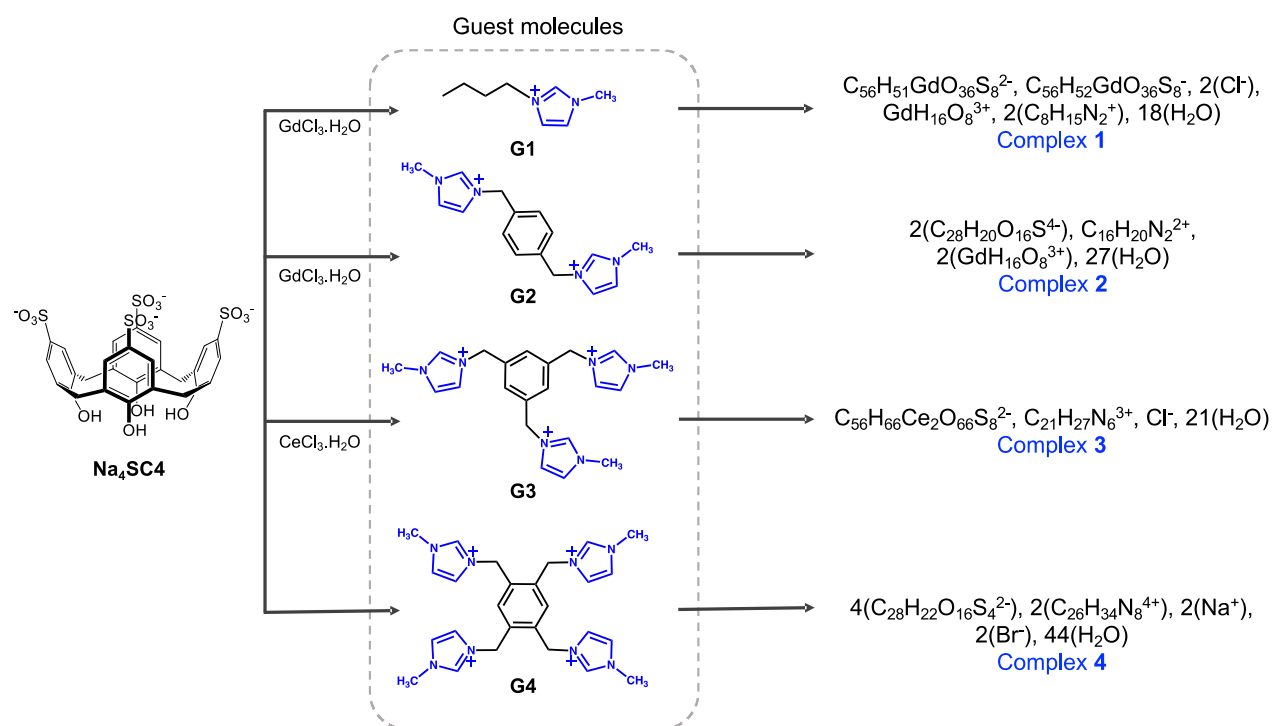


Supplementary Information

Hierarchical study of mono- and multicharged imidazolium encapsulation in *p*-sulfonatocalix[4]arene molecular capsule

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Scheme 1. Synthesis of inclusion complexes 1 to 4.

