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# Visualizing and Analyzing Structures of Coordination Polymers Synthesized in Ionic Liquids

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## *Introduction*

Synthesis of metal organic frameworks can result in different products based on the solvent that is used. One option is to use ionic liquids (ILs, or room temperature molten salts) to create novel metal organic coordination polymers.[1] Using databases such as Sci-Finder Scholar, and Cambridge Structural Database, our group analyzed metal organic polymers synthesized in ILs with the goal of cataloging the topology of the structures, the connectivity of the organic ligands,the overall net structures, and the roles of the ILs in the syntheses.

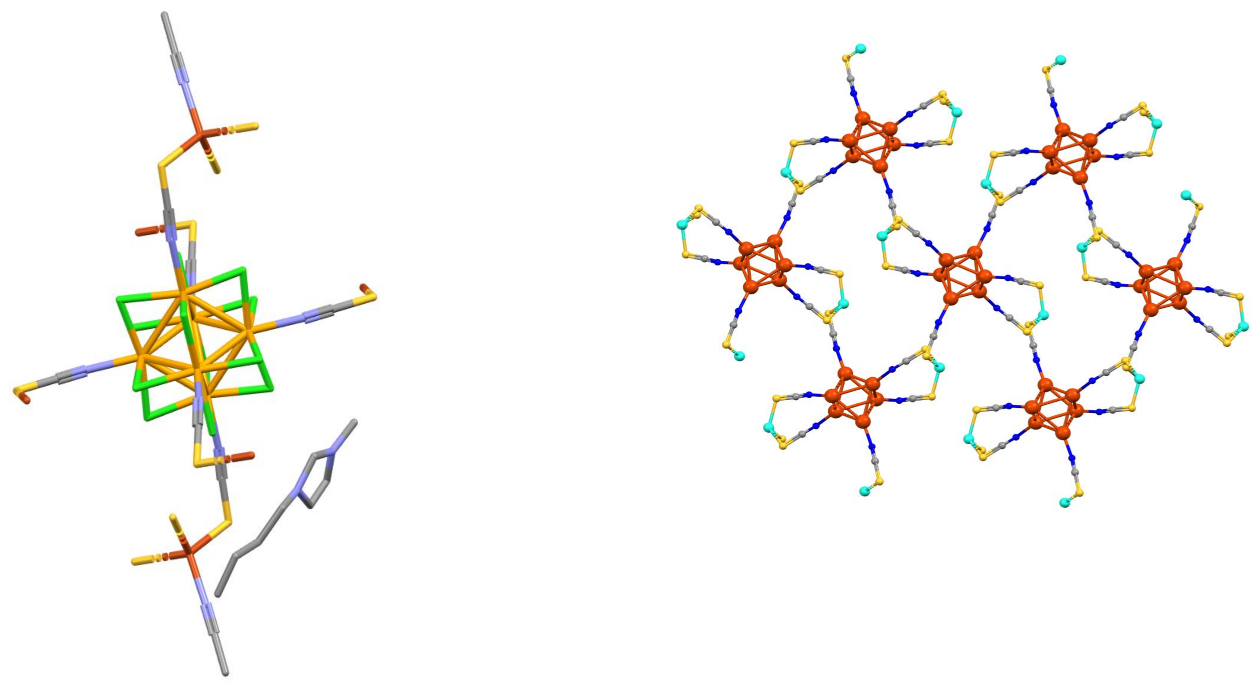


***Figure 2:*** Structures from the Pigorsh et. al paper. The left photo shows the[BMIM][$Nb_6Cl_{12}(NCS)_6\{Cu(CH_3CN)\}_2$] monomer with the EMIM, whereas the right photo shows the net connections of of the polymer.

