

Supplementary Information

Coordination and supramolecular assemblies of Mono-hydroxylated octamethylcucurbit[6]uril with alkali and alkaline earth metal ions in the presence of polychloride cadmium anions
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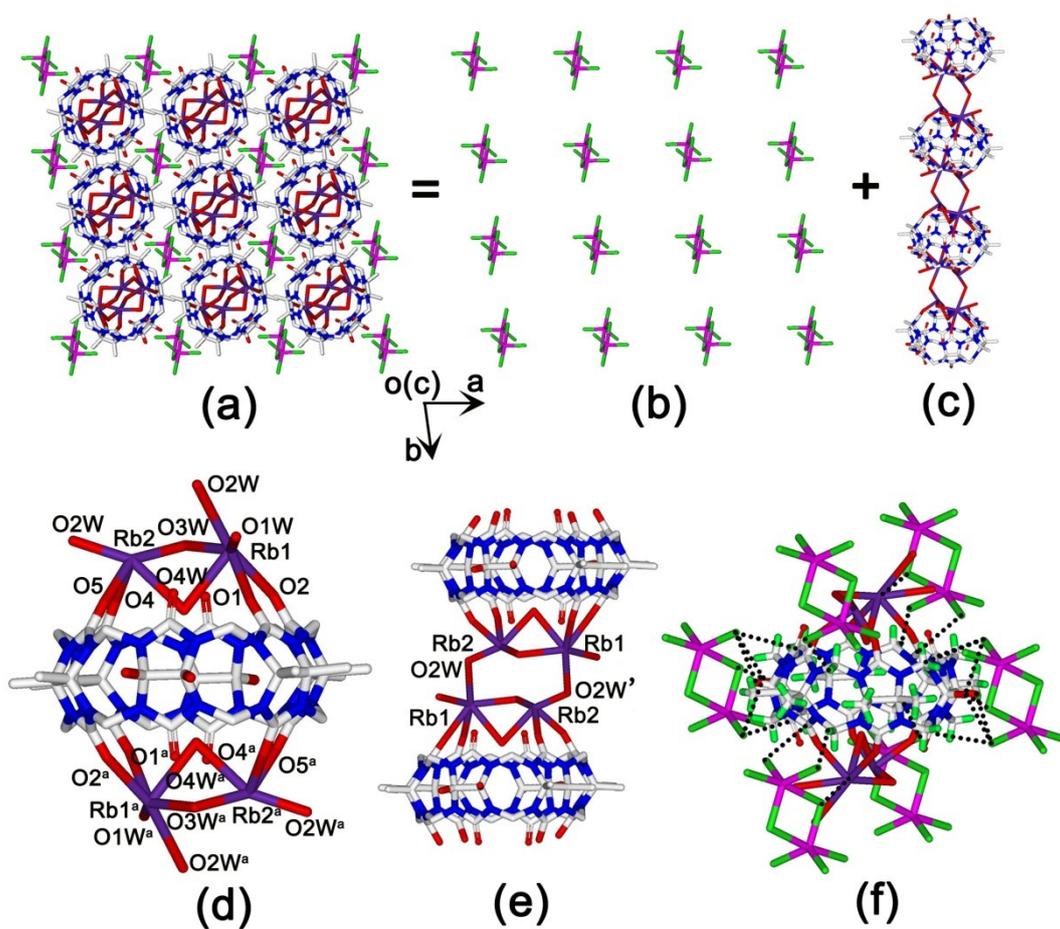


Figure S1. Crystal structure of **3**: (a) Overall view of the supramolecular assembly constructed of $[\text{Cd}_2\text{Cl}_8]^{4-}$ and $(\text{OH})\text{OMeQ}[6]/\text{Rb}^+$ complexes along the crystallographic c axis; (b) $[\text{Cd}_2\text{Cl}_8]^{4-}$ -based square grid-like framework along the crystallographic c axis; (c) an $(\text{OH})\text{OMeQ}[6]/\text{Rb}^+$ complex-based supramolecular chain linked by shared interaction with O2W molecules; (d) detailed interactions in an $(\text{OH})\text{OMeQ}[6]/\text{Rb}^+$ complex; (e) detailed interactions between two $(\text{OH})\text{OMeQ}[6]/\text{Rb}^+$ complexes; (f) interactions of an $(\text{OH})\text{OMeQ}[6]/\text{Na}^+$ complex with six $[\text{Cd}_2\text{Cl}_8]^{4-}$ anions.

