Electronic Supplementary Information for Manuscript Entitled: Ionic Dimeric Pyrogallol[4]arene Capsules

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Information comprises:

- Selected tables of bond distances for **1·CsCl** and **2·CsCl**.
- Additional figures as outlined in the manuscript.

Table S1. Selected interatomic distances (Å) with s.u.s in parentheses for **1·CsCl**.

Cs(1)-O(10)$^{(a)}$	3.072(4)	Cs(1)-O(6)$^{(b)}$	3.098(4)
Cs(1)-O(12)	3.199(4)	Cs(1)-O(1)	3.207(4)
Cs(1)-N(1)	3.228(6)	Cs(1)-O(11)$^{(a)}$	3.286(4)
Cs(1)-O(13)	3.344(5)	Cs(1)-O(2)	3.354(4)
Cs(1)-O(14)	3.368(5)	Cs(1)-O(5)$^{(b)}$	3.393(4)
Cs(1)-Cl(2)	3.5732(19)	Cs(1)-C(2)	3.586(5)
O(5)-Cs(1)$^{(b)}$	3.393(4)	O(6)-Cs(1)$^{(b)}$	3.098(4)
O(10)-Cs(1)$^{(c)}$	3.072(4)	O(11)-Cs(1)$^{(c)}$	3.286(4)

Key giving operations for symmetry related atoms:

(a) 1-x, 1/2+y, 1/2-z
(b) 1-x, 1-y, 1-z
(c) 1-x, -1/2+y, 1/2-z

Table S2. Selected interatomic distances (Å) with s.u.s in parentheses for **2·CsCl**.

Cs(1)-O(11)$^{(a)}$	3.084(5)	Cs(1)-O(3)$^{(b)}$	3.132(6)
Cs(1)-O(2)$^{(b)}$	3.144(5)	Cs(1)-O(8)$^{(c)}$	3.245(6)
Cs(1)-O(6)$^{(d)}$	3.258(6)	Cs(1)-O(1)	3.392(6)
Cs(1)-Cl(1)	3.512(3)	Cs(1)-O(2)	3.567(6)
Cs(1)-O(7)$^{(c)}$	3.756(7)	Cs(1)-Cs(1)$^{(b)}$	5.687(3)
O(2)-Cs(1)$^{(b)}$	3.144(5)	O(3)-Cs(1)$^{(b)}$	3.132(6)
O(6)-Cs(1)$^{(d)}$	3.258(6)	O(7)-Cs(1)$^{(e)}$	3.756(7)
O(8)-Cs(1)$^{(e)}$	3.245(6)	O(11)-Cs(1)$^{(a)}$	3.085(5)

Key giving operations for symmetry related atoms:

(a) 1-x, 1-y, 1-z
(b) 1-x, 2-y, 1-z
(c) -1+x, +y, +z
(d) 2-x, 2-y, 1-z
(e) 1+x, +y, +z

