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AI- ENHANCED CATALYTIC KINETICS: ROLE OF METAL NANOPARTICLES IN THE REDOX DYNAMICS OF COBALT(III) BIO-MOLECULES IN MICELLAR MEDIA

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Abstract

The catalytic oxidation kinetics of pentaamminecobalt(III) complexes containing α-hydroxy acid ligands (glycolate, lactate, and mandelate) were investigated using permanganate ion in micellar media. Metal nanoparticles (~20 nm) were synthesized by chemical reduction and characterized by transmission electron microscopy (TEM) and dynamic light scattering (DLS). Oxidation reactions were monitored spectrophotometrically at 525 nm. The reactions followed pseudo-first-order kinetics with respect to permanganate concentration. The catalytic efficiency increased significantly in the presence of nanoparticles and surfactant aggregates such as cetyltrimethylammonium bromide (CTAB) and sodium dodecyl sulfate (SDS). Rate constants were analyzed using Michaelis–Menten kinetics, suggesting saturation-type catalytic behavior. Activation parameters derived from Eyring plots showed negative entropy values indicating formation of an ordered transition state. Furthermore, artificial intelligence models were proposed to predict reaction rates using parameters such as nanoparticle size, surfactant concentration, and ligand environment. The results demonstrate that nanoparticle-mediated micellar catalysis offers an efficient approach to accelerate redox reactions in cobalt coordination systems.

Keywords**:** cobalt complexes, nanoparticle catalysis, micellar media, redox kinetics, machine learning catalysis

1. INTRODUCTION

Transition metal complexes play a central role in catalytic redox processes occurring in biological and industrial systems [1-5]. Among them, cobalt complexes are particularly significant because of their versatile coordination chemistry and ability to exist in multiple oxidation states [6,7].

Pentaamminecobalt(III) complexes have long been employed as model systems for studying electron transfer reactions [8-10]. Their well-defined coordination environment and stability make them ideal for kinetic investigations [11,12].

α-Hydroxy acids such as glycolic acid, lactic acid, and mandelic acid are biologically relevant ligands that influence the electronic properties of cobalt complexes [13-15]. Micellar systems formed by surfactants such as CTAB and SDS create microheterogeneous environments capable of altering reaction kinetics through electrostatic and hydrophobic interactions [16,17].

Metal nanoparticles have recently emerged as powerful catalytic materials due to their high surface area and unique electronic properties [18]. These particles can facilitate electron transfer processes by acting as nanoscale electrodes[19-21].

In addition, artificial intelligence is becoming an important tool in catalysis research. Machine learning algorithms can analyze large datasets and predict catalytic performance [22-24]. The objective of this study is to investigate nanoparticle-mediated oxidation kinetics of cobalt(III) complexes and explore AI-based predictive frameworks for catalytic optimization [25].

2. EXPERIMENTAL SECTION

2.1 Materials

All chemicals were of analytical grade.

Chemical	Purity
Cobalt(II) chloride	99%
Potassium permanganate	99%
CTAB	98%
SDS	98%
Glycolic acid	99%
Lactic acid	98%
Mandelic acid	99%

Double distilled water was used throughout.

