



SUMMER RESEARCH PROJECT



Metal-ligand Single-atom Catalysts at Surfaces

FINAL REPORT

Naufran Neyas

**Department of Chemical Engineering
Indian Institute of Technology, Bombay**

Guide:

Professor Steven L. Tait

Tait Lab

**Professor of Chemistry
Indiana University Bloomington**

Department of Chemistry
IU Bloomington

Abstract

This Project investigates the development of single-atom catalysts (SACs) using cobalt on Al_2O_3 supports through an on-surface metal-ligand coordination strategy.

We conducted ultra-high vacuum experiments for precise surface analysis using photoelectron spectroscopy. SACs were also synthesised under ambient conditions and their activity was evaluated in reactors. Characterisation involved X-ray photoelectron spectroscopy (XPS), DRIFTS and inductively coupled plasma mass spectrometry (ICP-MS).

My work aims to prepare Cobalt-Ligand Coordinated SACs for higher selectivity to propene in the propane dehydrogenation (PDH) reaction.

Acknowledgments

I would like to express my heartfelt gratitude to the Indiana University Bloomington and Prof. Srinivasan Iyengar for selecting me for the prestigious Summer Research Program. This opportunity has been instrumental in shaping my research skills and broadening my scientific horizons.

I would like to thank Prof. Steven L. Tait for allowing me to work on this project in the Tait Lab at the Indiana University Bloomington. I would also like to extend my appreciation to Wanna Wondemagegn, for being a wonderful mentor.

TABLE OF CONTENTS

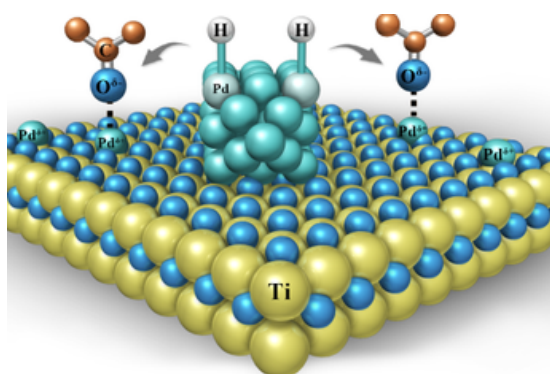
1. Introduction	3
1.1 Problem Statement	3
1.2. Single Atom Catalyst (SAC)	3
1.3. Advantages of using Single Atom Catalysts (SACs)	3
2. Preparation of Single Atom Catalysts(SACs)	4
2.1 Chemicals and Reagents	4
2.2 Chemical Reactions	6
2.3 Procedure	7
3. Characterisation of Single Atom Catalysts(SACs)	7
3.1 Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)	7
3.2 CO-Adsorption DRIFTS Technique	12
3.3 Inductively coupled plasma mass spectrometry (ICP-MS)	14
4. Propane Dehydrogenation Reaction (PDH)	16
4.1 PDH reaction with CO ₂ flow	16
4.2 Packing of Catalyst for Activity Test	17
4.3 Activity Test for Cobalt SACs	18
5. Effects of Ligands and Supports on Catalytic Activity	20
5.1 Effects of Ligands on Catalytic Activity	20
5.2 Effects of Supports on Catalytic Activity	21
Conclusions	22
Bibliography	23

1. Introduction

1.1 Problem Statement

Develop cost-effective **metal-ligand coordinated single-atom catalysts** on metal oxide supports to replace expensive noble metals for efficient and economically viable propane dehydrogenation.

1.2 Single Atom Catalyst (SAC)



A single-atom catalyst (SAC) features individual **metal atoms** dispersed on a **support material** at the atomic scale. This unique arrangement maximizes metal atom utilization, enhancing catalytic activity, selectivity, and stability. SACs are crucial in various chemical reactions.

Fig 1 :Single Atom Catalyst

1.3 Advantages of using Single Atom Catalysts (SACs)

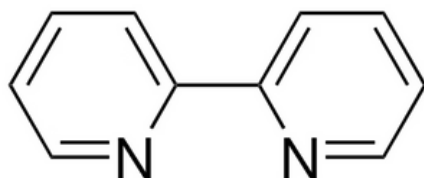
- **High Atom Utilization:** Every atom acts as a catalytic site, maximizing efficiency and reducing costs.
- **Superior Catalytic Activity:** Offers high turnover frequencies due to isolated active sites.
- **Enhanced Selectivity:** Uniform atomic dispersion leads to precise control over reaction pathways.
- **Stability and Longevity:** Resists sintering and remains stable under harsh conditions, extending lifespan.
- **Environmental Benefits:** Lowers metal usage and supports green chemistry by operating under milder conditions.
- **Versatility:** Suitable for a wide range of reactions, from hydrogenation to oxidation.
- **Improved Electronic Properties:** Unique electronic interactions enhance reaction mechanisms.

2. Preparation of Single Atom Catalysts(SACs)

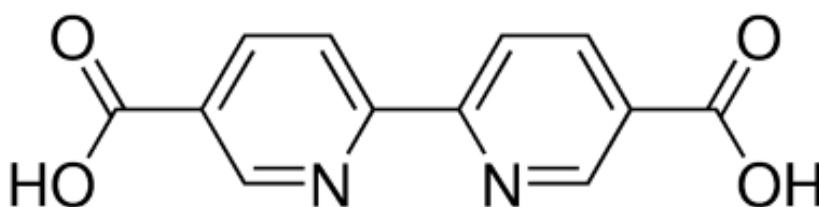
2.1 Chemicals and Reagents

2.1.1 Ligands

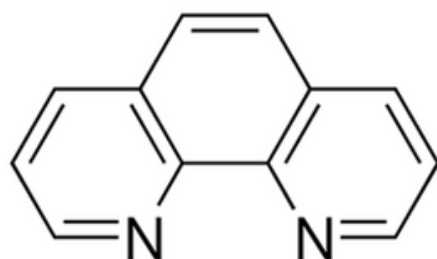
1) 2,2'-Bipyridine: $C_{10}H_8N_2$



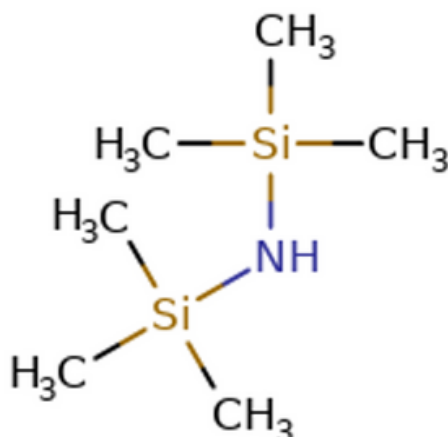
2) 2,2'-Bipyridine-5,5'-dicarboxylic acid : $C_{12}H_8N_2O_4$



3) 1,10-phenanthroline: $C_{12}H_8N_2$



4) Bis(trimethylsilyl)amine :- $HN(Si(CH_3)_3)_2$



2.1.2 Support



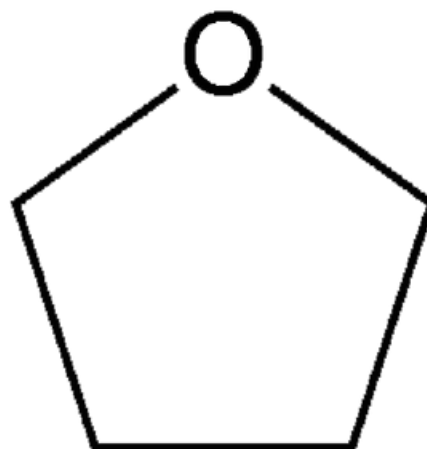
2.1.3 Cobalt Salt



2.1.4 Solvent

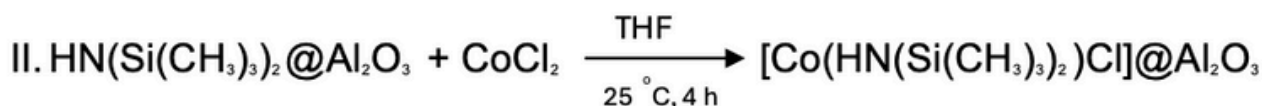
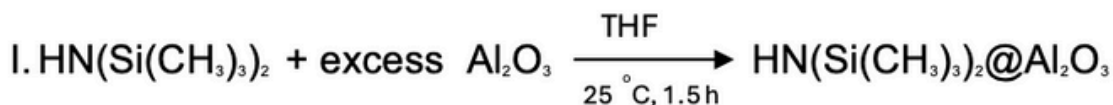
THF

