The Fifth Phase of Cu-mip

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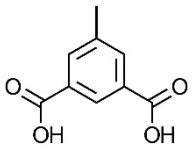
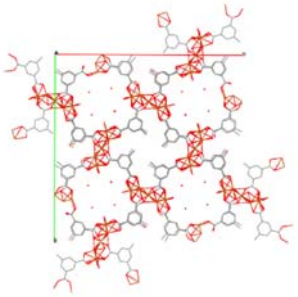
A fifth[1] phase of Cu-5-methylisophthalate (H_2mip shown below left) has been identified, with tetragonal unit cell dimensions a = 34.5 Å, c = 10.9 Å. For lovely crystals with clean diffraction patterns, the composition of the structural solutions are not clear. Several datasets have been collected on crystals from multiple batches, and all show the same connectivity (below right), however, the refinements are unsatisfactory and the precise space group and composition remain elusive.

What haven't I tried? Is this worth pursuing further? Would you publish this?





[1] a) T.-H. Chen, L. Wang, J. V. Trueblood, V. H. Grassian, S. M. Cohen, *J. Am. Chem. Soc.*, 2016, **138**, 9646; b) R.-Q. Zou, H. Sakurai, S. Han, R.-Q. Zhong, Q. Xu, *J. Am. Chem. Soc.*, 2007, **129**, 8402; c) Authors' own unpublished work