attacked in acidic or neutral medium. The mechanism of oxidation depends on the properties of the substrate and the pH of the reaction medium. Stable reduction product of permanganate in strongly alkaline medium is manganate ion, MnO_4^{2-} [25-27]. MnO_2 appears only after a long time i.e. after complete consumption of MnO_4^-.

In view of possible pharmaceutical importance of aminophylline and no literature on the oxidation of aminophylline by any oxidant and complexity of the reaction, detailed study of the reaction

becomes more important. Hence, we have studied the oxidation of aminophylline by potassium permanganate in alkaline media.

2. Experiment

2.1 Materials

All the chemicals used in the present study were of analytical reagent (AR) grade and were used as such without further purification. All solutions were freshly prepared in double-distilled water during the study. Aminophylline and potassium permanganate were obtained from a local chemical supplier. A stock solution of potassium permanganate was prepared by dissolving a suitable amount of the reagent in double-distilled water. The solution was allowed to stand, filtered when necessary, and standardized against standard oxalic acid solution by conventional procedures. Fresh permanganate solutions were prepared when required and standardized before use [28].

All solvents used in the study were checked for the absence of any significant absorption at the wavelength of analysis spectrophotometrically. Kinetic measurements were carried out under pseudo first order conditions with aminophylline in excess over potassium permanganate. The reaction rate was systematically investigated as a function of reactant concentrations, hydroxide ion concentration, ionic strength, temperature and solvent composition. The progress of the reaction was monitored spectrophotometrically by observing the decrease in absorbance of permanganate ion at 525 nm using double beam UV–Visible spectrophotometer (ELICO SL-210). All kinetic experiments were carried out in a thermostatically controlled environment and the temperature was maintained within ±0.5°C of the desired value.

2.2 kinetic Measurements

The kinetics of oxidation of aminophylline by potassium permanganate was studied under pseudo-first-order conditions with a large excess of aminophylline over permanganate concentration. The reaction was started by mixing thermostatically equilibrated solutions of potassium permanganate and aminophylline with the required concentrations of sodium hydroxide and sodium perchlorate. Sodium perchlorate was added to maintain a constant ionic strength during the kinetic runs.

The progress of the reaction was monitored spectrophotometrically by determining the decrease in the absorbance of permanganate ion at its characteristic absorption maximum, λ = 525 nm. The other components of the reaction mixture had no appreciable absorbance at this wavelength under the experimental conditions employed. Absorbance measurements were performed on a double beam UV-Visible spectrophotometer (ELICO SL-210) with a thermostatically controlled cell compartment. The reaction temperature was controlled within ±0.5°C of the set value.

3. Results and discussion

3.1 Influence of Aminophylline Concentration:

To investigate and analyse the effect of change in concentration of substrate, the concentration of Aminophylline was changed from 1.0×10^{-2} to 1.0×10^{-1} M keeping the concentration of [$KMnO_4$]= 1.0×10^{-3} M and [NaOH] = 1 M constant. The reaction has been studied under pseudo first order condition, so pseudo first order rate

constants were determined. It is clear that pseudo first order rate constants were found to decrease with increase in concentration of Aminophylline in irregular way. (**Table 1**) When initial rate is plotted against concentration of Aminophylline the trend line is linear with negative slope (**Fig.1**) When k vs [Aminophylline] is plotted it confirm fractional order of reaction. Thus, the reaction rate under pseudo first order is dependent on the concentration of the substrate.

Table 1: Pseudo first order rate constant at = 25^0C + 0.5^0C keeping variation in substrate (Aminophylline).