Tetrahydrofuran

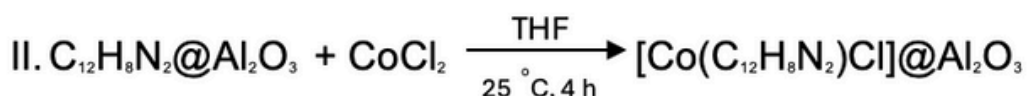
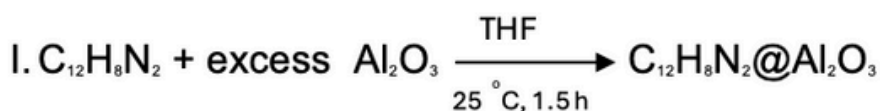


2.2 Chemical Reactions

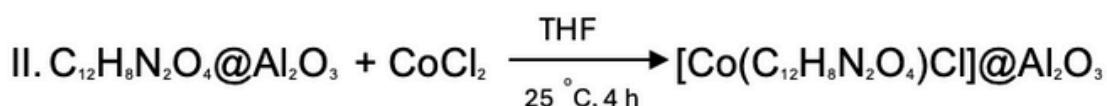
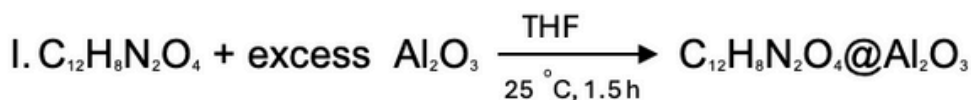
Reaction 1: Preparation of $[\text{Co}(\text{HN}(\text{Si}(\text{CH}_3)_3)_2\text{Cl})@\text{Al}_2\text{O}_3$ Ligand: Bis(trimethylsilyl)amine



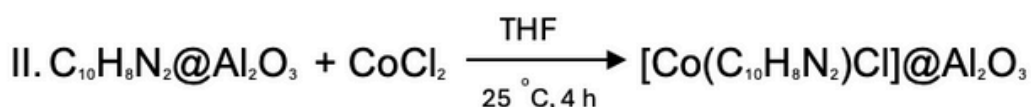
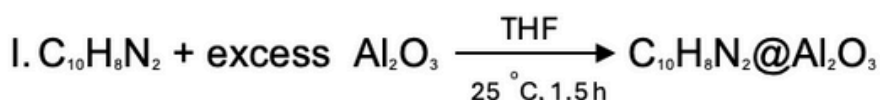
Reaction 2: Preparation of $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]@\text{Al}_2\text{O}_3$ Ligand: 1,10-phenanthroline



Reaction 3: Preparation of $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]@\text{Al}_2\text{O}_3$ Ligand: 2,2'-Bipyridine-5,5'-dicarboxylic acid



Reaction 4: Preparation of $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)\text{Cl}]@\text{Al}_2\text{O}_3$ Ligand: 2,2'-Bipyridine



2.3 Procedure

STEP 1

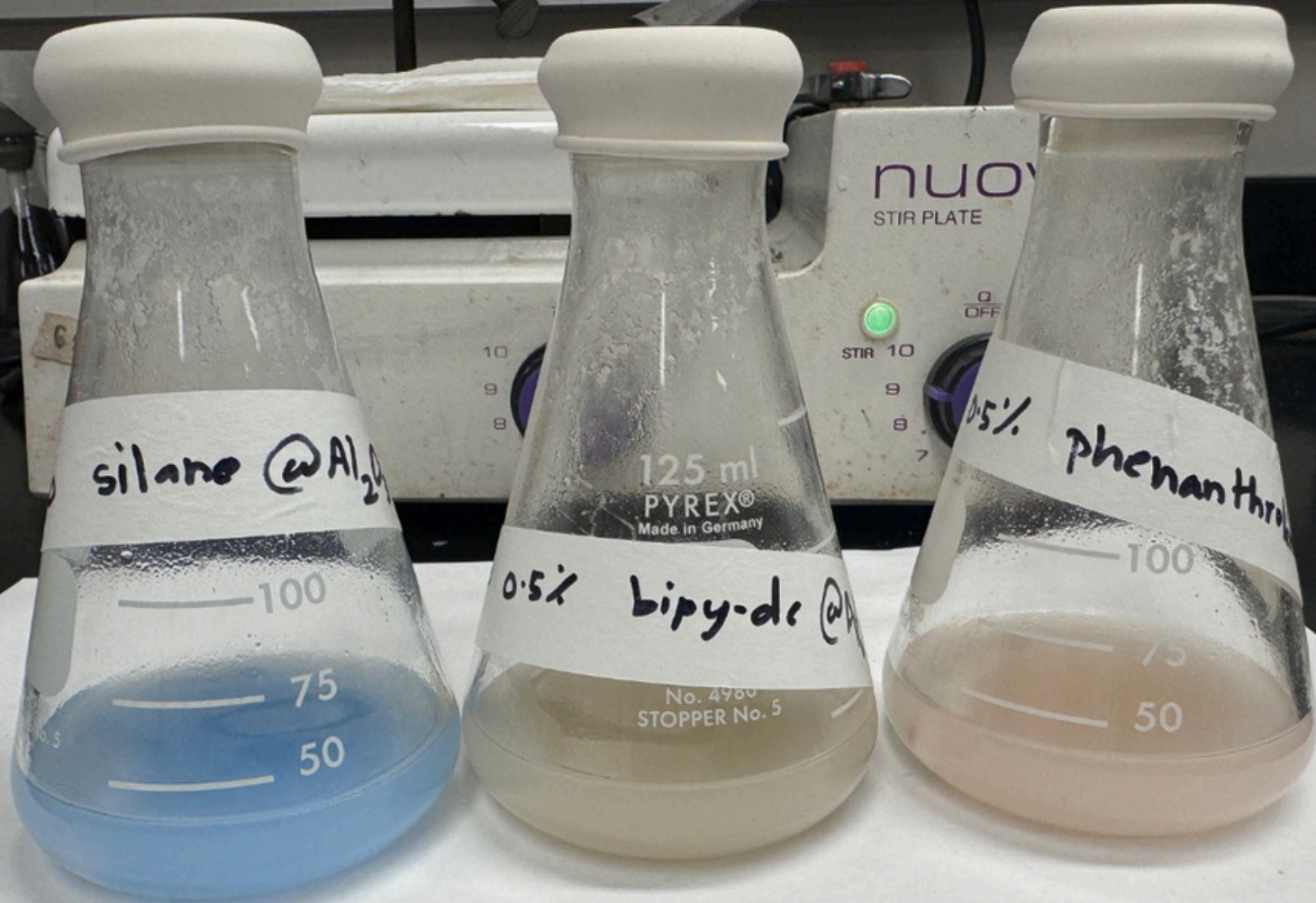
Initially, select one of the 4 ligands, Bis(trimethylsilyl)amine, 1,10-phenanthroline, 2,2'-Bipyridyl and 2,2'-Bipyridine-5,5'-dicarboxylic acid. Dissolve the ligand in 30.0 mL of THF solvent in a 125 mL reactor flasks. The mass of ligand is calculated for a 1:4 metal to ligand ratio for 0.5 and 1.0 wt% catalyst or a 1:1 ratio for 4 wt%.

