The supramolecular behavior of the polycatenated double-layer coordination polymer [Cd2(isonicotinate)4(pab)(H2O)] n (pab = 1,4-di-4-pyridyl-2,3-diaza-1,3-butadiene)

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The reaction mixture of pab and isonicotinate ligands with cadmium(II) nitrate under hydrothermal conditions generates a novel three-dimensional catenate framework, namely [Cd2(isonicotinate)4(pab) (H2O)]n (1) (pab = 1,4-di-4-pyridyl-2,3-diaza-1,3- butadiene). Single crystal X-ray diffraction shows that 1 possesses 2D bi-layer grids which are linked by pab pillars to give cuboidal subunits. The 2D bilayers are stacked and then concatenated to each other to form the 3D supramolecular framework. The most important interactions between the stacked layers involve the pivotal action of the water molecules through the formation of OH(water)/O(isonicotinate) H-bonds. Likewise, the concatenation produces strong H-bonding interactions that connect the entangled bilayers by using the non-aromatic CH groups of the pab pillar to give the CH(pab)/O(isonicotinate, water) arrangement. This supramolecular behavior of 1 is different from those observed in already known related cadmium complexes having