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Kinetic Study of Fast Brominations of Xylidine Using Competition Techniques

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Absract: *The competitive kinetics applied with assurance and determine the kinetic in milliseconds due to fast bromination reaction. Determination of kinetics is fundamental aspects for the design and operation of the reactor. Competition kinetic method was proposed to determine directly bromination rate constant of regioisomers of Xylidine.The specific reaction rates determined from this study are 1.7 x* $10^5M^{-1}S^{-1}$ *for 3,5 Xylidine, 1.4 x* $10^5M^{-1}S^{-1}$ *for 2,5 Xylidine* ***and*** *1.2 x* $10^5M^{-1}S^{-1}$ *for 2,3 Xylidine. Kinetic evidence gives information about mechanistic route.*

Keywords: *Regioisomers of Xylidine, Competitive kinetics, Bromine, Potassium nitrate, potassium iodide*

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I. Introduction

Kinetics of chemical reaction deals with the rate of chemical reaction, Chemical reaction is one or two step process usually involve collision between two reactants refer to as a bimolecular step or dissociation of a single reactant molecule which is refer as unimolecular. Kinetics study of chemical reaction is carried out analysis of elementary steps i.e. the reaction mechanism and determination of absolute rate of reaction. The rate of chemical reaction means the rate at which reactants are used up or equivalently the rate at which products are formed, In kinetic studies the kinetic parameters such as frequency factor, activation energy, stiochiometric concentration, enthalpy and entropic changes on the rate of reaction[1]

Experimental techniques have been developed to monitor reactions over timescale varying as few femto seconds (1Fs= 10^{-15}sec.) It is to monitor the kinetic study of a slow reaction occurring over minute to hour or longer and kinetic study of a fast reaction occur in few seconds or femto seconds therefore highly specialized techniques are used to study fastest reaction. In 2003, more than twenty US Army troops were allegedly exposed to 3,4-xylidine during the operation of Iraq, leading to a number of health complaints.[2]

A kinetic experiment essentially consists of mixing the reactants and initiating reaction on a timescale that is negligible to that of reaction and then monitoring concentration of reactants and products as the function of time. Reaction in pharmaceutical industries is known for their complexities, reaction with intermediate product are common in these industries.[3] For kinetic study of a fast reaction a large number of techniques have been developed as Flow Techniques, Flash photolysis techniques, Relaxation Method, Life time methods, Absorption Spectroscopy, Competition Techniques. The competition techniques are necessitated to study the kinetics of these brominations of aromatic substrate due to their rapidity.

Competition Techniques-

In Competitive Techniques A and B react with C However A and B do not react with each other but competition take place with A and B react with C Where C is insufficient quantity although A and B are large amount, if the rate constant for one of the competitive reaction is known, the other can be determined.

II. Experimental Method:

The Competition ratio V-v/v is maintained to be near to unity In titration **v** Cm^3 of sodium thiosulphate in the iodometric titration corresponds to the bromine reacted with potassium iodide V-v is corresponds to that reacted Xylidine in the competition. The Competition ratio V-v/v is arranged as that of near about 1. By using the following equation K can be calculated

Determination of Specific Reaction rate

Set I

10 ml 0.0025 M Br_2 + 40 ml KI 0.04 M + 50 ml H_2O **Vs** 0.005 M Na_2S_2O = **V Cm^3**

Set II

10 ml $Br_2$0.0025 M+40 ml KI 0.04 M+50 ml Xylidine 0.01 M **Vs** 0.005M $Na_2S_2O_3$ = **v Cm^3**

Table 1: Bromination of 2,5 Xylidine (Initial Conc.of the reactants in 100 Cm^3

Sr.no.	Reactant	Concentration
1	Bromine	0.0025
2	2,5 Xylidine	0.01
3	Potasium Iodide	0.04

Titrate Values V = 8.2 Cm^3 v = 4.5 Cm^3

Table 2: Bromination of 2,3 Xylidine (Initial Conc.of the reactants in 100 Cm^3

Sr.no.	Reactant	Concentration
1	Bromine	0.0025
2	2,3 Xylidine	0.01
3	Potasium Iodide	0.04