STEP 2

Next, add 300 mg of Al_2O_3 to each ligand solution and stir the mixture for 1.5 hours at 25 °C. Subsequently, slowly (30-40 seconds) add required amount of cobalt dichloride (salt crystals) to each solution to complex with the ligands, and continue stirring the mixture for 4 hours (shorter and longer times were also tested) at 25 °C. Immediately after adding the cobalt salt to the solution, the colour changes from white to the final colour of the solution within a few minutes.

STEP 3

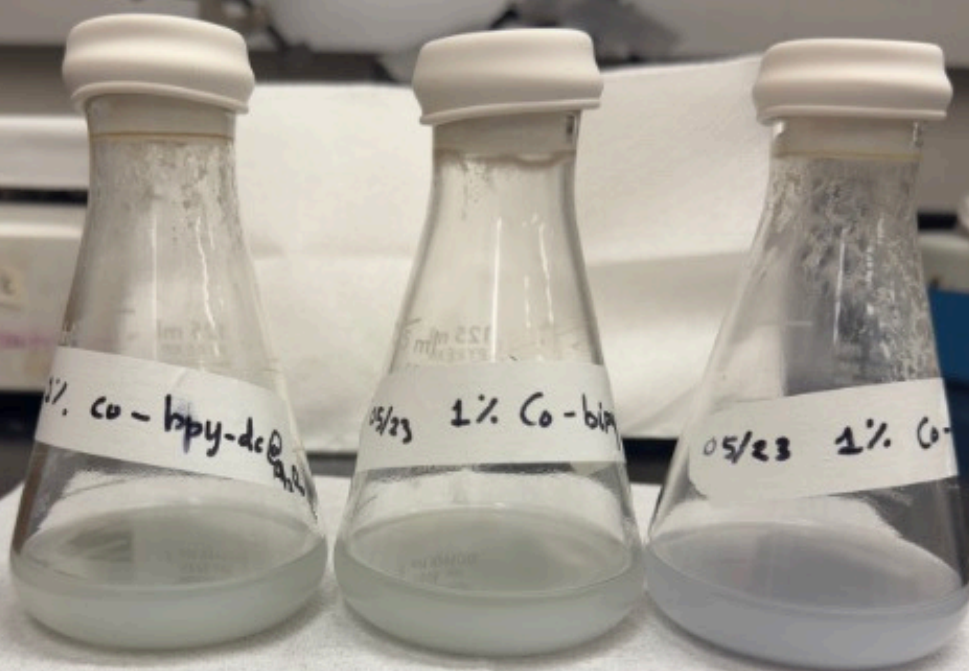
After the stirring, the mixture is centrifuged, and the solid residue is separated, rinsed three times with THF, and then dried in the oven at 55 °C for 24 hours. Finally, we obtain powdered catalysts.



0.5% $[\text{Co}(\text{HN}(\text{Si}(\text{CH}_3)_3)_2)\text{Cl}]\text{@Al}_2\text{O}_3$

0.5% $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]\text{@Al}_2\text{O}_3$

0.5% $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$



1% $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]\text{@Al}_2\text{O}_3$

1% $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$

1% $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$

3. Characterisation of Single Atom Catalysts(SACs)

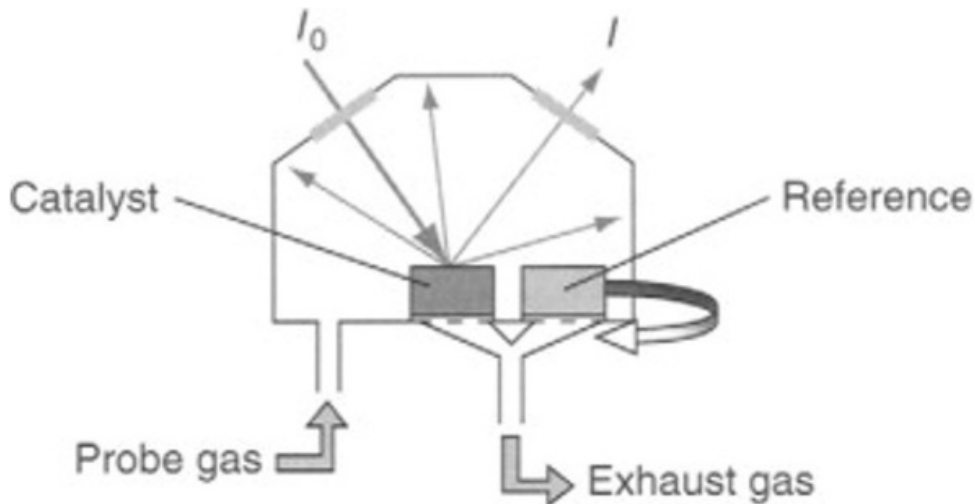
3.1 Diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)

3.1.1 Introduction

Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) is a technique used to study the surface of solid materials by analyzing how they absorb infrared light.

3.1.2 Working Principle

- Infrared light is directed at a sample.
- The sample reflects some of this light diffusely (in all directions).
- The reflected light is collected and analysed to determine which wavelengths were absorbed by the sample.



3.1.3 Inference

- Molecular Information: Helps identify different molecules on the sample's surface.
- Surface Chemistry: Provides insights into the chemical composition and interactions on the material's surface.

3.1.4 Applications

Used in catalyst research, material science, and surface chemistry to understand reactions and interactions at the molecular level.

