Probing Metal Organic Frameworks with ^{17}O NMR at 35.2 T

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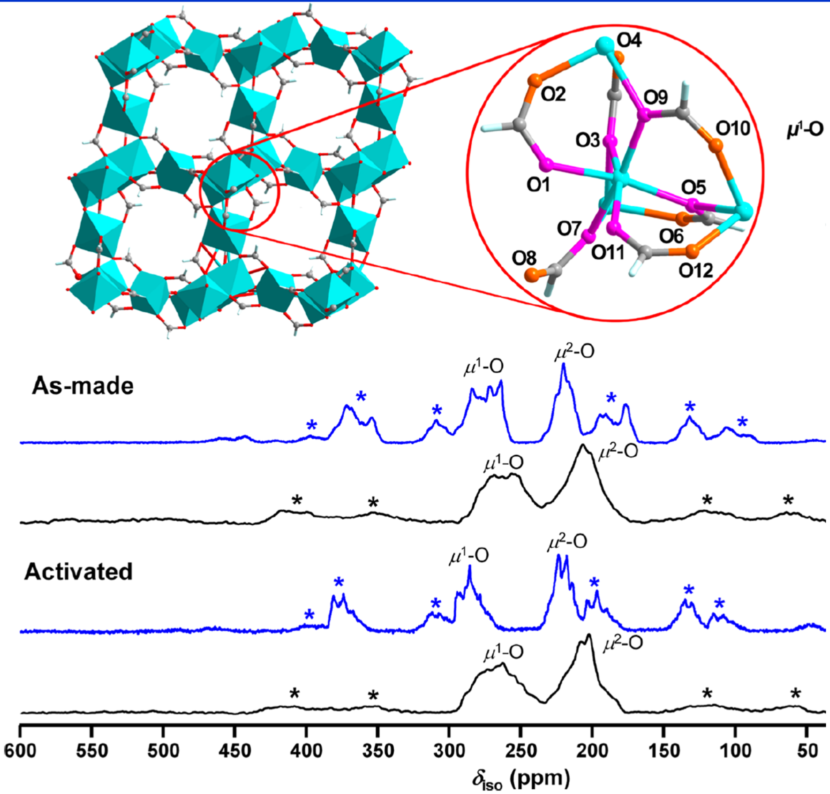
Metal-organic frameworks (MOFs) are a new generation of porous materials prepared via self-assembly of metal ions and organic linkers. MOFs have the properties of high thermal stability, permanent porosity, framework flexibility, and exceptionally high surface areas. *MOFs promise many potential applications in catalysis, drug delivery, chemical separation, gas adsorption and storage, fuel cells, and even, potentially, classical and quantum data storage*.

Solid-state nuclear magnetic resonance (NMR) of oxygen and metal atoms can typically determine the molecular structure of MOFs as well as the interactions between the MOFs and guest molecules like hydrogen, carbon dioxide and methane. *Oxygen-17 (^{17}O) NMR can help to identify the different types of oxygen sites in the framework; however, ^{17}O is a challenge for NMR* because it (i) has low natural abundance, (ii) low NMR frequency, and (iii) broad spectral lines from its quadrupolar interaction.

The MagLab's series-connected hybrid (SCH) magnet dramatically enhances ^{17}O NMR signal and spectral resolution…more than any other spectrometer in the world. This allows for the resolution of 12 unique oxygen sites in a α-$Mg_3(HCOO)_6$ MOF, including the observation of structural differences between as-made and activated (solvent removed) phases of this MOF.



(top) The α-$Mg_3(HCOO)_6$ metal-organic framework that contains twelve unique oxygen sites. **(bottom)** Oxygen-17 Magic Angle Spinning NMR spectra at 35.2 T (in blue) and at 21.1T (in black). *Note that the twelve unique oxygen sites (asterisks) are only resolved in the MagLab's unique 35.2T Series Connected Hybrid Magnet.*

Facilities and instrumentation used: NMR/MRI facilities and the 35.2T Series Connected Hybrid

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