[Aminophylline]	[$KMnO_4$]	[NaOH]	k
1×10^{-2}	1×10^{-3}	1M	1.41×10^{-2}
2×10^{-2}	1×10^{-3}	1M	1.29×10^{-2}
3×10^{-2}	1×10^{-3}	1M	1.32×10^{-2}
4×10^{-2}	1×10^{-3}	1M	1.22×10^{-2}
5×10^{-2}	1×10^{-3}	1M	1.48×10^{-2}
6×10^{-2}	1×10^{-3}	1M	1.39×10^{-2}
7×10^{-2}	1×10^{-3}	1M	1.43×10^{-2}
8×10^{-2}	1×10^{-3}	1M	1.26×10^{-2}
9×10^{-2}	1×10^{-3}	1M	1.23×10^{-2}

The observed rate constants were 1.22×10^{-2} to 1.48×10^{-2} s^{-1}. There were some fluctuations but the overall trend in **Fig. 1** indicates a slight increase in the rate of reaction with increasing aminophylline concentration. The plot of k vs. [Aminophylline] is approximately linear with positive slope showing the effect of substrate concentration on the rate of oxidation. The behavior is consistent with the participation of aminophylline in the rate-determining step of the reaction. The rate constant increased with increasing substrate concentration, showing a positive dependence of the reaction rate on the concentration of aminophylline. So, the oxidation of aminophylline by alkaline potassium permanganate is a reaction of fractional order concerning the substrate, which indicates the formation of a possible intermediate complex before the electron transfer step.(28)

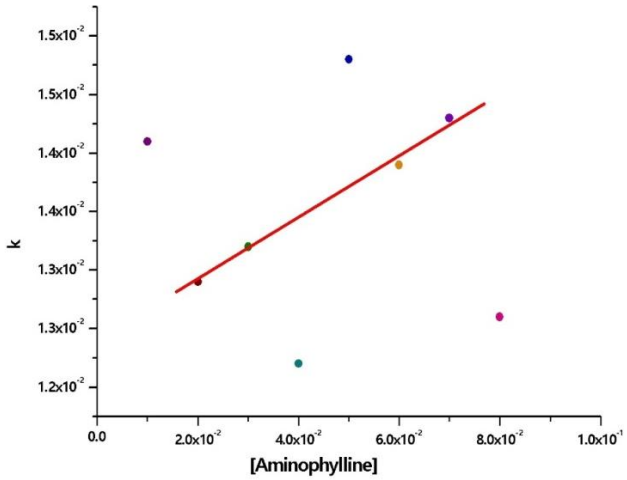


Fig. 1: Variation of Conc. of Aminophylline

3.2 Effect of variation of oxidant ($KMnO_4$) concentration: -

To evaluate and study the effect of variation of oxidant, the concentration of $KMnO_4$ was varied in the range of $1x10^{-4}$M to $9 x10^{-4}$M. The concentration of substrate [Aminophylline] was kept constant at 0.1 M and concentration of base NaOH 1M and temperature was kept constant $25^0C + 0.5^0C$ in thermostat.

Table 2: Pseudo first order rate constant at = $25^0C + 0.5^0C$ keeping variation in oxidant ($KMnO_4$).

[Aminophylline]	[$KMnO_4$]	[NaOH]	k
0.1M	1×10^{-4}	1M	1.46×10^{-2}
0.1M	2×10^{-4}	1M	1.38×10^{-2}
0.1M	3×10^{-4}	1M	1.34×10^{-2}
0.1M	4×10^{-4}	1M	1.33×10^{-2}
0.1M	5×10^{-4}	1M	$1.36x 10^{-2}$
0.1M	6×10^{-4}	1M	1.24×10^{-2}
0.1M	7×10^{-4}	1M	1.25×10^{-2}
0.1M	8×10^{-4}	1M	1.28×10^{-2}
0.1M	9×10^{-4}	1M	1.22×10^{-2}

