Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Salt formation affects the conformational and assembly properties of *p*-carboxylatocalix[4]arenes

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Information included:

- Additional figures to aid discussion.
- Powder X-ray diffraction patterns (observed and calculated) for **7**.

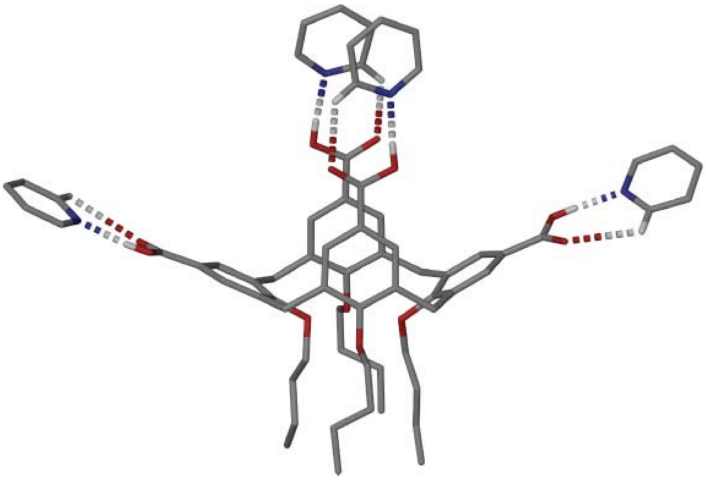

Figure S1. Formation of the Py···CO_2H heterosynthon between tetra-*O*-butoxy *p*CO_2[4] and pyridine. Note that the fully pinched-cone conformation is retained and the Py does not gain access to the potential cavity presented by the calixarene.

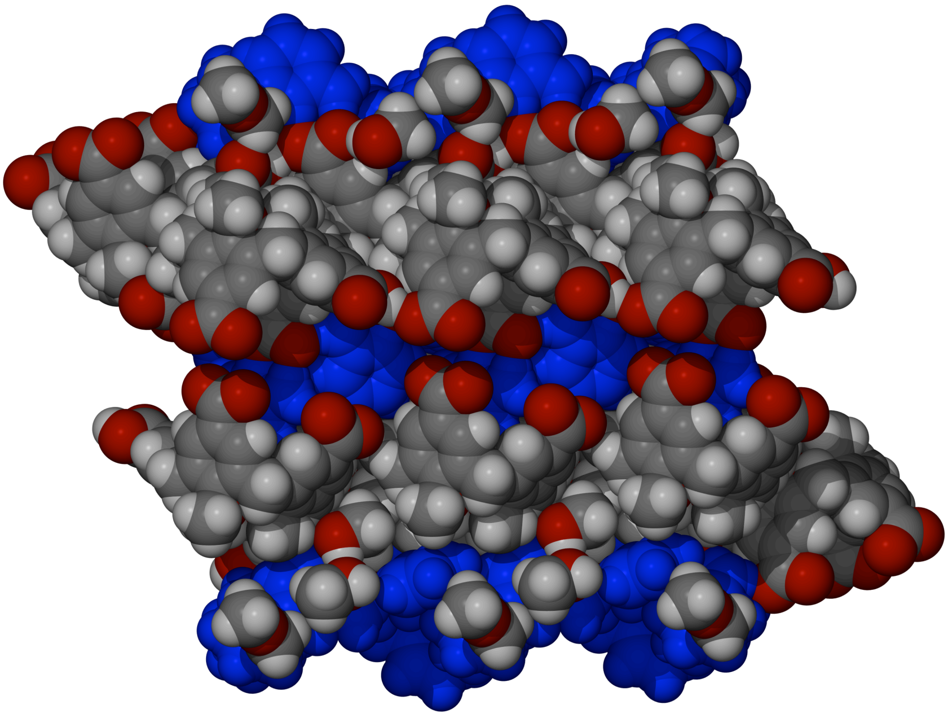

Figure S2. Space filling representation of the anti-parallel bi-layer packing motif found in the crystal structure of the salt formed between **1** and 2-AP (**5**). H2-AP cations are illustrated in blue, and in MeOH / **1** carbon atoms are shown in grey, oxygen atoms in red and hydrogen atoms in light grey.

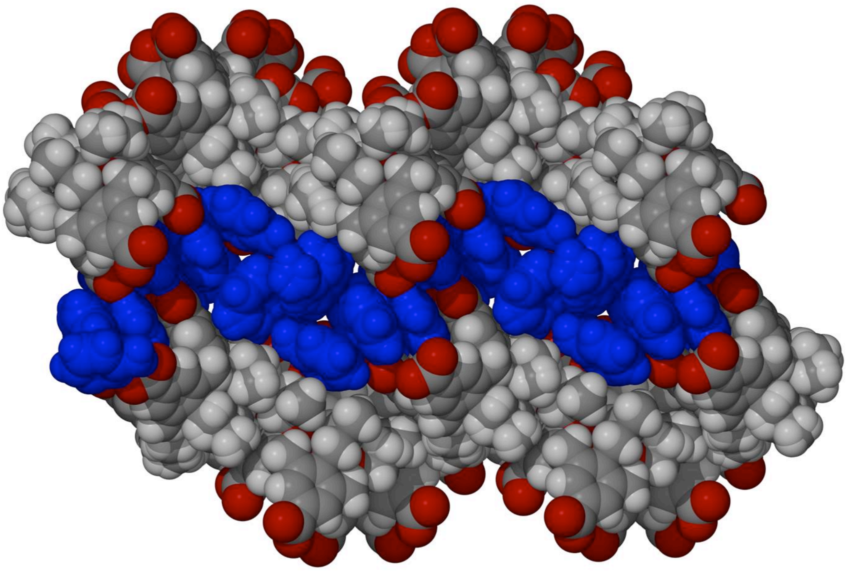

Figure S3. Space filling representation of the wave-like bi-layer motif found in the crystal structure of **6**. H2-AP cations are illustrated in blue. C, O and H atoms of the calixarenes are shown in grey, red and light grey respectively.

