



## Effect of Cetyltrimethyl Ammonium Bromide on the Kinetics of Iodination of Aniline by Iodine

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### ABSTRACT

Kinetics of the Iodination of aniline by iodine has been studied conventionally. The reaction shows second order kinetics. The effect of various concentration of cetyl trimethyl ammonium bromide has been investigated. It is observed that cetyl trimethyl ammonium bromide inhibits the reaction below critical micelle concentration. The inhibition coefficient has been evaluated and discussed.

**Keywords** : kinetics, Iodination, cetyltrimethyl ammonium bromide, micelle, Aniline

### INTRODUCTION

The investigation of micellar catalysis has provoked a great interest during last few decades, since the study of micelle catalyzed reaction might provide a basic interpretation of some aspect of catalysis.<sup>1-4</sup> The continuing research interest in the area of micelle formation, structure and their role in reaction catalysis reflects the importance of the subject. The extensive study and publications in the book summarize much of the knowledge about micelles.<sup>5-14</sup>

On the other hand, there are certain cationic surfactant like cetyltrimethyl ammonium bromide, that can affect the rate of aroniatic substitution reactions and plays important role in chemistry due to their ability to catalyze or inhibit certain reactions.<sup>15-17</sup>

The purpose of this paper is to show the effect of cetyl trimethyl ammonium bromide (CTAB) on the kinetics of iodination of aniline by iodine.

### EXPERIMENTAL

#### Preparation of solutions

The solutions were prepared for each set of experiments. Doubly distilled water was used for preparing various solutions of  $5.0 \times 10^{-2}$  M iodine and aniline were prepared along with 0.1 M cetyl trimethyl ammonium bromide and 0.1 M sodium iodide.

#### Critical micelle concentration

Critical micelle concentration of cetyltrimethyl ammonium bromide was determined by measuring absorbance of acridine orange ( $1.0 \times 10^{-3}$  M) in various concentrations of CTAB ranging from  $6.0 \times 10^{-3}$  M to  $13.0 \times 10^{-3}$  M.

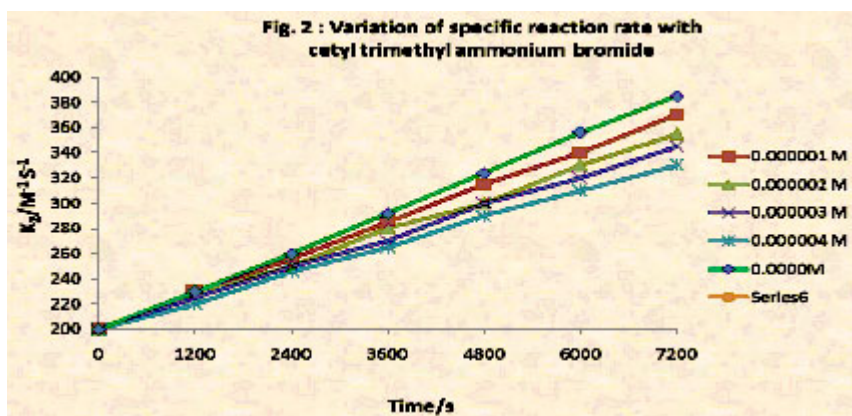
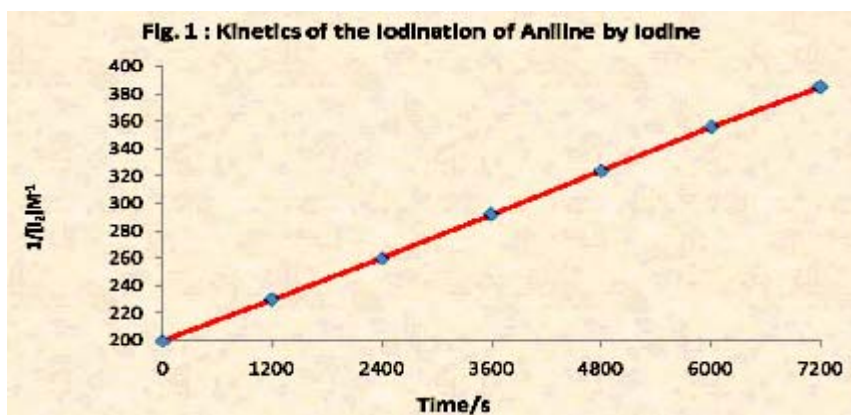
Table – 1 : Kinetics of Iodination of Aniline by Iodine

Concentration of Aniline	:	$5.0 \times 10^{-3}$ M	
Concentration of Iodine	:	$5.0 \times 10^{-3}$ M	
Concentration of Sodium iodide	:	$5.0 \times 10^{-2}$ M	
Concentration of sodium thiosulphate	:	$2.5 \times 10^{-2}$ M	
Volume of reaction mixture titrated for each estimation of unreacted iodine	:	25.0 cm <sup>3</sup>	
Temperature	:	25.0 <sup>o</sup> c	

