Electronic Supplementary Material (ESI) for RSC Advances.

Functional heterocyclic molecular inclusion in *p*-sulfonatocalix[5]arene and lanthanide(III) complexes

Irene ling,[*a] Alexandre N. Sobolev[b] and Colin L. Raston[*c]

Supporting Information

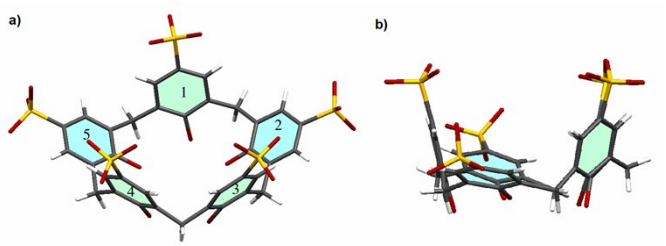

Figure S1. SC5 in all three complexes retains the cone conformation but differ in their splaying effect as judged by dihedral angles formed by aromatic rings and basal plane. (The numbering corresponds to the phenyl rings listed in Table S1 (Supporting Information)).

Table S1: Dihedral angles between the aryl plane and the basal plane of calixarene and lower rim O…O distances for complexes **1**, **2** and **3**.

Dihedral angles	Ring 1	Ring 2	Ring 3	Ring 4	Ring 5
Complex 1: Calix A	90.1(4)	31.4(5)	54.8(5)	74.0(4)	35.8(4)
Calix B	89.7(6)	33.1(4)	57.7(4)	74.5(4)	36.2(4)
Complex 2: Calix A	94.0(4)	34.6(3)	52.9(4)	73.0(4)	35.3(3)
Calix B	96.7(3)	34.4(3)	56.7(3)	76.2(3)	31.1(3)
Complex 3: Calix A	81.7(2)	31.3(2)	64.0(2)	73.3(2)	29.2(2)
Calix B	80.9(2)	30.5(2)	68.0(2)	67.1(2)	22.1(2)
Calix C	78.4(2)	31.3(4)	66.6(3)	67.9(3)	26.6(2)
Lower rim O…O distance	1	2	3	4	5
Complex 1: Calix A	2.75	3.65	2.90	3.47	2.89
Calix B	2.96	3.73	2.90	3.60	2.98
Complex 2: Calix A	2.76	3.75	2.81	3.61	2.88
Calix B	2.82	3.68	2.90	3.53	2.85
Complex 3: Calix A	2.77	3.54	2.92	3.43	3.20
Calix B	2.74	3.60	2.87	3.48	2.94
Calix C	2.73	3.42	2.90	3.35	3.08

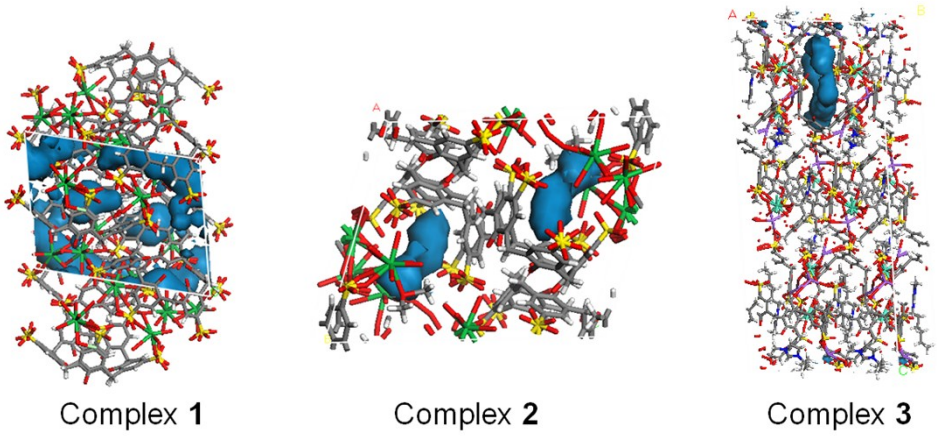

Figure S2. Internal volume calculated for complexes **1** (270 Å^3), **2** (285 Å^3) and **3** (312 Å^3).

