# "Exploration of Supramolecular Chemistry of Some Transition Metal Complexes with N, O Donor Ligands"

*Project Submitted to Midnapore City College*
*for the Partial Fulfillment of the Degree of*
*Master of Science (Chemistry)*
*Submitted*
*By*

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Under supervision of

Dr. Prankrishna Manna

**DEPARTMENT OF PURE AND APPLIED SCIENCE**
**MIDNAPORE CITY COLLEGE**
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West Bengal, India

**2023**

# Declaration

I do hereby declare that the present Master thesis entitled **"Exploration of Supramolecular Chemistry of Some Transition Metal Complexes with N, O Donor Ligands"**embodies the original research work carried out by me in the Department of pure and applied Sciences, Midnapore City College, Paschim Medinipur, West Bengal, India under the supervision of Dr.Prankrishna Manna, Assistant Professor, Department of pure and applied Sciences(Chemistry), Midnapore City College,Kuturiya, Bhadutala, Paschim Medinipur, Pin-721129, West Bengal, India.

No part thereof has been submitted for any degree or diploma in any University.

Date:

Place: Midnapore City College, Paschim Medinipur

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# Approval Sheet

This project report entitled **"Exploration of Supramolecular Chemistry of Some Transition Metal Complexes with N, O Donor Ligands"** by Sangita Pati, Stuti Bhattacharya, Soumili Mahata, Soumya Bhattacharya, Mangal Saren, Bappaditya Pal, Ayan Chakraborty, Souvik Paul, Sumon Mukherjee, Atanu Jana, Gobinda Mahata, Ram Kumar Giri, Subha Shannigrahi, Sougata Mohanta, Shyamali Mahata, approved for the degree of M.Sc. (Chemistry).

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(Name: Dr. Prankrishna Manna)

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(Name: Dr. Kuntal Ghosh)

(Signature of Director)
(Name: Dr. Pradip Ghosh)

Date: _____
Place: _____

# Acknowledgement

I would like to thank my thesis advisor Dr. Prankrishna Manna of the Department of Pure and Applied Sciences at Midnapore City College. The door to Dr. Manna office was always open whenever I ran into a trouble spot or had a question about my research or writing. He consistently allowed this paper to be my own work, but steered me in the right the direction whenever he thought I needed it.

I would also like to thank the other Faculties (Dr. Avishek Ghosh and Dr. Jagannath Pal) and other non-teaching staffs for their support to carry out this research project. Without their passionate participation and input, the validation survey could not have been successfully conducted.

Finally, I must express my very profound gratitude to my parents for providing me with unfailing support and continuous encouragement throughout my years of study and through the process of researching and writing this thesis. This accomplishment would not have been possible without them.
Thank you.

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## Abstract

Nature adores functional self-assembly, which relies on weak interactions rather than on covalent interactions. Self-assembly possesses a reversible and self-correcting cooperative process that responds to changes in environmental conditions (solvent, pH, temperature, concentration, etc.). Consequently, these assemblies often build host complexes that are very efficient for uptake and release of guests under controlled conditions.

In the context of supramolecular self-assembly and crystal engineering, various types of interactions are being exploited to build up multidimensional networks. These compounds find wide applications in the field of catalysis, non linear optics, electrical conductivity, biological recognition, and molecular sieves. A wide variety of extended networks can, however, be obtained by connecting metal complexes via non-covalent forces, e.g strong and weak conventional hydrogen bonds.

A large number of complexes involving acyclic and macrocyclic frame works are often assembled through metal coordination of suitable bridging ligands. The assembly process of these frameworks is highly influenced by a number of factors, e.g., the coordination nature of the metal ions, the structural and functional characterization of organic ligands, the nature of the solvent, temperature and pH of the reaction medium, metal-ligand ratio, template and counterions. A subtle alteration in any of these factors might result in new complexes with different structural topologies and functions.

Attempts will be made to obtain single crystals of first row transition metal complexes to determine their crystal structures by x-ray crystallography and then it is planned to investigate spectral behavior, detailed magnetic interactions, electrochemical properties, catalytic and biological activities, if any.

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# Chapter 1: Introduction

## 1. Introduction

Molecular synthesis is a technology that chemists use to make molecules by forming covalent bonds between atoms. Molecular self-assembly is a process in which molecules (or parts of molecules) impulsively form ordered aggregates and involves no human intervention; the interactions involved usually are noncovalent. In molecular self-assembly, the molecular structure determines the structure of the assembly Molecular self-assembly is omnipresent in chemistry, materials science, and biology and has been so long before self-assembly emerged as a discrete field of study and as a synthetic strategy.

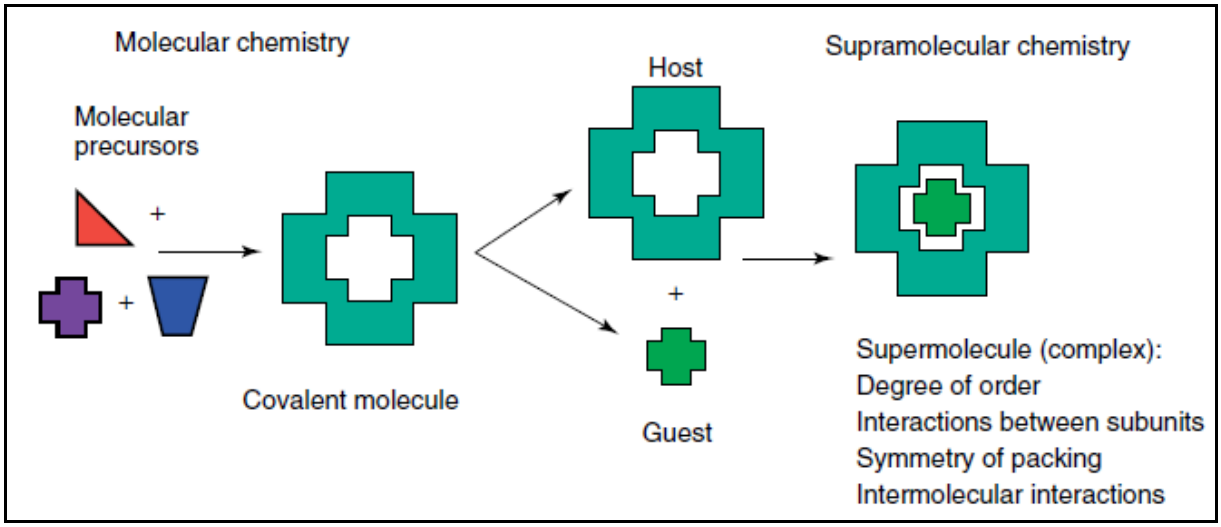



Fig 1: Supramolecular chemistry from molecular chemistry.

The concept of supramolecular chemistry has attracted lots of attention from chemists, biologists, and material scientists, where they utilize the noncovalent interactions, including hydrogen-bonding interaction, π–π stacking interaction, electrostatic interaction, van der Waals force, and hydrophobic/hydrophilic attraction, to explain the systems from easy to complicated. Besides the hydrogen bonds as directional non-covalent interactions responsible for organization and design of the supra-molecular architectures in solids, the C–H···π, (S. Karthikeyan, et al. 2013) π···π, (Christopher A. Hunter, 1990) lone pair···π, (Martin Egli, Sanjay Sarkhel, 2007) anion···π (De-Xian Wang, Mei-Xiang Wang, 2013) and cation···π (A.Subha Mahadevi, G.Narahari Sastry, 2013) interactions are also the important molecular forces whose nature is still a matter of discussion. Interactions of the type C–H···π provide weak but directional packing motifs which aid in the evaluation of molecular assemblies.

Other than the C–H···π interactions and the hydrogen bonds, the π···π interactions and lone pair···π (lp···π) interactions undoubtedly play important roles in determining the crystal packing, molecular assemblies and structures of large biological systems. Moreover, cation···π interactions, as well as anion···π interactions are also widely regarded as stabilizing interactions for a number of bio(macro)molecules, molecular recognition and supramolecular assemblies. These types of noncovalent interactions play a significant role in modern chemical research and are now-a-days considered as cornerstones in supramolecular chemistry, materials science and even in biochemistry.

