Electronic Supplementary Material (ESI) for Chemical Communications

Locking the free-rotation of a prochiral star-shaped guest molecule inside a two-dimensional nanoporous network by introduction of chlorine atoms.

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1. Lattice parameters measurements on drift-free STM images

As we sometime observe on our STM images of the TrisK networks, the 2D lattices progressively evolve from a regular to a slightly distorted hexagonal arrangement. Such a lattice distortion arises from thermal drift during data acquisition, as confirmed by the STM image of Fig. S1.

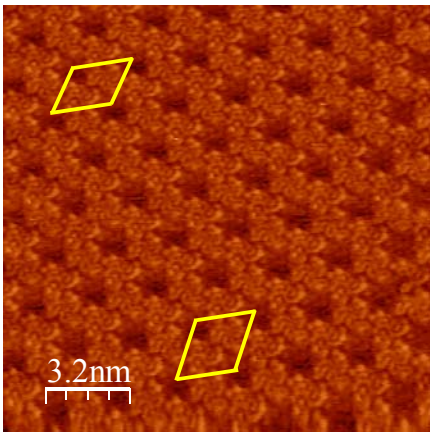

Fig. S1 Typical STM image (16×16 nm^2; V_s=+1.0 V; I_t=10 pA) of the empty honeycomb TrisK-3Cl network showing a vertical distortion of the 2D lattice due to thermal drift. The two rhombic unit cells materialized in yellow are substantially different in the upper (a=2.7 nm; b=1.9 nm; γ=57°) and the lower (a=2.7 nm; b=2.4 nm; γ=60°) part of image.

Therefore, in order to avoid any misinterpretation we perform the measurement of the (a,b,γ) lattice parameters on drift-free images such as in Fig. S2.

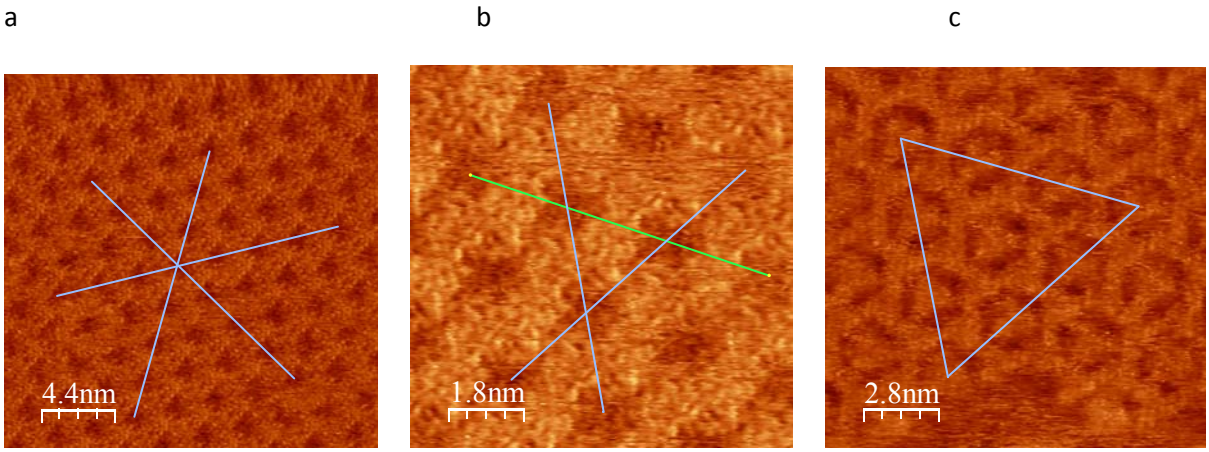

Fig. S2 (a,b) Drit-free STM images of the empty TrisK-3Cl network. The measured (a,b) lattice parameters are identical all over both images (a=b=24 Å; γ=60°). (c) Drift-free STM image of the filled TrisK-3Cl network and height profiles along the three blue lines showing that the hexagonal symmetry of the nanopores is regular and the lattice parameters of the rhombic cell are identical (a=b=29 Å; γ=60°).

2. Large scale model of the TrisK-3Cl filled network

For the sake of clarity in the model presented in Fig.3b of our article we deliberately omitted to draw the C3H7 chains of the TrisK-3Cl molecules. However, in order to discuss the possible interactions responsible for the locking of the central trapped molecule it is necessary to draw them. Therefore Fig.S3 is a large scale model showing that interactions can take place between the C3H7 chains of the trapped molecule and the inner atoms of the peripheral molecules constitutive of the cavities. These interactions may involve either steric hindrance and/or weak CH…Cl bonds between the H-atoms of the C3H7 chains and the Cl-atoms of the peripheral molecules.

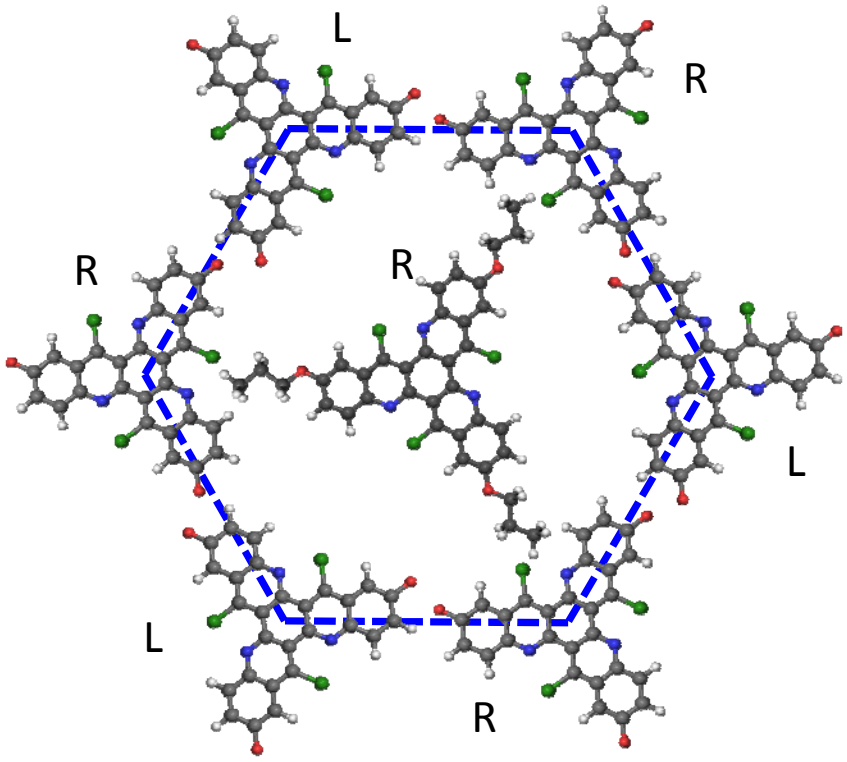

Fig. S3 Model of the hexagonal 2D molecular arrangement with alternate left (L) and right (R) handed TrisK-3Cl molecules (Cl-atoms are in green). The C3H7 chains of the trapped molecule are represented. The model shows the possible interactions between the C3H7 chains of the trapped molecule and the inner atoms (H and Cl) of the peripheral molecules.