Why does the 2,2'-bipyridine-4-methyl-3,3'-dicarboxylic acid not form MOFs: synthesis, crystal structure and properties of a new organic ligand.

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Streszczenie

2,2′-Bipyridine-4-methyl-3,3′-dicarboxylic acid monohydrate (**1**) is introduced as a new organic ligand. Synthesis, structure and properties (TGA, IR, NMR) are characterized. **1** includes an extensive hydrogen bonding network with formation of various graph-set motifs, such as R 2 2 (18) R22(18) or R 10 12 (40) R1210(40) . In contrast to the related compounds, **1** does not participate in formation of MOFs. This is rationalized based on DFT calculations showing that the most plausible conformations of **1** do not favour coordination of a metal ion.

Słowa kluczowe

single crystal structure analysis, organic ligands, x-ray diffraction, hydrogen bonding

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