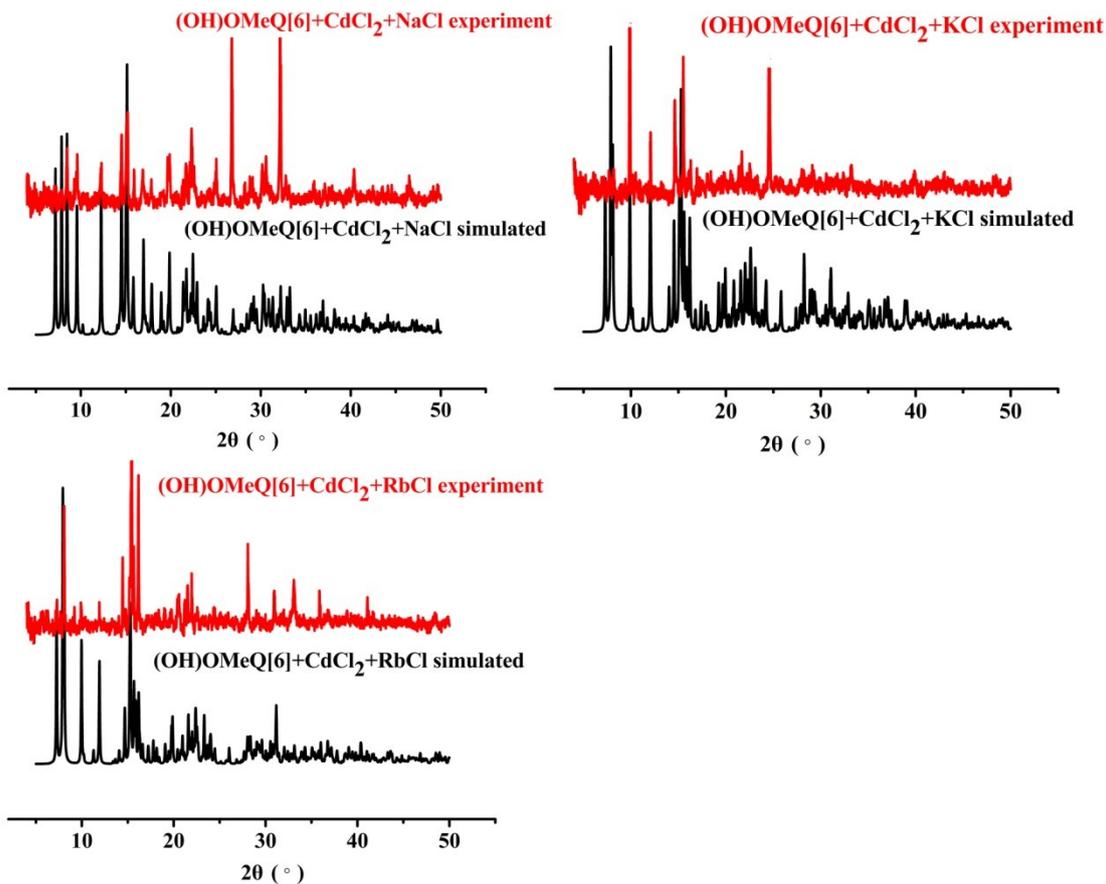


Figure S2. Powder X-ray diffraction (PXRD) patterns of crystals of 1–3 in comparison with the respective simulations.

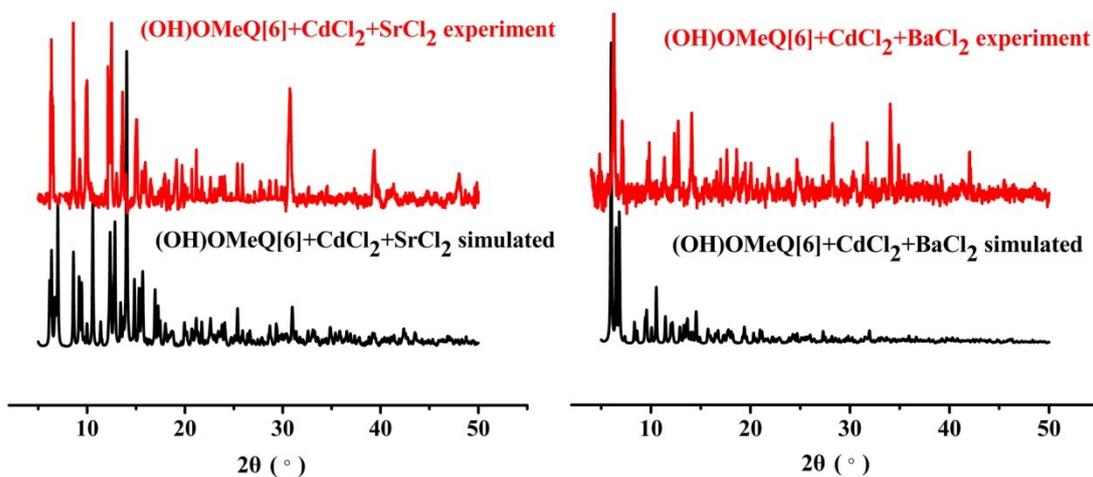


Figure S3. Powder X-ray diffraction (PXRD) patterns of crystals of compounds 4 and 5 in comparison with the respective simulations.