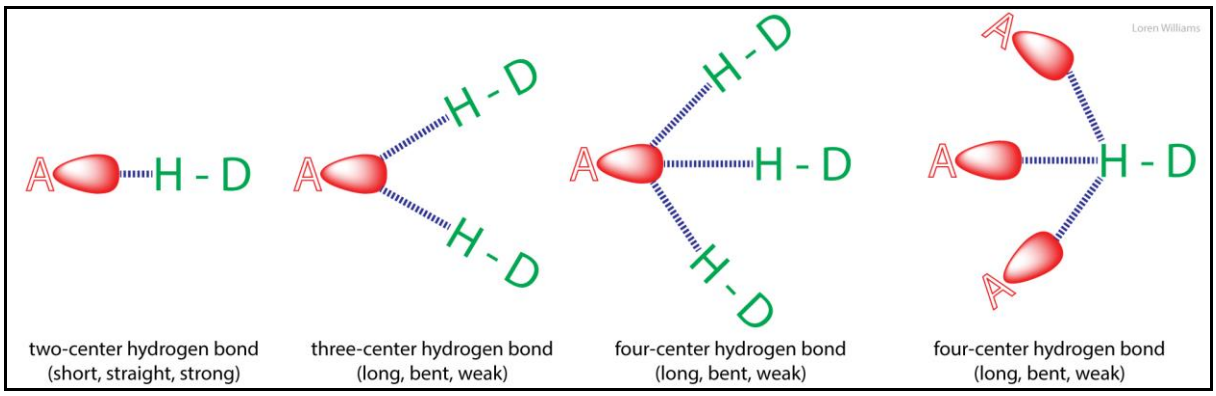



Fig 2: Illustrates two-, three- and four-center hydrogen bonds. The two-center hydrogen bond is closest to an 'ideal' hydrogen bond, and is stronger than the other types. The four-center hydrogen bonding scheme on the right is observed in crystalline ammonium, where one acceptor lone pair has to accommodate three donors.

**Supramolecular interactions:**

**Anion···π interactions:** Anion-π interactions are defined as favourable non-covalent contacts between electron-rich anions and electron-deficient aromatic systems (π-acid).

**Cation···π interaction:** Cation···π interaction is a noncovalent molecular interaction between the face of an electron-rich π system and an adjacent cation. Cation-π interactions are important in protein structure. The guanidinium group of arginine and the ε-$NH_3^+$ of lysine engage in cation- π interactions with aromatic protein sidechains. A favorable cation- π pair contributes as much to protein stability as a good hydrogen bond or an electrostatic (charge-charge) interaction. Tryptophan is the most frequent π system in protein cation- π pairs while

arginine is the most frequent cation. Tryptophan and arginine can form extended coplaner assemblies.

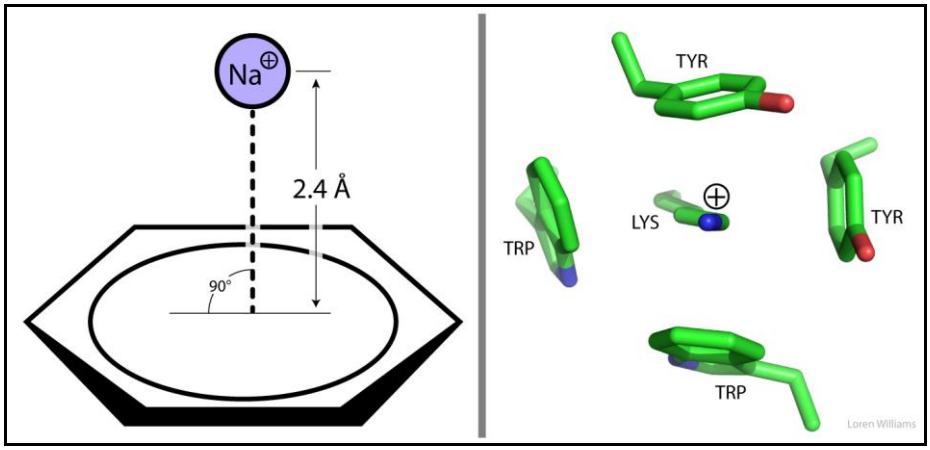



Fig 3: (Left) shows the optimal geometry for a cation- π interaction between a $Na^+$ cation and benzene.

The distance from the $Na^+$ to the center of the ring is 2.4 Å (ionic radius of $Na^+$ = 0.9 Å, vdw radius of C ($r_C$) = 1.7 Å). (Right) The ε-$NH_3^+$ of a lysine engages in cation- π interactions with two tryptophan sidechains and two tyrosine sidechains in a protein (glucoamylase, PDB ID 1GAI).

**Lone pair···π interaction:** Lone pair···π interaction is one of the most important supramolecular interactions recognized by the scientific community. Supramolecular As (lone pair)···π interactions provide stability to their crystal structures often leading to supramolecular chains and prevailing over As···X secondary contacts. The interaction (8 kJ $mol^{-1}$) arises from polarization induced in the aryl ring by the As-lone pair plus the weak sharing of these electrons with the ring-C atoms. Architectures based on (lone pair)···π(aryl) interactions provide stability to crystal structure.

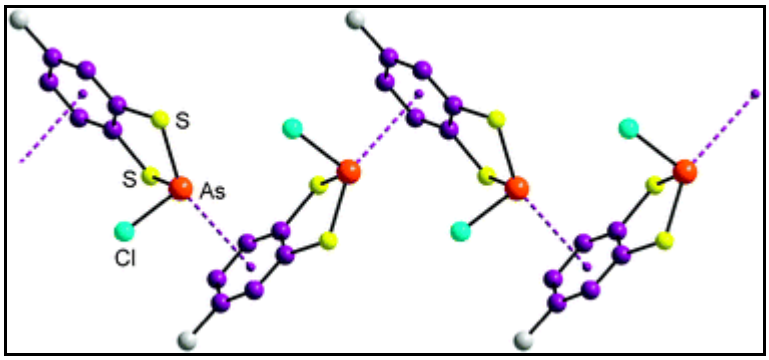



Fig 4: lone pair···π interactions provide stability to their crystal structures often leading to supramolecular chains and prevailing over As···X secondary contacts.

**π···π and C–H···π Interactions:** Aromatic–aromatic or π–π interactions are important non-covalent intermolecular forces similar to hydrogen bonding. Although π···π interactions are accepted as weak, they have been recognized to play an important role in the folding and the thermal stability of proteins. C–H···π interaction can also be considered as the weakest of hydrogen bonds that occurs between C–H groups and electron pairs in a π system.

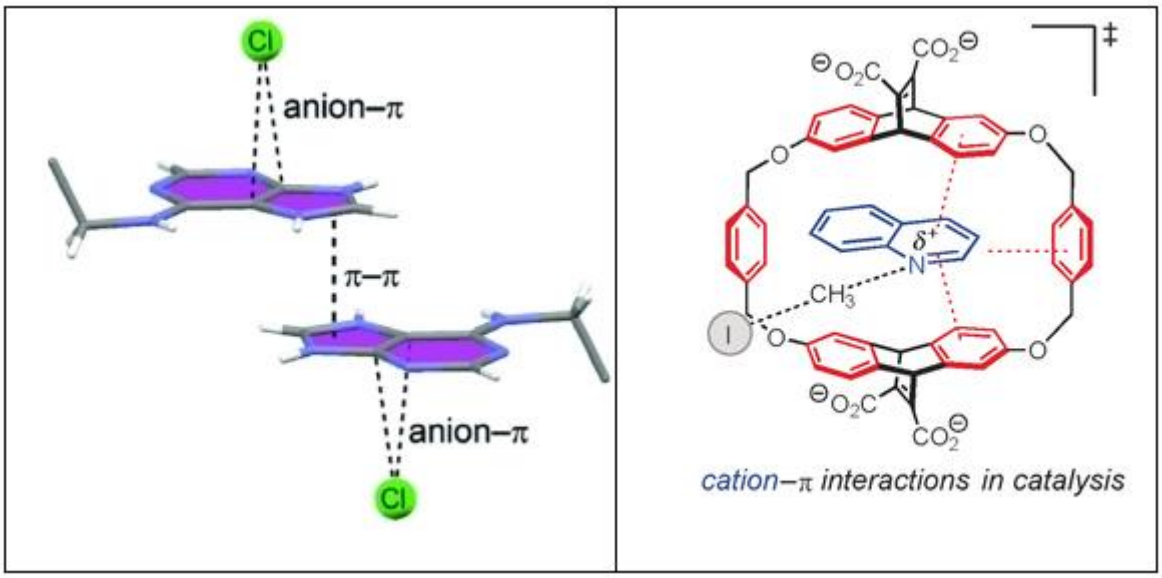



Fig 5: pi-pi or aromatic-aromatic interactions (left) and cation-pi interactions in catalysis(right).

