Electronic Supporting Information

Structural characterization of inclusion complexes of *para*-sulphonato-calix[8]arene with 1,2-bis(4-pyridyl)-ethane and 1,3-bis(4-pyridyl)-propane. New 'double cone' and 'up-flat-down' conformations of *para*-sulphonato-calix[8]arene

B. Lesniewska,[*a] F. Perret,[b] K. Suwinska[ac] and A. W. Coleman[*d]

[a] *Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, PL-01 224 Warszawa, Poland, e-mail blesniewska@ichf.edu.pl. Corresponding author. Tel: +48 22 343 3232, Fax: +48 22 343 3330.*
[b] *ICBMS, CNRS UMR4246, University Lyon 1, Villeurbanne, F69622, France, e-mail florent.perret@univ-lyon1.fr.*
[c] *Faculty of Biology and Environmental Sciences, Cardinal Stefan Wyszynski University, Wóycickiego 1/3, PL-01 938 Warszawa, Poland, e-mail ksuwinska@ichf.edu.pl, k.suwinska@uksw.edu.pl.*
[d] *LMI CNRS UMR 5615, University Lyon 1, Villeurbanne, F69622, France, e-mail antony.coleman@adm.univ-lyon1.fr. Corresponding author. Tel: +33 4 7243 1027, Fax: +33 4 7244 0618.*

[*] Corresponding author. Tel: +33 4 7243 1027. Fax: +33 4 7244 0618. E-mail: antony.coleman@adm.univ-lyon1.fr, blesniewska@ichf.edu.pl

a

b

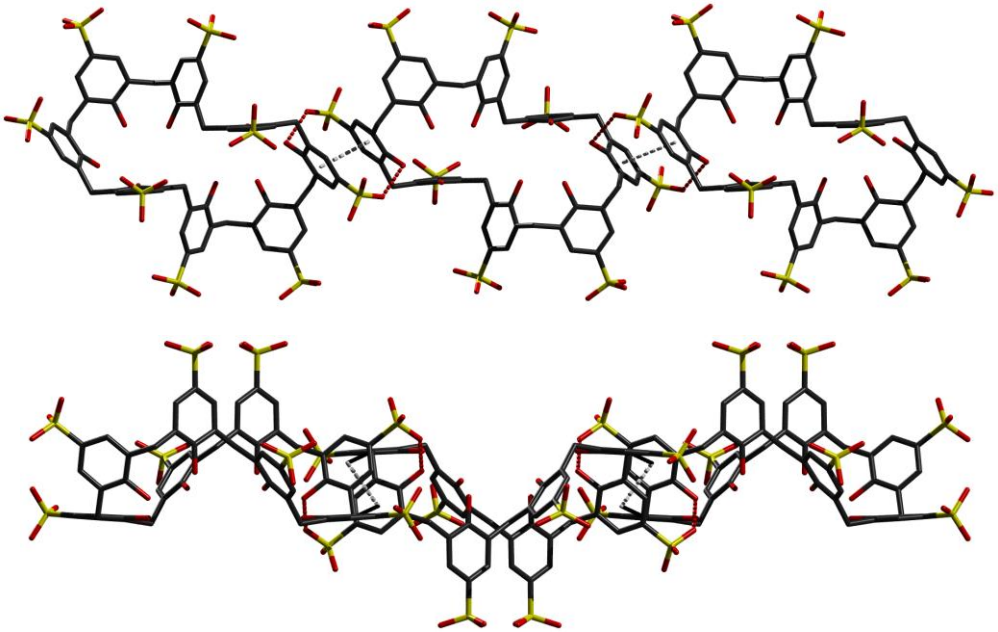
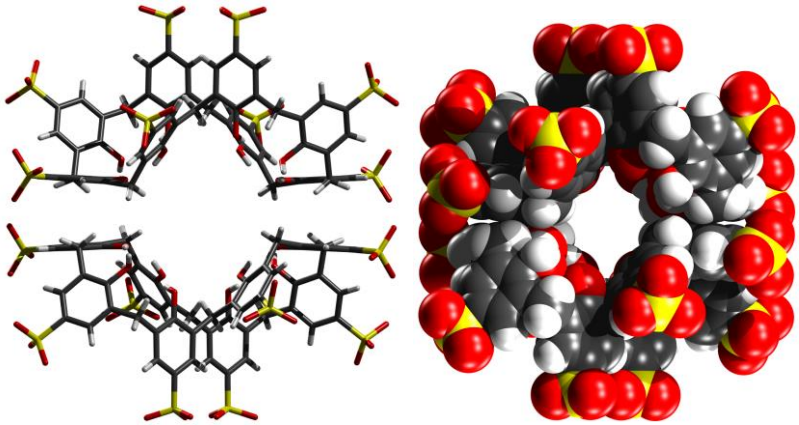
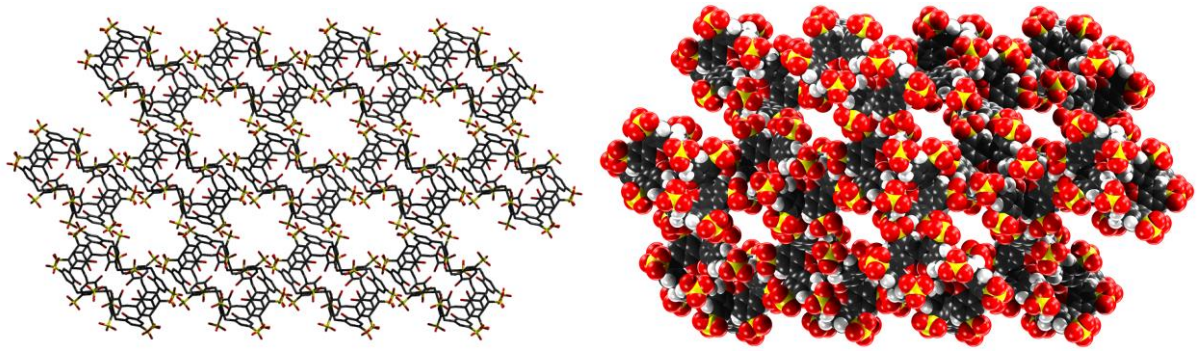


