Topologic features of Three Structures Based on I…Base Halogen Bonding

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The halogen bonding, that is the $n \rightarrow \sigma^*$ electron donation from Lewis bases to halogen atoms (Lewis acids) is an interaction that has attracted an increasing attention, especially in haloperfluorocarbons were the heavy halogen atom (I, Br) is highly polarized¹. We have recently studied the three component structure of the cryptate K.2.2.2 with KI and 1,8-diiodo-perfluorocatane showing a very unusual borromean assembly of the superanion². We present here other three halogen-bonded supra-molecular arrays showing unusual topologic features: the assembly of tetra(4-pyridyl)pentaerythritol . 1,4-diiodo-octafluorobutane 1, tetra(4-pyridyl)pentaerythritol . 1,8-diiodo-hexadecafluorooctane 2, and tetra(4-pyridyl)pentaerythritol . tetra(4-iodo-tetrafluorophenyl)pentaerythritol 3. The three structures present macrocyclic interpenetrate assembly. 1, 2, 3 show 2D 5-fold 4⁴ layers, 8-fold diamondoid class IIIa topologies, respectively.

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