

MOF functionalization via solvent-assisted ligand incorporation: phosphonates vs carboxylates.

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Solvent-assisted ligand incorporation (SALI) is useful for functionalizing the channels of metal–organic framework (MOF) materials such as NU-1000 that offer substitutionally labile zirconium(IV) coordination sites for nonbridging ligands. Each of the 30 or so previous examples relied upon coordination of a carboxylate ligand to achieve incorporation. Here we show that, with appropriate attention to ligand/node stoichiometry, SALI can also be achieved with phosphonate-terminated ligands. Consistent with stronger M(IV) coordination of phosphonates versus carboxylates, this change extends the pH range for retention of incorporated ligands. The difference in coordination strength can be exploited to achieve stepwise incorporation of pairs of ligands—specifically, phosphonates species followed by carboxylate species—without danger of displacement of the first ligand type by the second. Diffuse reflectance infrared Fourier-transform spectroscopy suggests that the phosphonate ligands are connected to the MOF node as $\text{RPO}_2(\text{OH})^-$ species in a moiety that leaves a base-accessible $-\text{OH}$ moiety on each bound phosphonate.

Adres publiczny

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<https://www.acs.org/content/acs/en.html>

