

# Kinetic study of Fast brominations of regioisomers of Chloroacetanilide using Competition Techniques

J.B.Bhore\*, Bhaskar Gatkul

Arts ,science and commerce college Indapur, Dist-Pune, Maharashtra, India.

jayashrigatkul@yahoo.com; jijau.vishwabala@gmail.com

**ABSTRACT** - 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 Chloroacetanilid Xylidine. The specific reaction rates determined from this study are  $1.7 \times 10^5 \text{M}^{-1}\text{S}^{-1}$  for *P*-Chloroacetanilide,  $1.8 \times 10^5 \text{M}^{-1}\text{S}^{-1}$  for *M*-Chloroacetanilide and  $1.3 \times 10^5 \text{M}^{-1}\text{S}^{-1}$  for *O*-Chloroacetanilide Kinetic evidence gives information about mechanistic route.

**KEYWORDS** - Regioisomers of Chloroacetanilide, Competitive kinetics, Bromine, Potassium nitrate, potassium iodide

## I. INTRODUCTION

Regio-isomers of Chloroacetanilide in the three competition reactions studied with the aim of maintaining the competition ratio nearly 1 and in view of the observed rapidity of the reactions. The concentrations of both the competitors are large and almost constant compared to that of bromine in the competition. The rate of reaction is an expression relating the rate of reaction to the concentration of the relating species present which may include reactant, product and catalyst<sup>1</sup>

Chloroacetanilide in which amide group is electron donating group it exerts +I effect and orienting ortho and para isomers. The reaction rate is influenced by certain external factors such as concentrations of the reacting substances, temperature and pressure.<sup>2</sup>

The Competition ratio  $V-v/v$  is operate in such manner as that of approximately 1. By using the equation rate constant can be calculated. Fast reaction will have a low activation energy, but if the reactants are present in low concentrations the rate of reaction will be small<sup>3</sup> The competition techniques are necessitated to study the kinetics of these brominations of aromatic substrate due to their rapidity.<sup>4</sup>

## II. EXPERIMENTAL METHOD

**Table 1 : Bromination of 2-chloroacetanilide**

Initial concentrations of the reactants in 100 ml reaction mixture

Sr. No.	Reactant	Concentration/M
1	Bromine	0.0025
2	2-chloroacetanilide	0.01
3	potassium iodide	0.04

Titre values  $V = 8.6 \text{ ml}$   $v = 4.9 \text{ ml}$

**Table 2 : Bromination of 3-chloroacetanilide:**

Initial concentrations of the reactants in 100 ml reaction mixture

Sr. No.	Reactant	Concentration/M
1	Bromine	0.0025
2	3-chloroacetanilide	0.01
3	potassium iodide	0.04

Titre values  $V = 8.6 \text{ ml}$   $v = 4.2 \text{ ml}$

**Table 3 : Bromination of 4-chloroacetanilide:**

Initial concentrations of the reactants in 100 ml reaction mixture

Sr. No.	Reactant	Concentration/M
1	Bromine	0.0025
2	4-chloroacetanilide	0.01
3	potassium iodide	0.04

Titre values  $V = 8.6 \text{ ml}$   $v = 4.5 \text{ ml}$

## III. OBSERVATION

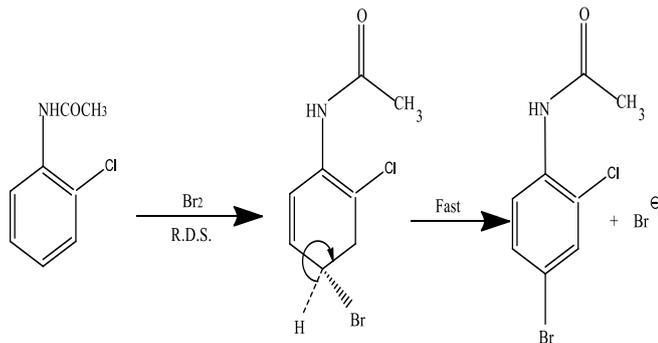
Velocity constant  $K$  can be calculated with the help of following equation

$$\frac{k_1 [\text{Chloroacetanilide}]^x [\text{Br}_2]^y}{k_2 [\text{K I}] [\text{Br}_2]} \times \frac{V-v}{v}$$

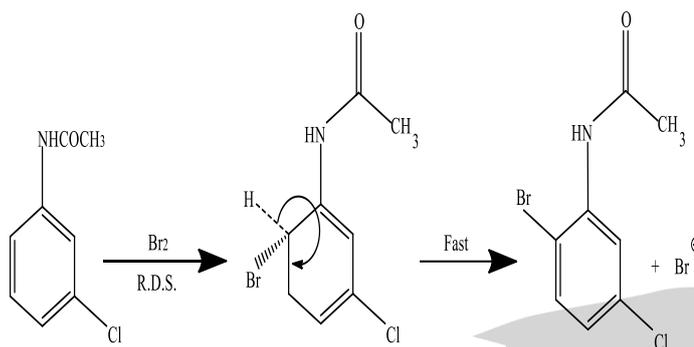
When  $x$  and  $y$  are both taken as 1, over a variation of the concentration range of Chloroacetanilide, the velocity constant values  $k_1$  obtained for the bromination of Chloroacetanilide are found to be constant suggesting an overall order of second for the reaction in all the two reactions studied. The velocity constant values obtained.