Figure 1. *para*-Sulphonato-calix[8]arene anions linked together by O–H···O (2.560 Å) and π–π (centroid–centroid distance: 3.611 Å) interactions in infinite chains; (a) view along [100] axis (b) view along [010] axis.

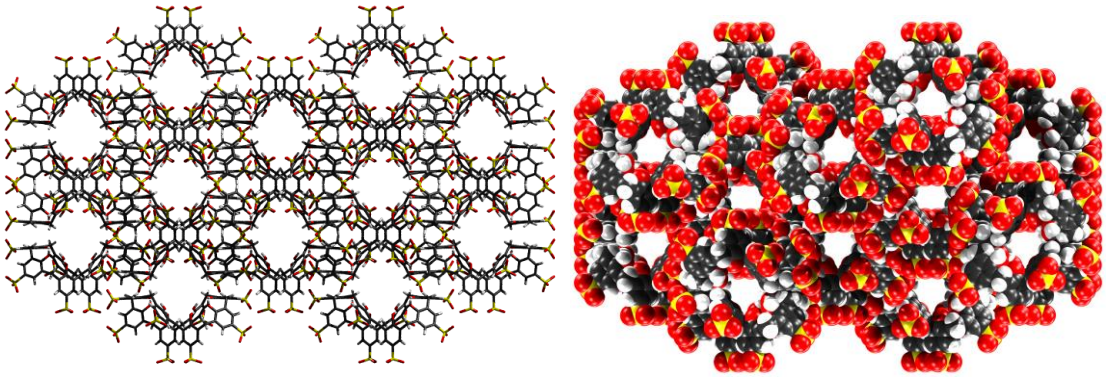


a *b*

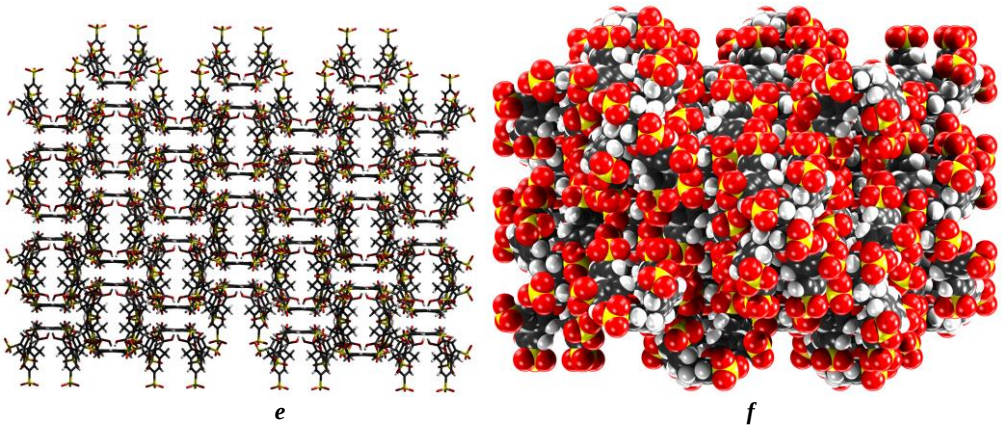
Figure 2. Molecular capsule formed by two *para*-sulphonato-calix[8]arene anions; (a): stick model (b): spacefill model.



