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# Kinetic study of oxidation reactions using Chromium (VI) Complexes TBC-1 and TAC-2

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## Abstract

**Background:** The chromium (VI) complexes have been extensively employed as oxidizing agents in organic reactions and kinetic studies have offered valuable information concerning the behavior of reactions and their mechanism of action.

**Purpose:** The current work will focus on studying the kinetics of oxidation processes that are catalyzed by the Chromium (VI) complexes TBC-1 and TAC-2.

**Methodology:** UV-Visible spectrophotometric monitoring was done through kinetic studies whereby the time-dependent variation in absorbance was recorded under experimental control. The influence of substrate concentration, oxidant concentration and temperature on the rate of reaction was experimented with, and observed rate constants were assessed under pseudo-first-order conditions.

**Findings:** The oxidation reactions were of pseudo-first-order kinetics. The measured rate constants were found to be increased with the concentration of the substrate, concentration of the oxidant and temperature. Arrhenius-type behaviour in temperature-dependent studies meant that an activated complex was involved. Comparison of the kinetic studies showed that the reaction rate of the TBC-1 complex was very slightly higher than that of TAC-2 under the same conditions.

**Conclusion:** The kinetic findings pass the test that Chromium (VI) complexes TBC-1 and TAC-2 are useful in catalyzing oxidation reactions, and the rate of the reactions depends on concentration and temperature parameters. The results give a mechanistic understanding of the Chromium (VI)-based oxidation systems and point to the role of ligand environment in determining the reaction kinetics.

Chromium (VI) complexes are complexes of chromium, which is the element with a central role in the semiconductor industry. <| human | > Chromium (VI) complexes are complexes of chromium, the element whose key role is played in the semiconductor industry.

**Keywords:** Chromium (VI), TBC-1, TAC-2, industry, oxidation, reaction kinetics, conditions

## Introduction

Oxidants based on chromium (VI) have been used extensively in the synthesis of organic compounds since they are powerful oxidizing agents and capable of being predicted in their reaction orders <sup>[1, 2]</sup>. The reactions of the Chromium (VI) species with organic substances tend to take place in electron-transfer reactions, which result in effective oxidation under mild conditions. Discrete Chromium (VI) organic complexes have gained growing popularity over the past years due to their greater stability and adjustable reactivity <sup>[3, 4]</sup>.

Kinetic studies are essential in determining the mechanistic pathways of the Chromium (VI)-mediated oxidation reactions. The parameters, including the order of the reaction, the rate constants and activation energy are also of great interest in terms of the nature of intermediate species and the rate-limiting step <sup>[5, 6]</sup>.  $\alpha$ ,  $\beta$ -Unsaturated carbonyls and other related substrates are especially interesting because of their conjugated systems, which play a role in their reaction with oxidizing agents <sup>[7, 8]</sup>.

The synthesized, characterized Chromium (VI) complexes TBC-1 and TAC-2 of Paper-1 provide a superior surface upon which the kinetics can be assessed because they are structurally stable and exhibit the ability to oxidize <sup>[3, 9, 10]</sup>. Nevertheless, little has been done in terms of investigations, at the kinetic level, of their oxidation behavior <sup>[11-14]</sup>.

Hence, the current paper is limited to the kinetic analysis of oxidation reactions involving Chromium (VI) complexes TBC-1 and TAC-2 under controlled experimental conditions with an emphasis on exploring their reaction mechanism and efficiency in relation to each other.

## Materials and Methods

### Materials and Chemical Reagents

The kinetic investigations applied Chromium (VI) complexes of TBC-1 and TAC-2.

The previously synthesized and characterized TBC-1 and TAC-2 chromium (VI) organic complexes were directly utilized in the current study (Paper-1). All the organic substances, as well as solvents, were of analytical grade and were not purified. The solution preparation was done with distilled water.

### Instrumentation

#### UV Visible spectrophotometer: Shimadzu UV-1800.

- Thermostatic Water Bath
- Analytical Balance ( $\pm 0.0001$  g)
- Hot Plate Magnetic Stirrer.

### Kinetic Procedure

Kinetic measurements were conducted under pseudo first order conditions when the substrate concentration was held in large excess over the concentration of the Chromium (VI) complex. The course of the oxidation reaction was followed spectrophotometrically by observing the variation of the absorbance with time at the respective wavelength of the reacting species<sup>[15]</sup>.

The reaction was started by the addition of a known quantity of Chromium (VI) complex solution into the already-mixing reaction mixture at the required temperature. The values of absorbance were obtained at set time intervals until the reaction had attained completion.

### Rate Constants

Rate constants are determined by measuring the solution times of the holograms corresponding to the various angular positions of the light beam.