Titrate Values V = 8.2 Cm^3 v = 4.8 Cm^3

Table 3: Bromination of 3,5 Xylidine (Initial Conc.of the reactants in 100 Cm^3

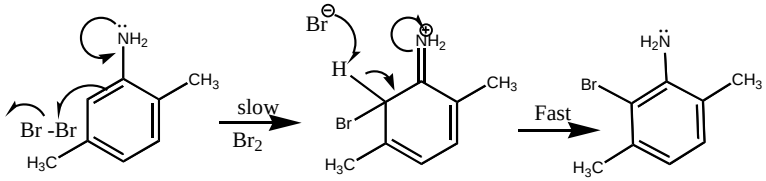
Sr.no.	Reactant	Concentration
1	Bromine	0.0025
2	3.5 Xylidine	0.01
3	Potasium Iodide	0.04

Titrate Values V = 8.2 Cm^3 v = 4.2 Cm^3

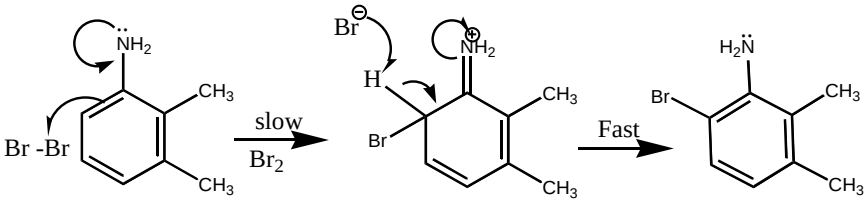
Mechanism - bromination of Xylidine:

Fig. 1 Mechanism - bromination reaction of Xylidine

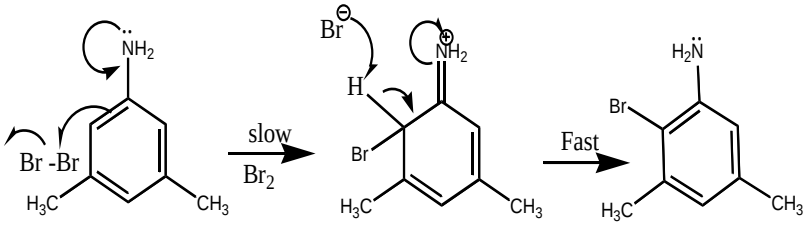
I.Bromination of 2,5 Xylidine by molecular bromine



II. Bromination of 2,3 Xylidine by molecular bromine



III. Bromination of 3,5 Xylidine by molecular bromine



III. Result and Discussion:

In Competitive Techniques Xylidine and KI react with Br_2 However Xylidine and KI do not react with each other but competition take place with Xylidine and KI react with Br_2 Where Br_2 is insufficient quantity although Xylidine and KI are large amount, 'With the help of competition techniques kinetics and experiment results calculated by competition method, kinetics to find out rate constant of reaction species with target comp'.[4] The appropriate concentration of each of three region-isomers of xylidine in the reaction with maintaining the competition ratio approximately one, the velocity constant calculated for bromination of region-

isomers of xylidine quantitatively justify the speculated relative reactivity of region-isomers of xylidine in aqueous medium in electrophilic aromatic substitution react ion. 'The absorption band could be assigned to this vibrations have the same polarization characterize as those of bands due to known planar vibration'[5] With the help of velocity constant assigned as 3,5 xylidine is the fast reaction followed by 2,5 xylidine, that of 2.3 xylidine as slowest reaction. The rate at which bromination reaction occur can provide important information concerning the mechanism.[6]

Table 4: The velocity constant for bromination of Regioisomers of Xylidine

Sr.No.	Regioisomers of Xylidine	Velocity constant for bromination $10^5 M^{-1} S^{-1}$
1	2,3Xylidine	**1.2**
2	2,5Xylidine	**1.4**
3	3,5Xylidine	**1.7**

IV. Conclusion:

The competition techniques are necessitated to study the kinetics of these brominations due to their rapidity. The rate of bromination for 2,5 Xylidine, 2,3 Xylidine and 3,5 Xylidine influence due to Steric hindrance. The rate of bromination of 3,5 Xylidine is fastest than 2,3 Xylidine, that of 2,5 Xylidine is Slowest. The research quantitatively complies with the principles of electrophilic aromatic substitution reaction.
Stereochemistry principles that are quantitatively hitherto speculated.[7] Kinetic study for the bromination of Regioisomers of Xylidine by Competitive techniques is reliable and challenging technique

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