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# Coordination polymers as functional materials

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## INTRODUCTION & AIM

The advanced synthesis of coordination polymers is fascinating due to its resulting structural diversity and vast opportunities to design new functional magnetic materials.

The physicochemical properties of coordination polymers result from a combination of synthesis conditions and properties of simple, well-known precursors [1,2,3].

This generates the possibility to model the electrical, magnetic, and optical properties of coordination polymers. These could find application as luminescent materials, catalysts, sensors, ion exchangers, and as magnetic materials. An important research topic in recent years is the luminescent properties of these materials.

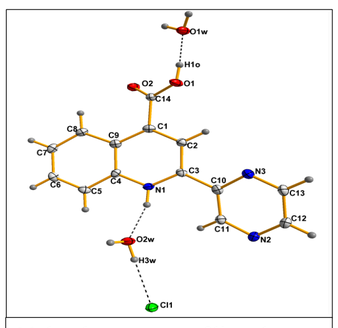
In comparison with organic compounds that are used, e.g., in the manufacturing of OLED-type diodes, inorganic coordination compounds prevail as they possess a much higher thermal stability, widening the operational temperature range.

Depending on the valence electrons' configuration, the luminescent properties of coordination polymers are governed by MLCT (metal–ligand charge transfer), LMCT (ligand–metal charge transfer), LLCT (ligand–ligand charge transfer), or IL (inter-ligand charge transfer) states.

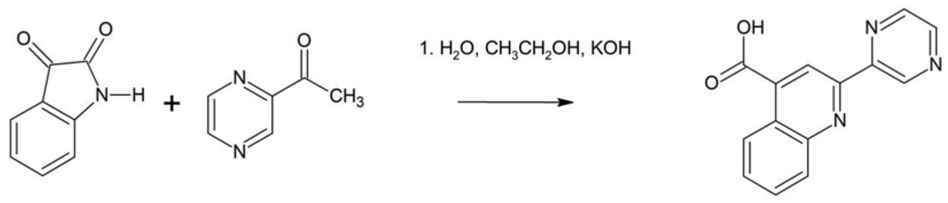
Herein, we present novel coordination polymers based on copper ions and organic aminocarboxylate ligands. For these compounds, the complexation of copper ions results in the amplification of emissions and an increase in the maximum emission shift.

## METHOD

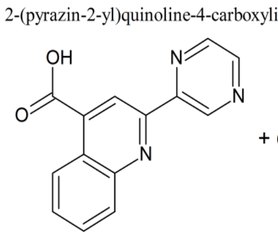
**Pressure reactor Berghof BR100.**




Molecular structure of ligand, thermal displacement of thermal ellipsoids at 50% probability level.