Time/s	Volume of thiosulphate.cm <sup>3</sup>	Unreacted Iodine, [I <sub>2</sub> ]/10 <sup>-3</sup> M	1/[I <sub>2</sub> ]/M <sup>-1</sup>
0	16.0	5.00	200
1200	13.9	4.35	230
2400	12.3	3.85	260
3600	10.9	3.42	292
4800	9.9	3.09	324
6000	9.0	2.81	356
7200	8.3	2.60	385

Slope of the graph of  $1/[I_2]$  versus time = specific reaction rate,  $k_2 = 0.026 \text{ M}^{-1} \text{ S}^{-1}$



### Kinetic study

The rate of reaction is followed by determining the unreacted iodine from the iodine-aniline ( $5.0 \times 10^{-3}$  M each) system at various time intervals. The reciprocal of concentration of unreacted iodine was plotted versus time. (Table 1 and Fig. 1) Similar rate determinations were made in presence of various concentrations of cetyl trimethyl ammonium bromide and the plot of unreacted iodine versus time was plotted (Fig. 2).

### RESULTS AND DISCUSSION

In order to study the kinetics of Iodination of aniline by iodine, equally concentrated aniline and iodine were mixed together. The final concentration of each reactant was  $5.0 \times 10^{-3}$  M. The unreacted iodine was titrated against  $2.5 \times 10^{-3}$  M sodium thiosulphate using freshly prepared starch as an indicator. Reciprocal of unreacted iodine was plotted versus time. A straight line graph

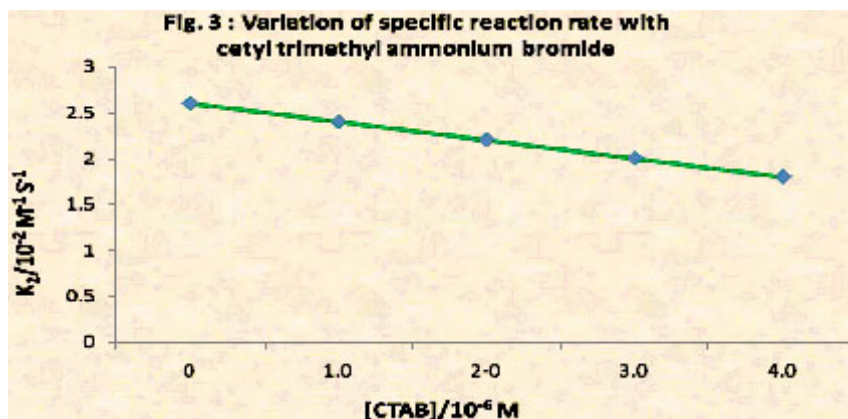
was obtained (Table 1 and Fig. 1). The second order rate constant evaluated from this graph is  $0.026 \text{ M}^{-1} \text{ S}^{-1}$ .

In the following stages of the study, the effect of micellar media on the rate of reaction was investigated. For this purpose, critical micelle concentration of cetyl trimethyl ammonium bromide (CTAB) was determined in presence of equally concentrated aniline and iodine : The CMC of CTAB in presence of  $5.0 \times 10^{-3}$  M aniline and iodine was found out to be  $1.0 \times 10^{-3}$  M from the absorption versus concentration of CTAB graph using acridine orange as colouring agent.

The  $1/[I_2]$  versus time graph (Fig. 2) was plotted with the observed unreacted iodine values during the reaction of  $5.0 \times 10^{-3}$  M aniline and iodine solutions in the presence of CTAB in different concentrations in order to see its effect on second order kinetics. The second order rate constants were

**Table 2 : Kinetics of Iodination of Aniline by iodine : in presence of CTAB**

Concentration of Aniline	:	$5.0 \times 10^{-3}$ M
Concentration of Iodine	:	$5.0 \times 10^{-3}$ M
Concentration of Sodium iodide	:	$5.0 \times 10^{-2}$ M
Temperature	:	$25.0^\circ\text{C}$
<b>[CTAB]/<math>10^{-6}</math> M</b>		<b>Specific reaction rate <math>k_2/10^{-2} \text{ M}^{-1} \text{ S}^{-1}</math></b>
-		2.6
1.0		2.4
2.0		2.2
3.0		2.0
4.0		1.8



evaluated. The dependence of these rate constants on CTAB concentration has been shown in Table 2 and Fig. 3.

The critical micelle concentration of CTAB does not affected by  $5.0 \times 10^{-3}$  M aniline and iodine. It indicates that iodine solubilization do not occur within the micelles. Hence the tri-iodide formation in presence of iodide ion is resonable to consider, since cetyl trimethyl ammonium bromide favours the formation of tri-iodide ion and stabalize it.

Fig. 2 shows that the presence of CTAB in the reaction medium, though at much lower concentration than critical micelle concentration, leads to the inhibition of the iodination of aniline by iodine. Fig. 2 and Fig. 3 leads us to conclude that the iodination of aniline is inhibited by the cetyl trimethyl ammonium bromide.

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