# Chapter 2: Literature Review

## 2. Literature Review

**A short review on transition metal malonate complexes:**

Synthesis of metal malonate complexes:

**Synthesis of {[M($C_3H_2O_4$)($H_2O$)$_4$]·$NO_3$}n(M = Gd, Tb, Ho) (1–3)**

The compounds 1–3 were synthesized by reacting 0.225 g (0.5 mmol) of M($NO_3$)$_3$· 6$H_2O$ (M = Gd, Tb, Ho) dissolved in 5mL de-ionized water and 0.156 g (1.5mmol) of malonic acid in 20mL ethanol. The solutions were stirred for 2 h at room temperature. The pH of the reaction mixture was adjusted between 5 and 6 with 0.1M NaOH solution. The solutions were filtered and kept at ambient temperature (or in the refrigerator) for crystallization. The crystals appeared in the solution after 2–3 weeks. The complexes **1, 2,** and **3** were obtained as light yellow, colorless, and light pink crystals, respectively.

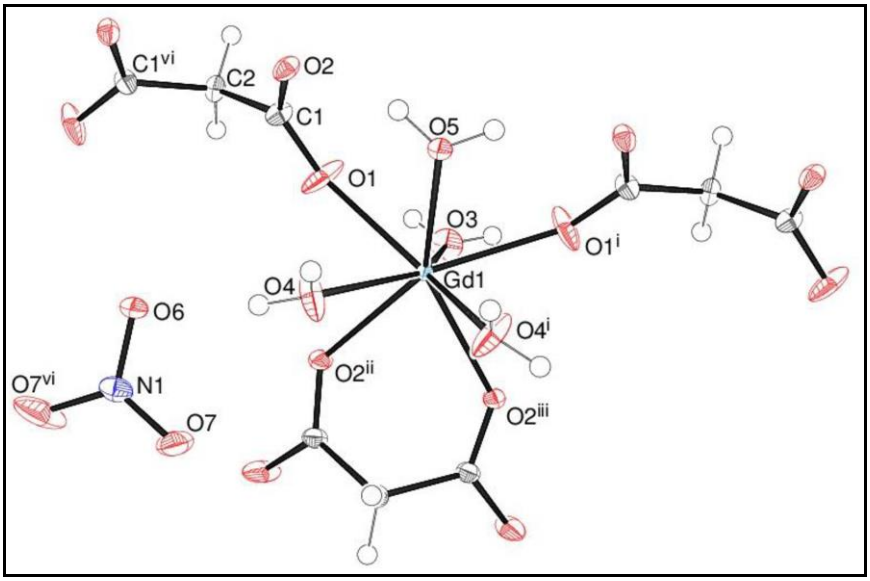



Fig 6: The asymmetric unit of 1 (50% displacement ellipsoids) expanded to show the full metal coordination sphere.

**Synthesis of [Er($C_3H_2O_4$)($C_3H_3O_4$)($H_2O$)$_2$]$_n$ (4)**

Malonic acid (0.104 g, 1 mmol) and $ErCl_3$· 6$H_2O$ (0.137 g, 0.5 mmol) were separately dissolved in 20mL ethanol and 10mL deionized water, respectively. The solutions were mixed and stirred for 2 h in a round-bottom flask at room temperature. During stirring, 0.1M NaOH

solution was used to maintain the pH of the mixture between 5 and 6. After 10 days, pink crystals of 4 appeared in solution, which were isolated by filtration and rinsed with methanol.

**Synthesis of $\{[Eu_2(C_3H_2O_4)_2(C_3H_3O_4)_2(H_2O)_6]\cdot 4H_2O\}_n$ (5)**

To a solution of 0.183 g (0.5 mmol) of $EuCl_3\cdot 6H_2O$ in 10mL deionized water was added 0.104 g (1 mmol) of malonic acid dissolved in 25mL ethanol. The solutions were mixed in round bottom flask and stirred for 3 h at room temperature at a pH of 5–6 maintained by using 0.1M NaOH solution. After 2 weeks, colorless crystals of 5 were recovered by filtration and rinsed with methanol.

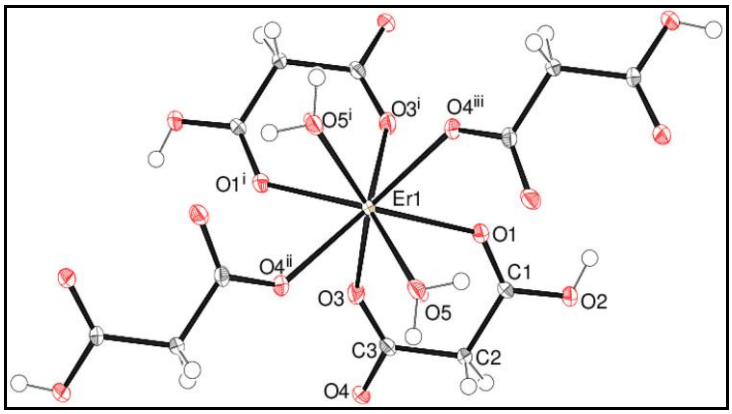



Fig 7 : The asymmetric unit of 4 expanded to show the full metal coordination sphere.

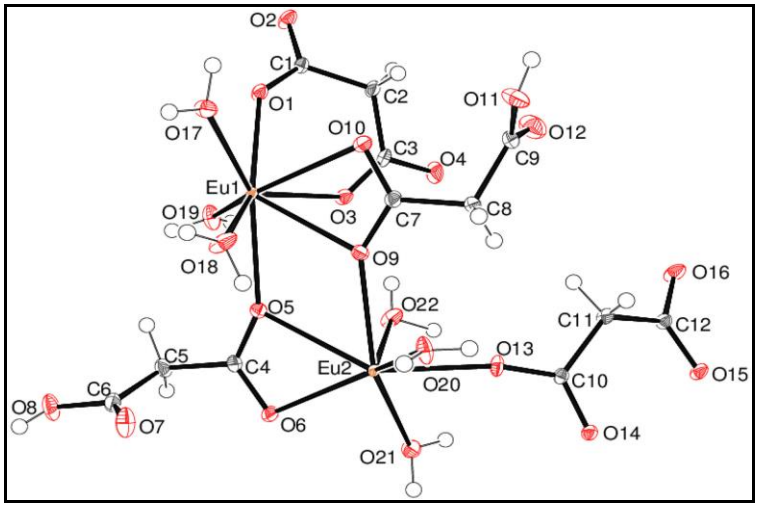



Fig 8: The asymmetric unit of 5 with the non-coordinated water molecules of crystallization omitted for clarity.

**Synthesis of Mg (II)-Malonate-2-Aminopyridine-Nitrate complex:**

Magnesium (II) nitrate hexahydrate (0.256 g, 1.0 mM) dissolved in 25 mL of water was allowed to react with malonic acid (0.208 g, 2.0 mM) in water (25 mL) at 60 °C, resulting in a clear colorless solution. A warm aqueous solution (20 mL) of 2-aminopyridine (0.376 g, 4.0 mM) was added dropwise to the above colorless solution with continuous stirring. The reaction mixture thus obtained was further heated at 60 °C for an hour with continuous stirring the resulting solution was then cooled down to room temperature (the pH of this solution was 3.7) and kept unperturbed for the slow evaporation of the solvent. After a few weeks, flat, colorless single crystals suitable for X-ray analysis were obtained. The crystals were collected by filtration, washed with cold water, and dried in air.