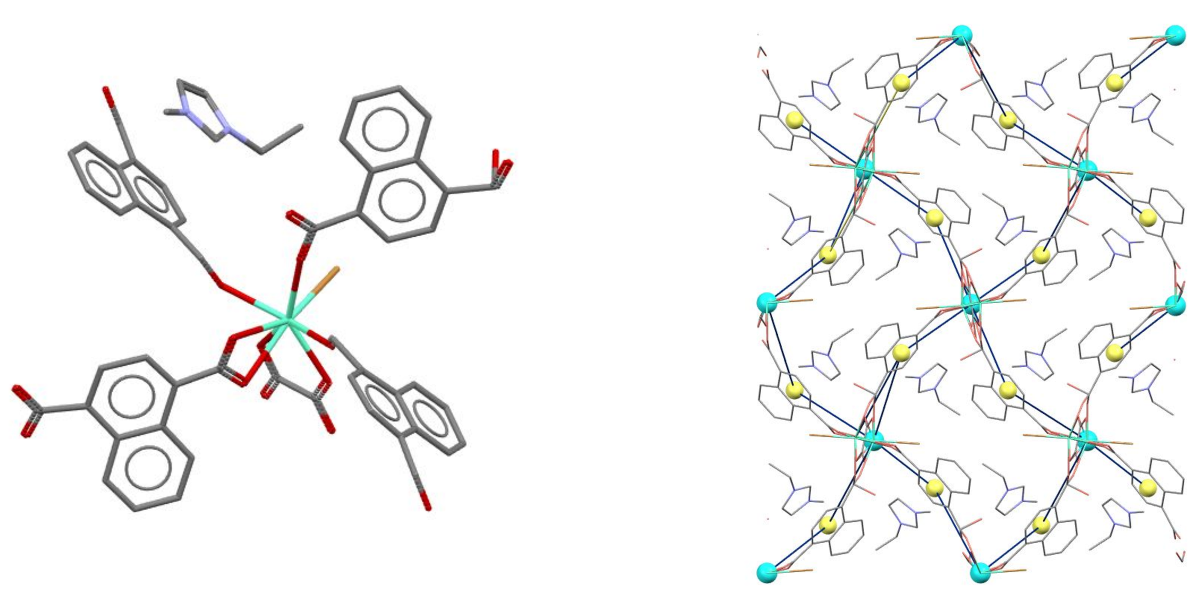


***Figure 3:*** The left photo shows the{(EMIM)[Eu(1,4-ndc)(ox)0.5Br]}$_n$ monomer centered around the EU atom and the photo on the right shows the net connections between the Eu atoms and the carbon rings

## *Methods*

Our methods consisted of using three different databases: Sci-Finder Scholar, Conquest, and Mercury.

Sci-Finder Scholar → Conquest (CSD) → Mercury

**Sci-Finder Scholar**
- Used to find relevant papers
- Searched using keywords and phrases such as "Ionic liquid syntheses" or "Mixed ligand coordination Polymers

**Conquest (CSD)**
- Used to find compounds from papers
- Could search for compound
  - Formula, structure, author
- Would give us a 'hitlist' of results under six letter reference codes
  - Ex: OROKAJ

**Mercury**
- Used ref code to find and edit structure
- Created net structures through connecting centroids
- Created centroids in Mercury and then turned them into "dummy atoms" in CIF file which allowed for creation of Net figures