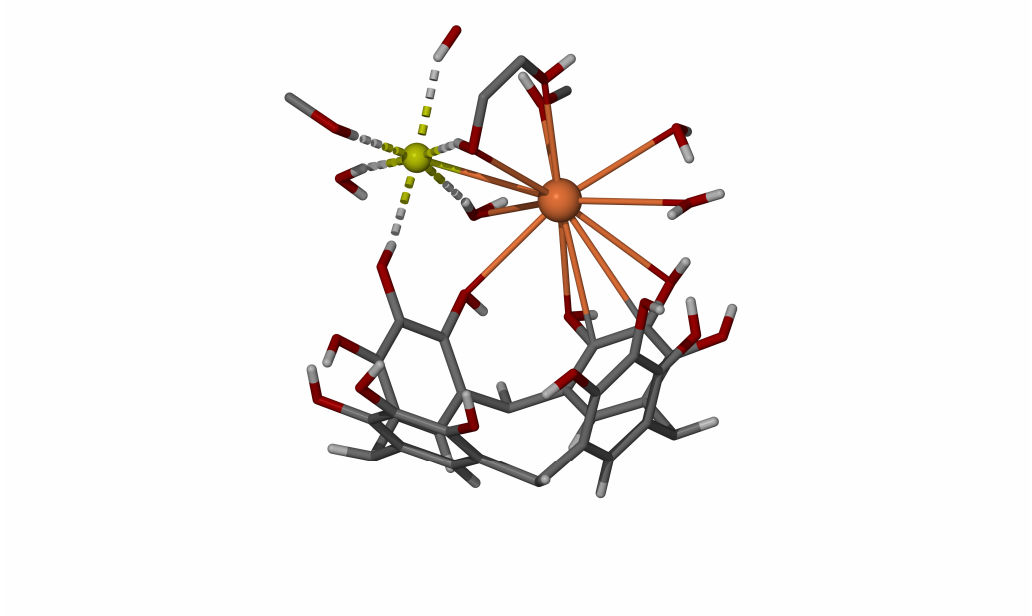

Figure S1. Hydrogen bonding associated with the chloride in **1·CsCl**.

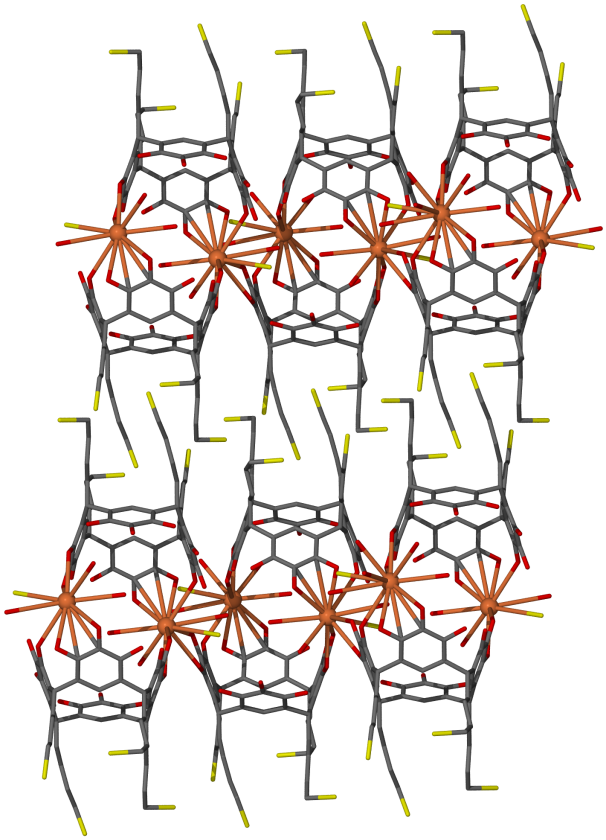

Figure S2. The extended bi-layer structure in **1·CsCl**.

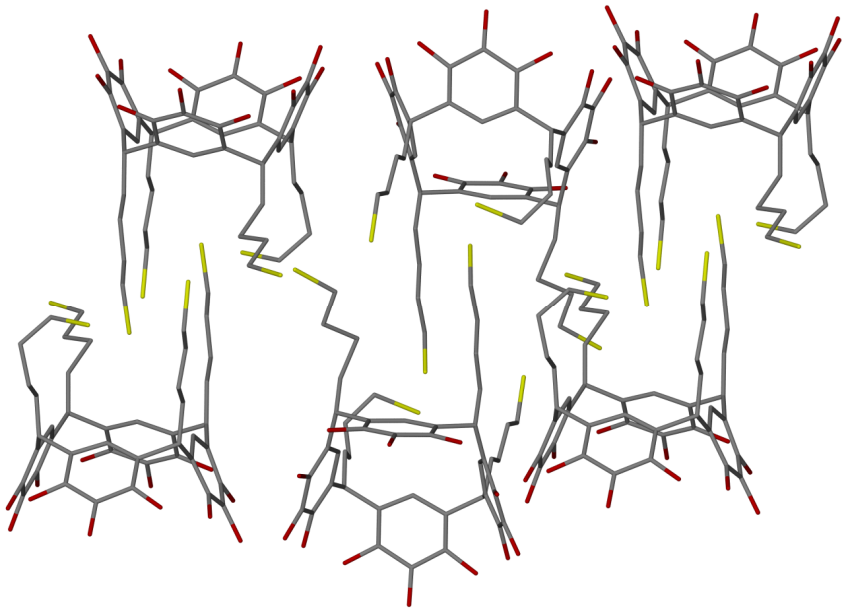

Figure S3. Extended bi-layer structure formed when **1** is crystallised from methanol.[15]

