MS30 Advanced porous materials : MOFs, COFs, SOFs....and what else?

MS30-05

Dynamic Behaviour of a Tetrapyridine-Based Crystalline Supramolecular Organic Framework

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Abstract

In recent years, supramolecular organic frameworks (SOFs) have emerged as an important class of functional porous materials, alongside metal-organic frameworks (MOFs) and covalent organic frameworks (MOFs)[1-2]. Herein we report a dynamic responsive SOF obtained through the self-assembly of rigid aromatic tetrahedral molecules (tetra-4-(4-pyridil)phenylmethane, **TPPM**) *via* van der Waals interaction and non-conventional hydrogen bonds. It presents a responsive behaviour, in its crystalline form, based on the reversible switch from an empty to a filled phase framework and *vice-versa*, when exposed to specific organic solvents vapours and heat, respectively.

The phase transition between filled and empty phase goes through a single-crystal to single-crystal path, despite that after the solvent removal the obtained phase presents high defectivity and nanometric crystalline domains. The Empty phase single crystals were too small and defective to be characterized by standard X-ray diffraction experiments. Their crystal structure could be determined only by 3D electron diffraction (3D ED)[3-4] working in low dose mode with a parallel nanobeam of 150 nm in size, which matches perfectly with the grain size of the compound. The structural model obtained ab-initio by 3D ED was also refined taking into account dynamical scattering to a final R-value of 13%, with thermal parameters that mimic the rotational flexibility of the biarylic wings.

References

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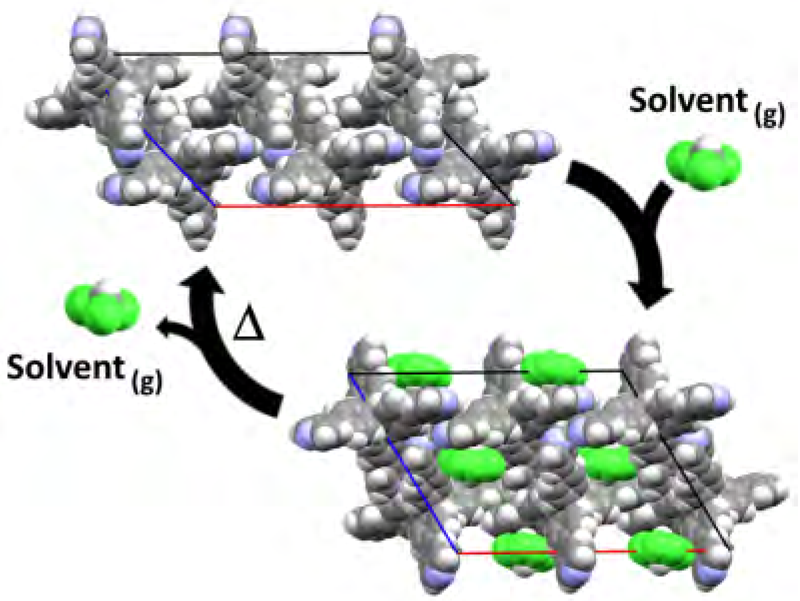
Dynamic Behaviour of the proposed SOF



3D ED Reciprocal Space Reconstruction