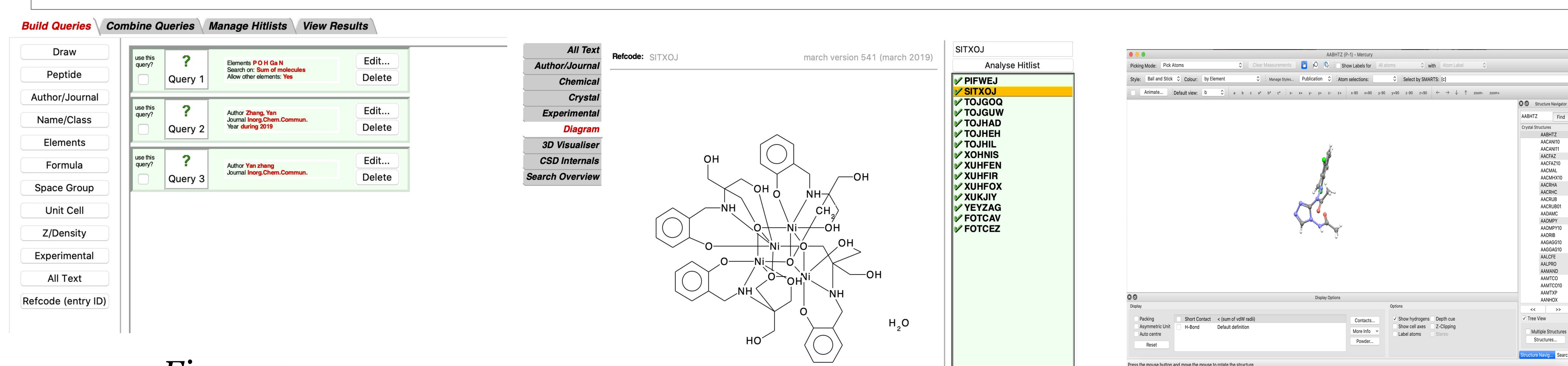


Figure 1a. Figure 1b. Figure 1c.

***Figure 1:*** The databases used in our research. Figure 1a and 1b show the program conquest, and figure 1c shows the program Mercury.

## *Results*

| Formula | Reference # | Ref code | IL | Role of IL | 1D, 2D, 3D? | Ligand | Net | Interesting properties |
|---|---|---|---|---|---|---|---|---|
| [BMIM][$Nb_6Cl_{12}(NCS)_6\{Cu(CH_3CN)\}_2$] | 2 | OROKAJ | [BMIM][PF6] | Cation/ Medium | 3D bridged compound | Isothiocyanato ligands n-bonded to cluster unit | Ligands n bonded to cluster units (cluster bound) | H-bonds between layers |
| {(EMIM)[Eu(1,4-ndc)(ox)0.5Br]}$_n$ | 3 | EMUTUD | [EMIM]Br | Cation | 2D layers that form 3D framework | Bromide ion as terminal ligand | 6 connected PCU net | Exhibit lanthanide luminescence emissions |
| [$M_2(TBAPy)(H_2O)_2$]·(Guests)$_x$ (M = Co, Zn) | 4 | KUJYUM | [RMIM]Br (R= ethyl, propyl, butyl) | Medium (increases yield) | 2D layers stack to form 3D network | TBAPy ligand bridging and monodentate to each metal | 4,4 - net Square grid | Temperature dependent fluorescence |
| [$Mn_2(ptptp)(suc)_{0.5}(H_2O)_3$] • Br • $0.5H_2O$ | 5 | EFEFUS | [BMIM]Br or [$P_{14}$]Br | Anion donor and structure regulator | 1D helical structure forms 3D supramolecular network | Ptptp ligand and suc ligand are bridging | N/A | Anti-ferromagnetic properties |

## *Results discussion*

- Role of IL divided into cation donor, anion donor, medium.
- Many compounds form 3D frameworks or networks
  - 2d structures can stack to form 3D layers
- Some have interesting properties that can be applied to useful things
  - Luminescence
  - Fluorescence

## *Future Work*

For our future work, we have two major projects:

1. Continue our work analyzing new structures synthesized in ionic liquids and to use the topology program TOPOS Pro as another tool to analyze the structures. We plan on writing a review paper incorporating the different structures using the visuals we created.
2. Identify systems with $Na_3$SIP ligands that can be adapted to ionic liquids in order to synthesize new products and to do those reactions in a lab setting.