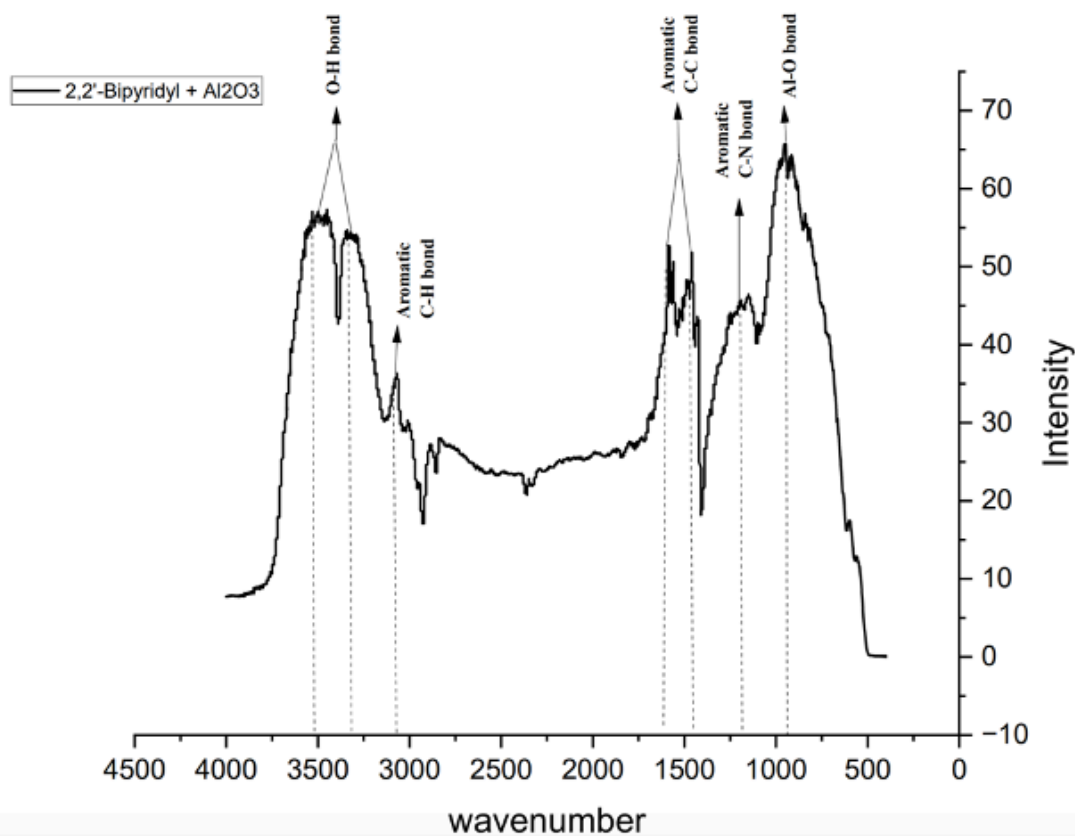


Figure 1. DRIFTS spectra collected for 2,2'-Bipyridine on Al₂O₃ support.

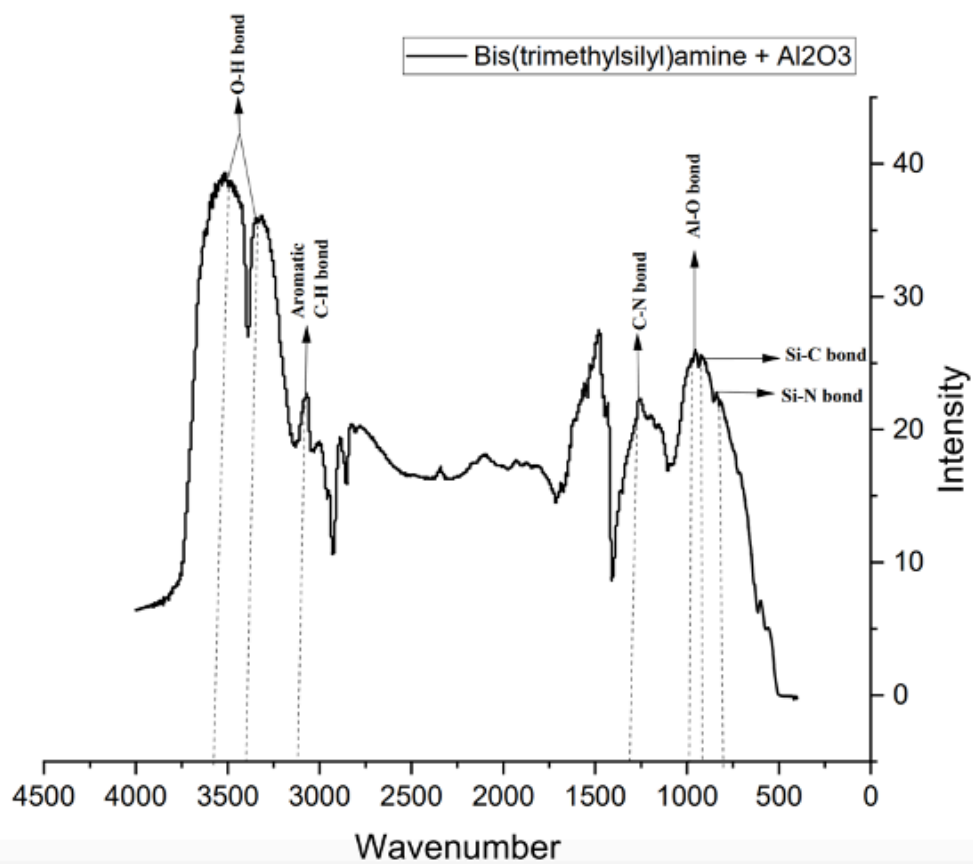


Figure 2. DRIFTS spectra collected for Bis(trimethylsilyl)amine on Al₂O₃ support.

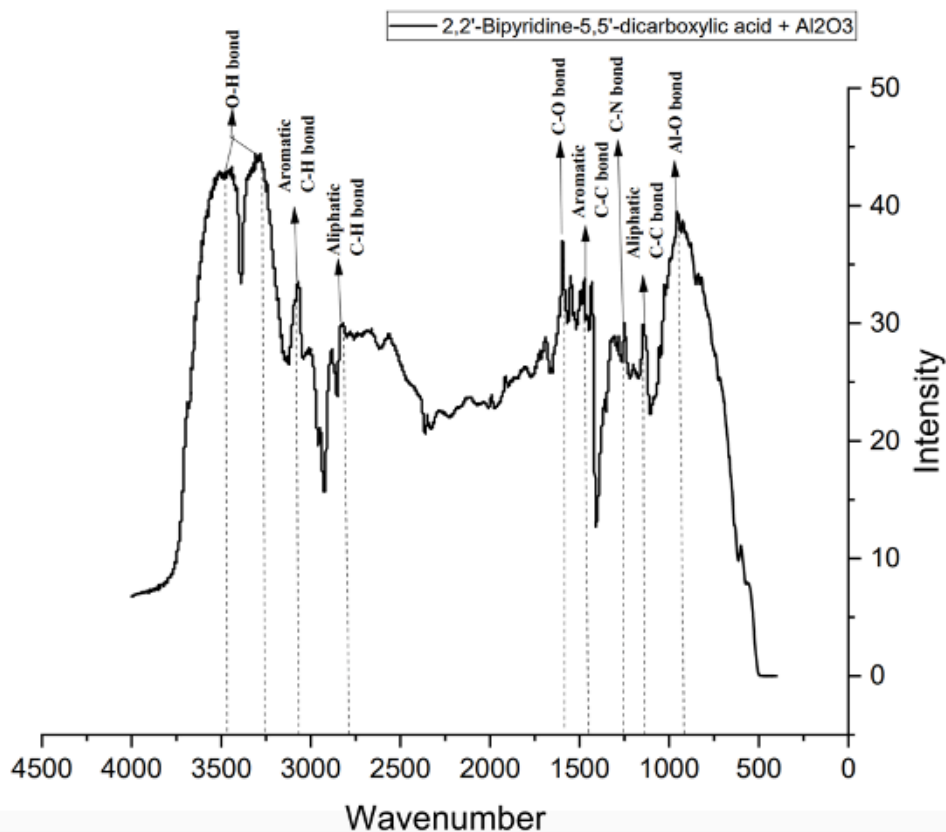


Figure 3. DRIFTS spectra collected for 2,2'-Bipyridine-5,5'-dicarboxylic acid on Al₂O₃ support.

