Purification of Water by the Removal of Metal Cations Using Thiophene Containing UiO-66

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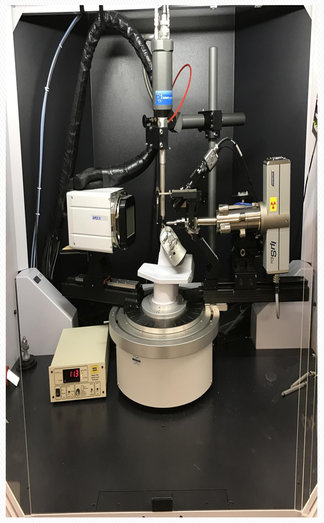
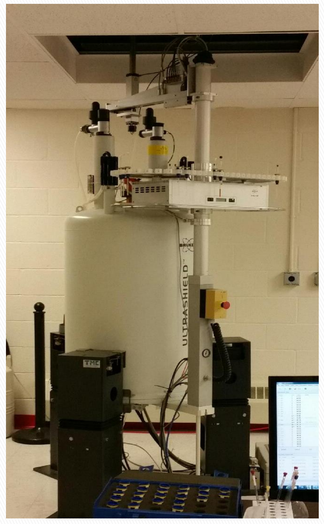
Abstract

The construction of a Thiophene-containing version of the common Metal Organic Framework (MOF) UiO-66 was performed by a linker exchange using 2,5-thiophenedicarboxylic acid. This MOF was targeted due to its projected ability to absorb metal cations from aqueous media into the MOF's pores from contaminated water. The purpose of this is to be able to use this framework to purify water which could then avoid incidents such as the unsanitary water conditions in Flint, Michigan.

Introduction

A metal organic framework (MOF) is a molecule that has metal node connected between organic linkers that form a cage like structure. Most MOF's use carboxylate linkers that can bind to a node and form a crystalline structure that can then be analyzed via an X-Ray Crystal Diffraction (XRD). In the research being conducted, we exchanged a linker from the common MOF UiO-66 with 2,5-Thiophenedicarboxylic acid. In creating this new Thiophene containing UiO-66 compound, the goal is then to test this product in a solvent containing metal cations to purify the liquid. The application of this research is to create a product that can remove harmful metals from drinking supplies such as the one plaguing Flint, Michigan. With this research, a promising method of saving both water and lives could be developed.

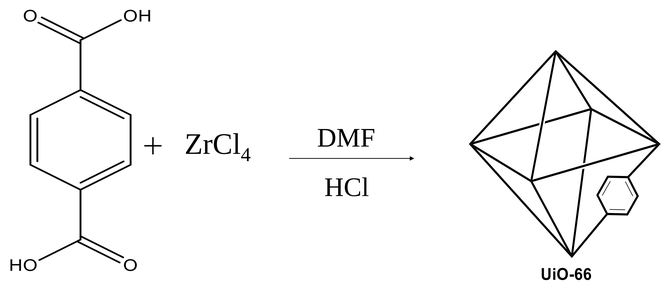




Making UiO-66

- Make Solution of 0.125g of $ZrCl_4$ mixed with 5 mL of DMF and 1 mL of HCl
- Sonicate for 20 minutes
- Make solution of 0.123g terephthalic acid mixed with 10 mL of DMF
- Add to already sonicated solution and sonicate for 20 more minutes
- Place in 80ºC oven for 24 hours.
- Decant the liquid off top layer and clean with DMF & Methanol

