

Small Agents to Direct Improved MOF Structures

Scientific Achievement

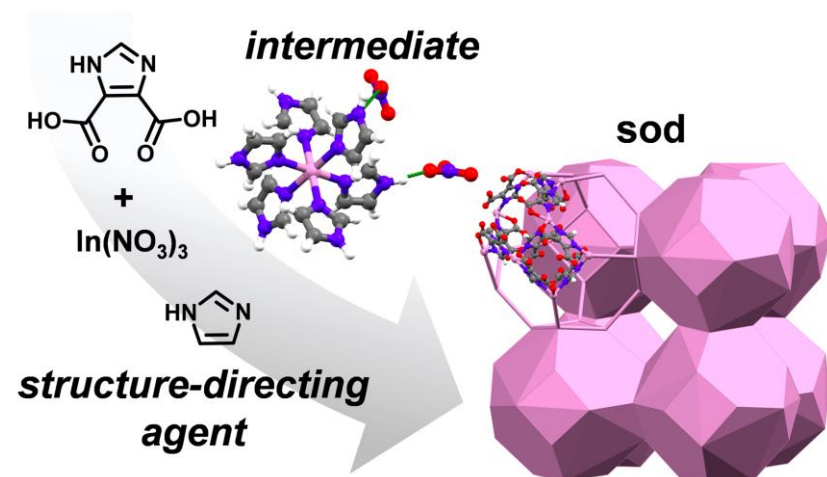
Scientists revealed that structure-directing agents (SDAs) influence the structure formation during the synthesis of a metal organic framework (MOF).

Significance and Impact

Customized MOFs are used for gas separation and catalysis; understanding how SDAs direct MOF formation will allow for more rational and straightforward design of MOFs.

Research Details

- In situ X-ray diffraction and small-angle X-ray scattering revealed formation of a molecular intermediate composed of the SDA and metal salt during the reaction.
- The intermediate persisted in both solid and liquid phases, confirming it is integral to MOF formation despite its absence in the final MOF structure.
- In situ x-ray diffraction was performed at the XPD beamline at NSLS-II.



A structure-directing agent reacts with indium nitrate, $\text{In}(\text{NO}_3)_3$, to generate a key molecular intermediate that directs the formation of a 3-D sodalite (sod) structured framework material.

Sinnwell MA, Miller QRS, Palys L, Barpaga D, Liu L, Bowden ME, Han Y, Ghose S, Sushko ML, Schaefer HT, Xu W, Nyman M, Thallapally PK. *J Am Chem Soc.* **142**, 17598–17606 (2020).

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