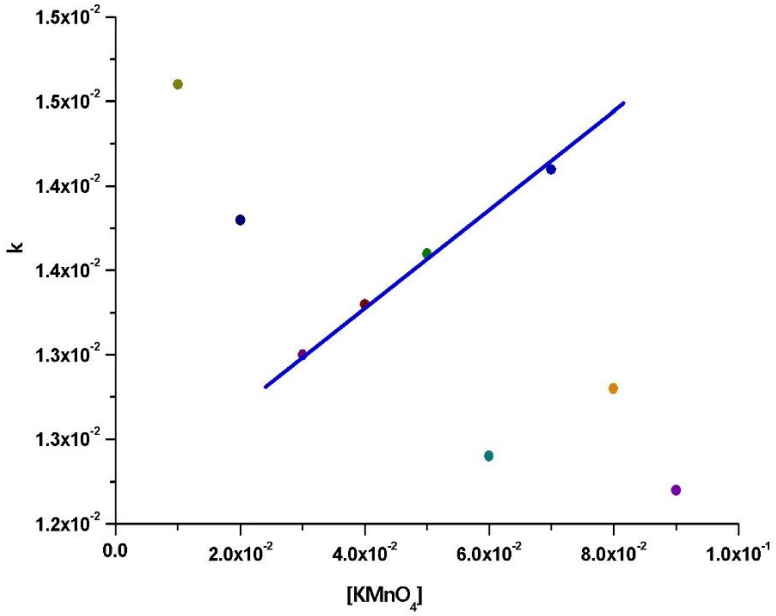


Fig. 2: Variation of Conc. of $KMnO_4$

It is clearly seen that pseudo first order rate decreases with increasing the concentration of $KMnO_4$ in irregular manner (**Table 2**). When we plotted the concentration $KMnO_4$ versus rate constant the trend line is linear with negative slope. (**Fig. 2**) Hence the rate of reaction under pseudo first order rate depends on the concentration of oxidant. (29)

The observed rate constants decreased slightly overall from 1.46 x 10^{-2} s^{-1} to 1.22 x 10^{-2} s^{-1} with increasing permanganate concentration. At intermediate concentrations there were minor fluctuations, but generally the reaction rate is not much enhanced by increasing the concentration of $KMnO_4$. The plot of k vs. [$KMnO_4$] (**Fig. 2**) is almost linear with a small negative slope indicating a weak inverse dependence of the observed rate constant on the concentration of the oxidant. (30)

This behavior indicates that the oxidation reaction is not simply first order with respect to permanganate ion. The decrease of k values with increasing oxidant concentration may be due to the formation of less reactive intermediate species or change in the distribution of active permanganate species in alkaline medium. Thus under the experimental conditions used the reaction is of a fractional or inverse fractional order with respect to the potassium permanganate concentration.

3.3 Effect of variation of NaOH concentration: -

To study the effect of variation of concentration of sodium hydroxide (NaOH), in the experimental sets the concentration of NaOH was varied in the range of 0.1M to 0.9 M, keeping constant concentration i.e. [Aminophylline]= 0.1M and [$KMnO_4$] = 1 x 10^{-3} M, at the 25^0C + 0.5^0C constant temperature. As the reaction has been studied under pseudo first order condition for varying [NaOH] was made and pseudo first order rate constants were calculated (**Table 3**).

Table 3: Pseudo first order rate constant at = 25^0C + 0.5^0C keeping variation in NaOH concentration.

[Aminophylline]	[KMnO4]	[NaOH]	k
0.1M	1×10^{-3}	0.01M	1.04×10^{-2}
0.1M	1×10^{-3}	0.02M	1.17×10^{-2}
0.1M	1×10^{-3}	0.03M	1.04×10^{-2}
0.1M	1×10^{-3}	0.04M	1.03×10^{-2}
0.1M	1×10^{-3}	0.05M	1.04×10^{-2}
0.1M	1×10^{-3}	0.06M	1.06×10^{-2}
0.1M	1×10^{-3}	0.07M	1.20×10^{-2}
0.1M	1×10^{-3}	0.08M	1.09×10^{-2}
0.1M	1×10^{-3}	0.09M	1.20×10^{-2}

It is clear from that pseudo first order rate constants increases with increases in concentration of NaOH in irregular manner confirming the first order dependence with respect to Base. Hence the reaction under pseudo order rate depends on the concentration of base. We plot initial rate with conc. of NaOH. The trend line is linear with positive slope. (**Fig.3**)

