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## Kinetic And Mechanistic Study Of Oxidation Of Some Organic Substrates By Benzimidazolium Fluorochromate : A Review

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### ABSTRACT

*The study of the organic compounds is of immense importance both from mechanistic and synthetic point of view. In this paper we discuss about the chemical Kinetics along with oxidation of some organic substrates by Benzimidazolium Fluorochromate (BIFC). BIFC is an efficient and clean oxidant for alcohols under various solvent conditions.*

**Keywords:** Benzimidazolium Fluorochromate, Alcohols, Kinetic and Mechanistic, Oxidation





## 1. INTRODUCTION

A survey of literature gives the kinetics of oxidation of Alcohols by various oxidizing reagent have been studied<sup>21</sup>. Large number of alcohols is commercially available as well as can be early prepared. The rate of change of concentration of any one of the reactants or products per unit time known as rate of reaction.

Chemical Kinetics is the branch of chemistry which studies the rate of reaction where by various chemical reaction take place in different condition such as Nature of the reactants, concentration of reactants, Temperature, presence of catalyst, Surface area of the reactants etc. Kinetics takes into consideration the time required for transformation of reactants from one state to another. Many researchers<sup>18-20</sup> had made very important work in chemical kinetics.

Kinetic study covers the effect of concentration, Temperature and Pressure on different types of reaction. Based on the type of reaction so many types of experimental techniques had been used to investigate. Kinetics is useful in study of gas, liquid and solid phase reaction. Especially liquid phase reaction is studied the most due to higher interest of organic and inorganic chemists particularly engineers from Industry<sup>2-5</sup>. Many Kinetic factors such as concentration, catalyst, dielectric constant<sup>6-11</sup>, salt<sup>11-14</sup>, ionic strength, temperature<sup>15</sup> and free radicals<sup>16,17</sup> were accounted by various Researchers.

## 2. MATERIALS AND METHODS

In Kinetic study, So many methods are used for the basis on time period or half-life period of reactions completion. Different kinetic methods are as listed below.

SEE TABLE ON NEXT PAGE

## 3. RESULT AND DISCUSSION

The study of organic compounds is of immense importance both from mechanistic and synthetic point of view. Halochromates<sup>1-5</sup> have been used as mild and selective oxidizing reagent in synthetic organic chemistry. A number of new Halochromates like Pyridinium Halochromate<sup>6</sup>, Quinolinium Chlorochromate<sup>7</sup>, 2-Bipyridinium Chlorochromates<sup>8</sup>, Pyridinium Fluorochromates<sup>9</sup>, Quinolinium Fluorochromates<sup>10</sup>, Quinolinium bromochromate<sup>11</sup>, pyridinium Chlorochromate<sup>12</sup>, Imadazolium Fluorochromates<sup>13</sup> have been used to study the kinetics and mechanism of oxidation of various organic compounds. But a newly synthesized and developed oxidizing agent is Benzimidazolium Fluorochromates<sup>14</sup>. This reagent is more efficient and stronger oxidizing agent. Oxidation of alcohols by Benzimidazolium Fluorochromates(BIFC) leads to the corresponding formation of aldehyde. So, we are interested to select Benzimidazolium Fluorochromates as oxidizing agent for the proposed kinetic study.

### Synthesis of Benzimidazolium Fluorochromate

BIFC has been prepared by the method described in the literature<sup>1</sup>, from benzimidazole 40%(23.6 gm; 0.2 mole), hydrofluoric acid(4mL;0.23mole) and chromium trioxide(20gm;0.2 mole) in the molar ratio 1:1.3:1 at 0°C. BIFC is obtained as yellow orange crystals. It is non hygroscopic, light insensitive and stable on storage.