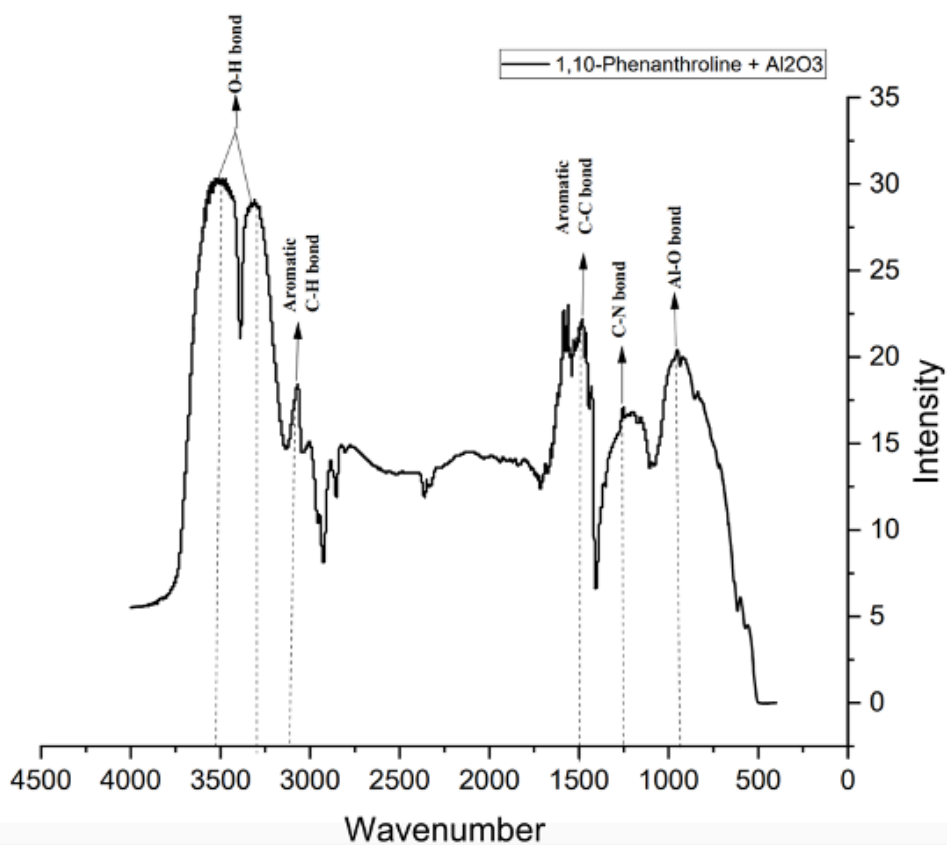


Figure 4. DRIFTS spectra collected for 1,10-phenanthroline on Al₂O₃ support.

3.2 CO-Adsorption DRIFTS Technique

3.2.1 Introduction

The CO-adsorption test is used to analyse the surface properties and active sites of catalysts by measuring how carbon monoxide interacts with the surface. It is particularly useful for **detecting single-atom catalysts** by identifying unique adsorption patterns indicative of isolated metal atoms.

3.2.2 Working Principle

- The CO adsorption test detects single-atom catalysts by exposing them to CO gas and analysing adsorption using infrared spectroscopy or temperature-programmed desorption.
- Single atoms show distinct adsorption behaviour, with unique binding energies and spectral features.
- This test differentiates single atoms from clusters and bulk metal, confirming the catalyst's structure and ensuring its functionality.

3.2.3 CO-Adsorption Test on $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]\text{@Al}_2\text{O}_3$

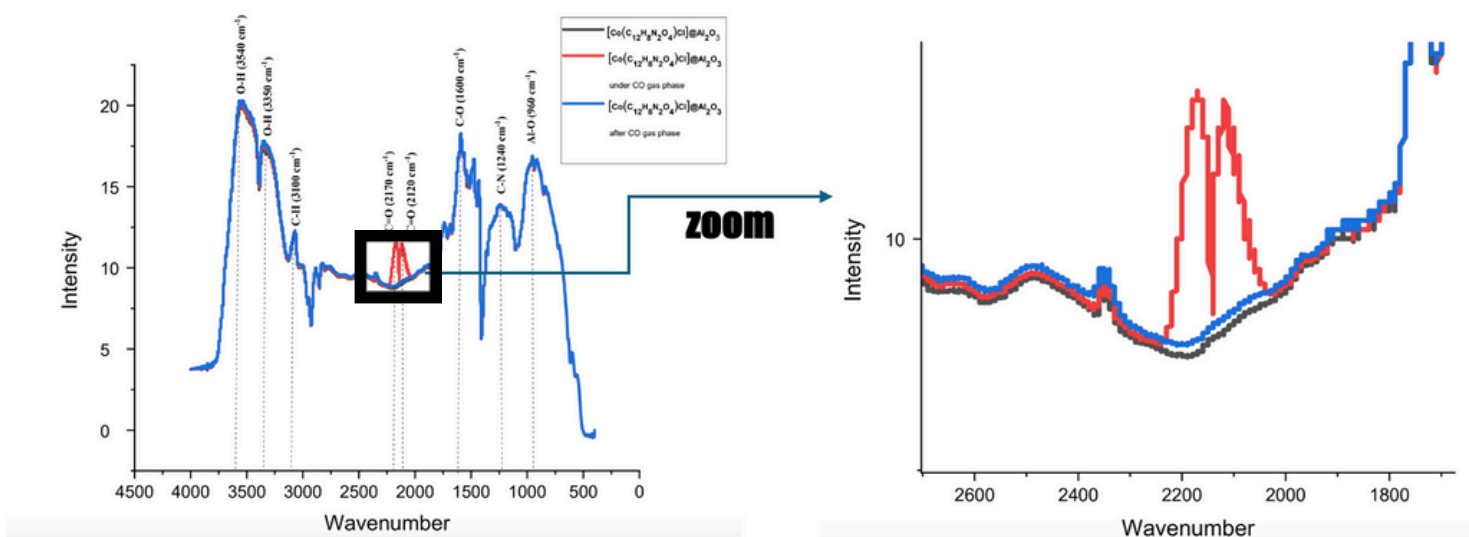
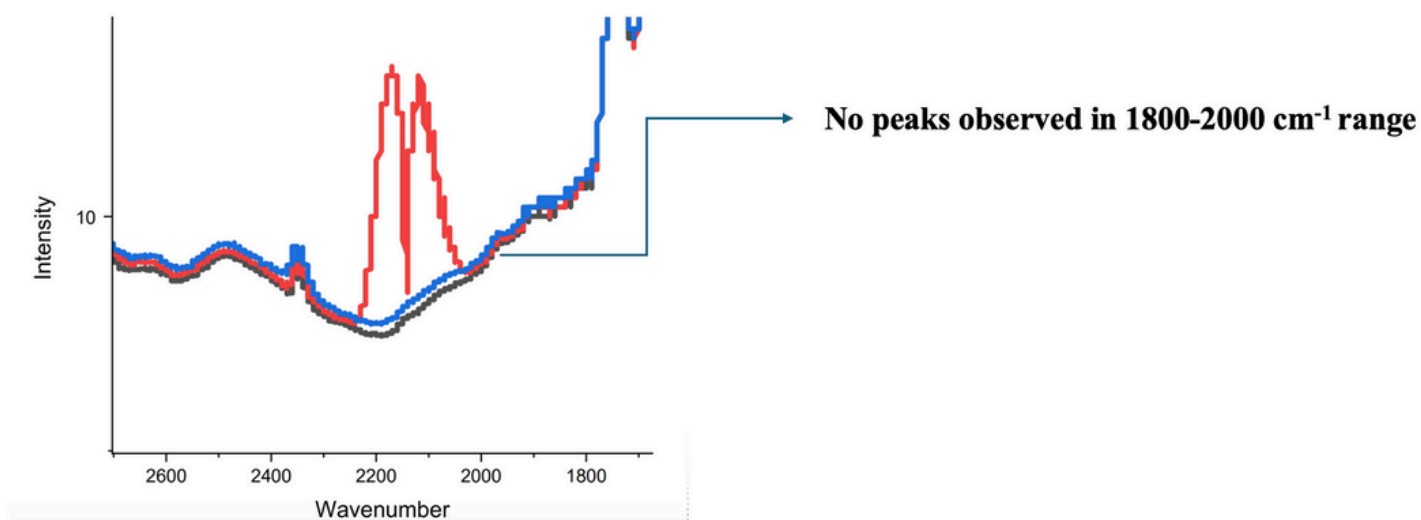


Figure: CO adsorption DRIFTS measurement was conducted after heat treatment at 1200°C under Ar. For CO adsorption the sample was exposed to 10% CO with Ar flow gas for 15 minutes at 300°C, and data was collected during and after CO exposure.