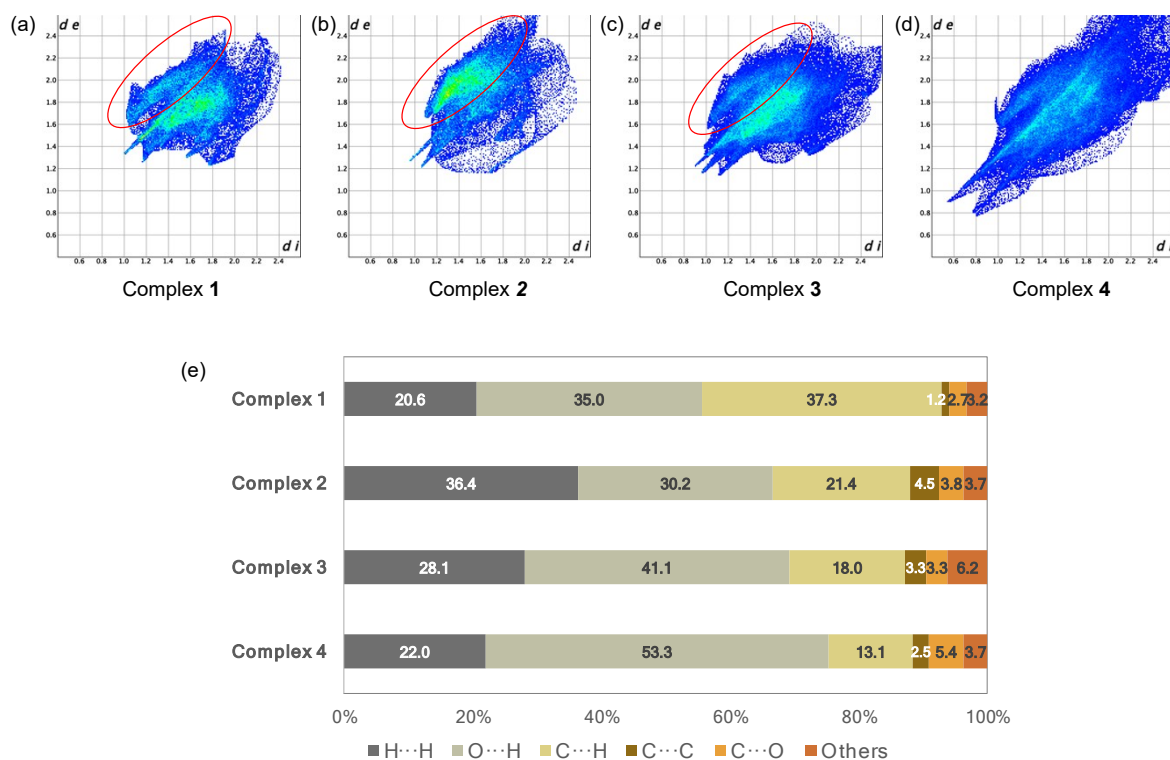


Figure S1. (a-d) Fingerprint plots generated from the Hirshfeld surfaces mapped on 1-butylimidazolium (G1), 3,3'-(1,4-phenylenebis(methylene))bis(1-methylimidazolium) (G2), 3,3',3''-(benzene-1,3,5-triyltris(methylene))tris(1-methylimidazolium) (G3), and 3,3',3''',3''''-(benzene-1,2,4,5-tetrayltetrakis(methylene))tetrakis(1-methylimidazolium) (G4) for complexes **1** to **4**. (e) Relative percentage contributions of different interactions (C–H...H–C, C–H...O, C–H...C, C...C, C...O and other minor contacts) to the overall cations' Hirshfeld surface.

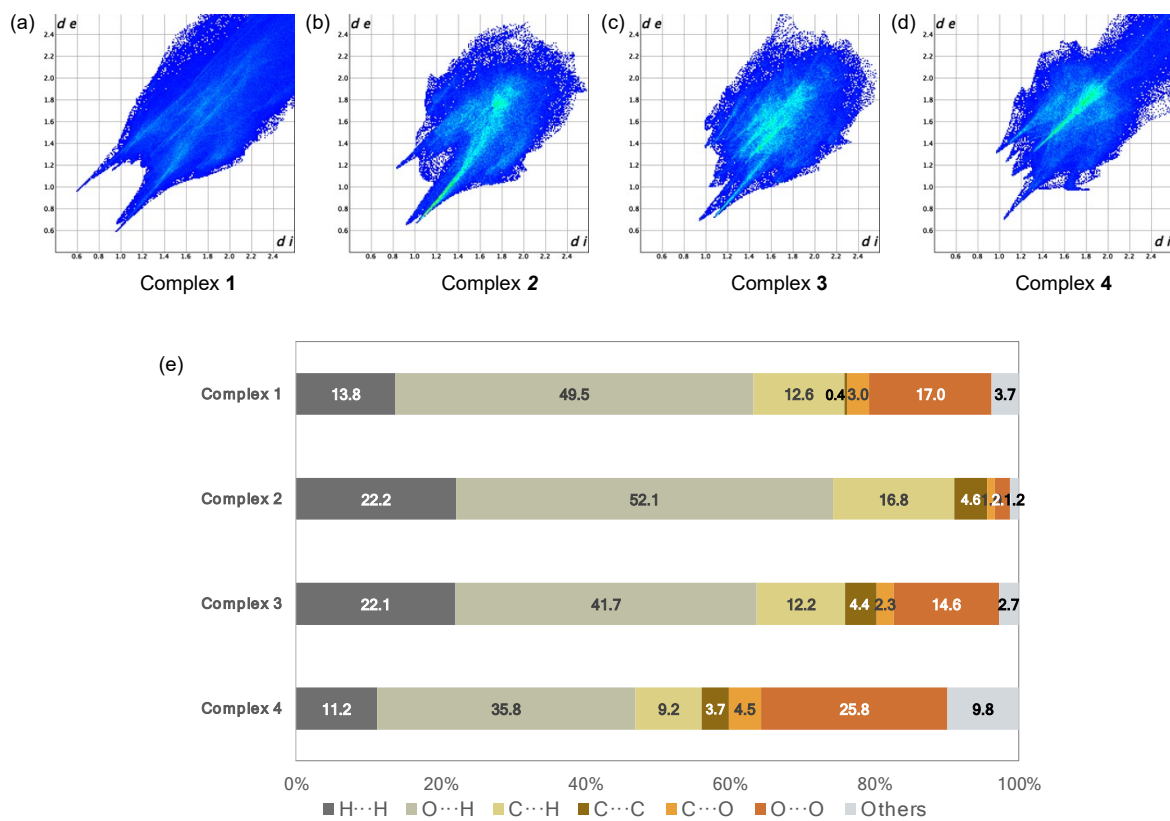


Figure S2. (a-d) Fingerprint plots generated from the Hirshfeld surfaces mapped on *p*-sulfonatocalix[4]arene (SC4) for complexes **1** to **4**. (e) Relative percentage contributions of different interactions (C–H...H–C, C–H...O, C–H...C, C...C, C...O, O...O and other minor contacts) to the overall SC4 Hirshfeld surface.