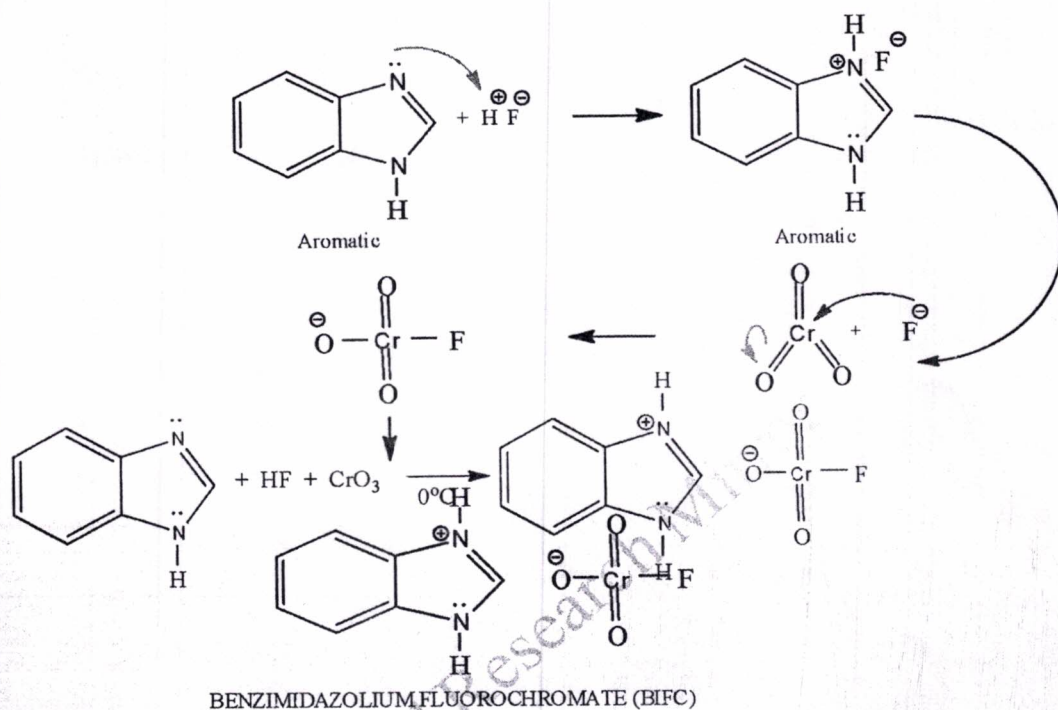


Sr. No.	Method	Time scale	Kinetic Parameters
1	Conventional	$\geq 10$ s	The reactants are mixed together in a batch reactor and Concentration Vs time is measured
2	Stopped flow	$\geq 10^{-1}$ s	Set of continuously flow system in which reactants are feed into the reactor and flow out again so quickly that there is negligible reaction followed by stopping the flow for reactant to react and lastly calculated conversion Vs time.
3	Conventional flow system	$\geq 10^{-3}$ s	Continuously reactants are feed into a reactor and the steady state reaction rate was measured
4	Pressure Jump and Temperature Jump by Eigen	$\geq 10^{-6}$ s	The reactants are mixed at such a low temperature that the reaction rate is negligible. CO <sub>2</sub> lasers used suddenly to heat the reaction, concentration Vs time measured then the reactant concentration Vs time measured.
5	NMR	$10^{-2}$ - $10^9$ s	Initiate a change with magnetic pulse and then the decay of spins measured by NMR
6	Flash photolysis by Porter	$10^{-9}$ - $10^{10}$ s	Reactants are placed into a vessel under conditions where reaction is negligible. Pulse a laser flash lamp to start reaction. The reactant conc. Vs time was measured.
7	Molecular Beam by Hersch Feld	$10^{-9}$ - $10^{13}$ s	Direct Beams of reactants towards each together in a vacuum system and measure the steady state reaction rate.
8	Femto spectroscopy by Ahmed Zewel	$10^{-15}$ s	Life time reaction can be studied.
9	Spectrophotometric Method by Arnold O. Beckman	$\geq 10$ s	Oxidation reaction at different concentrations with respect oxidant and Substrate and also measured different kinetic parameter like concentration, temperature etc.





### \* Mechanism of Benzimidazolium Fluorochromate (BIFC)



### Characteristics of Benzimidazolium Fluorochromate (BIFC)

Molecular formula of BIFC is  $\text{C}_7\text{H}_7\text{N}_2\text{CrFO}_3$ , Its Molar mass is 238 g/mol, BIFC is appeared in Yellow-orange crystals, Melting point  $-195^\circ\text{C}$ , Solubility-slightly soluble in alcohol, acid and water, Its crystal structure-Heterocyclic, Flash point-Non-flammable. It is non-hygroscopic, light insensitive and stable on storage. BIFC is an effective and clean oxidant for alcohols.

