Synthesis of UiO-66 Metal Organic Frameworks
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Introduction
- Metal organic frameworks are composed of a regular array of positively charged metal ions surrounded by organic molecules called linkers. The metal ions act as nodes which bind the linkers together. The structure of a MOF is hollow, which results in a large internal surface area.
- MOFs are currently being studied for CO\textsubscript{2} capture based on its structure, stability, selectivity, and excellent adsorption capacity. In an industrial environment with several other gases, these characteristics make MOFs a viable option.
- Two MOF candidates were synthesized and analyzed: one established for over a decade, UiO-66, and UiO-66-SO\textsubscript{3}H, a newer MOF with minimal research for CO\textsubscript{2} capture.

Experimental
- UiO-66 was synthesized by dissolving equimolar amounts of ZrCl\textsubscript{4} and terephthalic acid in dimethylformamide or DMF. This mixture was then heated for 24 hours at 120°C. The resulting solid was dissolved within DMF, centrifuged several times, and dried overnight in a vacuum oven at 90°C.
- UiO-66-SO\textsubscript{3}H was synthesized by mixing ZrCl\textsubscript{4} and 2-sulfoterephthalic acid where both of which were previously dissolved in DMF. 1 mL of acetic acid was added, and the mixture was placed into an autoclave and heated at 120°C for 40 hours. The precipitate was then centrifuged within DMF twice and methanol once, and placed in a vacuum oven overnight at 100°C.
- The final product: UiO-66 is on the left and UiO-66-SO\textsubscript{3}H is on the right.

Results
- X-Ray Diffraction (XRD):
  - The XRD data for UiO-66 and UiO-66-SO\textsubscript{3}H was measured between 5° and 70° at a rate of .5° min.
  - The peaks measured are consistent with the literature values, and the similarity of the first two peaks demonstrate that UiO-66-SO\textsubscript{3}H is crystalline and maintained the UiO-66 structure.

Density Functional Theory (DFT)
- The tabular data is derived from DFT, an analysis method based on molecular modeling, and provides accurate values for microporous materials, the material type of the MOFs.

Conclusions
- UiO-66 and UiO-66-SO\textsubscript{3}H were successfully synthesized.
- The significant reduction in surface area and pore volume is plausibly due to the sulfination of UiO-66.

Future Research
- Varying the molar ratio of acetic acid to ZrCl\textsubscript{4} in the UiO-66-SO\textsubscript{3}H synthesis has yet to have been done, and its impact undetermined.
- This new UiO-66-SO\textsubscript{3}H could be superior in CO\textsubscript{2} capture applications, potentially due to improved adsorption capabilities from this change in the molar ratio.

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References