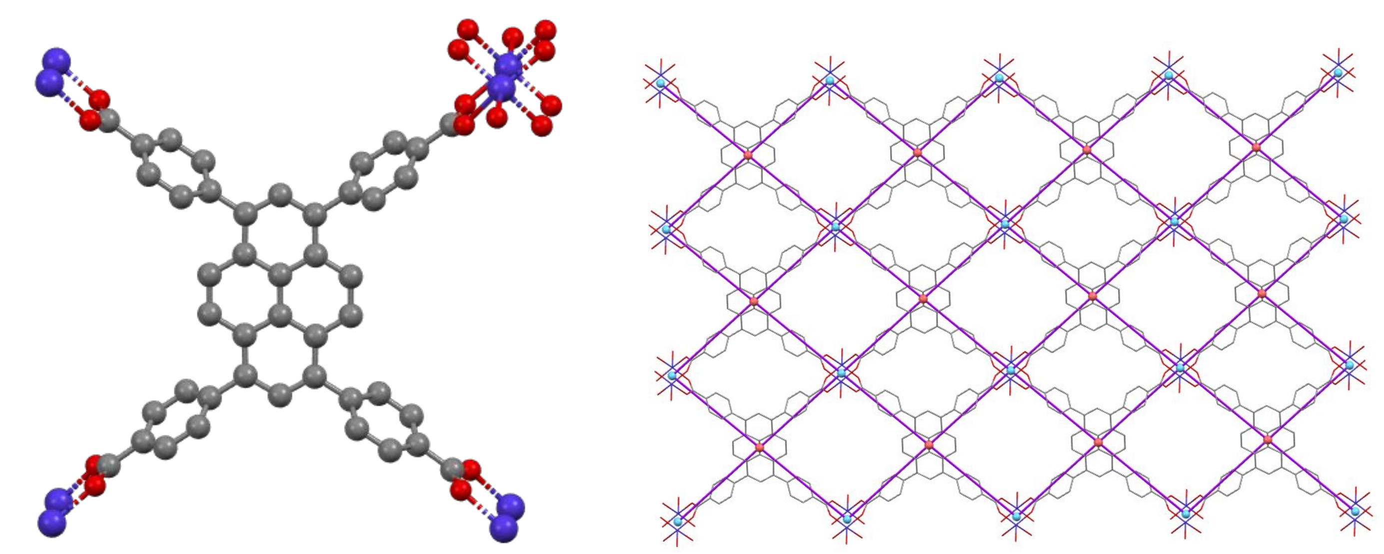
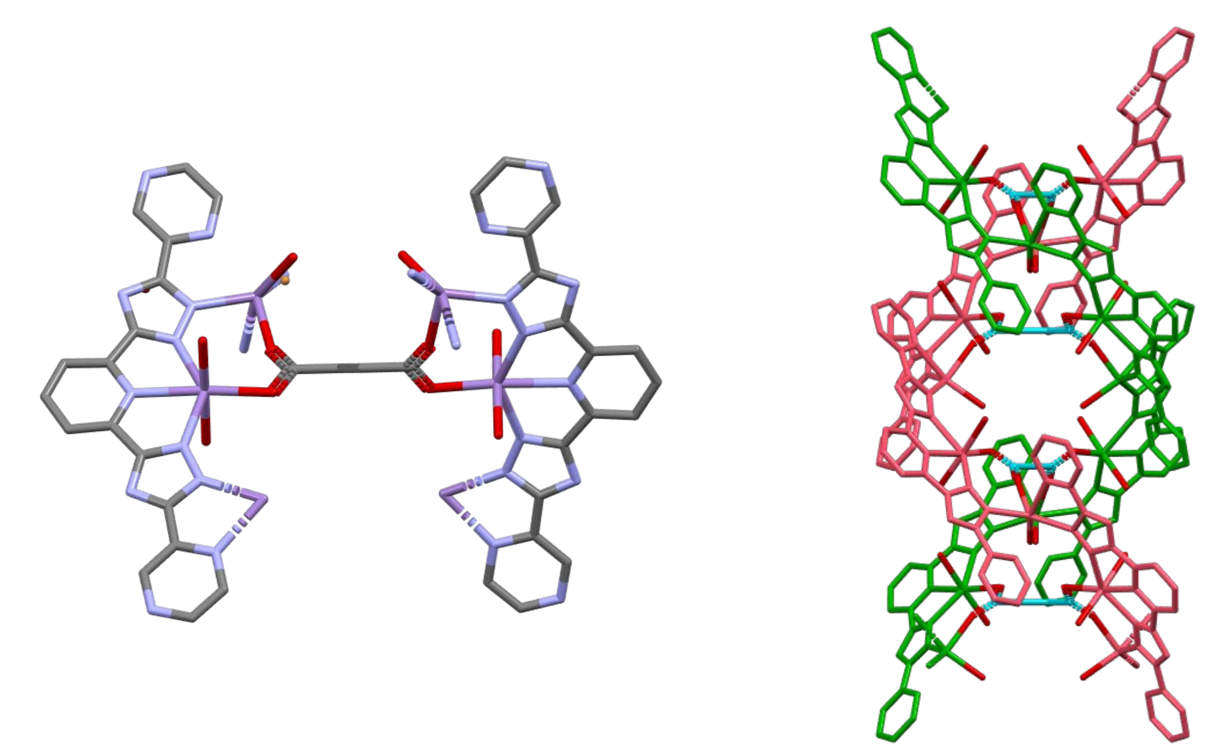