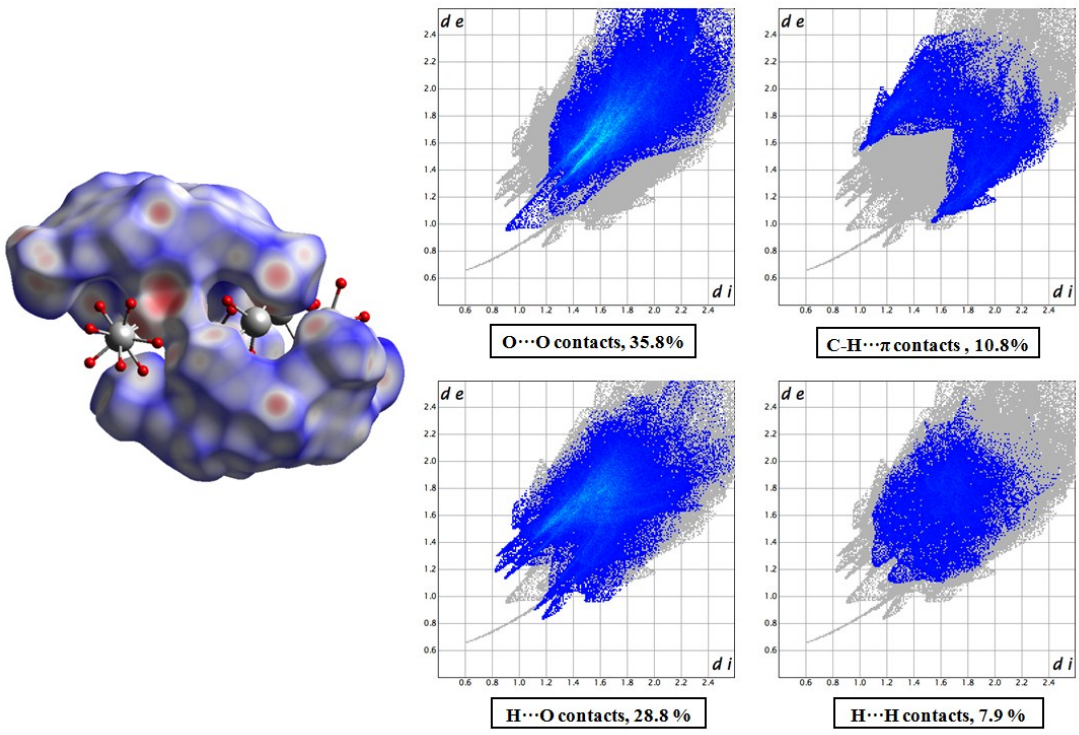

Figure S3. Hirshfeld surface for SC5 anions in complex **1** along with corresponding fingerprint plots showing all close intermolecular interactions (right).