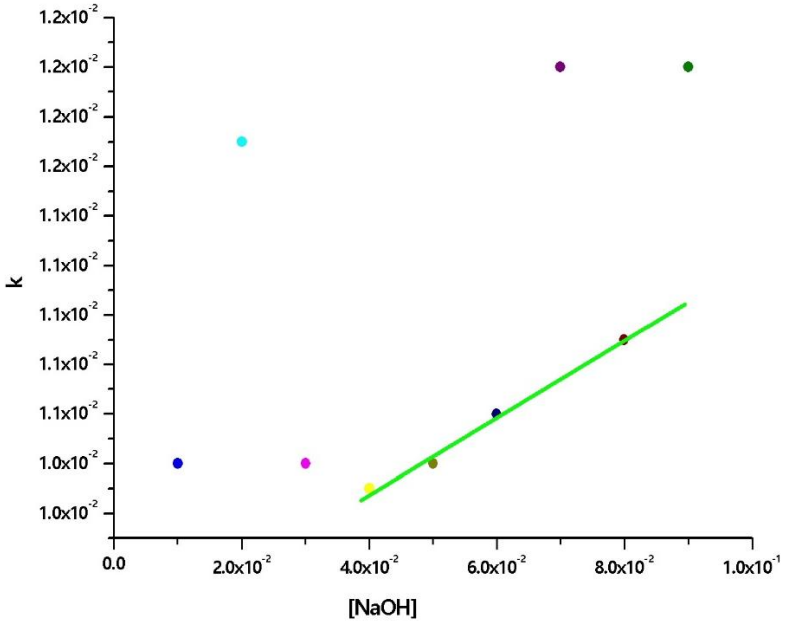


Fig. 3: Variation of Conc. of NaOH

The observed rate constants were increased from 1.04 × 10^{-2} s^{-1} at 0.1 M NaOH to 1.22 × 10^{-2} s^{-1} at 1.0 M at 1.0 M NaOH. Although some fluctuation was observed at intermediate alkali concentrations, the general trend clearly indicates an increase in the rate of reaction with increasing concentration of hydroxide ions. The plot of k versus [NaOH] has a positive slope, indicating that the mechanism of the reaction involves hydroxide ions which catalyze the oxidation.(31) In alkaline medium the rate of the reaction is enhanced, probably because more active manganate or hydroxylated permanganate are formed which facilitate the electron transfer from aminophylline to the oxidant. The rate constant dependence on hydroxide ion concentration indicates a positive fractional order reaction in alkali concentration. Thus, hydroxide ions play an important role in the rate of oxidation of aminophylline by potassium permanganate in alkaline medium.

3.4 Effect of variation of temperature: -

The effect of temperature was studied keeping constant concentration of all reactants such as [$KMnO_4$] = 1 x 10^{-3} M, [Aminophylline] = 0.1 M and [NaOH] = 1 M. The temperature variation was varied in the range of 25^0C to 55^0C. (**Table 4**) The energy of activation was calculated by using the Arrhenius Equation, $K = Ae^{-E_a}/RT$

by solving this equation we get $Log\ K = Log\ A - 2.303\ E_a/RT$

$$\Delta H = E_a - RT$$

The temperature dependence of rate constant can be given as;

$$k = k_B\ /Te^{-\Delta G/RT}$$

by solving this equation, we get

$$Log\frac{k_1}{T} = -\frac{\Delta H}{2.303RT} + Log\frac{K_b}{h} + \frac{\Delta S}{2.303R}$$

Rearranging this equation, we get

$$\Delta S = 2.303 \times R\ (Log\frac{K_1}{T_2} + \frac{\Delta H}{2.303RT} - Log\frac{K_b}{h})$$

The modest enthalpy of activation and higher rate constant of slow step indicate that the oxidation presumably occurs by an inner sphere mechanism. The free energy change (ΔG), enthalpy changes (ΔH) and entropy change (ΔS) was determined.