***Figure 4:*** Structures from the Huang et. al study. The left image is the [$M_2(TBAPy)(H_2O)_2$]·(Guests)$_x$ (M = Co, Zn) monomer. The right image shows how the monomers connect to form a 2D layer with 4,4 net square grid structure (as shown by the purple lines).



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## *Acknowledgments*

We would like to express our gratitude and appreciation to the Department of Chemistry and Biochemistry, the Science Research Fellows Program, Caroline Gilson, Tiffany Hebb, and Gina Federighi for supporting this project.

## *References*

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(2) Pigorsch, A. and Köckerling, M. *Cryst. Growth Des.* **2016**, *16* (8), 4240-4246.

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# ***Results***

| **Formula** | **Reference#** | **Ref Code** | **Ionic Liquid** | **Role of IL** | **1D, 2D, 3D?** | **Ligand** | **Net** | **Interesting properties** |
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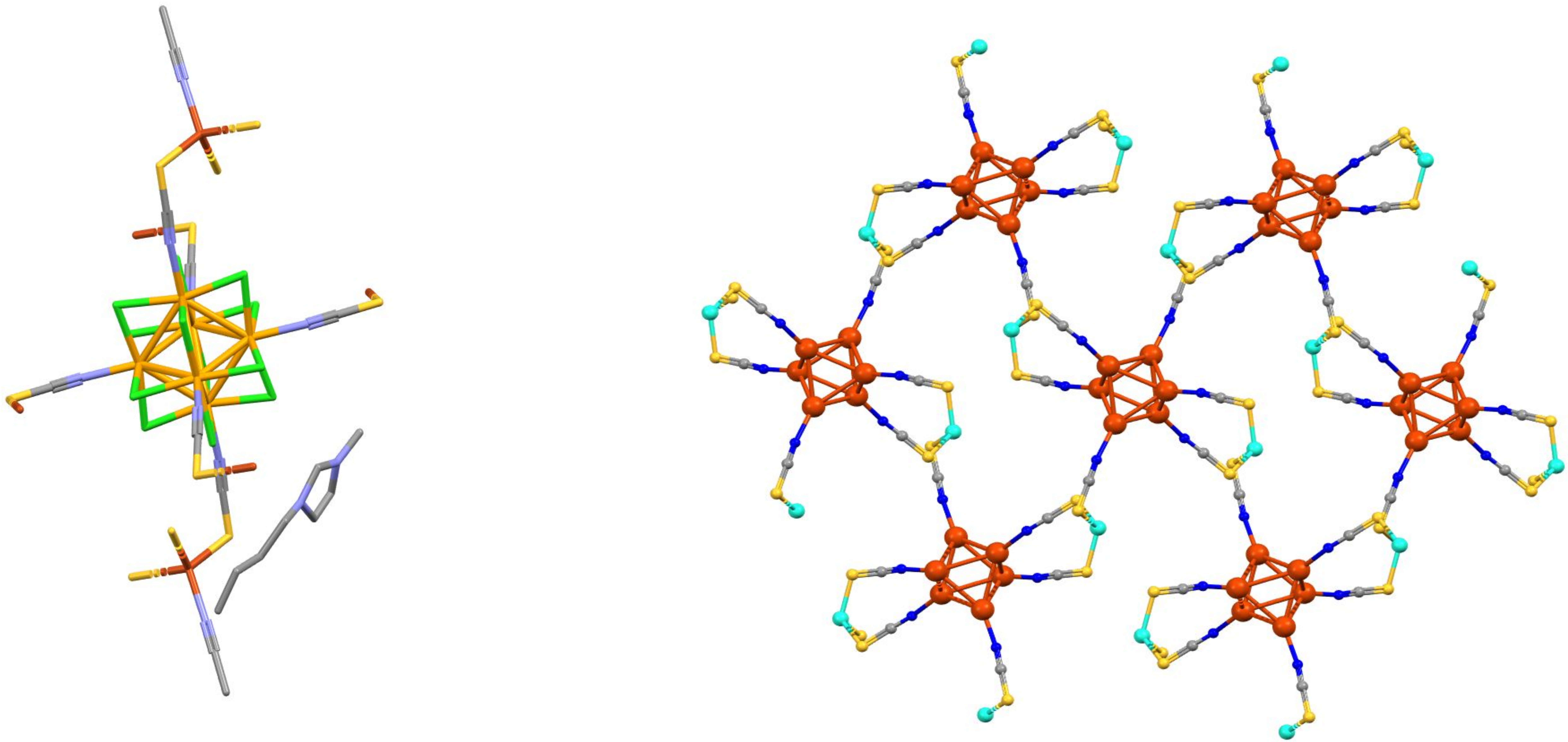

