Fall 10-2020

Conceptualizing and Analyzing Metal-Organic Frameworks and the Role of the Ionic Liquid

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CONCEPTUALIZING AND ANALYZING METAL-ORGANIC FRAMEWORKS AND THE ROLE OF THE IONIC LIQUID

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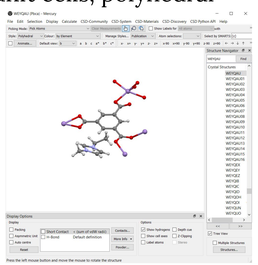
Introduction

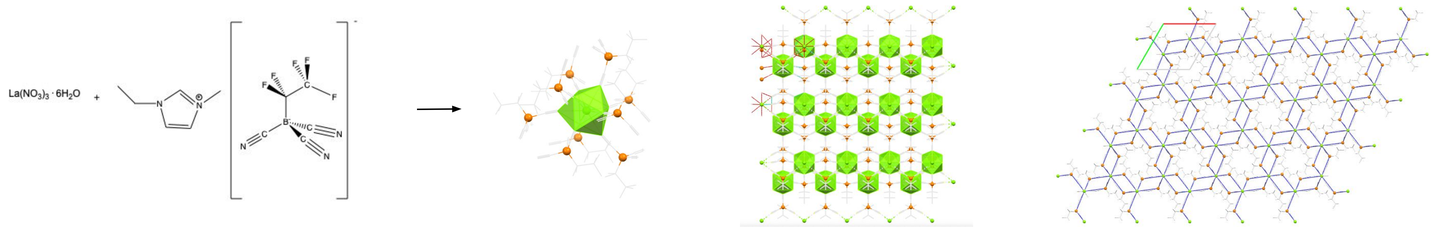
The synthesis of metal-organic frameworks, or MOFs, can be manipulated by changing the solvent medium to an ionic liquid (IL), which is a room temperature molten salt. Different MOFs can result from reactions done in ILs than those synthesized in traditional solvents. Ionic liquids can be incorporated into the final structure either with the role of the ionic liquid as the cation, anion, or a ligand to the metal ion.[1] We analyzed previously published structures of MOFs synthesized in ILs to determine the connectivity of the metals and ligands, the overall net structure of the solid, and the role of the ionic liquid in these syntheses.

Methods

- Searched Scifinder Scholar and Google Scholar for "MOFs in ionic liquid"
- Retrieved structural data from Cambridge Structural Database using ConQuest
- Analyzed crystal structure in Mercury
- Utilized structural data to create new figures in Mercury to convey information effectively
  - Created figures showing unit cells, polyhedral geometry
  - Net structures were created through the use of cif (crystallographic information file) files and the enCIFer program

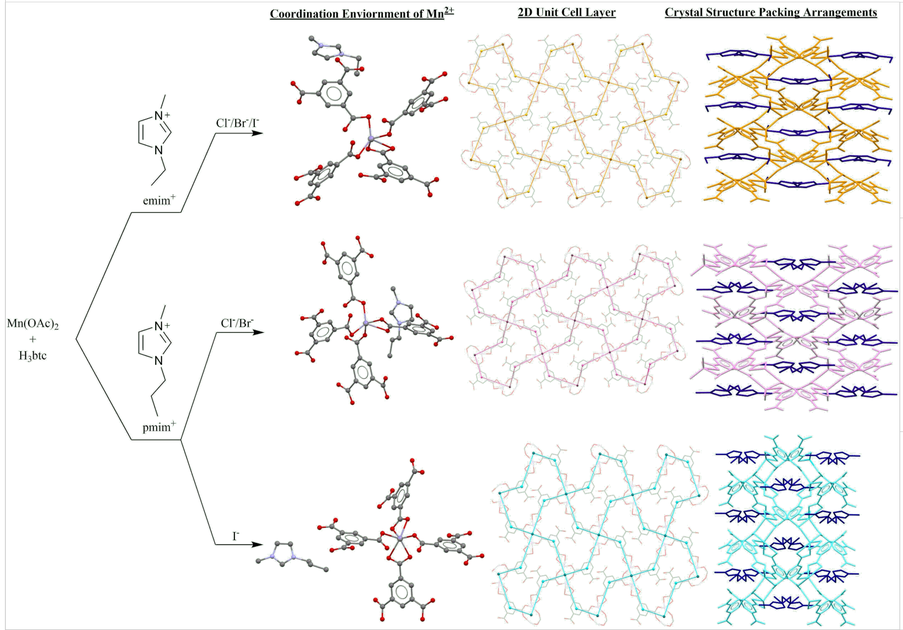


$[La\{C_2F_5B(CN)_3\}_3]$ [3]



- IL:[emim]Cl
- Ligand bridging: 9 separate bridging ligands coming off of one La^{3+}
- Ligand plane: 3 La^{3+} connected by the one ligand
- Coordination number of Metal: 9
- Geometry of metal: Tricapped octahedron

[emim][Mn(benzene-1,3,5-tricarboxylic acid)] and [pmim][Mn(benzene-1,3,5-tricarboxylic acid)] [2]



- IL: [emim]Cl, [emim]Br, or [emim]I
- Ligand Bridging: 1 bidentate connection, 2 monodentate connections to bridging 2 separate Mn^{2+}, 1 monodentate connection
- Ligand Plane: 2 Mn^{2+} above plane, 2 Mn^{2+} below plane
- Coordination number of Metal: 5
- Geometry of metal: Distorted square pyramid

- IL: [pmim]Cl or [pmim]Br
- Ligand Bridging: 1 bidentate connection, 2 monodentate connections bridging 2 separate Mn^{2+}, 1 monodentate connection
- Ligand Plane: 1 Mn^{2+} in plane, 2 Mn^{2+} above plane, 1 Mn^{2+} below plane
- Coordination number of Metal: 5
- Geometry of metal: Distorted square pyramid

- IL: [pmim]I
- Ligand Bridging: 2 separate bidentate connections, 2 monodentate connections bridging 2 separate Mn^{2+}
- Ligand Plane: 1 Mn^{2+} in plane, 2 Mn^{2+} above plane, 1 Mn^{2+} below plane
- Coordination number of Metal: 6
- Geometry of metal: Distorted octahedral

Future Work

- Further research analyzing new structures synthesized in ionic liquids
- Further research using the topology program TOPOS Pro to analyze geometrical and topological properties of MOFs
- Research will be used in upcoming review paper written on our findings, using the structures and figures created with Mercury and ChemDraw.

Results

- [emim][Mn(btc)] and [pmim][Mn(btc)] incorporates the cation into the structure while $[La\{C_2F_5B(CN)_3\}_3]$ incorporates the anion of the ionic liquid in both of the final structure
- Both structures have a 'net' structure with cavities
- Both structures are in a 3D framework

Acknowledgments

We would like to express our gratitude and appreciation to DePauw University Librarians Tiffany Hebb and Caroline Gilson, DePauw's Department of Chemistry and Biochemistry, and the DePauw FDC Student-Faculty Research Fund.

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