

**MS30-2-7 Pillarplexes - Porous Organometallic Synthons in Crystal Engineering**  
**#MS30-2-7**

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**Abstract**

Pillarplexes[1] (Fig. 1A), supramolecular organometallic complexes (SOCs),[2] are self-assembled by two macrocyclic NHC ligands and eight coinage metal ions (AgI and AuI) and can act as tubular metallocavitands with remarkable properties (Fig. 1B): intrinsic photoluminescence, tunable solubility via anion exchange and shape-selective host abilities towards linear molecules. Furthermore, they can also be applied as building blocks in mechanically interlocked rotaxanes[2] (Fig. 1C) and show potential in the biological context.[3]The pillarplexes can also be potentially applied as synthons in crystal engineering. Hereby, a variety of non-covalent interactions can occur, ranging from hydrogen bonding, pi-stacking to metallophilic contacts (Fig. 2A).[4] Via chemical modification of the rim of the pillarplexes a higher flexibility can be introduced while preserving the porosity of the cavitand.[5] In detail, we were able to observe a shape-adaptive behaviour of the pillarplex in the solid state, mainly driven by hydrogen bonding. The modified rim of the pillarplexes induces less steric repulsion, resulting in a lower energy penalty upon compression as rationalized by DFT calculations.

**References**

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