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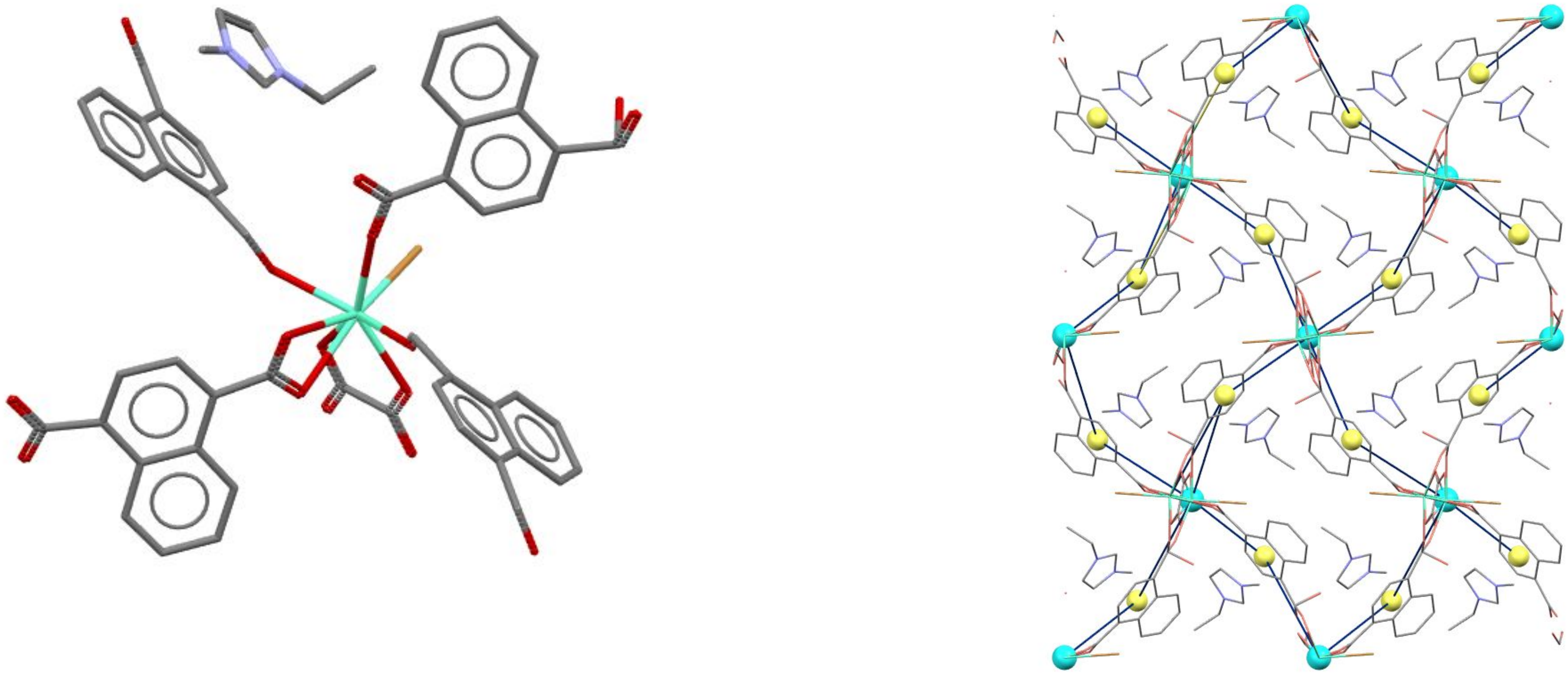