The effect of temperature on oxidation of aminophylline by potassium permanganate has been studied in the temperature range 25°C to 55°C keeping the concentrations of aminophylline, potassium permanganate and sodium hydroxide constant. As shown in Table 4, the pseudo-first-order rate constant increased from 1.26 × 10^{-2} s^{-1} at 25°C to 2.02 × 10^{-2} s^{-1} at 55°C. The rate constant increases with temperature, indicating a thermally activated process. The kinetic energy of the reacting species increases at higher temperature and this results in more effective collision and hence, faster electron transfers between aminophylline and permanganate ion. Such a behaviour is in agreement with the Arrhenius theory and confirms that the temperature has a positive effect on the rate of oxidation.(32)

Table 4: Pseudo first order rate constant at different temperatures:

Temp.	[Aminophylline]	[$KMnO_4$]	[NaOH]	k
25°C	0.1M	1 x 10^{-3}	1M	1.26 x 10^{-2}
30°C	0.1M	1 x 10^{-3}	1M	1.63 x 10^{-2}
35°C	0.1M	1 x 10^{-3}	1M	1.75 x 10^{-2}
40°C	0.1M	1 x 10^{-3}	1M	1.87 x 10^{-2}
45°C	0.1M	1 x 10^{-3}	1M	1.89 x 10^{-2}
50°C	0.1M	1 x 10^{-3}	1M	1.90 x 10^{-2}
55°C	0.1M	1 x 10^{-3}	1M	2.02 x 10^{-2}

From **Table 5** it is clear that the rate of reaction increases with increase in temperature. From this the energy of activation was calculated to be 10833.84812 J/mole. This activation energy was used to calculate the enthalpy of activation (ΔH) using equation ΔH = Ea — RT. The value of ($\Delta \mathbf{H}^{\#}$) decreases with increase in temperature and ($\Delta \mathbf{G}^{\#}$) increases with increase in temperature. The average (ΔH), (ΔG) and (ΔS) was found to be 8252.04 J/mole, 86802.07 J/mole and -256.2766 J/mole respectively. Then from this, we calculate the entropy of activation. (**Table 6**)

Table 6: Thermodynamic parameter of the kinetic oxidation process:

T	k	$\Delta H^{\#}$ (KJ $mole^{-1}$)	$\Delta S^{\#}$ (J $mole^{-1}$)	$\Delta G^{\#}$ (KJ $mole^{-1}$)
298	1.26 x 10^{-2}	8355.98	-271.17	83203.89
303	1.63 x 10^{-2}	8314.40	-251.91	84641.86
308	1.75 x 10^{-2}	8272.83	-252.62	86086.51
313	1.87 x 10^{-2}	8231.25	-253.32	87519.84
318	1.89 x 10^{-2}	8189.68	-253.99	88959.84
323	1.90 x 10^{-2}	8148.10	-254.65	90400.48
328	2.02 x 10^{-2}	8106.53	-255.29	91841.77
Average		8252.04	-256.27	86802.07

3.5 Effect of variation of solvent concentration: -

The effect of solvent composition on the oxidation of aminophylline by potassium permanganate has been studied using acetic acid, acetone, ethyl acetate and n-hexane at different solvent percentage (20-60%) keeping all other reaction conditions constant. Results in **Table 7** show that the reaction rate is strongly affected by the nature and concentration of the solvent. The rate constants in acetic acid and n-hexane media were weakly dependent on the solvent percentage. On the other hand, acetone exhibited a significant increase in rate constant from 0.0136 to 0.0374 s^{-1} with the increase of its proportion. Ethyl acetate gave the highest rate constants, but a slow decrease was observed with increasing solvent concentration. These findings indicate the importance of the solvent polarity and the solute-solvent interactions

in the oxidation process in relation to the stability of the reaction intermediates and the electron-transfer step. Thus the solvent environment has a strong effect on the rate of oxidation of aminophylline.(33)