The integrated first-order rate equation was used to compute observed rate constants ( $k_{obs}$ ):

$$\ln \frac{A_0}{A_t} = k_{obs} t$$

**$A_0$  and  $A_t$  are the values of the absorbance at time zero and at time  $t$ , respectively**

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The substrate concentration effect was examined by changing the substrate concentration and maintaining the concentration of the Chromium (VI) complex and the other reaction parameters constant. The same was done with the influence of the concentration of the oxidants where the concentration of TBC-1 or TAC-2 was varied at a constant concentration of the substrate. Studies were carried out using a temperature range of 298-313 K in order to determine the thermal characteristics of the reaction system. All kinetic experiments were done in three replicates and analysis was done using average values of the rate constants.

### Results

Kinetic behavior of oxidation reactions between complexes of Chromium (VI), TBC-1 and TAC-2, was methodically studied under controlled experimental conditions, through UV-Visible spectrophotometric studies. The rate of the reaction was analyzed depending on the concentration of substrates and oxidants, and temperature so as to explain the kinetic properties of the system.

### Concentration of Substrate Effect

The concentration of substrate on the rate of oxidation was experimented with the TBC-1 complex when other experimental parameters were kept constant. The observed rate constant ( $k_{obs}$ ) in the results summarized in Table 1 indicates a constant rise in rate constant with an increase in the substrate concentration. The  $k_{obs}$  values rose with the increased concentration of substrate as it was changed to  $0.100 \text{ mol L}^{-1}$  instead of  $0.025 \text{ mol L}^{-1}$  and the  $k_{obs}$  values increased to  $6.71 \times 10^{-4} \text{ s}^{-1}$  -  $1.78 \times 10^{-4} \text{ s}^{-1}$  (Table 1). The fact that the rate constant increases linearly with the concentration of substrate shows that the reaction rate is dependent on the substrate concentration in the first order. This action implies that the generation of a temporary complex between the substrate and the Chromium (VI) center preceding the rate-limiting step occurs.

**Table 1:** Effect of substrate concentration on reaction rate (TBC-1)

| Substrate Concentration ( $\text{mol L}^{-1}$ ) | $k_{obs} (\text{s}^{-1}) \times 10^{-4}$ | $\log k_{obs}$ |
|-------------------------------------------------|------------------------------------------|----------------|
| 0.025                                           | 1.78                                     | -3.75          |
| 0.050                                           | 3.42                                     | -3.47          |
| 0.075                                           | 5.06                                     | -3.30          |
| 0.100                                           | 6.71                                     | -3.17          |

Figure 1 shows how the concentration of the substrate affects the rate constant recorded in the oxidation reaction by the TBC-1 complex. The rate of reaction to  $k_{obs}$  is found to rise linearly with the concentration of substrate, which

confirms that the rate of the reaction depends on substrate concentration in the first-order. This activity favors the influence of the coordination of the substrate to the Chromium (VI) center, before the rate-determining step.

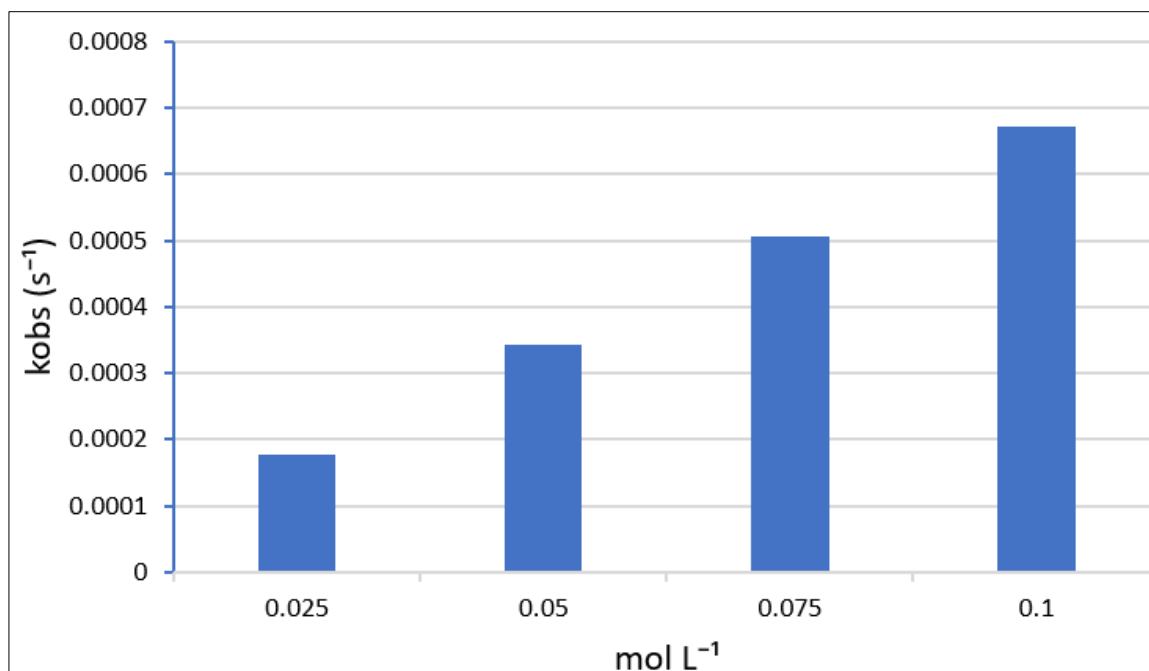


**Fig 1:** Substrate concentration effect on the rate constant of oxidation reaction mediated by Chromium (VI) complex TBC-1 in constant temperature and constant oxidant concentration.