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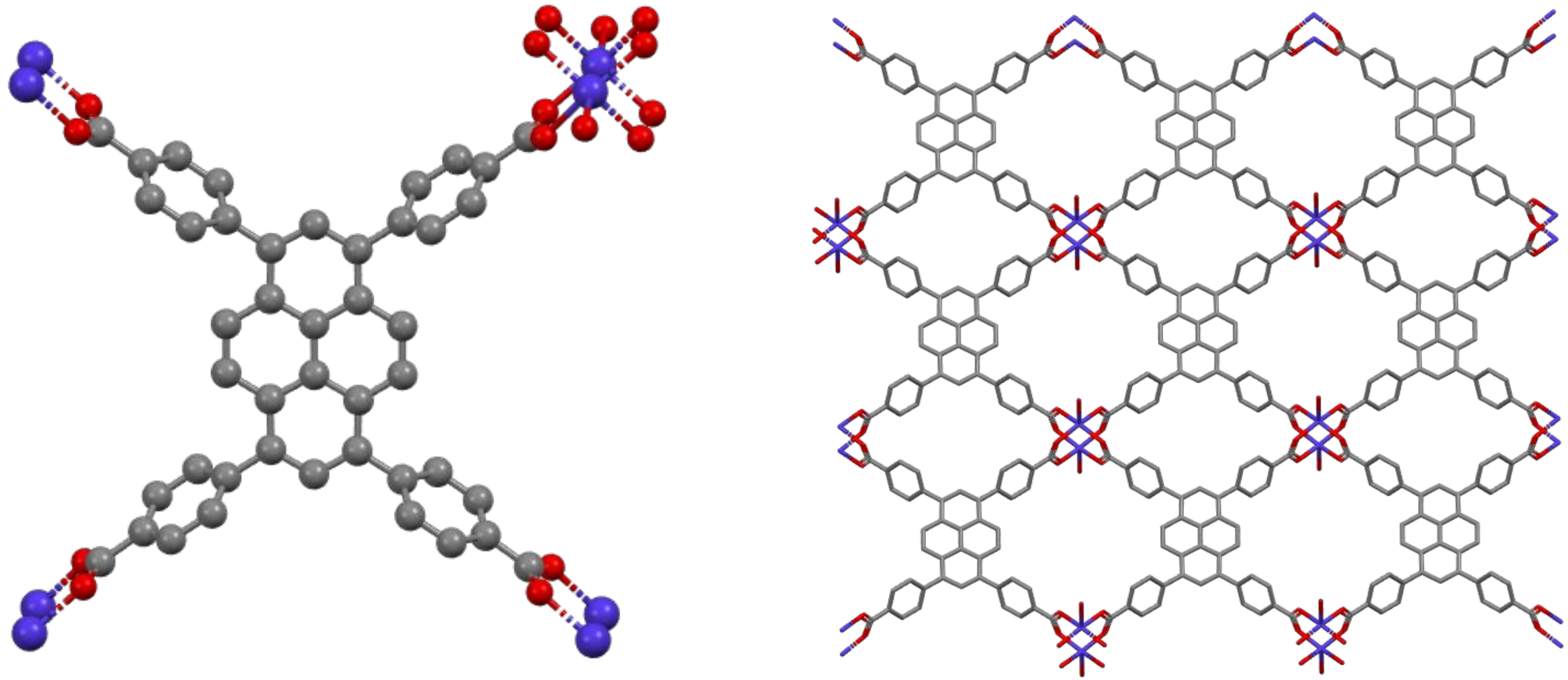