HL = 2-(pyrazin-2-yl)quinoline-4-carboxylic acid



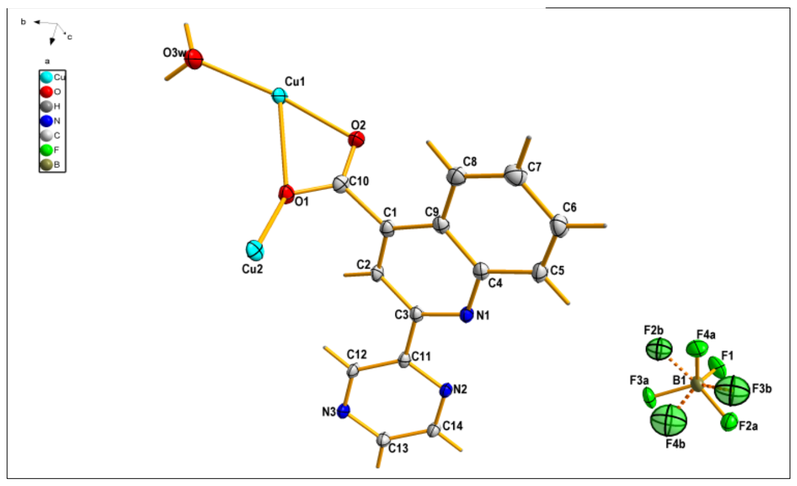

+ $Cu(BF_4)_2 \cdot nH_2O + H_2O$

Autoclave Berghof BF100
165 °C, 5 days

$\{[Cu_3(L)_2(H_2O)_2][BF_4]_2\}_n$

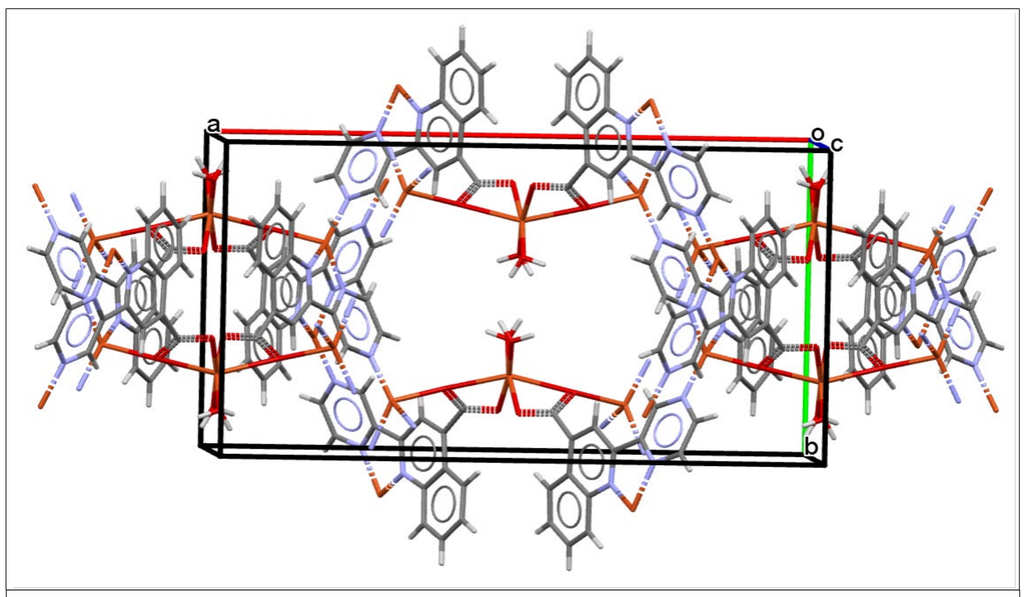
**Crystal data**

| | |
|---|---|
| **Molecular weight** | **900.77** |
| **Crystal system, space group** | **Orthorhombic *Pbcn*** |
| a [Å] | 21.9637(8) |
| b [Å] | 12.4106(3) |
| c [Å] | 11.5844(4) |
| a [Å] | 21.9637(8) |
| V [Å$^3$] | 3157.71(18) |
| Z | 4 |

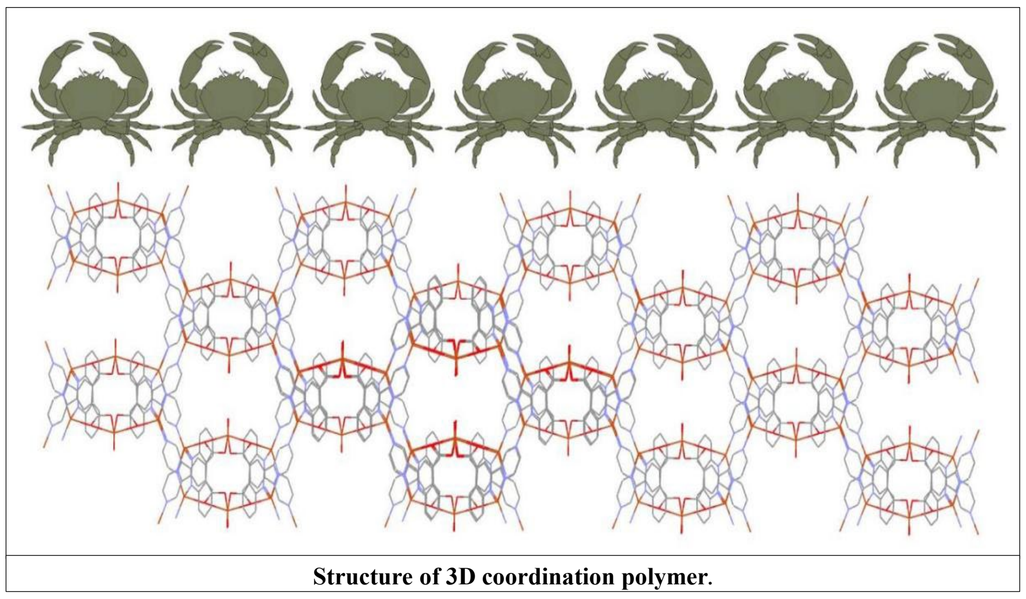



## RESULTS & DISCUSSION

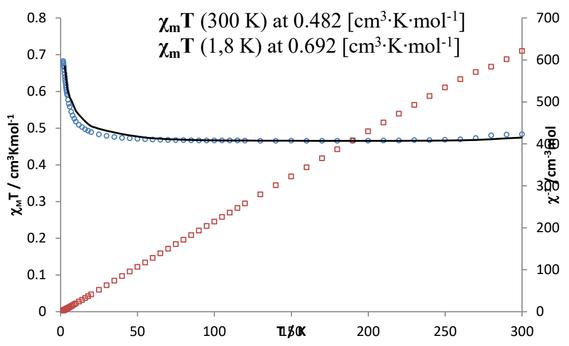
$\{[Cu_3(L)_2(H_2O)_2][BF_4]_2\}_n$




**Crystal structure packing in [001] direction.**



**Structure of 3D coordination polymer.**




Cu1-Cu1$^{iv}$((iv) -x, -y+2, -z)) is 8.573(2) Å.

## CONCLUSION

- Novel coordination polymers based on copper ions and organic aminocarboxylate ligands have been synthesized.
- Structure and magnetic / emission properties have been characterized.
- Complexation of copper ions results in the amplification of emissions and an increase in the maximum emission shift.

## FUTURE WORK / REFERENCES

Literature

[1] S.R. Batten, S.M. Neville, D.R. Turner, Coordination Polymers: Design, Analysis and Application, School of Chemistry, Monash University, Victoria, Australia, (2009)

[2] B. Moulton, M. J. Zaworotko, Chem. Rev. 101, 1629 (2001)

[3] A.Kochel, M . Hołyńska, K. Twaróg, A. Jezierska, J.J., Panek and J. Wojczyński, Acta Cryst. C78, 405 (2022)