3.2.4 Observations



- Linear and Bridge CO adsorption peak expected 1900-2000 cm^{-1} and 1800-1900 cm^{-1} respectively.
- Adsorbed CO as linear or bridged on Cobalt is not observed, this maybe due to Co being not accessed or blocked by the ligands.

3.3 Inductively coupled plasma mass spectrometry (ICP-MS)

3.3.1 Introduction

ICP-MS (Inductively Coupled Plasma Mass Spectrometry) is a highly sensitive and precise analytical technique for detecting and quantifying trace elements and isotopes in various samples. It ionizes the sample with plasma and measures the mass-to-charge ratio of ions.

3.3.2 Working Principle

- **Sample Introduction:** The sample is introduced into the instrument, often in liquid form, via a nebulizer which creates a fine aerosol.
- **Ionization:** The aerosol is introduced into an inductively coupled plasma (ICP) torch, where it is ionized at high temperatures (6000-10000 K).
- **Ion Extraction:** The ions produced in the plasma are extracted into the mass spectrometer through a series of cones (sampler and skimmer).
- **Mass Analysis:** The extracted ions are separated based on their mass-to-charge ratio using a mass analyzer, typically a quadrupole or time-of-flight (TOF) system.
- **Detection:** The ions are detected by an ion detector, usually a dynode or Faraday cup, which converts the ions into an electrical signal.
- **Data Processing:** The signals are processed to quantify the concentrations of the elements and isotopes present in the sample.

3.3.3 Experimental Results

No.	Catalysts	Co Wt.% prepared	ICP-MS Data (%)
1	$[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$	0.5	0.34
2	$[\text{Co}(\text{HN}(\text{Si}(\text{CH}_3)_3)_2)\text{Cl}]\text{@Al}_2\text{O}_3$	0.5	0.42
3	$[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]\text{@CeO}_2$	0.5	0.13
4	$[\text{Co}(\text{HN}(\text{Si}(\text{CH}_3)_3)_2)\text{Cl}]\text{@CeO}_2$	0.5	0.10
5	$[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$	1.0	0.47
6	$[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$	1.0	0.56
7	$[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2\text{O}_4)\text{Cl}]\text{@Al}_2\text{O}_3$	1.0	0.61

3.3.4 Observations

- 0.5 wt% Co SACs prepared on Al_2O_3 support has more Co-Ligand complex coordinated to it as compared to CeO_2 support.
- 0.5 wt% Co SACs prepared on Al_2O_3 support has retained more Cobalt as compared to 1 wt% Co SACs prepared on Al_2O_3 .

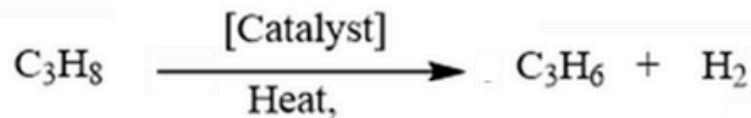
3.3.5 Conclusion

- Al_2O_3 is a better support as compared to CeO_2 due to its higher surface area, which provides more anchoring sites for the Co-ligand complexes.
- 0.5 wt% Co SACs on Al_2O_3 retain more cobalt than 1 wt% Co SACs due to better dispersion, stronger metal-support interactions, and reduced sintering. Higher loadings lead to site saturation, cobalt agglomeration, and weaker stability, resulting in less effective cobalt retention and performance..

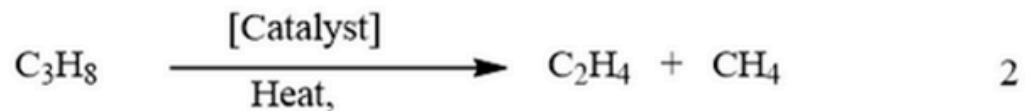
4. Propane Dehydrogenation Reaction (PDH)

4.1 PDH reaction with CO₂ flow

Main Reaction Path



Undesired Side Reaction



$$\text{C}_3\text{H}_8 \text{ Conversion (\%)} = \frac{\text{C}_3\text{H}_6 + \text{C}_2\text{H}_4 + \text{C}_2\text{H}_2 + \text{C}_2\text{H}_6 + \text{CH}_4}{\text{C}_3\text{H}_8 + \text{C}_3\text{H}_6 + \text{C}_2\text{H}_4 + \text{C}_2\text{H}_2 + \text{C}_2\text{H}_6 + \text{CH}_4} \times 100\%$$

$$\text{C}_3\text{H}_6 \text{ Selectivity (\%)} = \frac{\text{C}_3\text{H}_6}{\text{C}_3\text{H}_6 + \text{C}_2\text{H}_4 + \text{C}_2\text{H}_2 + \text{C}_2\text{H}_6 + \text{CH}_4} \times 100\%$$