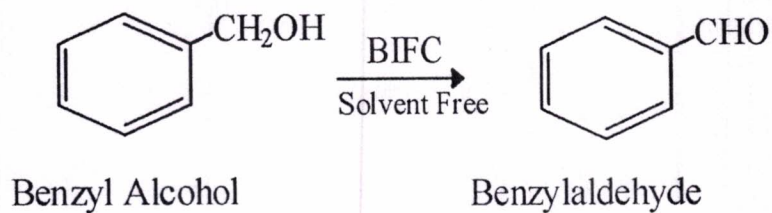
### Mechanism

Oxidation of alcohol by BIFC is an acid catalysed reaction. The oxidation of alcohols yields the corresponding aldehyde as the product.

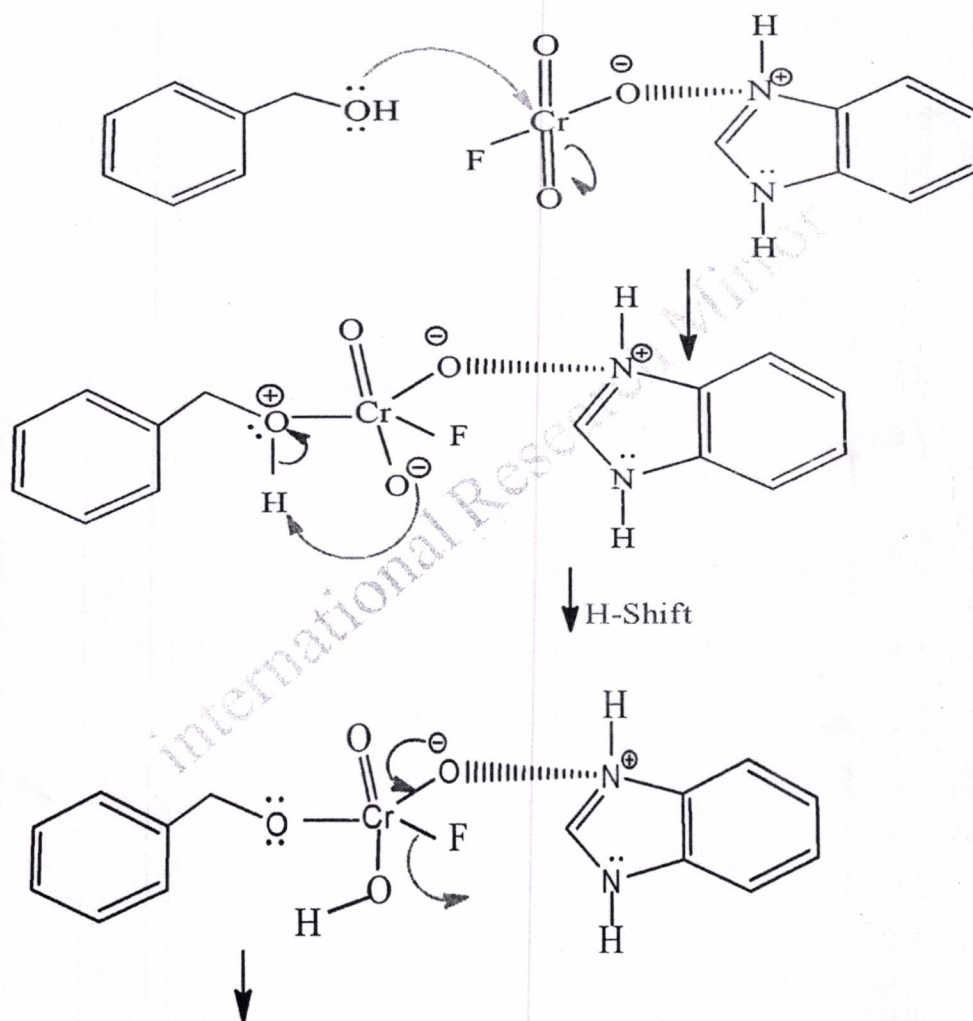
#### 1) Mechanism of Oxidation of Benzyl Alcohol with BIFC