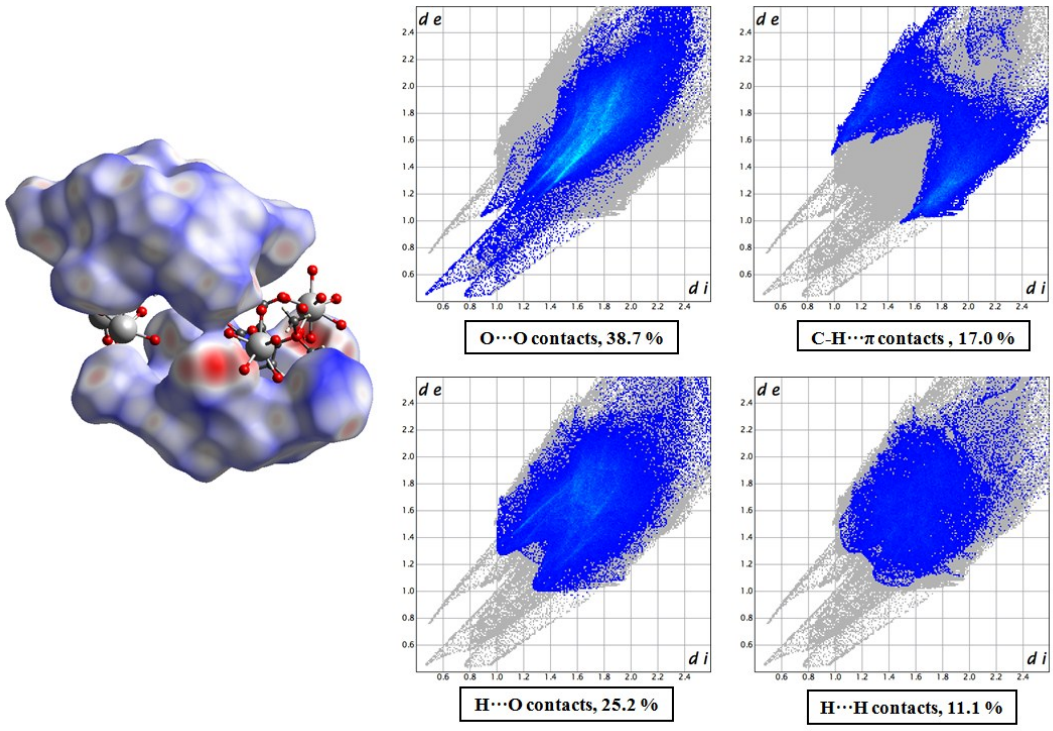

Figure S4. Hirshfeld surface for SC5 anions in complex **2** along with corresponding fingerprint plots showing all close intermolecular interactions (right).

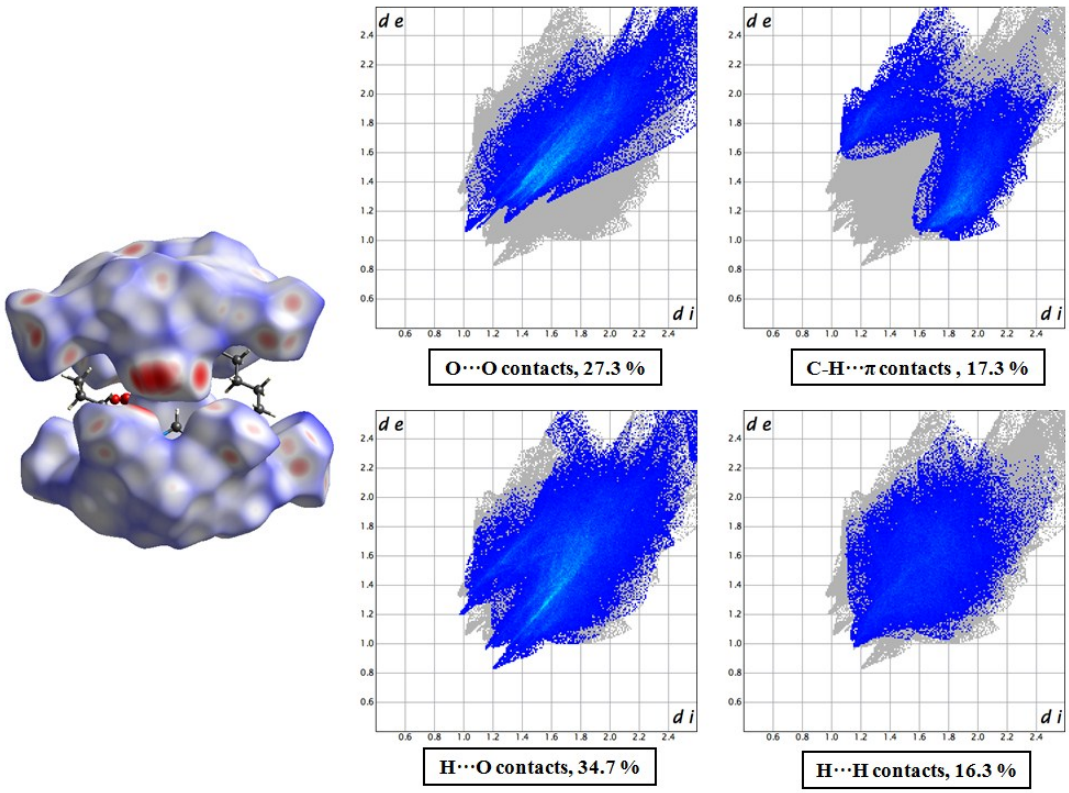

Figure S5. Hirshfeld surface for SC5 anions in complex **3** along with corresponding fingerprint plots showing all close intermolecular interactions (right).