4.2 Packing of Catalyst for Activity Test

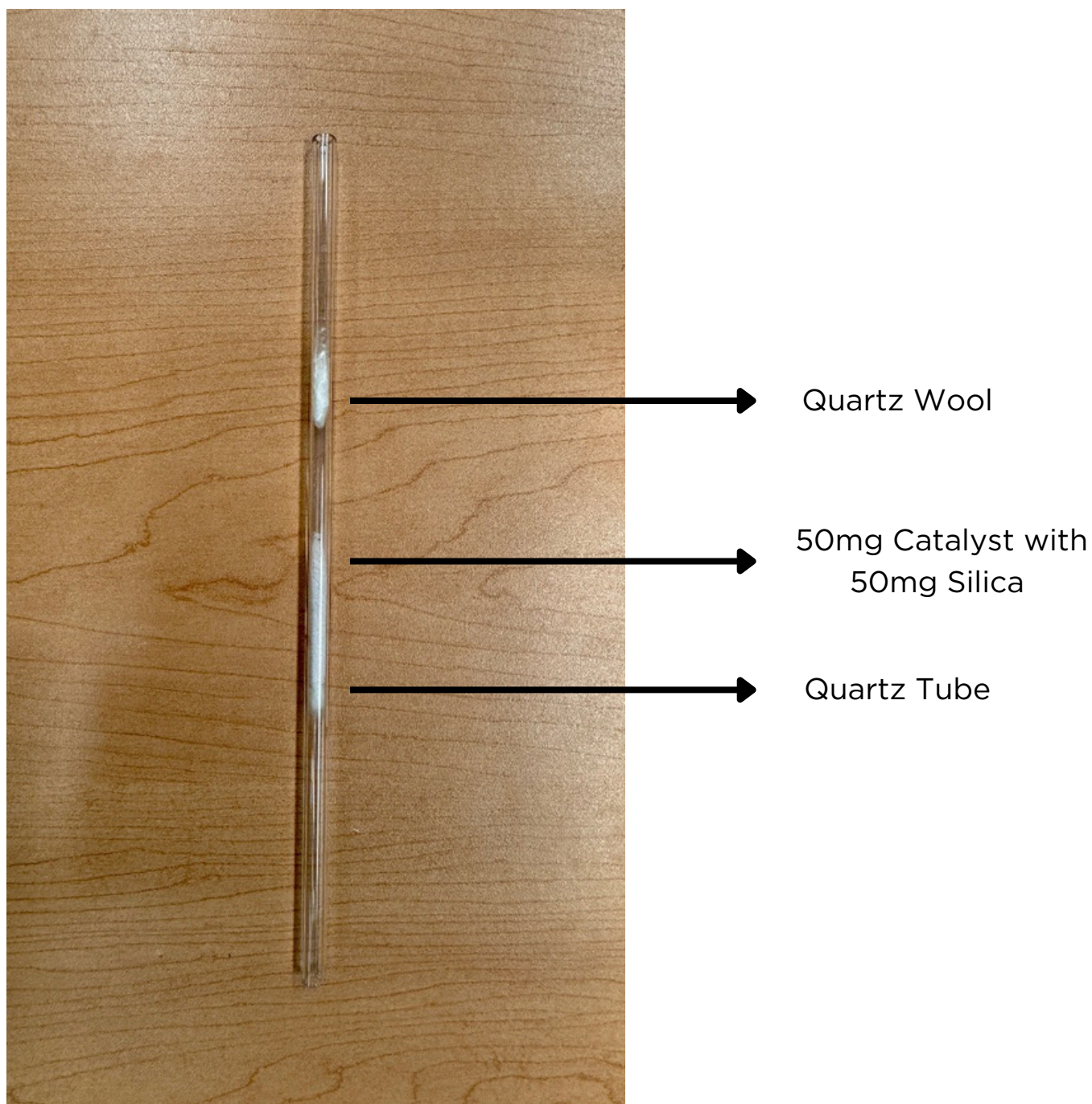


Figure: 50mg of Catalyst is mixed with 50mg of silica gel calcined (mesh 60-200) diluent and packed with quartz wool in a quartz tube

4.3 Activity Test for Cobalt SACs

The propane cracking ion and PDH products ions peak during the propane dehydrogenation reaction and overlapping the mass fragment of each production, and quantitative analysis was challenging using the mass spec technique. The profile spectrum of each compound measured in our mass spec is compared with the NIST data. Hence, the abundant ion peaks of each compound were selected for the product identification and quantitative analysis of the data. The products detected from PDH that are directly driven from $^{29}\text{C}_3\text{H}_8$ propane are $^{41}\text{C}_3\text{H}_6$, $^{27}\text{C}_2\text{H}_4$, $^{15}\text{CH}_4$, $^{26}\text{C}_2\text{H}_2$, and $^{30}\text{C}_2\text{H}_6$. Therefore, the propane dehydrogenation products were quantitatively determined by correcting each compound ion peak, multiplying the experimental intensity by the relative abundance %, and subtracting the contributor.

The PDH reaction setup was prepared by purging residual gases using the empty cell for 30 minutes and confirming that the gas lines were clean from the previous reaction. In the reactor quartz tube, 50 mg of catalyst powder was mixed with 15 mg of SBA-15 silica diluent packed using quartz wool. Reaction data collection began with baseline data collection using only Ar gas flow at 30 °C for 15 minutes, followed by pretreatment at 4% H_2 with Ar at 30 °C for 30 minutes. For comparison, baseline data were collected at the end of the reaction with only Ar gas flow at 30 °C for 15 minutes.

The PDH reactivity of the Co-ligand SACs catalyst was tested under different reactant concentrations and reaction conditions. The performance of the catalyst was evaluated at 3% and 4/5% C_3H_6 and 3% and 4/5% CO_2 at 100 °C, 200 °C and 300 °C. The performance of the $[\text{Co}(\text{bipy})(\text{Cl})]@\text{Al}_2\text{O}_3$ and $[\text{Co}(\text{Phen})(\text{Cl})]@\text{Al}_2\text{O}_3$ catalyst is presented in Figures 1 and 2. The experimental data for each compound were normalized by dividing the intensity of the compound by the Ar intensity. Propane conversion and selectivity to propylene were calculated using the formula. Each compound's m/z experimental reading was corrected by considering the ratio of cracking ions and contributions from other compounds identified from the NIST database.

4.3.1 Activity Test for $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$

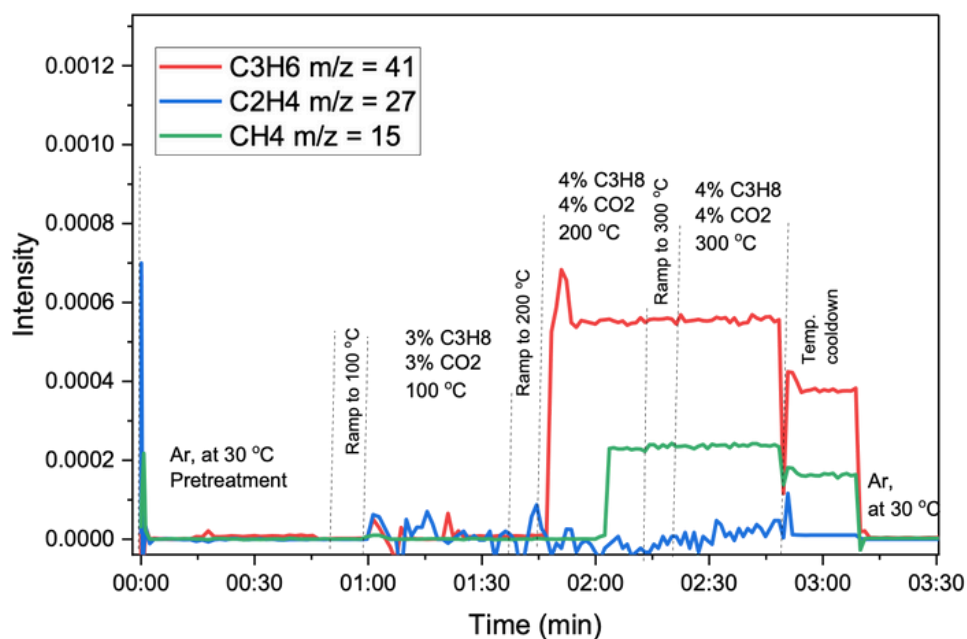


Figure 1: PDH reaction major products of C_3H_6 , C_2H_4 , and CH_4 were obtained using $[\text{Co}(\text{bipy})(\text{Cl})]\text{@Al}_2\text{O}_3$ catalyst in different reaction conditions. Reaction conditions: 3% and 4% C_3H_8 (1.2 & 1.6 sccm), 3% and 4% CO_2 (1.2 & 1.6 sccm) under Ar balance up to 40 sccm at 100, 200 and 300 °C using the catalyst for 3.5 h. In the reactor cell, 50 mg of catalyst powder was mixed with 15 mg SBA-15 silica diluent packed using quartz wool.

