

Chains, layers, channels, and more: supramolecular chemistry of potent diphosphonic tectons with tuned flexibility. The generation of pseudopolymorphs, polymorphs, and adducts.

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Streszczenie

Naphthalene-1,5-diphosphonic acid [$C_{10}H_6(PO_3H_2)_2$, $H_4NDP(1,5)$, **1**] and its more flexible counterpart, naphthalene-1,5-bis(methylphosphonic) acid [$C_{10}H_6(CH_2PO_3H_2)_2$, $H_4NDP(1C,5C)$, **2**], have been synthesized, characterized, and used as building blocks in supramolecular assemblies with 4-(*N,N*-dimethylamino)pyridine (DMAP) and morpholine. The two acids generate two distinct solvatomorphs each, with and without dimethyl sulfoxide (DMSO) molecules. The two adducts of $H_4NDP(1,5)$ with DMAP (**3A** and **3B**) reveal conformational polymorphism caused by the rotation of phosphonic groups. The two adducts of $H_4NDP(1C,5C)$ show unexpected structural diversity, generating a symmetric hydrogen bond and creating a layered structure, **4A**, or a channel structure, **4B**. The adducts of both acids with morpholine (**5A** and **5B**) allow for observing the influence of the conformational flexibility of the acids on the dimensionality of a final hydrogen bond network, which is in general higher for $H_4NDP(1C,5C)$. The structural motifs and trends are analyzed in terms of the geometric criteria of these interactions. For the first time, Hirshfeld surface analysis has also been applied for the investigation of supramolecular interactions of phosphonic acids in different protonation states.

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