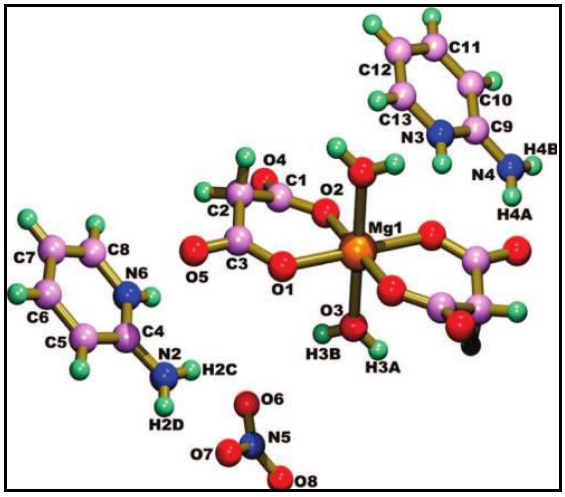



Fig 9: Representation of the molecular structure of 1. Unlabeled atoms are generated by the inversion operation (*-x*, 1 - *y*, 1 - *z*).

**Synthesis of Cu (II)-Malonate-2-Amino-4-methyl pyridine complexes:**

Copper (II) chloride dihydrate (0.170 g, 1.0 mmol) was dissolved in 20 mL of water and allowed to react with malonic acid (0.208 g, 2.0 mmol) in water (25 mL) at 60°C. A warm aqueous solution (20 mL) of 2-amino-4-methylpyridine (0.432 g, 4.0 mmol) was added dropwise to the above solution with continuous stirring. Finally, a warm aqueous solution (20 mL) of ammonium hexafluorophosphate (0.652 g, 4.0 mmol) was added to it under stirring conditions. The reaction mixture thus obtained was heated at 60 °C for an hour with continuous stirring. The resulting blue solution was then cooled to room temperature and filtered to remove any undissolved materials. Mother solution was then left unperturbed for

crystallization at room temperature. Block-shaped blue single crystals suitable for single-crystal X-ray structure analysis were obtained after a few weeks. The crystals were separated by filtration, washed with ice-cold water, and then air-dried**.**

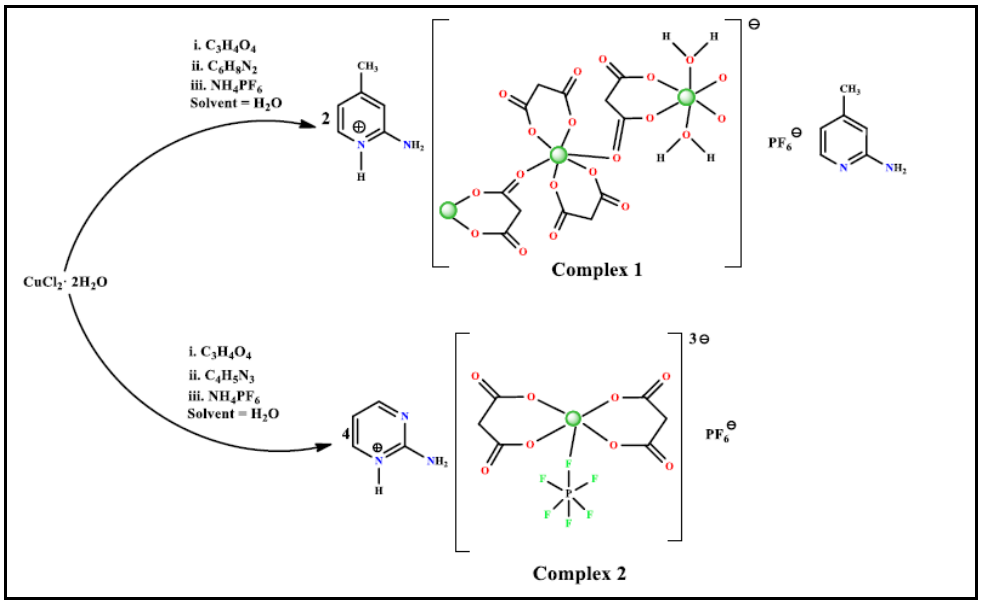



Fig 10: Scheme of the reactions for the preparation of the complexes.

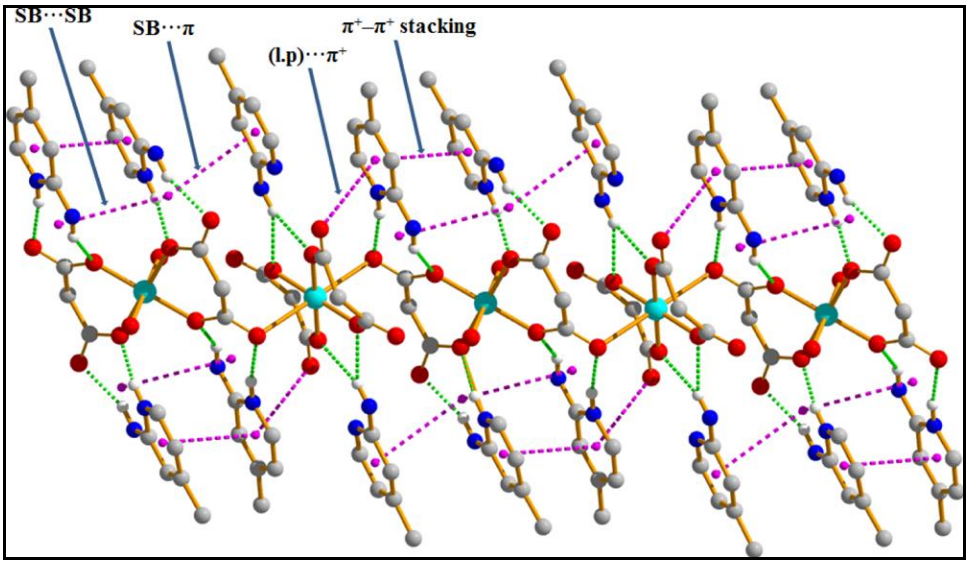



Fig 11: Perspective view of the extended supramolecular SB···SB/ SB···π and lone-pair (lp)···π+/+π+–π+ networks in complex 1.

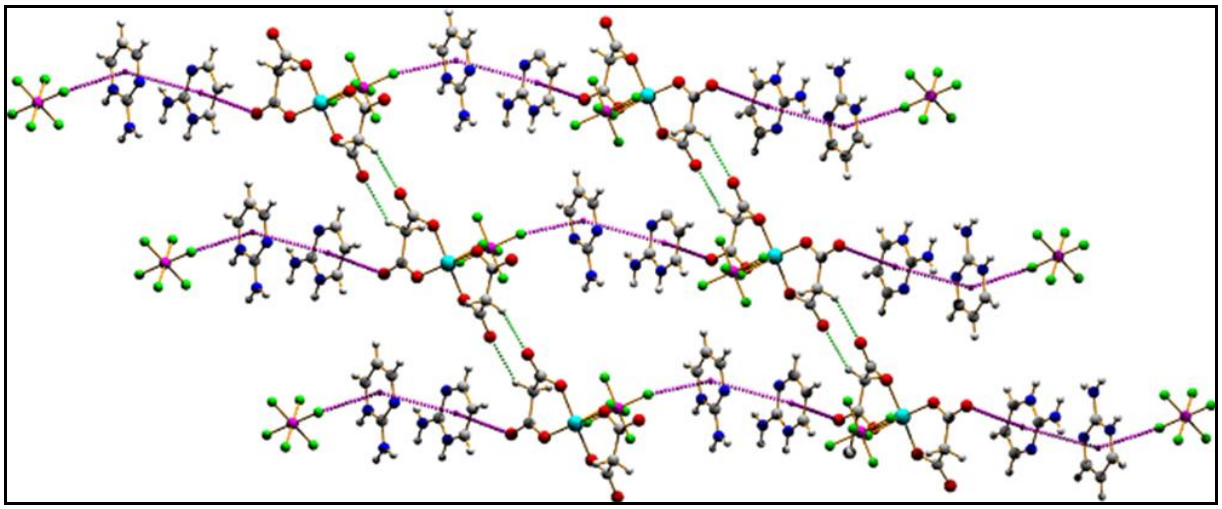


Fig 12: Perspective view of the layered structure in complex 2 generated through the extended lone-pair (lp)···π+/π+–π+/π+···anion network**.**