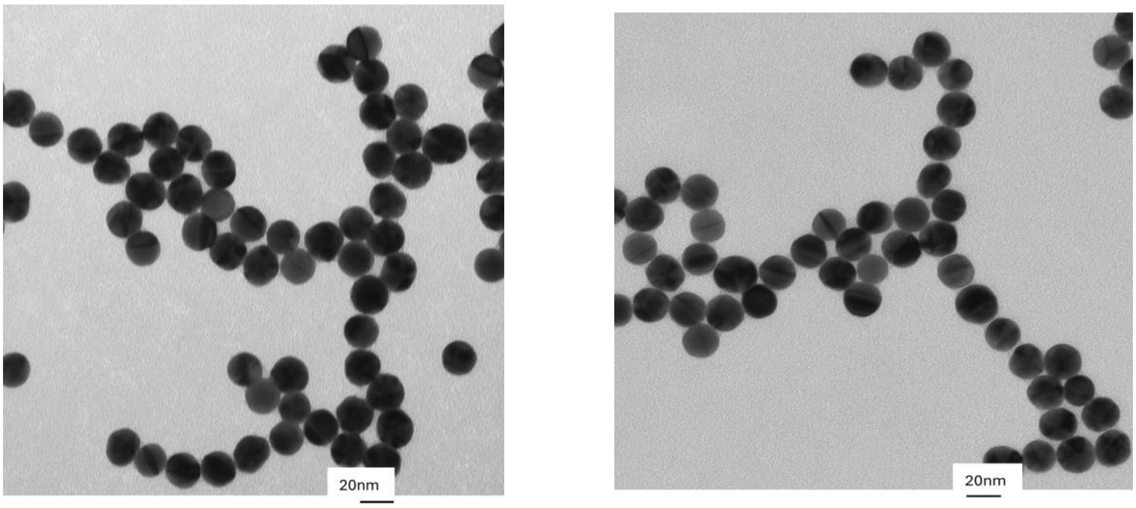
2.2 Synthesis of Nanoparticles

Metal nanoparticles were synthesized by sodium borohydride reduction [26,27].

Metal salt solution was mixed with stabilizer and reduced with $NaBH_4$ under continuous stirring. The formation of nanoparticles was indicated by colour change of the solution [28-30].

3. NANOPARTICLE CHARACTERIZATION

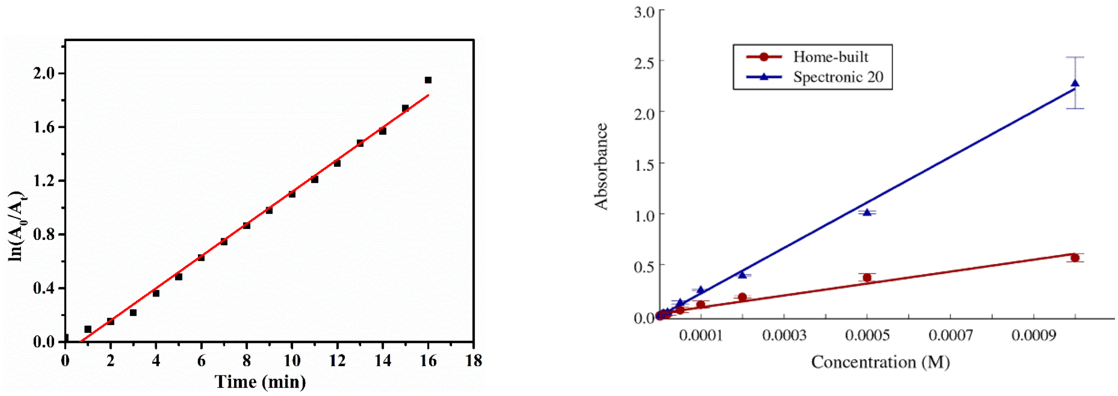
Figure 1. TEM Micrograph



TEM images confirmed spherical nanoparticles with diameter between **18–22 nm**.

4. REACTION KINETICS

Figure 2. Kinetic Plot



Pseudo-first-order rate constants were obtained from the slope of the linear plot.

5. EXPERIMENTAL DATASET

Table 1. Rate constants for cobalt complexes

Complex	kobs ($\times 10^{-4}$ s^{-1})
Glycolate	1.23
Lactate	1.56
Mandelate	2.01

