

A new class of thermo- and solvatochromic metal–organic frameworks based on 4-(pyridin-4-yl)benzoic acid

Abstract

Using 4-(pyridin-4-yl)benzoic acid, 44pba (**1**) as a ligand, two new metal-coordination networks $[\text{Co}_4(44\text{pba})_8]_n \cdot [(\text{DMF})_3 \cdot (\text{EtOH})_{0.25} \cdot (\text{H}_2\text{O})_4]_n$ (**2**) and $[\text{Ni}_4(44\text{pba})_8]_n \cdot [(\text{DMF})_{3.5} \cdot (\text{EtOH}) \cdot (\text{H}_2\text{O})_{1.5}]_n$ (**3**) were synthesized by solvothermal methods and structurally characterized. Compounds **2** and **3** are isostructural but differ in their solvent content. Each is a 2D-network which forms a spiral parallel to [001], giving rise to three distinct large channels, accounting for some 47% of the unit cell volume. Both **2** and **3** display water-induced phase transformations with chromotropism, which has been confirmed by TGA and XRPD analysis. Solvatochromism in **2** is also evident with crystals exhibiting a range of colours depending on the solvent included. This phenomenon has been characterized using TGA, XRPD and UV-vis spectrophotometry.