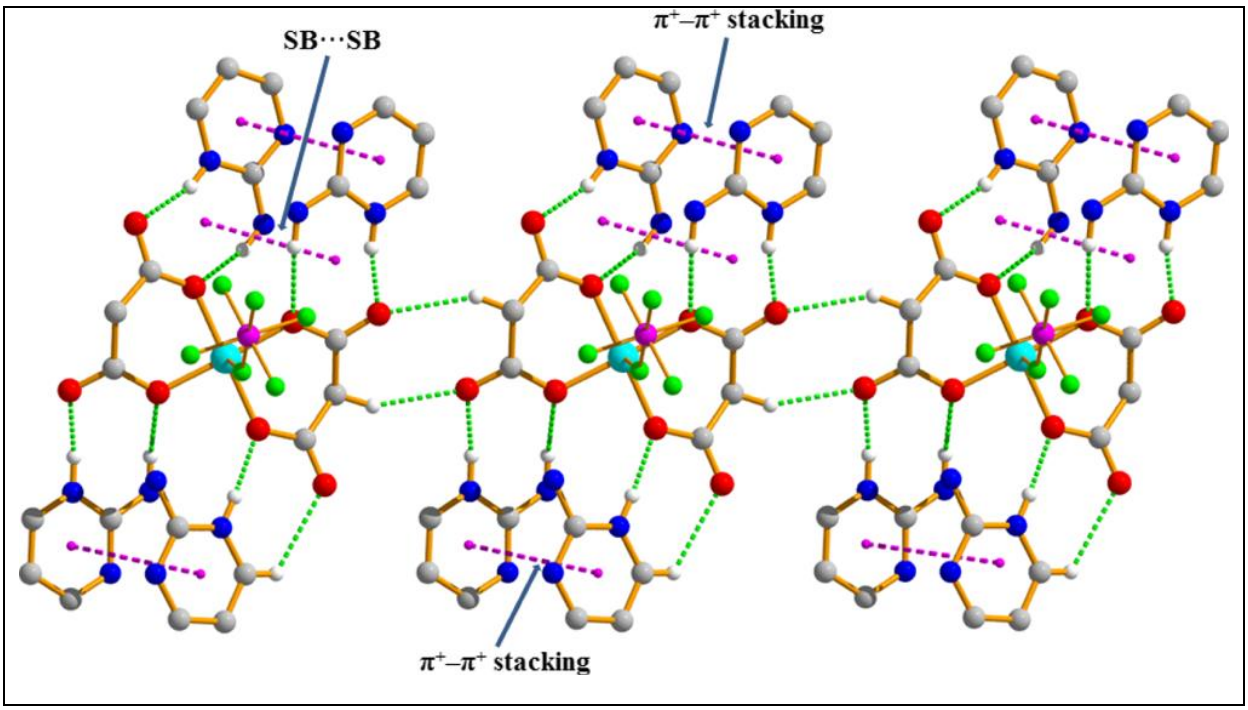



Fig 13: Supramolecular framework generated through SB···SB and π+–π+ interactions in complex 2.

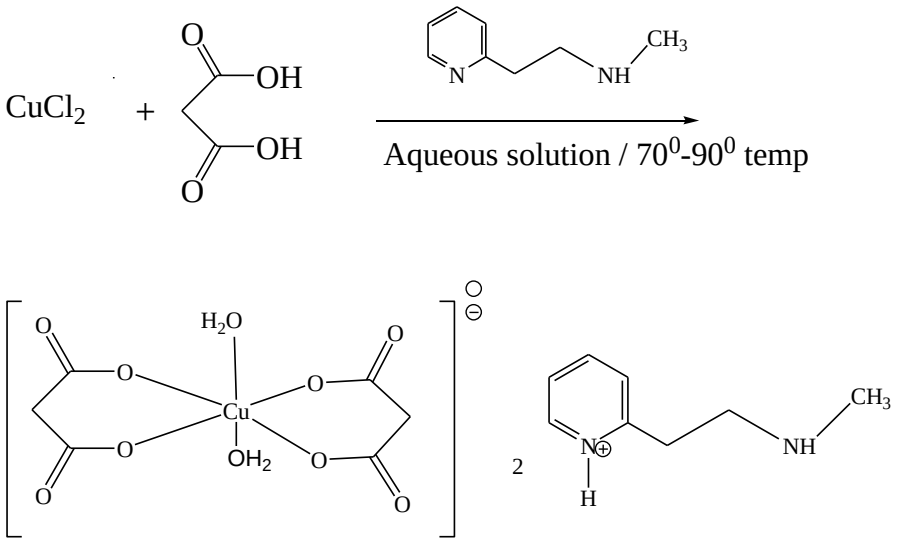
The protonated pyrimidine nitrogen atom of four 2-aminopyrimidine of moieties is in contact with the three carbonyl and one carboxylate oxygen atoms, and three-amine nitrogen atoms from the 2-aminopyrimidine moieties are interconnected with the carboxylate oxygen atoms of the malonate moieties. Thus, two SB units are interconnected by a separation distance of 3.532 Å (Fig 6). Moreover, the molecular packing is such that the π+−π+ stacking interactions50−52 between the aminopyrimidine rings are optimized with an interplanar spacing of 3.407 Å and a ring-centroid separation of 3.971(2) Å. In the opposite side, the pyrimidine rings are interconnected through the π+−π+ stacking interactions with a ring-centroid separation of 3.766(2) Å and an interplanar spacing of 3.361 Å. The combination of C−H···O h interactions results in a 2-D supramolecular framework in the (110) plane.

# Chapter 3: Aims and Objective

## 3. Aims and Objective

The broad area of research in the group is supramolecular chemistry and bioorganic chemistry. We are interested in understanding how molecules interact, how they recognise each other, how they fold and how they can assemble into larger, multi-component systems. Supramolecular chemistry focuses on the intermolecular interactions between molecules, such as hydrogen bonding, the hydrophobic effect, metal-ligand coordination, interactions and electrostatic effects. The goal of our research is to understand the role of non-covalent interaction in biological and chemical systems, to utilise supramolecular interactions to manipulate biological systems, and to take inspiration from biology to build new and complex chemical architectures, host-gest systems and adaptive materials. We are interested to synthesis a series of transition metal complexes of carboxylic acid with auxiliary ligands of suitably positioned donor sites. The synthesized compounds will be thoroughly characterized by standard analytical techniques, viz. elemental analysis, X-ray diffraction analysis (XRD), FTIR study. Syntheses of transition metal complexes, spectroscopic and electrochemical characterization of the synthesized metal complexes, preparation of single crystals and single crystal X-ray structure determination of these synthesized complexes. The biological activity of synthesized complexes will be examined under various conditions. Finally, it will be tried to explore supramolecular features of synthesized metal complexes. The outcome of the proposed project work will be submitted in various journals of repute for publication.

Scheme 1:



# Chapter 4: Methods & Materials

## 4. Methods & Materials:

All of the chemicals were procured from the Sigma Aldrich, India. First row transition metal salt of Co, Cu, Ni, Zn (like nitrates, chlorides, carbonates etc.). Different auxiliary ligands, malonic acid and its derivatives.

**Experimental Procedure:**

(a) Purchase of chemicals.

(b) Experimental instrument set up.

(c) Synthesis of compound (chemical reaction).

(d) Purification of compounds.

(e) Preparation of single crystals.

(f) Structure determination.

(g) Characterization of synthesized compound.

