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## Halogen bonded polypseudorotaxanes based on a pillar[5]arene host†

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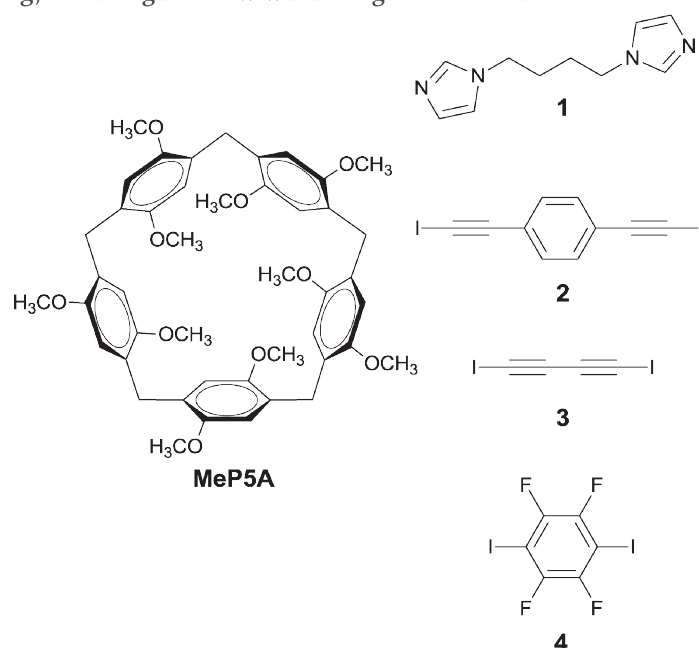
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Two crystalline supramolecular polypseudorotaxanes were obtained by combining permethylated pillar[5]arene as a macrocyclic wheel with 1,4-bis(1-imidazolyl)butane and 1,4-bis(iodoethynyl)benzene or 1,4-diiodo-1,3-butadiyne linked by C–I...N halogen bonds and creating a polyrotaxane axis. The resulting highly ordered supramolecular arrays were characterized by X-ray crystallography.

The synthesis of mechanically interlocked catenane and rotaxane assemblies has become a recent challenge in supramolecular chemistry not only for their unique structures but also due to their potential applications as molecular devices and functional materials.<sup>1,2</sup> Among numerous interlocked structures constructed and studied in last few decades, polymers comprising rotaxane units have attracted considerable attention in the fields of materials science and nanotechnology.<sup>2,3</sup> Polyrotaxanes and polypseudorotaxanes are constructed by threading macrocyclic rings, including cyclodextrins, crown ethers, cucurbiturils, calixarenes or pillararenes onto covalent type linear chains like polyethers, polyesters or polyamides, employing a variety of synthetic protocols. On the other hand, considerable efforts have been directed to the design of supramolecular polymers bearing rotaxane units self-assembled by highly directional and cooperative non-covalent interactions such as hydrogen bonding, host–guest interaction,  $\pi$ – $\pi$  stacking or metal–ligand coordination.<sup>3–8</sup> Due to the reversible, self-repairing and tunable nature of these interactions more advanced and useful

supramolecular structures can be obtained in a relatively simple way. However, the vast majority of these studies have been performed in solution, where the molecules are in a constant flux, and the degree of oligomerization and the structure of oligomers are strongly concentration dependent.<sup>3–6</sup> Despite the fact that for future applications materials with high and controllable structural regularity are required, there are very few well-characterized examples of crystalline polyrotaxanes including 1D, 2D and 3D arrays assembled by hydrogen bonding, metal–ligand or  $\pi$ – $\pi$  stacking interactions.<sup>8</sup>



In this paper, we report the synthesis and structural characterization of two crystalline supramolecular polypseudorotaxanes by combining permethylated pillar[5]arene (MeP5A) as a macrocyclic wheel with 1,4-bis(1-imidazolyl)butane (1) and 1,4-bis(iodoethynyl)benzene (2) or 1,4-diiodo-1,3-butadiyne (3) linked by halogen bonds and creating a polyrotaxane axis. Pillararenes, a new family of macrocyclic hosts, due to their symmetrical structure and rigid electron-rich cavity are ideal candidates as host molecules for the construction of rotaxanes or

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† Electronic supplementary information (ESI) available: Experimental details, geometry of halogen and hydrogen bonds and crystal structure of MeP5A-1-4<sub>2</sub>. CCDC 1465200, 1465201 and 1469513 contain the supplementary crystallographic data for this paper. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c6ce01416j