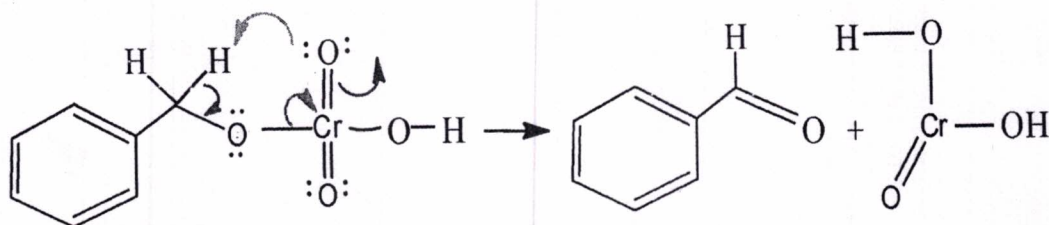
### 1) Mechanism of Oxidation of Benzyl Alcohol with BIFC



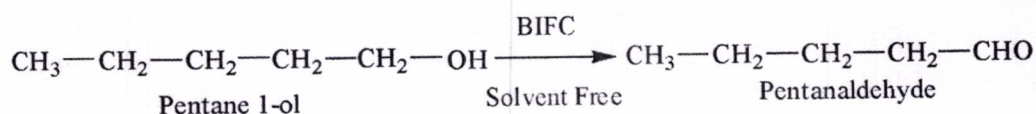
### \* Mechanism of Oxidation of Benzyl Alcohol with BIFC