**Instrumentation for experiments and characterization**

Characterization techniques

- Elemental analysis
    - CHNS Analyzer

    Structural Analysis
    - Fourier Transform Infra Red Spectrometry (FTIR)
    - X-ray Diffraction Spectrometry (XRD)

    Thermal Analysis
    - Thermogravimetric Analyser (TGA)
    - Differential Thermal Analyser (DTA)

    Interaction Analysis
    - DFT calculation
    - NCI analysis
    - Hirshfeld surface analysis

**Schedule of project work:**

| | | Number of Weeks | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Sl. No. | **Activity Description** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** | **10** | **11** | **12** | **13** | **14** | **15** | **16** | **17** | **18** | **19** | **20** | **21** | **22** | **23** | **24** |
| 1 | Project Initiation and Planning | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | Step I Literature survey or review work | | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | Step II Research problem finalized | | | | | | | | | | | | | | | | | | | | | | | | |
| 4 | Step III Experimental instrument set up | | | | | | | | | | | | | | | | | | | | | | | | |
| 5 | Step IV Synthesis of compound | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | Step V Purification of compounds | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | Preparation of single crystals | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | Final Report | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | Implementation | | | | | | | | | | | | | | | | | | | | | | | | |
| 10 | Final inspection | | | | | | | | | | | | | | | | | | | | | | | | |

# Chapter 5: Results

**5.Results:**

**Synthesis of compound:**

**Materials**

All reactions were carried out in aerobic conditions and in water as the solvent. Malonic acid, Nickel(II) nitrate hexahydrate, Cobalt(II) chloride hexahydrate, 2-aminopyridine, Methyl-(2-pyridin-2-yl-ethyl)-amine, Sodium hydroxide, and all other chemicals were of reagent grade quality, purchased from Sigma-Aldrich Chemical Co. and used without further purification. Freshly boiled, doubly distilled water was used throughout the present investigation.

**Synthesis of compound (1)**

Cobalt(II) nitrate hexahydrate (0.291 g, 1.0 mmol) dissolved in 25 mL of water was allowed to react with malonic acid (0.208 g, 2.0 mmol) in water (25 mL) at 60°C resulting in a clear pink solution. A warm aqueous solution (20 mL) of Methyl-(2-pyridin-2-yl-ethyl)-amine (0.5 ml, 4.0 mmol) was added drop wise to the above solution with continuous stirring. The pH of the resulting solution was adjusted to 5.5 by the addition of dilute aqueous NaOH. The reaction mixture thus obtained was further heated at 60°C for an hour with continuous stirring. The solution was then cooled to room temperature and filtered and left unperturbed for crystallization. After a few weeks, block shaped, pale brown single crystals suitable for X-ray analysis were obtained. The crystals were collected by filtration, washed with cold water and dried in air (Yield: 65%).

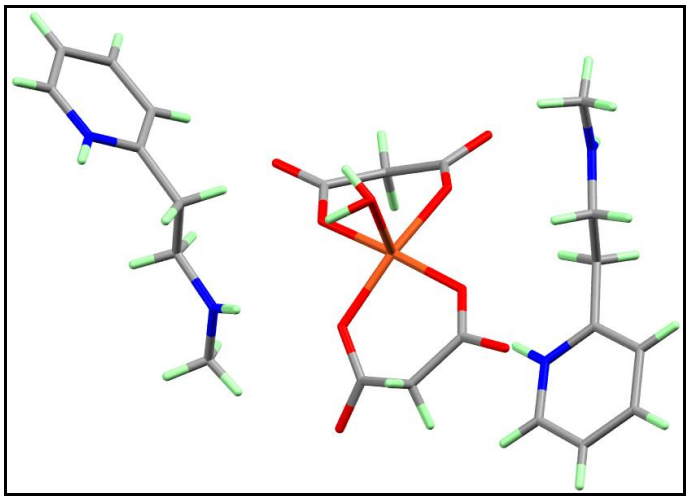


Fig. 14: X-ray single crystal structure of compound 1.

**Table 1: Crystallographic Data for complex 1**

| **Complex** | **1** |
|---|---|
| Formula | $C_{14}$ $H_{19}$ Cu $N_2$ $O_9$ |
| *M* | 803.58 |
| Crystal system | triclinic |
| Space group | *P n a* $2_1$ |
| *a*/ Å | 9.346(5) |
| *b*/ Å | 10.607(7) |
| *c*/ Å | 17.231(5) |
| *A* | 90.00 |
| *B* | 90.00 |
| *Γ* | 90.00 |
| *F*(000) | 417 |
| *V*/ $Å^3$ | 845.6(3) |
| *Z* | 4 |
| *T/K* | 100 |
| θ Min-Max [˚] | 1.8 to 26.4° |
| λ(Mo Kα)/ Å | 0.71073 Å |
| μ(Mo Kα)/ $mm^{-1}$ | 0.597 |
| Crystal Size [mm] | 0.18 × 0.20 × 0.30 |
| *R*1, *I*> *2σ(I)* (all) | 0.0311 |
| w*R*2, *I* > 2σ(*I*) (all) | 0.0792 |
| S(GOF) | 1.06 |
| Total reflections | 6739 |
| Independent reflections ($R_{int}$) | 3397(0.020) |
| Observed data [*I* > 2σ(*I*)] | 3098 |
| Min. and Max. Resd. Dens. [e/ $Å^3$] | -0.27, 0.34 |

# Chapter 6: Discussion

**Crystal structure description of complex 1.**

The complex **1** is essentially isomorphous and crystallized in the triclinic space group *P n a 2₁* with the asymmetric unit consisting of half of the molecular anion $[Cu(C_3H_2O_4)_2(H_2O)]^{2-}$, one crystallographically independent $C_8H_{13}N_2^+$ cation. The monomeric anionic units, that is, $[Cu(C_3H_2O_4)_2(H_2O)]^{2-}$ are interlinked to each other via strong self-complementary O5-H1O5···O2 hydrogen bonds which give rise to a $R_4^4(22)$ cyclic motif, ultimately generating an infinite 2D tape along the crystallographic *a* axis Fig 15.

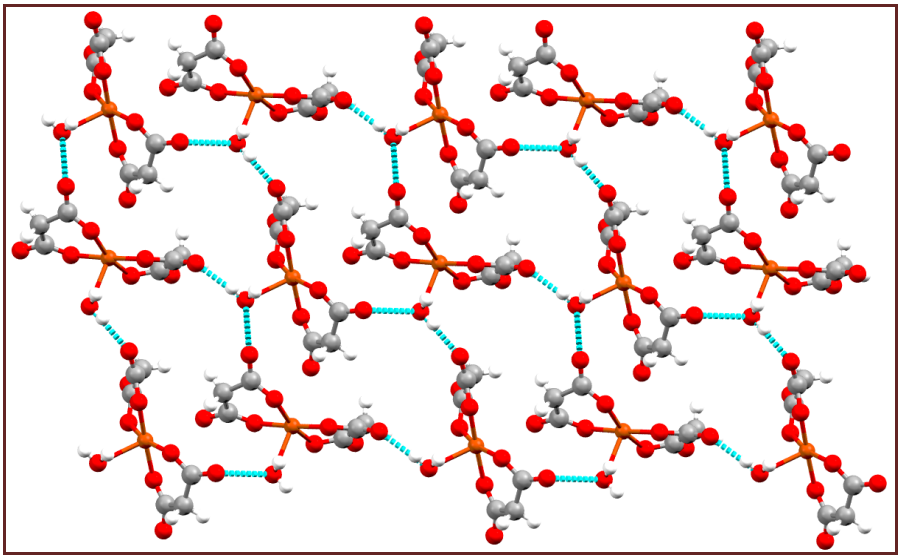


Fig 15: Formation of 2D tape in complex **1** through association of discrete $[Cu(mal)_2(H_2O)]^{2-}$ monomeric units by O5-H1O5···O2 hydrogen bonds.

Each monomeric anionic unit also recognizes three methyl-(2-pyridin-2-yl-ethyl)-aminium cations ($C_8H_{13}N_2^+$ cation) through doubly coordinated carboxylate ends, involving the hydrogen bonds N1–H1···O2, C3O4···H2N2, and C6–O7···H2N2 (Fig 16).

