Investigation of a Series of N-oxide Schiff-base Ligands Derived from 2-Pyridinecarboxaldehyde N-oxide and 1,2-Phenylenediamine, and Their Respective Metal Complexes

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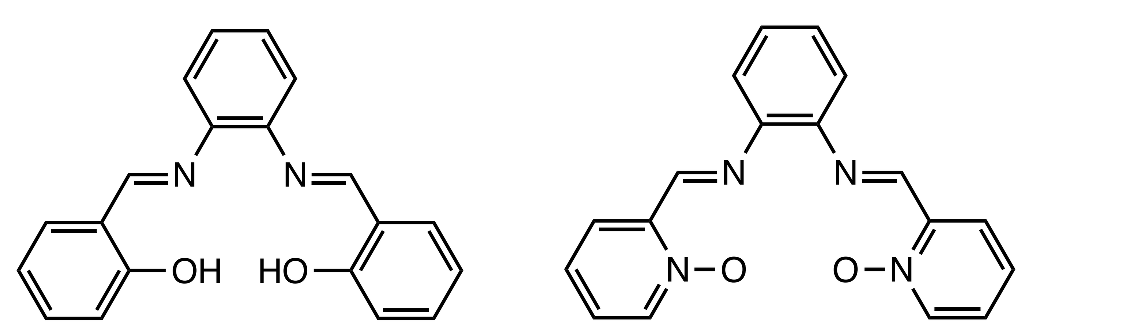
Background:

Organic ligands containing Schiff-base functionality have been of particular interest in coordination chemical studies.

The ligands in this study take inspiration from tetradentate salphen-type Schiff-base ligands, the complexes of which have applications in:

- **Industrial Catalysis** – Organic Chemical Transformations[1]
- **Biological Therapeutics** – Antibiotic, Anti-inflammatory, Anti-tumor Properties[2]
- **Photochemical Technology** – Development of OLED Displays[3]
- **Chemical Analysis** – Anion Receptors[4]



Salphen ("Classical" Tetradentate Schiff-base Ligand)

Poxphen (N-oxide Analogue of Salphen)

Although inspired by salphen-type ligands, all ligands in the study are distinguished by their N-oxide functionality. Not much is known about the structures and properties of N-oxide Schiff-base ligands compared to the extensive research done on their phenolate counterparts.

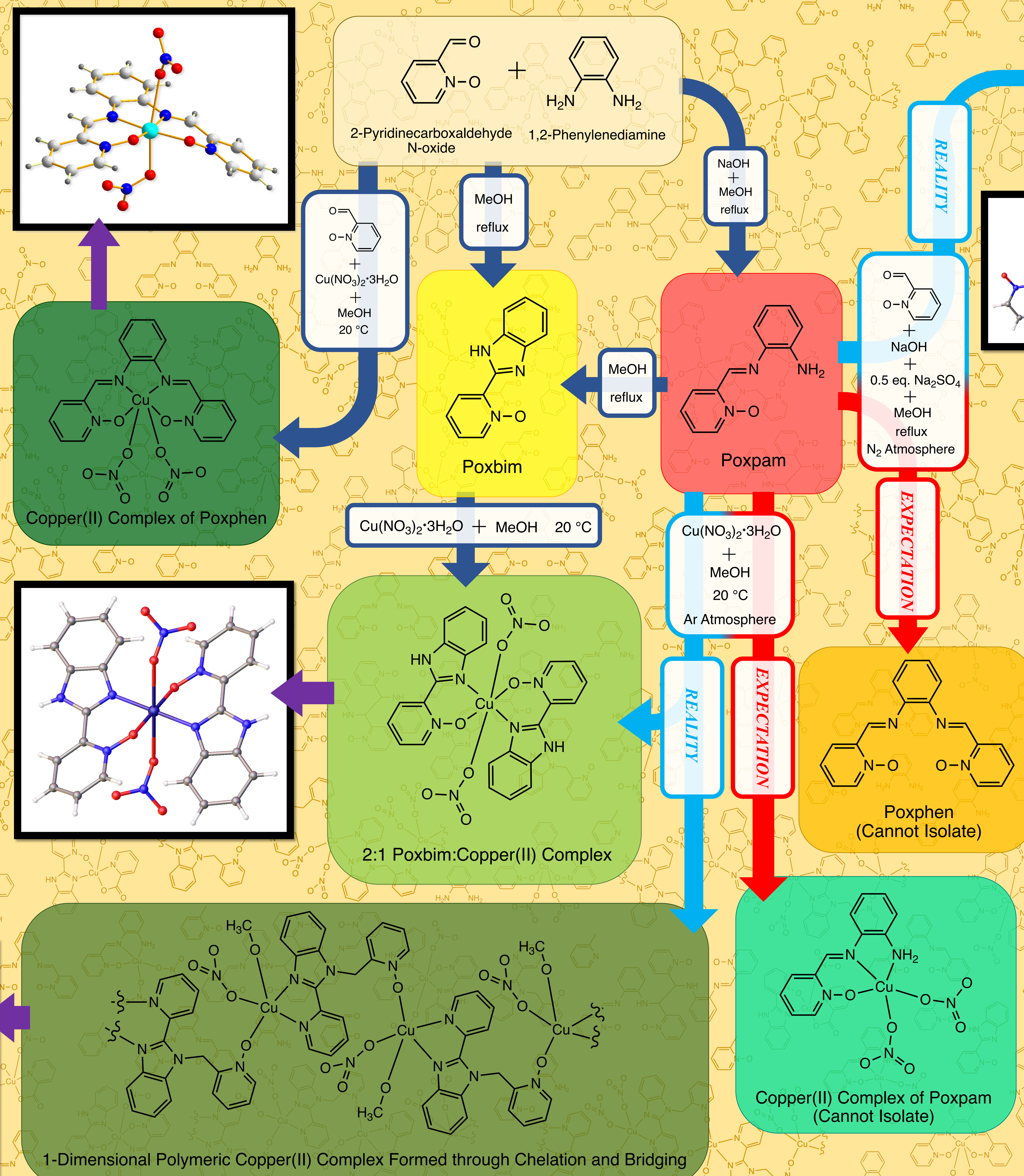
Methods & Results:

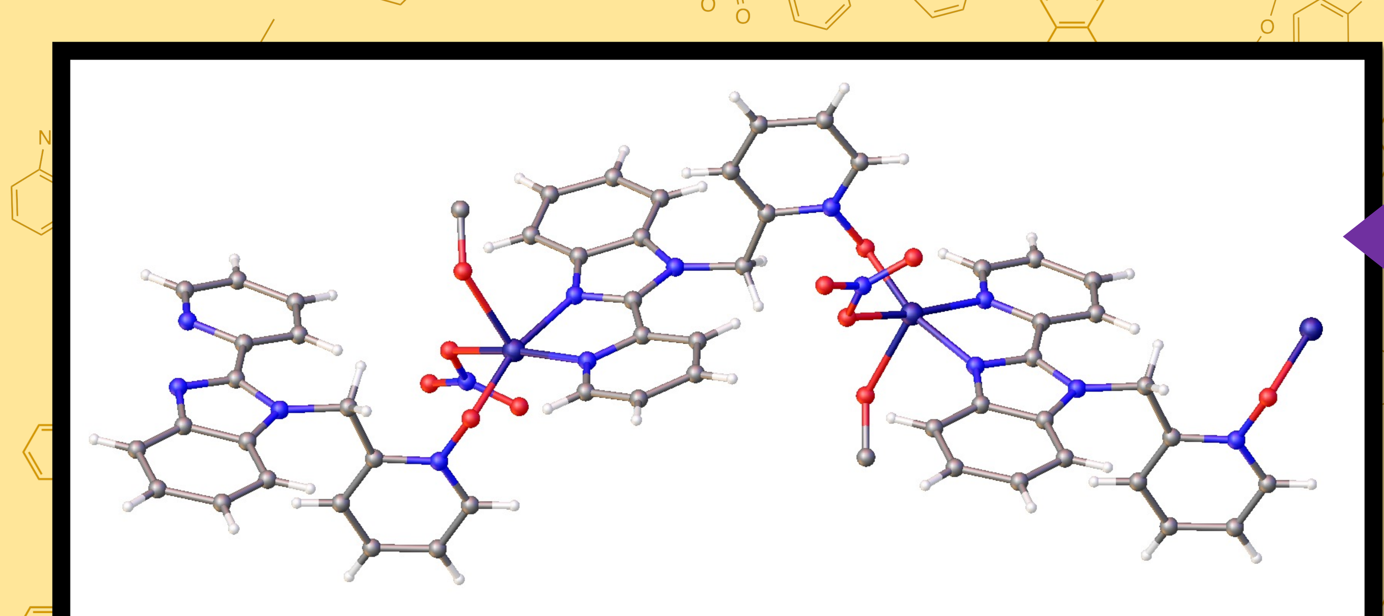
The following map outlines the series of synthetic pathways conducted to form various N-oxide Schiff-base ligands and coordination complexes:

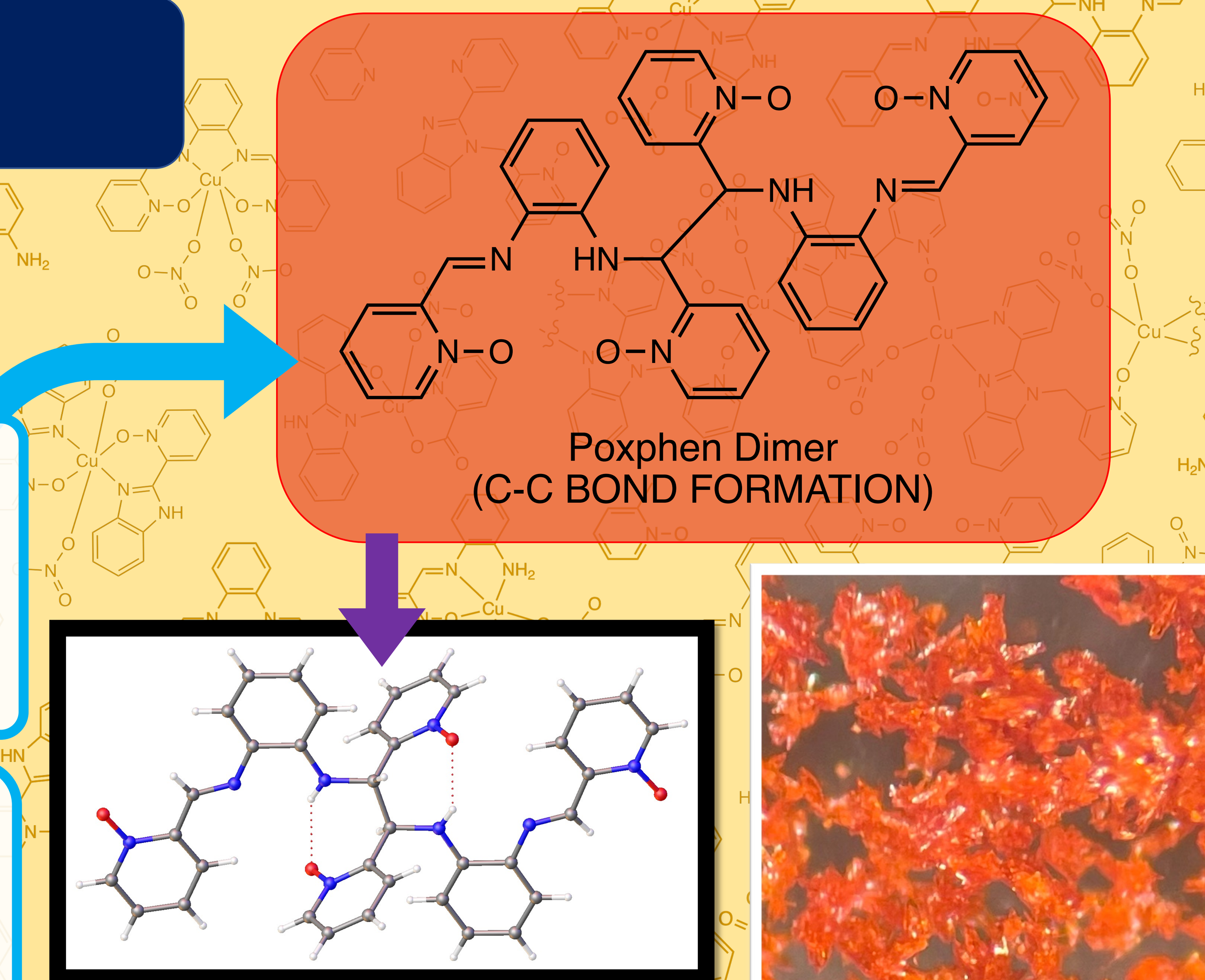
- Reactions with **dark blue reaction arrows** represent a repetition of results obtained by previous students in our research group.
- Reactions with **red reaction arrows** yield theoretical products that were expected to result from specific transformations.
- Reactions with **light blue reaction arrows** represent the experimental products obtained in contrast to the theoretical products.
- **Violet arrows** from certain species point toward their corresponding structures determined by X-ray crystallography.
  - Reagents, solvents, and conditions are listed near their respective reaction arrows.
  - Certain reactions were conducted in inert atmospheres. All reported syntheses were conducted in air unless otherwise specified.

All products obtained were characterized by X-ray crystallography, infrared spectroscopy, and melting point analysis (where applicable).

Synthetic Pathways & Results:







Conclusions & Project Outlook:

- Although the monomer of the tetradentate N-oxide analogue of salphen cannot be isolated, its dimer is synthesized through a carbon-carbon bond-forming reaction.
- Despite the inability to synthesize a copper(II) coordination complex with the tridentate poxpam ligand, a polymeric complex can be formed through formation of a different tridentate ligand *in situ* with bridging and chelating capabilities.
- Future endeavors could include further examining the formation of the carbon-carbon bond of the poxphen dimer, synthesizing complexes of the poxphen dimer, and exploring the synthesis and physicochemical properties of the newly-obtained polymeric complex with the novel tridentate ligand.

Acknowledgements:

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References:

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