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The solid-state structures of organic salts formed by calix[4]arene dihydroxyphosphonic acid with nucleic bases cations: adeninium, cytosinium, guaninium and uracilium

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Abstract

© 2018 Informa UK Limited, trading as Taylor & Francis Group. Calix[4]arene dihydroxyphosphonic acid has been demonstrated to possess an interesting range of biological properties, including atypical anti-cancer activity. The robustness of calix[4]arene dihydroxyphosphonic acid and its ubiquitous dimeric motif offers perspectives for pre-defined solid state complexation with small molecules. In the current article we describe co-crystals (organic salts) of calix[4]arene dihydroxyphosphonic acid with four nucleic base cations: adeninium, cytosinium, guaninium and uracilium. A number of characteristic interactions between the components in the four co-crystals are pointed out also using the Hirshfeld surface analysis. All the four co-crystals are based on layers of calix[4]arene dimers, alternating with layers of nucleic acid molecules. Two of the reported crystal structures (cytosinium and guaninium) are 1D channel-type structures, while the two others (adeninium and uracilium) represent 2D channel-type structures. In three out of four reported structures, interactions between the cations of nucleic bases are present generating 1D chains of cations. A constant motif is that the nucleic base is present in a type of cavity formed by one aromatic ring and a phosphonic acid moiety.

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Keywords

Calix[4]arene, co-crystal, Hirshfeld surface analysis, nucleic bases, X-ray analysis

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