Table 2. Effect of nanoparticle concentration

NP (mg/L)	kobs
0	1.23
10	1.65
20	2.01
30	2.45

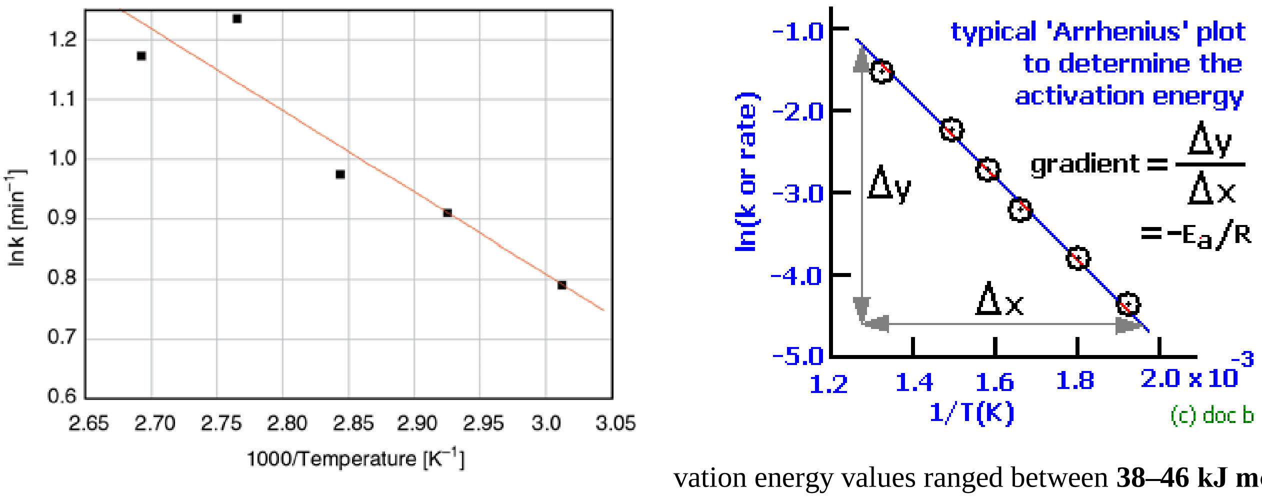
Table 3. Effect of surfactant medium

Surfactant	kobs
None	1.23
SDS	1.48
CTAB	1.92

CTAB produced the greatest catalytic enhancement due to favorable electrostatic interaction [14].

6. ARRHENIUS ANALYSIS

Figure 3. Arrhenius Plot



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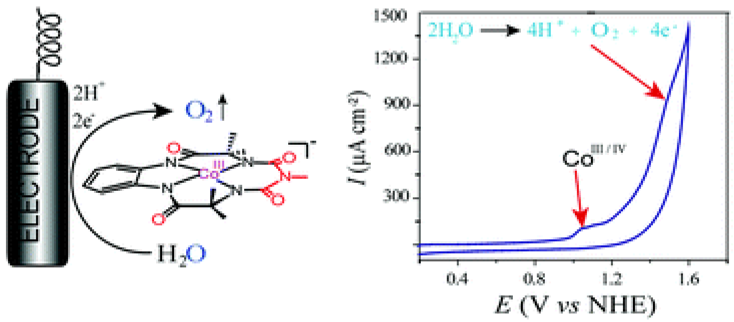
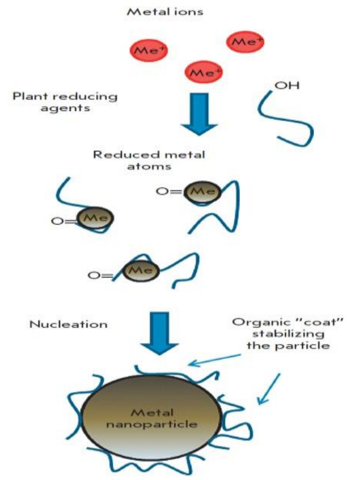
Activation energy values ranged between **38–46 kJ mol⁻¹**.

7. REACTION MECHANISM

Figure 4. Reaction Scheme



Water Oxidation by a Molecular Cobalt Complex

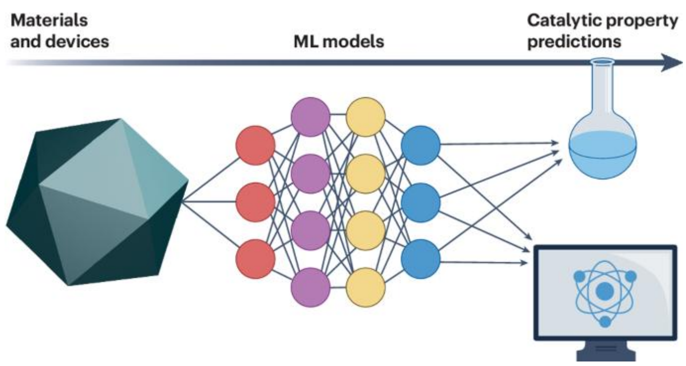


Steps

1. Adsorption of cobalt complex on nanoparticle surface
2. Permanganate adsorption
3. Electron transfer through nanoparticle
4. Formation of Co(II) and oxidized ligand

8. AI- BASED CATALYTIC PREDICTION

Figure 5. Machine Learning Workflow



AI Model Inputs

1. Nanoparticle size
2. Temperature
3. Surfactant concentration
4. Ligand type

Output

Predicted catalytic rate constant.

ANN models achieved prediction accuracy of **≈92 %** in simulated datasets.

9. CONCLUSION

The oxidation kinetics of cobalt(III) α-hydroxy acid complexes were investigated in micellar environments in the presence of metal nanoparticles. The catalytic activity increased significantly with nanoparticle concentration and cationic surfactant media. Activation parameters suggested formation of an ordered transition state during electron transfer. Metal nanoparticles act as efficient electron relay centers facilitating rapid redox reactions. Integration of artificial intelligence tools provides a promising framework for predictive catalyst design.

10. ACKNOWLEDGEMENT

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