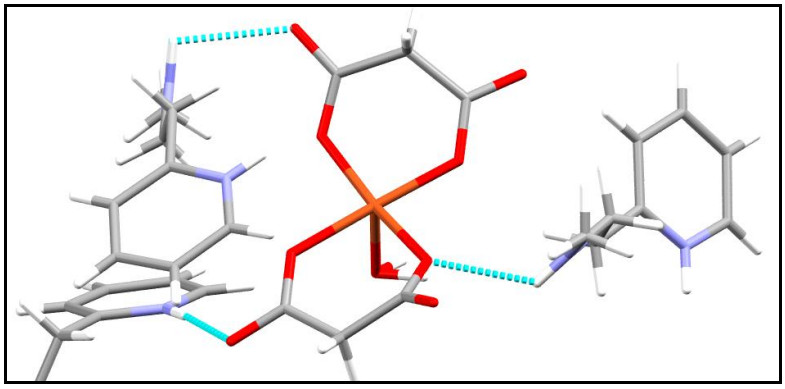


Fig 16: Each monomeric unit of complex **1** is also connected three methyl-(2-pyridin-2-yl-ethyl)-aminium cations the hydrogen bonds.

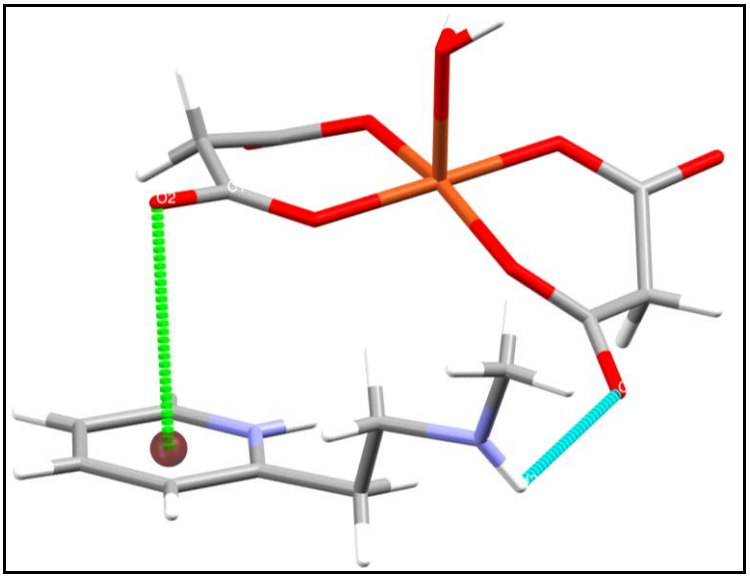


Fig 17: Each monomeric unit of complex **1** is also connected to methyl-(2-pyridin-2-yl-ethyl)- through lone pair····π.

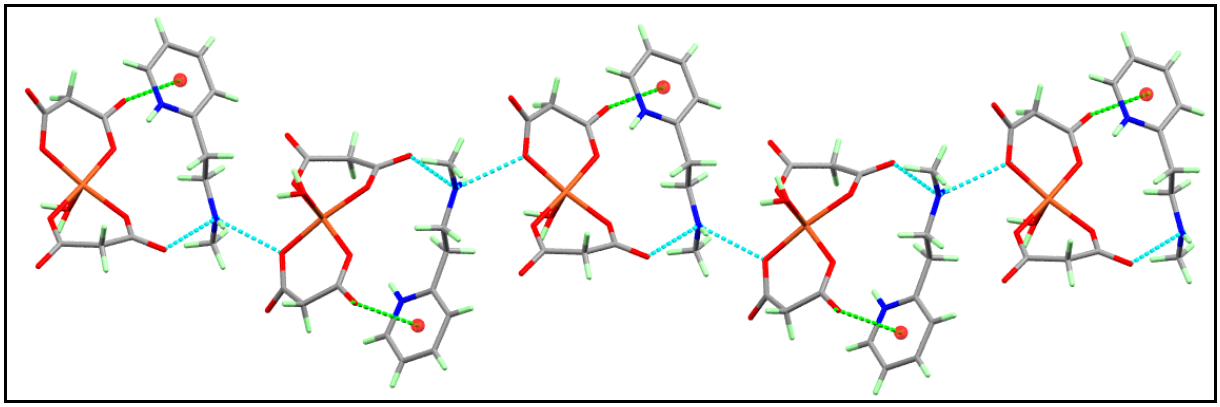


Fig 18: Formation of 1D supramolecular network involving lone pair····π, C6–O7···H2N2 and C3O4···H2N2 hydrogen bond interaction.

**Hirshfeld surface analysis**

Hirshfeld surfaces and the associated 2D-fingerprint plots were calculated using Crystal Explorer, which accepts a structure input file in CIF format. Bond lengths to hydrogen atoms were set to typical neutron values (C–H = 1.083 A, N–H = 1.009 A). For each point on the Hirshfeld isosurface, two distances $d_e$, the distance from the point to the nearest nucleus external to the surface, and $d_i$, the distance to the nearest nucleus internal to the surface, are defined. The normalized contact distance ($d_{norm}$) based on de and $d_i$ is given by

$$d_{\text{norm}} = \frac{d_{\text{i}} - r_{\text{i}}^{\text{vdw}}}{r_{\text{i}}^{\text{vdw}}} + \frac{d_{\text{e}} - r_{\text{e}}^{\text{vdw}}}{r_{\text{e}}^{\text{vdw}}}$$

where $r_i^{vdW}$ and $r_e^{vdW}$ are the van der Waals radii of the atoms. The value of $d_{norm}$ is negative or positive depending on intermolecular contacts being shorter or longer than the van der Waals separations. The parameter $d_{norm}$ displays a surface with a red-white-blue color scheme, where bright red spots highlight shorter contacts, white areas represent contacts around the van der Waals separation, and blue regions are devoid of close contacts.

The Hirshfeld surfaces of the title complex were analyzed to illuminate the nature of the intermolecular interactions and are illustrated in Fig. 9 showing the surfaces that have been mapped over de, dnorm, shape-index and curvedness. As expected, the dnorm surfaces of Fig. 9 reveal the close contacts of hydrogen bond donors and acceptors, but other close contacts are also evident. In dnorm surfaces, the large circular depressions (deep red) are the indicators of hydrogen bonding contacts whereas other visible spots are due to H…H contacts. The

dominant H…O interactions in the title crystal structure are evident in the Hirshfeld surface plots by the bright red area (Fig. 20) and light red spots are due to C–H…O interactions.

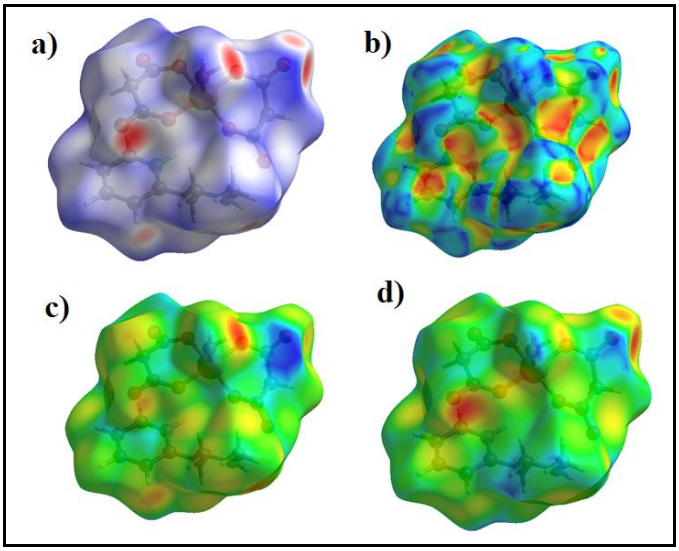



Fig 19: Hirshfeld surfaces mapped with a) $d_{norm}$; b) shape-index c) $d_i$ and d) $d_e$ for the title complex.