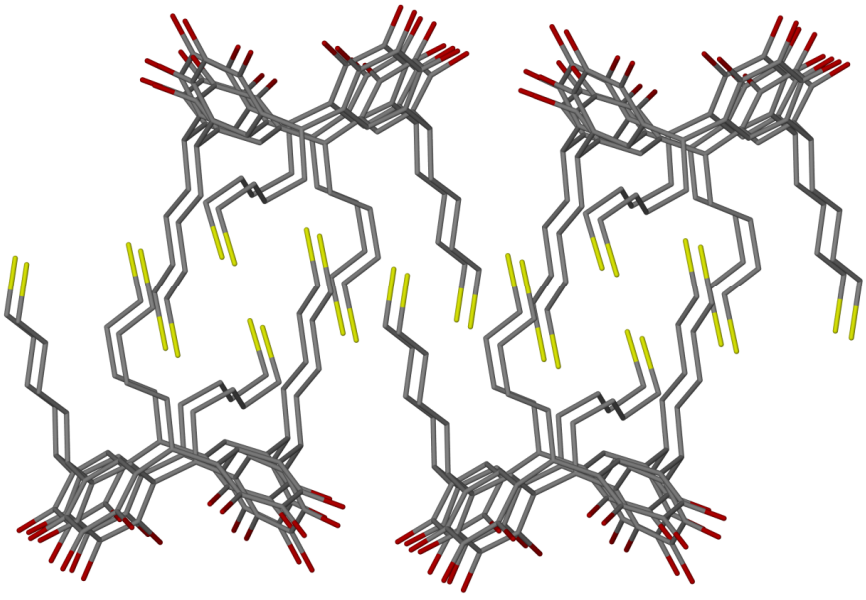

Figure S4. Extended bi-layer structure formed when **1** is crystallised from ethyl acetate.[15]

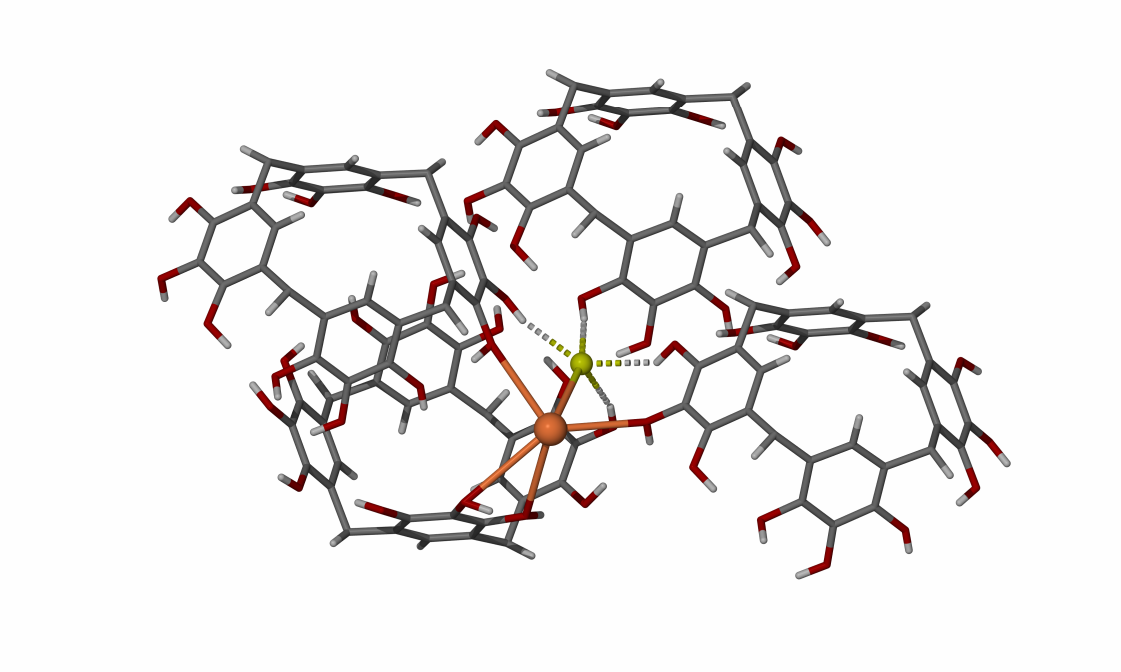

Figure S5. Hydrogen bonding associated with the chloride in **2·CsCl**.