### Fig.1 Mechanism of bromination reaction of Chloroacetanilide

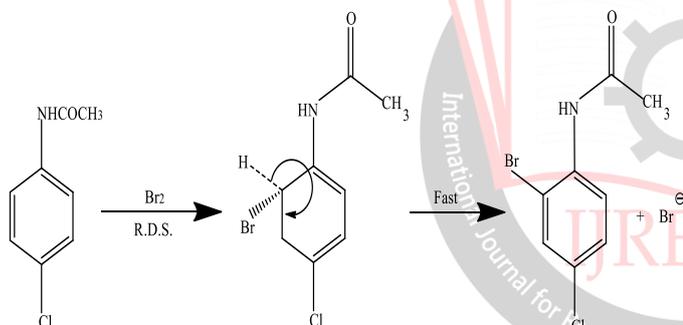
- I. Bromination of 2- Chloroacetanilide by molecular bromine



Bromination of 3-Chloroacetanilide by molecular bromine



II. Bromination of 4-chloroacetanilide by molecular bromine



#### IV. RESULT AND DISCUSSION

In chemical process the reactant is converted product in an individual steps<sup>5</sup> In Competition method Chloroacetanilide and KI react with Br<sub>2</sub> However Chloroacetanilid and KI do not react with each other but competition take place with Chloroacetanilide and KI react with Br<sub>2</sub> Where Chloroacetanilide and KI are large amount, 'With the help of competition techniques kinetics and experiment results calculated by competition method, Velocity constant calculated for bromination of region-isomers of Chloroacetanilide quantitatively justify the speculated relative reactivity of region-isomers of Chloroacetanilide in aqueous medium The rate at which bromination reaction occur can provide important information concerning the mechanism.<sup>6</sup>

In *m*-Chloroacetanilide amide group is activating group it activates ortho/para position therefore ortho/para product is major product. In bromination reaction bromine is incoming bulky group therefore alter of ortho position of amide group. The steric effect occurred in between bromine and amide acetanilide group.

In *p*-Chloroacetanilide acetamide is activating group and chlorine is deactivating group. Activating group activates ortho/para position therefore incoming bulky bromine group occupies oar ortho/para position and gives ortho/para product. Chlorine is deactivating group it gives *meta* product as major product thus bromination of *p*-Chloroacetanilide gives 6-bromo 4-Chloroacetanilide. These reactions are faster reaction than *o*-Chloroacetanilide and *m*-Chloroacetanilide. The velocity constant values obtained in this study for the bromination of the Regio isomers of chloroacetanilide quantitatively justify the determined relative reactivity of Chloroacetanilide in aqueous solution in electrophilic aromatic substitution reactions. The rate of bromination of *p*-chloroacetanilide is the greatest followed by *m*-Chloroacetanilide, that of *o*-Chloroacetanilide being the slowest.

#### V. CONCLUSIONS

The competition techniques are necessitated to study the kinetics of these brominations due to their rapidity. The rate of bromination for Ortho-Chloroacetanilide, Meta-Chloroacetanilide and Para-Chloroacetanilid influence due to Steric hindrance. The rate of bromination of Meta-Chloroacetanilid is fastest than Para-Chloroacetanilid that of Ortho-Chloroacetanilid is Slowest. The research quantitatively complies with the principles of electrophilic aromatic substitution reaction.

Stereochemistry principles that are quantitatively hitherto speculated.<sup>7</sup> Kinetic study for the bromination of Regioisomers of Chloroacetanilid by Competitive techniques is reliable and challenging technique

Table 4 : The relative reactivity of Chloroacetanilide evidenced from kinetic data for bromination

Regio isomer	Velocity constant for bromination /10 <sup>5</sup> M <sup>-1</sup> s <sup>-1</sup>
<i>o</i> - Chloroacetanilide	1.3
<i>m</i> - Chloroacetanilide	1.8
<i>p</i> - Chloroacetanilide	1.7

#### REFERENCES

- [1] .Dr.Claire vallance  
<https://vallanc//chem.ox.ac.uk.pdfs.kinetics>

- [2] [https:// Britanica.com/science/chemical-kinetics/measuring fast reaction.](https://Britanica.com/science/chemical-kinetics/measuring-fast-reaction)
- [3] H.E.Avery  
[https://springer.com/chapter/10.1007%2F978-1-349-15520-](https://springer.com/chapter/10.1007%2F978-1-349-15520-349-15520-)
- [4] Bhore J.B.and Dangat V.T. Fast Bromination of Regioisomers of Cresol International journal of science and Technology2014 Vol.2(4)142-144.
- [5] Shah et.al,Basic reaction kinetics and mechanism,DOI 10.5772 intechopen.70483
- [6] David s.Hage,Xiwel zheng et.al.J.Pharm.Biomed Anal2015sept 10;113;163-180
- [7] Jerry March'Advanced Organic Chemistry' Third Edition.p-448(1992)