Table 7: Pseudo first order rate constant at = 25^{0}C + in solvent concentration: 0.5^{0}C keeping variation

Percentage of Solvent	Rate constant (sec^{-1})			
	Acetic Acid	Acetone	Ethyl Acetate	N-Hexane
20%	0.0175	0.0136	0.0508	0.0183
30%	0.0155	0.0158	0.0469	0.0194
40%	0.0160	0.0237	0.0414	0.0201
50%	0.0147	0.0299	0.0407	0.0191
60%	0.0150	0.0374	0.0342	0.0189

3.6 Effect of variation of salts: -

The effect of the added salts on the oxidation of aminophylline by potassium permanganate was investigated by varying the concentrations of $Al(NO_3)_3$, KNO_3, KBr, KCl, and $Hg(Ac)_2$ from 1.0×10^{-2} to 1.0×10^{-1} M , while the concentrations of aminophylline, potassium permanganate and sodium hydroxide were kept constant. The pseudo-first-order rate constants are shown in **Table 8** to have very little variation with the concentration of $Al(NO_3)_3$, KNO_3, KBr, and KCl, indicating a negligible effect of ionic strength on the reaction rate. (34)

Table 8: Pseudo first order rate constant at = 25^{0}C + 0.5^{0}C **keeping variation in salts concentration:**

[Aminophylline] = 9 X10^{-3}M; [$KMnO_4$] = 3 X 10^{-3}M; [NaOH] = 1M; [Temp.] = 25^{0}C + 0.5^{0}C

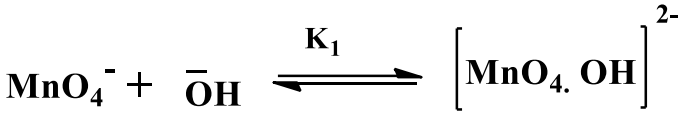
Concentration of Salt	Rate constant (sec-1)				
	$Al(NO_3)_3$	KNO_3	KBR	KCL	$Hg(Ac)_2$
1 x 10^{-2}	0.0124	0.0109	0.0119	0.0118	0.0202
2 x 10^{-2}	0.0127	0.0143	0.0120	0.0118	0.0167
3 x 10^{-2}	0.0116	0.0116	0.0129	0.0115	0.0122
4 x 10^{-2}	0.0130	0.0115	0.0129	0.0124	0.0205
5 x 10^{-2}	0.0139	0.0117	0.0122	0.0126	0.0168
6 x 10^{-2}	0.0126	0.0108	0.0118	0.0121	0.0156
7 x 10^{-2}	0.0132	0.0124	0.0130	0.0128	0.0170
8 x 10^{-2}	0.0120	0.0114	0.0141	0.0114	0.0148
9 x 10^{-2}	0.0118	0.0115	0.0143	0.0118	0.0172
10 x 10^{-2}	0.0119	0.0124	0.0123	0.0112	0.0194

In contrast, $Hg(Ac)_2$ showed significantly higher rate constants over the concentration range, indicating a pronounced catalytic effect on the oxidation. The rate increase may be attributed to specific interactions of the reaction intermediates with mercury(II) ions promoting electron transfer. The results indicate, in general, that oxidation of aminophylline is relatively insensitive to common electrolyte salts, but is greatly accelerated in the presence of mercury(II) acetate.

3.7 Proposed Reaction Mechanism of Aminophylline:

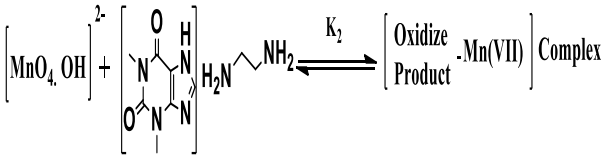
Step I: Formation of Reactive Permanganate Species (Fast Equilibrium):

In alkaline medium, permanganate interacts with hydroxide ions to form an activated species:



Step II: Formation of Intermediate Complex (Fast Equilibrium)