4.3.2 Activity Test for $[\text{Co}(\text{C}_{12}\text{H}_8\text{N}_2)\text{Cl}]\text{@Al}_2\text{O}_3$

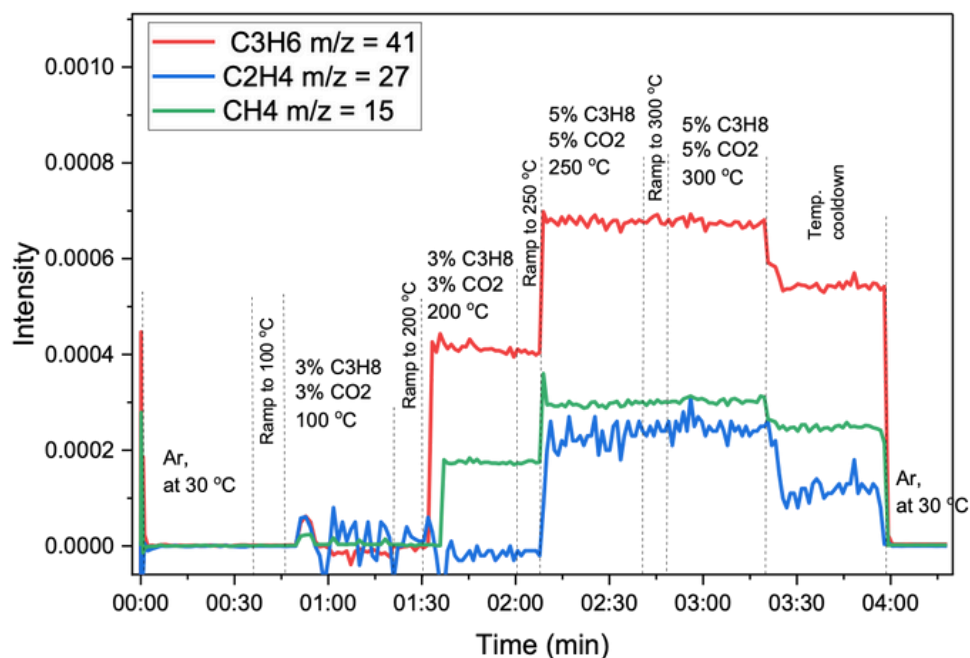


Figure 2: PDH reaction major products of C_3H_6 , C_2H_4 , and CH_4 were obtained using $[\text{Co}(\text{Phen})(\text{Cl})]\text{@Al}_2\text{O}_3$ catalyst in different reaction conditions. Reaction conditions: 3% and 5% C_3H_8 (1.2 & 2.0 sccm), 3% and 5% CO_2 (1.2 & 2.0 sccm) under Ar balance up to 40 sccm at 100, 200, 250, and 300 °C using the catalyst for 4.0 h. In the reactor cell, 50 mg of catalyst powder was mixed with 15 mg SBA-15 silica diluent packed using quartz wool.

5. Effects of Ligands and Supports on Catalytic Activity

5.1 Effects of Ligands on Catalytic Activity

5.1.1 Experiment

- 1% Co-Ligand coordinated SACs were prepared using 2,2'-Bipyridine-5,5'-dicarboxylic acid : $C_{12}H_8N_2O_4$ (strongly electron withdrawing group) and Bis(trimethylsilyl)amine :- $HN(Si(CH_3)_3)_2$ (strongly electron donating group) and their activity was tested under similar conditions.
- In the reactor quartz tube, 50 mg of catalyst powder was mixed with 15 mg of SBA-15 silica diluent packed using quartz wool. Reaction data collection began with baseline data collection using only Ar gas flow at 30 °C for 15 minutes, followed by pretreatment at 4% H_2 with Ar at 30 °C for 30 minutes.

5.1.2 Observations

- The catalytic performance of 1% $[Co(bpy-dc)Cl]@Al_2O_3$ resulted in a 27% (average) conversion, whereas 1% $[Co(silane)Cl]@Al_2O_3$ achieved a higher conversion of 38% (average). The propane conversion for the 1% $[Co(bipy)(Cl)]@Al_2O_3$ and 1% $[Co(Phen)(Cl)]@Al_2O_3$ catalysts are 29% and 31% respectively.
- The propene selectivity of 1% $[Co(bipy)(Cl)]@Al_2O_3$ and 1% $[Co(Phen)(Cl)]@Al_2O_3$ was greater than 50% on average, 4.3.1 and 4.3.2 (figures 1 & 2). However, 1% $[Co(bpy-dc)Cl]@Al_2O_3$ was 30% (average), while 1% $[Co(silane)Cl]@Al_2O_3$ had a propene selectivity of 23% (average).

5.1.3 Conclusion

- EDGs are generally more favourable for enhancing catalytic activity and stabilizing the catalyst, this is because EDGs generally increase the electron density around the metal centre, which can facilitate the adsorption of propane and improve the activation of C-H bonds.
- EWGs are beneficial for increasing selectivity and controlling reactivity, this is because EWGs can decrease the electron density around the metal centre, which helps in controlling the reactivity and improving the selectivity towards the desired product, propylene

5.2 Effects of Support on Catalytic Activity

5.2.1 Experiment

- 0.5% Co-Ligand coordinated SACs were prepared on Al_2O_3 and CeO_2 supports.
- Using ICP-MS technique, the Co wt% loaded on each support after the preparation was measured and compared to the theoretical value.

5.2.2 Observations

- 0.5 wt% Co SACs prepared on Al_2O_3 support have more Co-ligand complexes coordinated to them compared to those on CeO_2 support.
- Al_2O_3 support enhances the coordination of Co-ligand complexes more effectively than CeO_2 support.

5.2.3 Conclusion

- The higher coordination of Co-ligand complexes in 0.5 wt% Co SACs on Al_2O_3 compared to CeO_2 can be attributed to several factors. Al_2O_3 provides a higher surface area and more suitable anchoring sites, promoting better dispersion and stability of the Co-ligand complexes.
- Additionally, the surface chemistry of Al_2O_3 fosters stronger metal-support interactions, enhancing the retention and coordination of single-atom cobalt species.
- In contrast, CeO_2 may have fewer available sites and weaker interactions, leading to lower Co-ligand complex coordination.
- These factors collectively make Al_2O_3 a superior support for stabilizing single-atom cobalt catalysts.

Conclusions

In this project, Co-ligand coordinated single-atom catalysts were developed for the propane dehydrogenation (PDH) reaction. Different characterisation techniques confirmed the formation of stable Co-ligand SACs.

Activity tests demonstrated promising selectivity to propene. It was found that Al_2O_3 support enhances the loading of Co-ligand complex coordination compared to CeO_2 .

The effects of various ligands and supports on catalytic activity were systematically studied.

Bibliography

- **Characterisation Techniques:**

- Chorkendorff, I., & Niemantsverdriet, H. (2007). Concepts of Modern Catalysis and Kinetics. Wiley-VCH.
- Ertl, G., Knözinger, H., & Weitkamp, J. (Eds.). (1997). Handbook of Heterogeneous Catalysis. Wiley-VCH.
- Atkins, P., & de Paula, J. (2010). Physical Chemistry for the Life Sciences. Oxford University Press.

- **Single-Atom Catalysts and Metal-Ligand Coordination:**

- Liu, L., & Corma, A. (2018). Metal Catalysts for Heterogeneous Catalysis: From Single Atoms to Nanoclusters and Nanoparticles. Chemical Reviews, 118(10), 4981-5079.
- Flytzani-Stephanopoulos, M., & Gates, B. C. (2012). Single Atom Catalysts: Synthesis, Characterization, and Applications. Annual Review of Chemical and Biomolecular Engineering, 3, 545-568.

- **Catalyst Supports and their Effects:**

- Freund, H.-J., & Pacchioni, G. (2008). Oxide Ultra-thin Films on Metals: New Materials for the Design of Supported Metal Catalysts. Chemical Society Reviews, 37(10), 2224-2242.
- Rodriguez, J. A., & Goodman, D. W. (1992). The Nature of the Metal-Ceria Interface in Model Catalysts. Science, 257(5072), 897-903.

- **Propane Dehydrogenation (PDH) Reactions:**

- Sattler, J. J. H. B., Ruiz-Martinez, J., Santillan-Jimenez, E., & Weckhuysen, B. M. (2014). Catalytic Dehydrogenation of Light Alkanes on Metals and Metal Oxides. Chemical Reviews, 114(20), 10613-10653.
- Ding, K., Gulec, A., Johnson, A. M., et al. (2015). Identification of Active Sites in CO Oxidation and Water-Gas Shift over Supported Pt Catalysts. Science, 350(6257), 189-192.

- **General Catalysis and Surface Chemistry:**

- Thomas, J. M., & Thomas, W. J. (2015). Principles and Practice of Heterogeneous Catalysis. Wiley-VCH.
- Somorjai, G. A., & Li, Y. (2010). Introduction to Surface Chemistry and Catalysis. Wiley-Interscience.