#### Impact of concentration of oxidant

The rate constant of the reaction with the concentration of the oxidants was investigated in the case of the TAC-2 complex. The information provided in Table 2 shows that the rate constant observed increases in direct proportion to the concentration of oxidants. As the concentration of the

oxidant was changed to  $1.5 \times 10^{-3}$  to  $6.0 \times 10^{-3}$  mol L<sup>-1</sup>, the values of  $k$  changed to  $1.56 \times 10^{-4}$  s<sup>-1</sup> to  $6.13 \times 10^{-4}$  s<sup>-1</sup> (Table 2). Such a trend affirms pseudo-first-order kinetics to the Chromium (VI) oxidant with respect to the experiment conditions utilized as is consistent with a normal Chromium (VI)-mediated oxidation system.

**Table 2:** Effect of oxidant concentration on reaction rate (TAC-2)

| Oxidant Concentration (mol L <sup>-1</sup> ) | k <sub>obs</sub> (s <sup>-1</sup> ) × 10 <sup>-4</sup> | Log k <sub>obs</sub> |
|----------------------------------------------|--------------------------------------------------------|----------------------|
| 1.5 × 10 <sup>-3</sup>                       | 1.56                                                   | -3.81                |
| 3.0 × 10 <sup>-3</sup>                       | 3.02                                                   | -3.52                |
| 4.5 × 10 <sup>-3</sup>                       | 4.58                                                   | -3.34                |
| 6.0 × 10 <sup>-3</sup>                       | 6.13                                                   | -3.21                |

**Effect of Temperature:** Using the TBC-1 complex, temperature dependence of the oxidation reaction was investigated at a temperature range of 298-313 K. Table 3 indicates that further rise of temperature led to a significant rise in the observed rate constant. The  $k_{obs}$  was found to rise at 298 K to  $2.05 \times 10^{-4}$  s<sup>-1</sup> to  $4.96 \times 10^{-4}$  s<sup>-1</sup> at 313 K.

The similar trend in the values of  $\ln k_{obs}$  with temperature is an indication that the reaction is thermally activated (Table 3). The dependence of the rate constants on temperature indicates that a standard Arrhenius equation may be applied and indicates that an activated complex is likely to be involved in the oxidation reaction.

**Table 3:** Effect of temperature on reaction rate

| Temperature (K) | k <sub>obs</sub> (s <sup>-1</sup> ) × 10 <sup>-4</sup> | ln k <sub>obs</sub> |
|-----------------|--------------------------------------------------------|---------------------|
| 298             | 2.05                                                   | -8.49               |
| 303             | 2.78                                                   | -8.19               |
| 308             | 3.74                                                   | -7.89               |
| 313             | 4.96                                                   | -7.61               |

The Arrhenius plot, which was obtained based on temperature-dependent data of kinetic analysis of the oxidation reaction mediated by the TBC-1 complex, is displayed in Figure 2. Linear dependence of the  $\ln k_{obs}$  on

$1/T$  proves Arrhenius-type behavior which means that the reaction is carried out by a thermally activated transition state. The gradient of the plot can be applied to determine the activation energy of the reaction.