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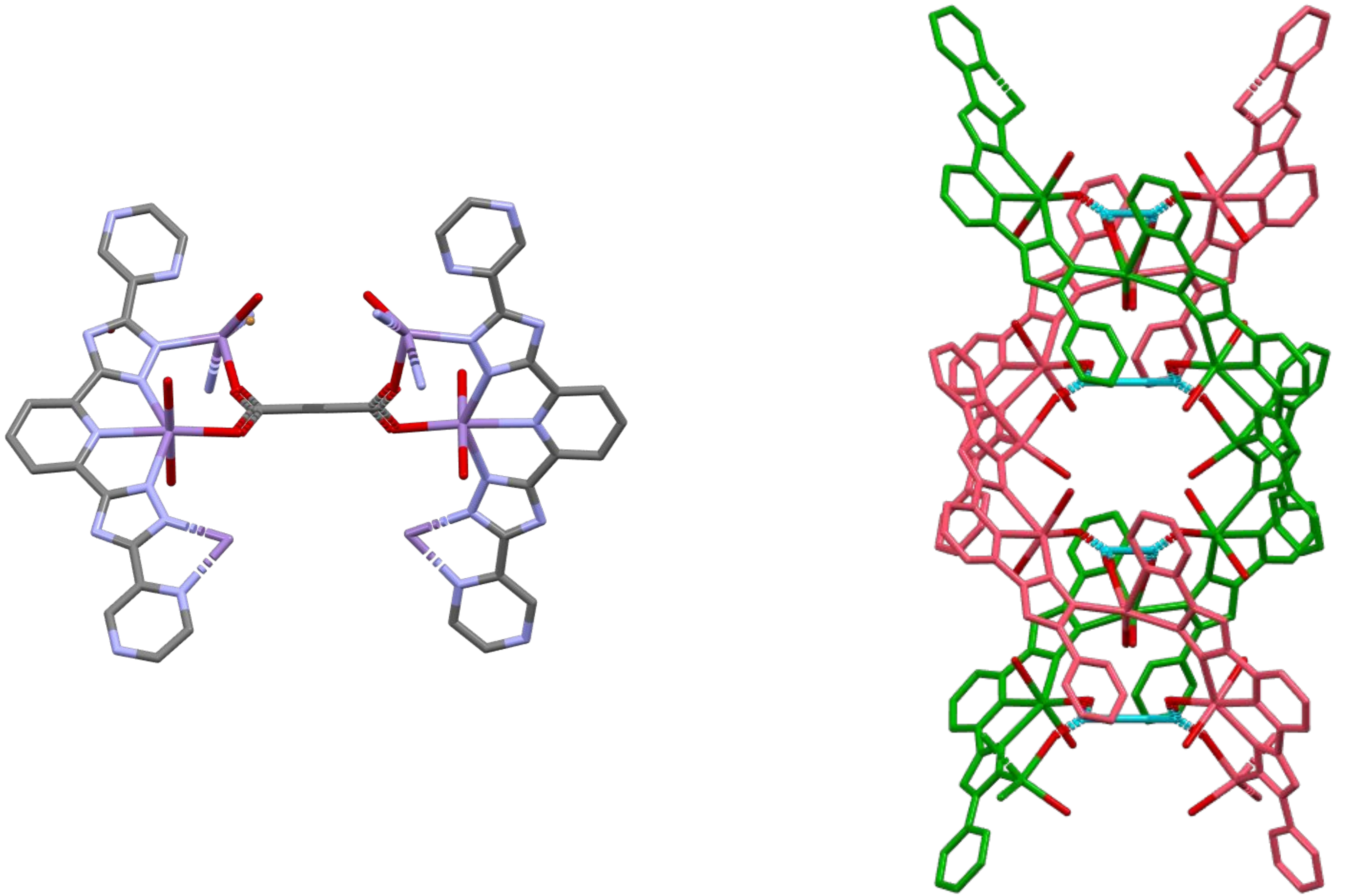

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