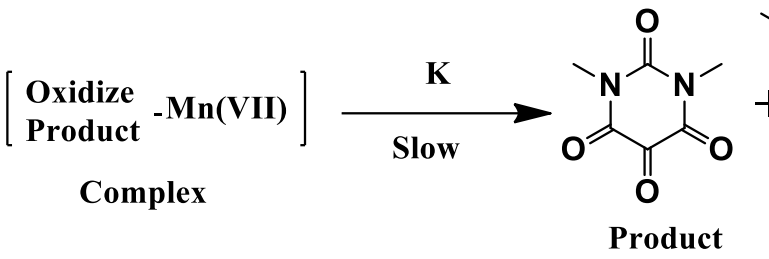
The activated permanganate species interacts with Aminophylline to form a coordination complex:



This step involves coordination through the hydroxyl or amino functional group of Aminophylline.

Step III: Electron Transfer and Decomposition (Slow Step)

The complex undergoes slow electron transfer, leading to bond cleavage and oxidation:



3.8 Possible Kinetic Mechanism for oxidation of aminophylline

$$[MnO_4^-] = [MnO_4^-] + [HMnO_4^{2-}]$$

$$= [MnO_4^-] + K[MnO_4^-][OH^-]$$

$$= [MnO_4^-]\{1+K_1[OH^-]\}$$

$$K = \frac{K_2 K\,[\text{aminophylline}][MnO_4^{-2}]}{1 + K_1[OH^-]}$$

$$\frac{Rate}{[MnO_4^-][\text{aminophylline}]} = \frac{K\,K_2}{1 + K_1[OH^-]}$$

$$\therefore \frac{1}{K_{Obs}} = \frac{1}{K\,K_2} + \frac{K_1[OH^-]}{K\,K_2}$$

Hence, the rate expression is verified by plotting $1/K_{obs}$ against $[KMnO_4]$, a strength line is observed. Under conditions of excess oxidant, the oxidation of aminophylline by alkaline potassium permanganate follows pseudo–first-order

kinetics. The reaction goes through the formation of an intermediate aminophylline–Mn complex, which breaks down slowly and sets the rate of the reaction.

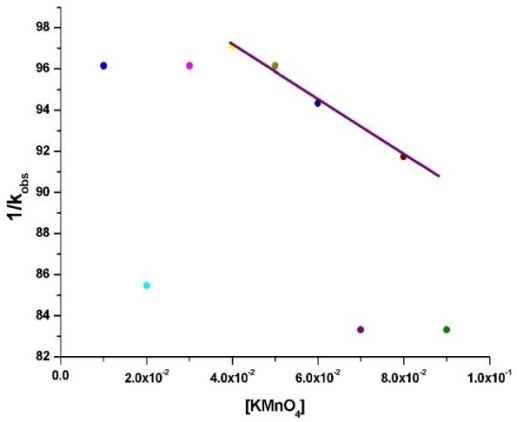


Fig. 4: Variation of [$KMnO_4$] Vs $1/k_{obs}$

4.Product Characterization via FTIR Spectroscopy

Following the complete consumption of the active permanganate ion, the primary oxidized fragment was carefully isolated via localized solvent extraction protocols and analyzed using Fourier-Transform Infrared (FTIR) spectroscopy. The diagnostic absorption spectra revealed several structurally defining shifts:

• **Carbonyl Architecture:** The spectrum displays an intense, sharp absorption band centered at 1653 cm^{-1} along with a secondary peak at 1598 cm^{-1}. These represent the highly conjugated asymmetric stretching frequencies of multiple carbonyl (C=O) functional groups localized within a highly symmetric cyclic alloxan nucleus.

