

## Poster Presentation

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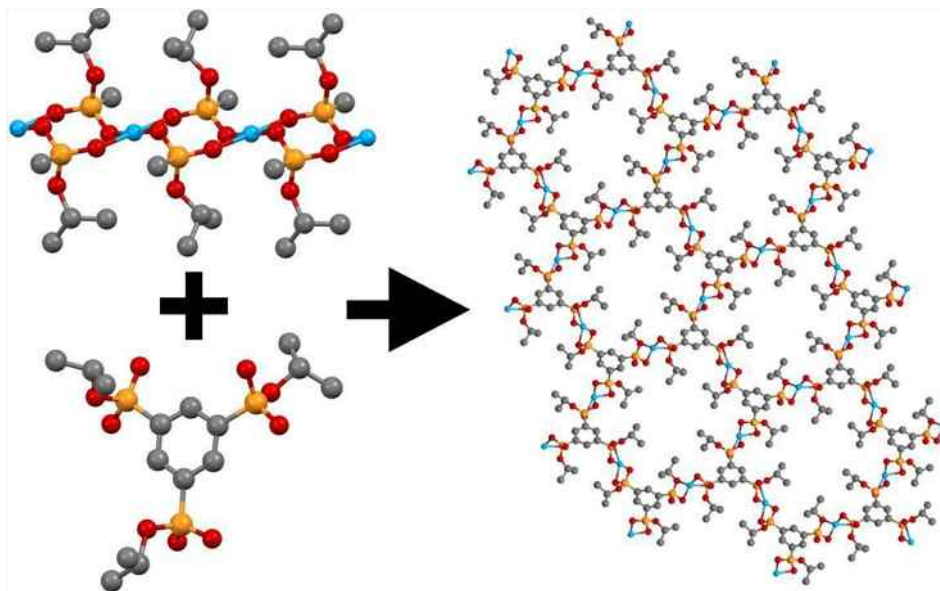
### Development of Phosphonate Monoesters Building Units in Metal-Organic Frameworks

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The use of predictable coordination geometries and the development of new ligands has allowed supramolecular chemists to design a plethora of new materials. Among these are metal-organic frameworks (MOFs), which are composed of ligands coordinating to metal atoms or clusters to generate a framework with potential porosity. MOFs exemplify supramolecular design strategy as their extended structure and tunable properties allow them to be applied for various applications.<sup>1</sup> To date, many MOFs utilize carboxylates as the coordinating group since they have well studied coordination geometries and thus predictable framework topologies. Though there are examples of carboxylate-based MOFs possessing water stability, most do not possess this key feature, hindering their application in industrial settings. Phosphonate monoesters (PMEs) have been investigated as a means to impart water stability to a MOF by kinetically shielding the linker-metal bond with the ester moiety.<sup>2</sup> Unfortunately, phosphonate monoesters have relatively unexplored coordination geometries, with most studies focusing on chloridronic acid and its derivatives, which do not typically form porous materials. In an attempt to establish building units based on PMEs, 1,4-benzenediphosphonate monoester ligands have been synthesized, coordinated to Cu(II), and characterized. It was found that while the methyl and ethyl analogues form similar 3-D structures with poor water stability,<sup>3</sup> the isopropyl analogue forms a layered material possessing water stability. The isopropyl analogue contains chains of Cu-PME, with the isopropyl esters lying directly above and below the Cu atoms, kinetically shielding this bond from water. This water stable building unit was predicted to generate a porous framework with non-linear ligands. To test this hypothesis, 1,3,5-benzenetriphosphonate monoisopropyl ester was synthesized and coordinated to Cu(II). Unfortunately, no single crystal of sufficient quality has been produced, though a predicted and refined structure matches well to various characterization techniques. As predicted, this material is porous and does not degrade in harsh humid conditions (353K and 90% relative humidity).

[1] Yaghi O., O'Keeffe M., Ockwig N. W., et al., *J. Nature* 2003, 423, 705., [2] Taylor J. M., Vaidhyanathan R., Iremonger S. S., et al., *J. Am. Chem. Soc.* 2012, 134, 14338., [3] Iremonger S. S., Liang J., Vaidhyanathan R., et al., *J. Am. Chem. Soc.* 2011, 133, 20048.



**Keywords:** phosphonate monoester, frameworks, MOFs