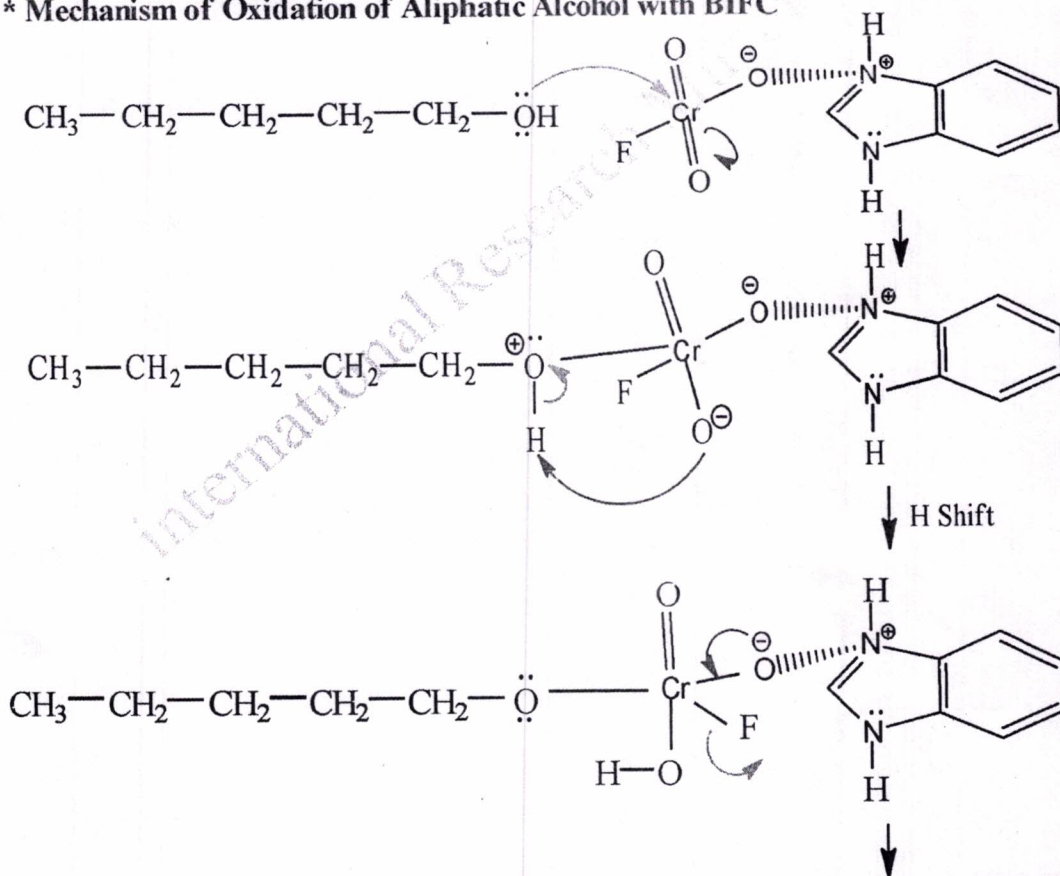


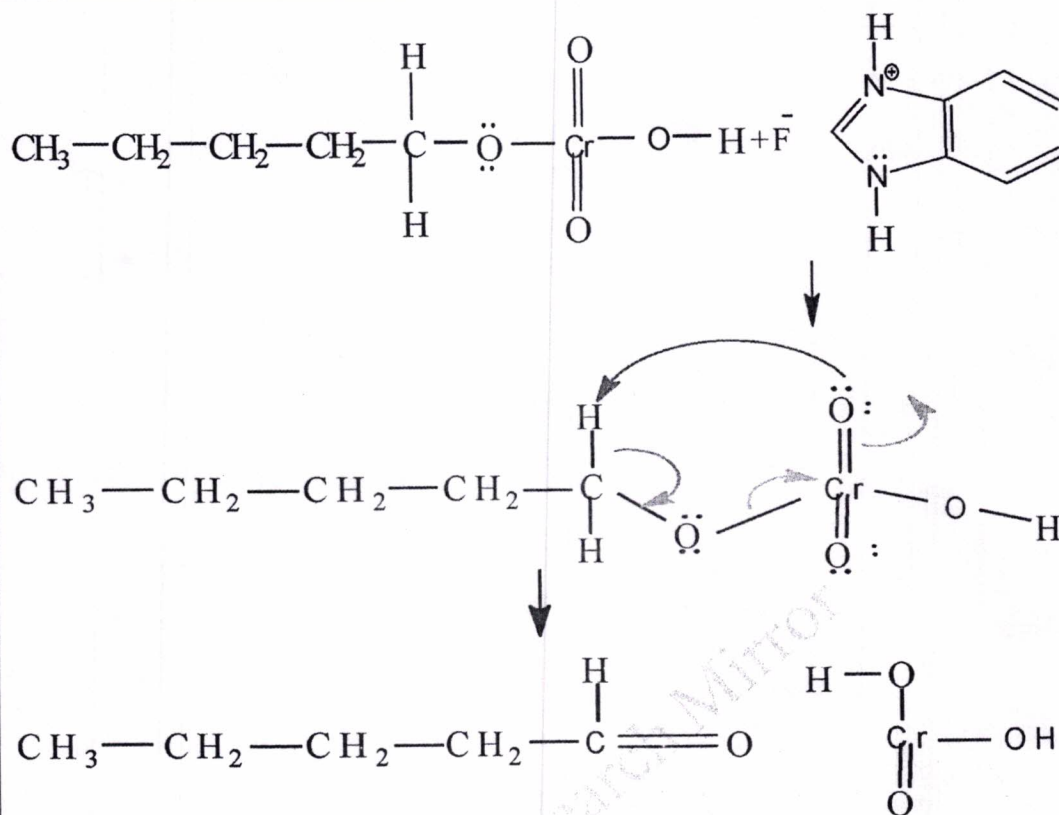


2) Oxidation of Aliphatic Alcohol with BIFC:-



\* Mechanism of Oxidation of Aliphatic Alcohol with BIFC





## 2. CONCLUSION

In this oxidation kinetic parameters the effect of ionic strength and solvent polarity suggest the participation of an ion and a neutral molecule in the mechanistic step. Alcohols are used in this oxidation, are of extrapure quality received from Merck and Fluka and Heraeus CHN-O-RAPID analyser was carried out its elemental analysis. The present method of estimation of alcohol<sup>10-11</sup> is expected to be based on the oxidation of primary alcohol to aldehyde and associated reduction of oxidation state Cr(VI) to Cr(III). Simple spectrophotometric method has been developed based on the oxidation of primary and secondary alcohol by BIFC. The reaction were performed by monitoring the

decreasing the concentration of Benzimidazolium fluorochromate spectrophotometrically using (Shimadzu UV-VIS) spectrophotometer (model UV-1800). The reaction was studied under Pseudo-First order condition by using an excess of substrate over Benzimidazolium Fluorochromate.  $k_{obs}$  are independent of initial concentration of Benzimidazolium Fluorochromate, the rate of reaction increases with increase in the concentration of alcohol but not linearly. Reaction rate depend on reductant concentration at different temperature and are calculated from double reciprocal plots. The rate of reaction constants,  $k_{obs}$ , are evaluated from the linear plots of  $\log [BIFC]$  vs time. The observed multivariate and simple linear regression analysis data was carried out by using the least-squares method.





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