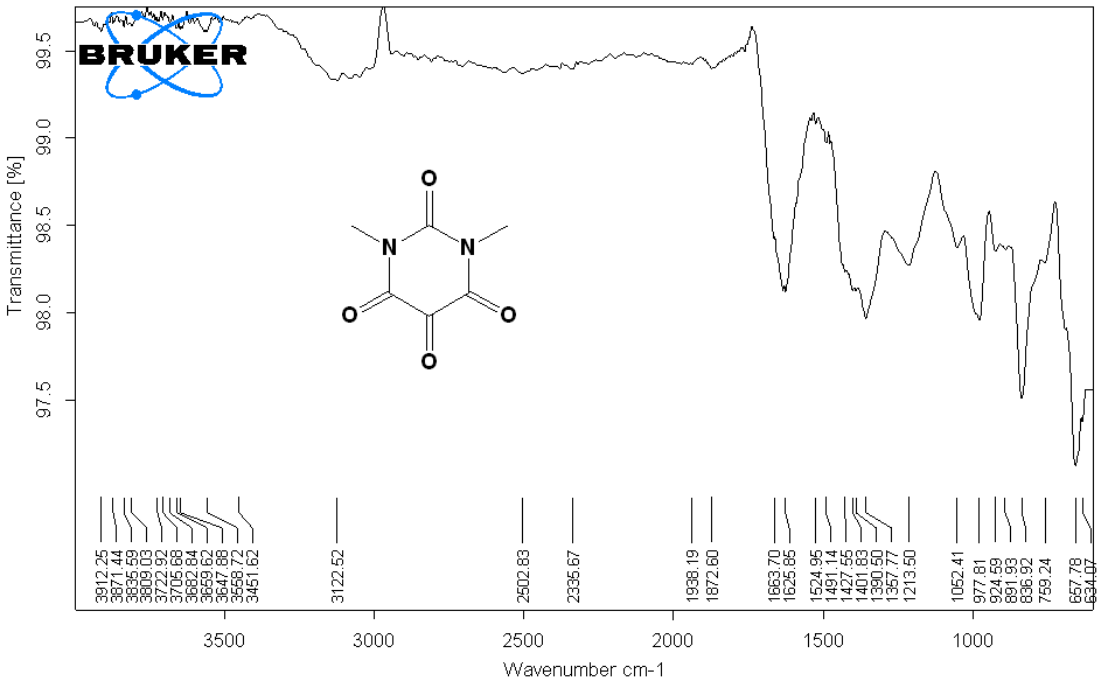
• **Absence of Protic Stretches:** Notably, the spectrum lacks any broad hydroxyl (O-H) stretching cascades in the 3200–3600 cm^{-1} zone, proving that no hydroxylated intermediates remain in the isolated structure.

• **Amine Modifications:** The total disappearance of primary or secondary N-H stretching bands near 3300–3500 cm^{-1} is in structural agreement with absolute methyl substitution at both nitrogen heteroatoms, further validated by distinctive methyl deformations at 1408 cm^{-1} and 1369 cm^{-1}.

• **Ring System Identifications:** Characteristic internal finger-print peaks emerging prominently at 1491 cm^{-1}, 1252 cm^{-1}, and 1072 cm^{-1} are attributed directly to the cyclic C-N stretching vibrations of the consolidated cyclic ureide heterocyclic block.

Conclusively, the overlapping infrared data rigorously confirms that the major oxidative degradation product of Aminophylline under alkaline potassium permanganate stress is 1,3-dimethylalloxan.

Fig. 4: The infra-red spectrum of oxidized product of Aminophylline



CONCLUSION

The chemical kinetics of the oxidation of Aminophylline by alkaline potassium permanganate were systematically resolved using UV-Visible spectrophotometry. The reaction follows a base-catalyzed fractional pathway with a negative entropy of activation, pointing to a rigid inner-sphere intermediate complex prior to the rate-limiting electron transfer. Under these alkaline conditions, the xanthine core undergoes oxidation to yield 1,3-dimethylalloxan. These findings provide critical quantitative insights into the chemical stability, metabolic simulation pathways, and oxidative degradation mechanics of this essential bronchodilator.

Conflict of Interest:

The authors declare that they have no conflict of interest.

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