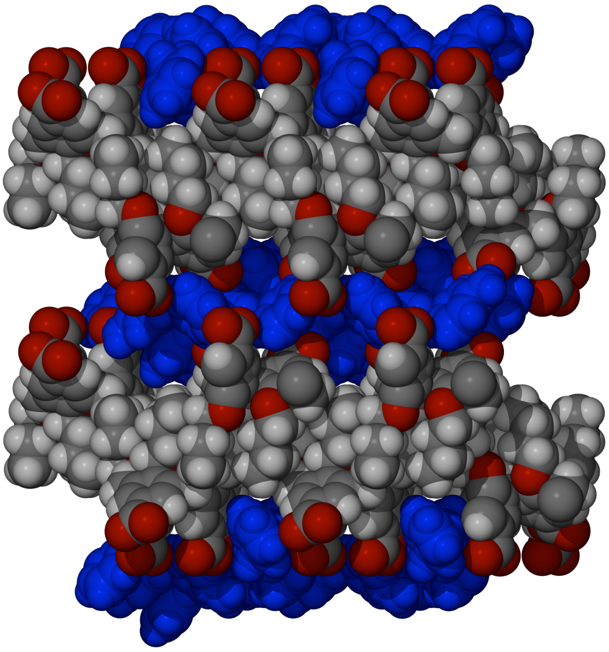

Figure S4. Space filling representation of the anti-parallel bi-layer array observed in the extended structure of **7**. H2-AP cations are illustrated in blue. C, O and H atoms of the calixarenes are shown in grey, red and light grey respectively.

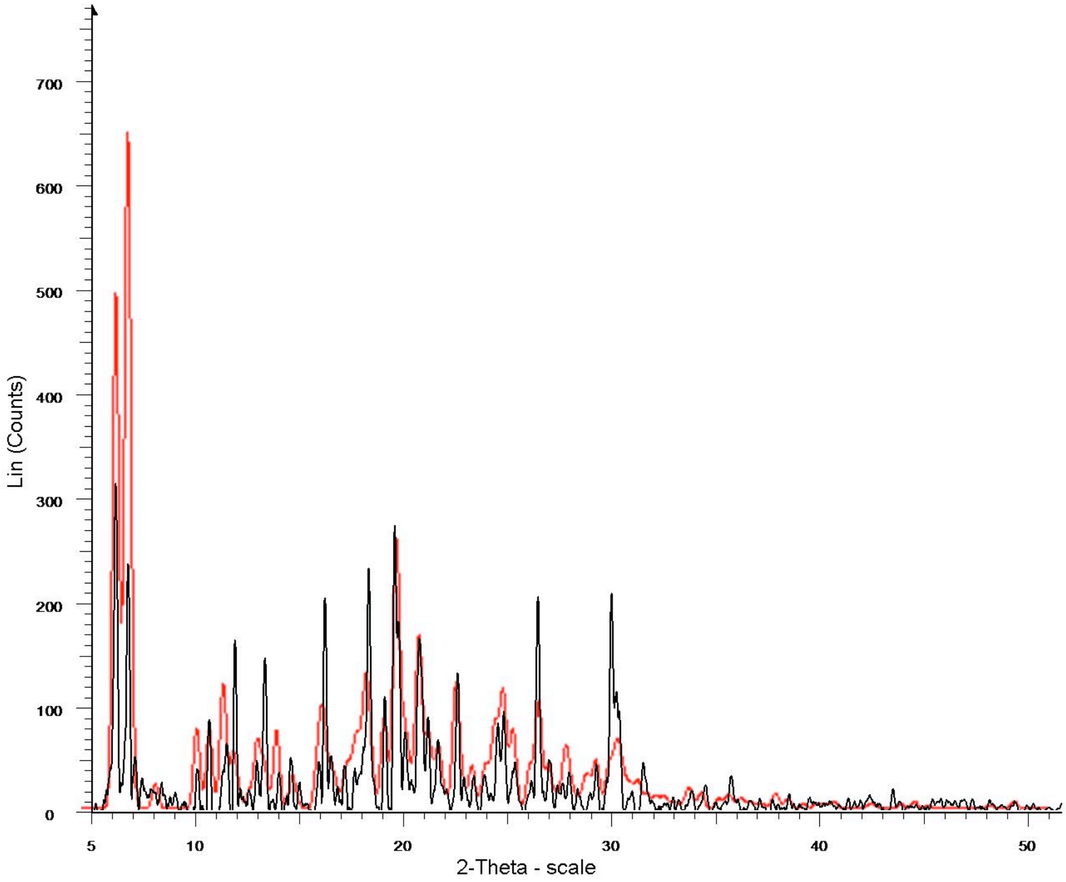

Figure S5. Overlay of experimental (black) and calculated (red, from single crystal structure) powder patterns for **7**.