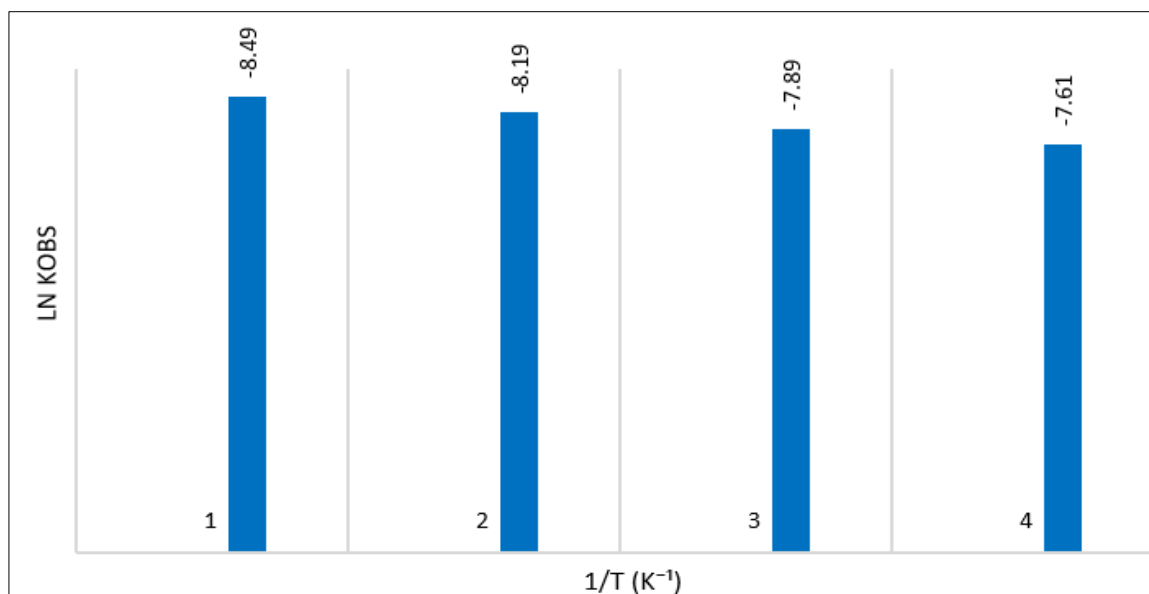


**Fig 2:** Arrhenius plot of  $\ln k_{\text{obs}}$  versus inverse temperature ( $1/T$ ) for the oxidation reaction mediated by Chromium (VI) complex TBC-1

### Comparative Kinetic Behaviour

The kinetic performance of the two Chromium (VI) complexes was composed of a comparative analysis of each under the same experimental conditions of 308 K. The results in Table 4 indicate that the observed rate constant of TBC-1 complex ( $5.06 \times 10^{-4} \text{ s}^{-1}$ ) is higher than that of TAC-2 ( $4.32 \times 10^{-4} \text{ s}^{-1}$ ). This reactivity difference can be explained by the differences in the ligand surrounding the Chromium (VI) center which could affect the rate of electron-transfer and interaction with the substrate (Table 4). The findings refer to the fact that TBC-1 has a little higher oxidative capacity under the same conditions as TAC-2.

**Table 4:** Comparative rate constants for TBC-1 and TAC-2

| Chromium (VI) Complex | $k_{\text{obs}} (\text{s}^{-1}) \times 10^{-4}$ | Reaction Conditions         |
|-----------------------|-------------------------------------------------|-----------------------------|
| TBC-1                 | 5.06                                            | 308 K, identical conditions |
| TAC-2                 | 4.32                                            | 308 K, identical conditions |

### Discussion

Kinetic information gained in the current research shows clearly that the oxidation reactions with the use of the Chromium (VI) complexes TBC-1 and TAC-2 correspond to pseudo-first-order kinetics. The variation of the rate with the concentration of substrate implies that the coordination to or association with the Chromium (VI) center takes place before the rate-limiting step. This action is usually found in oxidation reactions involving Chromium (VI) in which the development of a short-lived substrate-oxidant complex aids in electron transfer.

The fact that the rate constants appeared to increase with the concentration of the oxidant also indicates the presence of Chromium (VI) species in the rate-limiting step of the reaction. The kinetic data that have been collected depending on the temperature show that the oxidation process is thermally activated and the dependence of the  $\ln k_{\text{obs}}$  on temperature is characteristic of Arrhenius behavior. This indicates that oxidation is done using an activated transition state where the electron transfer of the substrate to the Chromium (VI) center takes place.

The kinetic comparative analysis shows that TBC-1 has a greater oxidative efficiency as compared to TAC-2 in the

same conditions. This disparity can be justified with reference to the effect of ligands which can cause changes in the redox potential and the accessibility of the Chromium (VI) center. In general, the kinetic findings are consistent with previously observed Chromium (VI) oxidation mechanisms and also prove the influence of ligand environment in regulating reaction rates.

### Conclusion

The current kinetic analysis shows that the oxidation reactions that are mediated by the Chromium (VI) complex, TBC-1 and TAC-2, under the experimental conditions are pseudo-first-order reactions. The rate of reaction rises steadily as the concentration of the substrate and the oxidant concentration rise, and this shows the effective involvement of both species in the oxidation process. Kinetic data (temperature-dependent) display Arrhenius-type behavior, with the oxidation reactions thought to occur through an activated transition state.

The relative kinetic analysis indicates that TBC-1 complex is more oxidatively efficient than TAC-2 under the same experimental conditions and this could be explained by the variations in the ligand environment that may affect the electron-transfer reactions. On the whole, the study can give a clear picture of the kinetic behavior of Chromium (VI)-mediated oxidation reaction and can add to the general knowledge of the mechanics of Chromium (VI) oxidation chemistry.

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