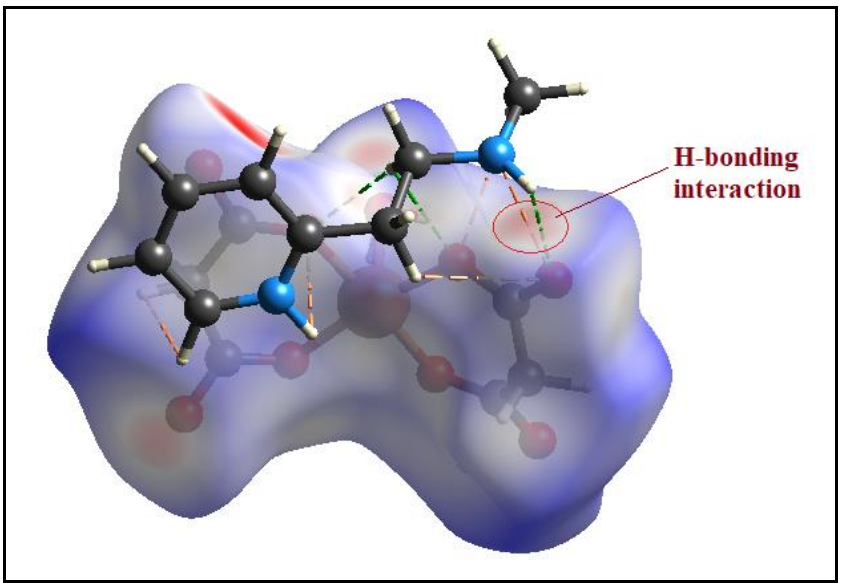



Fig 20: Hirshfeld surfaces plot of H-bonding interactions which are shown in red circle.

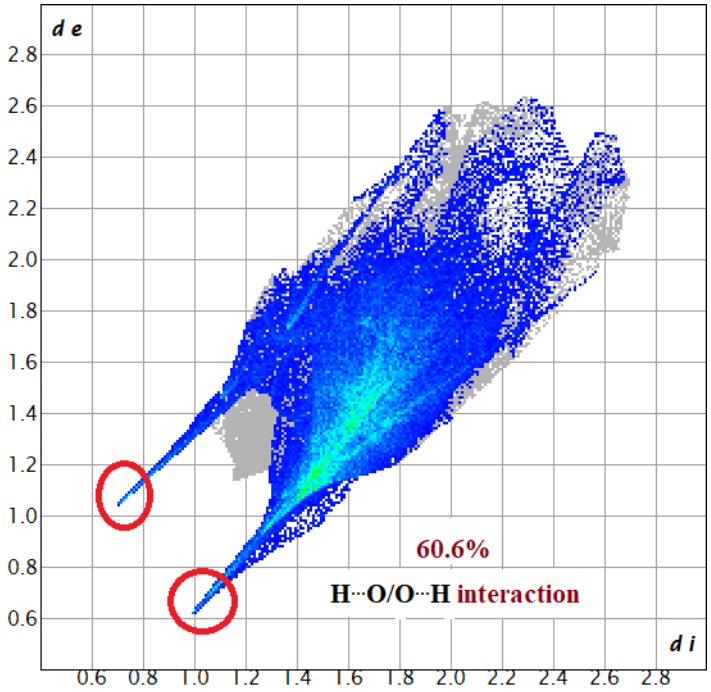



Fig 21: Hirshfeld surfaces fingerprint plot of H····O/O····H bonding interactions (60.6%) which are shown in red circle.

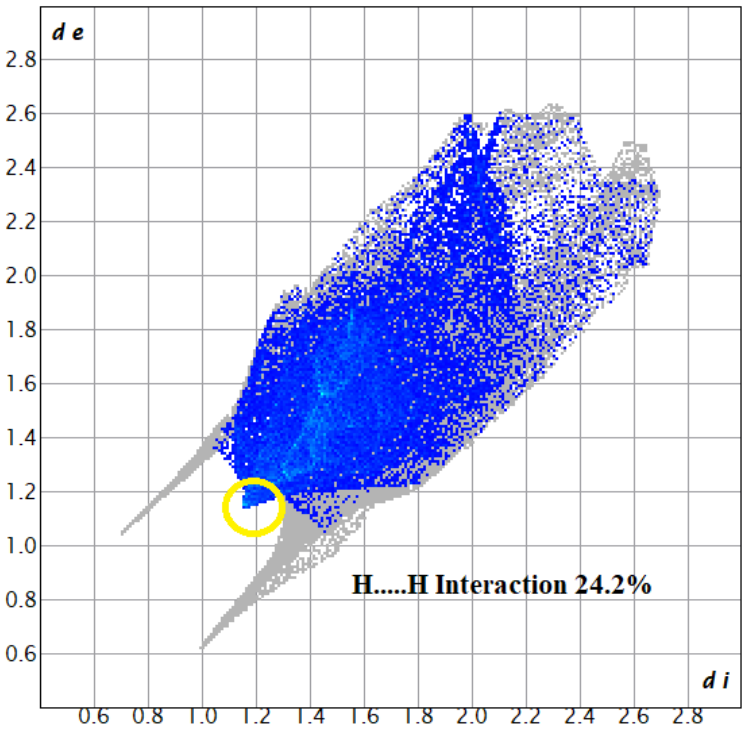



Fig 22: Hirshfeld surfaces fingerprint plot of H····H bonding interactions (24.2%) which are shown in yellow circle.

# Chapter 7: Conclusion

## 7. Conclusions:

The study of non-covalent interactions is crucial to understanding many biological processes that rely on these forces for structure and function. Biological systems are often the inspiration for supramolecular research. Supramolecular chemistry is also important to the development of new pharmaceutical therapies by understanding the interactions at a drug binding site. From our project work we understand about the different types of non-covalent interaction which is responsible for crystals packing by DFT calculation.

Finally, it is tried to explore supramolecular features of synthesized metal complex. The outcome of the proposed project work will be submitted in various journals of repute for publication. In summary,

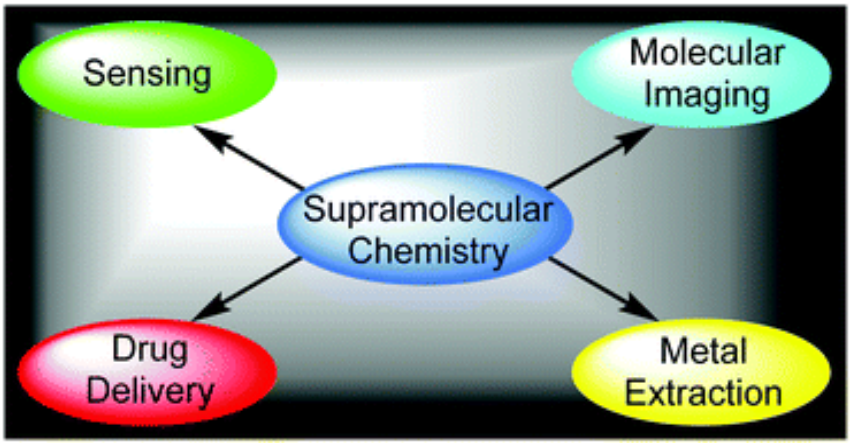
- Review works have been done.
- Finalization of project work.
- Planning of project work has been decided.
- Purchase of chemicals and instruments set up.
- Some chemical reactions have been performed.
- Single crystal suitable for X-ray have been obtain
- Crystal structure were established and
- Hirshfeld surfaces analysis has been done.

The study of non-covalent interactions is crucial to understanding many biological processes that rely on these forces for structure and function. Biological systems are often the inspiration for supramolecular research.Supramolecular chemistry is also important to the development of new pharmaceutical therapies by understanding the interactions at a drug binding site.From our project work we understand about the different types of non-covalent interaction which is responsible for crystals packing by DFT calculation.We can explore supramolecular chemistry include molecular self-assembly, molecular folding, molecular recognition, host–guest chemistry.Molecular devices exist at the boundary between supramolecular chemistry and nanotechnology, and prototypes have been demonstrated using supramolecular concepts.

# Chapter 8: Future Scope

## 8. Future Scope

Supramolecular chemistry is also significant to the development of new pharmaceutical therapies by understanding the interactions at a drug binding site. The area of drug delivery has also made critical advances as a result of supramolecular chemistry providing encapsulation and targeted release mechanisms. Developments in molecular and supramolecular design and engineering open perspectives towards the realization of molecular photonic, electronic and ionic devices, that would perform highly selective recognition, reaction and transfer operations for signal and information processing at the molecular level.



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