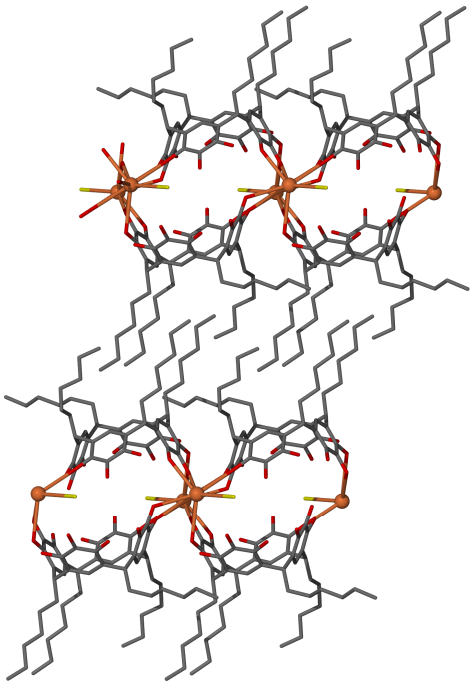

Figure S6. View of the fourth lower rim hexyl chain bending away from the base of the bowl-shaped molecule in the extended structure based on **2**.

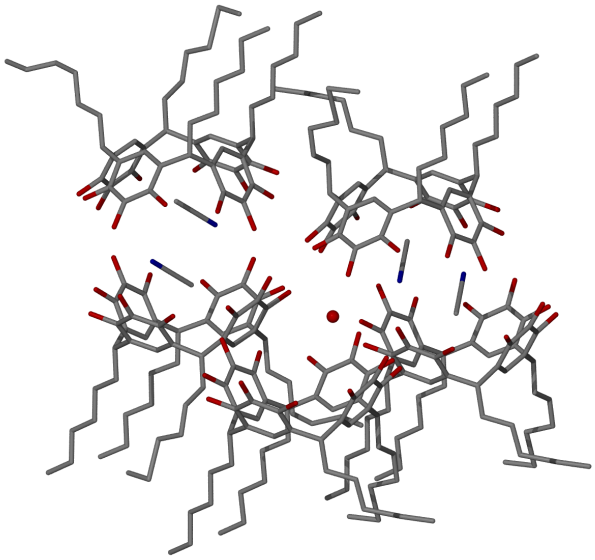

Figure S7. View of the water of crystallisation in the 'metal free' dimeric capsule structure based on 2 when crystallised from a acetonitrile.[13d]

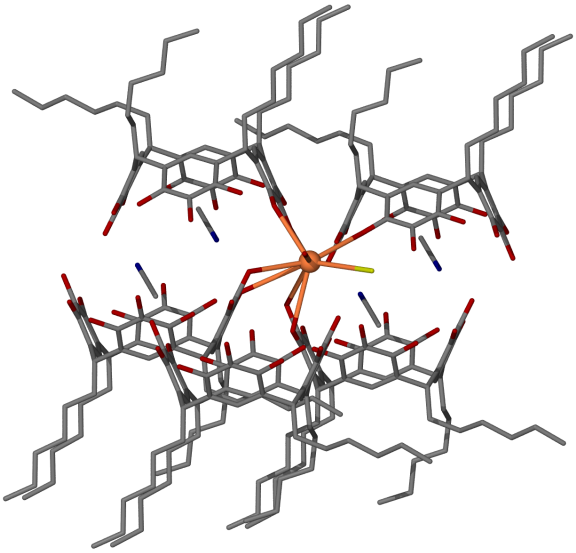

Figure S8. View of the close substitution of water of crystallisation in figure S7 for caesium in the dimeric capsule structure of **2·CsCl**.