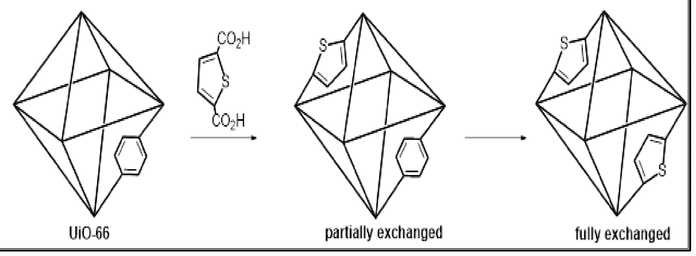
Reagents	Terephthalic acid	$ZrCl_4$	HCl	DMF
MW (g/mol)	166.13	73.09	36.46	73.09
Mass (g/mL)	0.123 g	0.125 g	1.0 mL	15.0 mL
Mmol	0.750	0.54	32.64	194.55
Eq	0.124 g	0.125 g	1.0 mL	15.0 mL

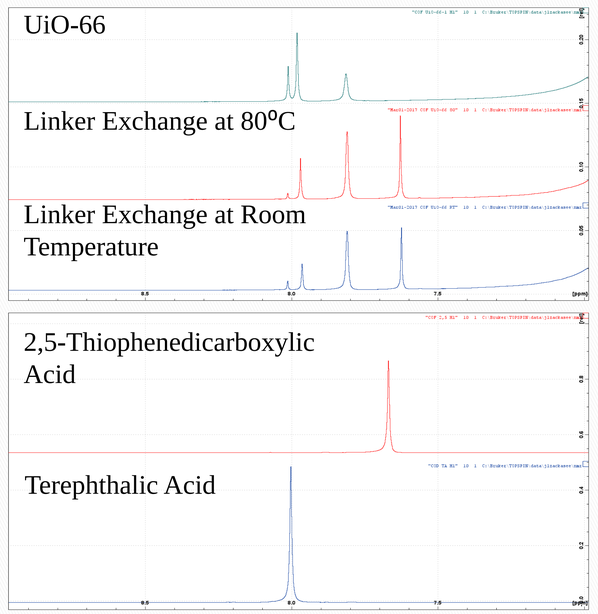


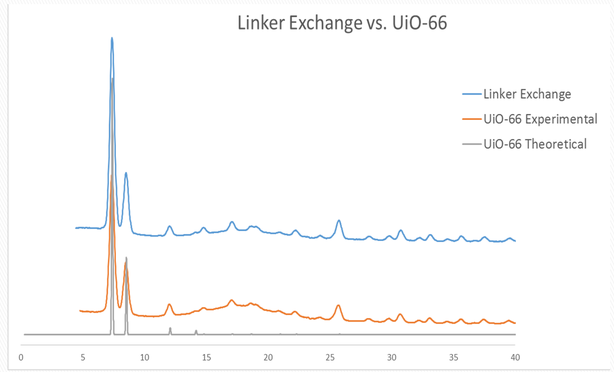
Linker Exchange

- Dry UiO-66 on pump with liquid nitrogen for 24 hours.
- Run powder diffractions and Proton NMR to ensure UiO-66
- Then dissolve 17mg of 2,5-thiophenedicarboxylic acid in 5mL of DMF
- Disperse 30mg of UiO-66 into solution and place in 80ºC oven for 24 hours
- Clean with DMF
- Run powder diffraction and Proton NMR to see if linker exchange was successful

Reagents	DMF	2,5-Thiophene-dicarboxylic acid	UiO-66
MW (g/mol)	73.09	172.16	n/a
Mass (g/mL)	5 mL	0.0170 g	0.03 g
mmol	64.988	0.0987	n/a
Eq 1	5 mL	0.0170 g	0.0297 g
Eq 2	5 mL	0.0088 g	0.0300 g
Eq 3	5 mL	0.0046 g	0.0300 g







Conclusion: Using the data from the XRD and NMR scans, it was determined that both the creation of UiO-66 and attempted linker exchange with 2,5 - thiophenedicarboxylic acid were successful. The next step is then to prove that this new linker is able to give UiO-66 the capabilities of water purification. To do so, further research will need to be conducted by running the thiophene linked MOF through a lead test to determine whether this new linker possesses the capability of storing metal cations. If this test is successful, this MOF will have the potential to reach the ultimate goal of becoming a new method of water purification.

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