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Design and Serendipity in the Construction of a Non-centrosymmetric Network Through π - π Interactions.

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The design and synthesis of non-centrosymmetric crystals is a difficult but important challenge in crystal engineering, due to their potential physical properties. We have used as strategy the design of non-centrosymmetric 2D networks organized through directional π - π interactions. To achieve this directionality we have used an organic molecule with two phenyl rings one of them being pentafluorinated, 5Fph, and a step (imidazol) as a geometric restriction to favor non-centrosymmetry interactions between the ph and the 5Fph rings. The 2D layers organize into a non-centrosymmetric 3D structure due to



ionic repulsions. The details of the above mentioned strategy as well as the crystal structure of the 1-benzyl-3-(2,3,4,5,6-pentafluorobenzyl)-1*H*-imidazolium bromide will be discussed.