a *b*



c *d*



e *f*

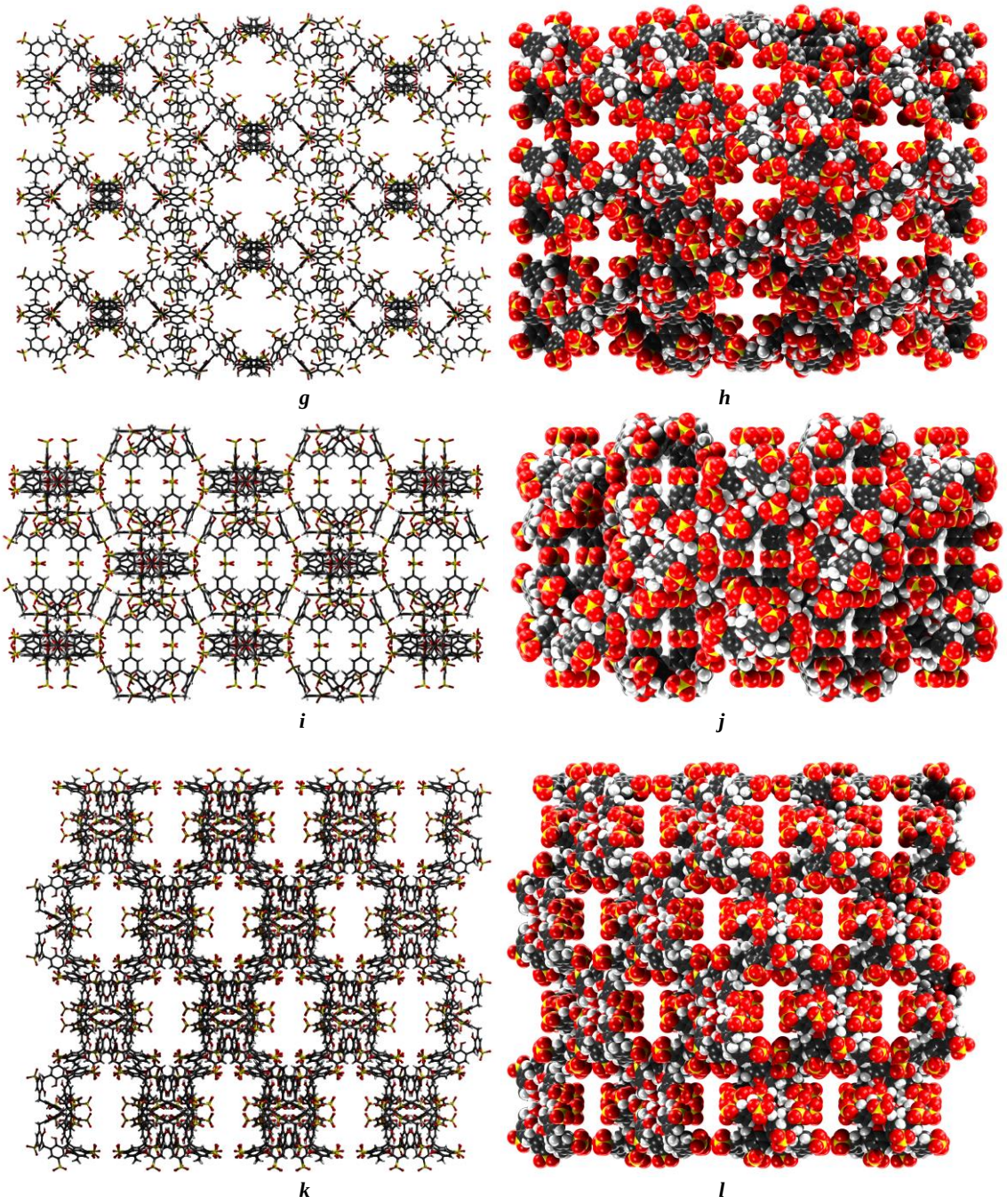


Figure 3. Packing of *para*-sulphonato-calix[8]arene anions: (a, b) view along [100] axis; (c, d) view along [010] axis; (e, f) view along [001] axis; (g, h) view along [110] axis; (i, j) view along [011] axis; (k, l) view along [101] axis.

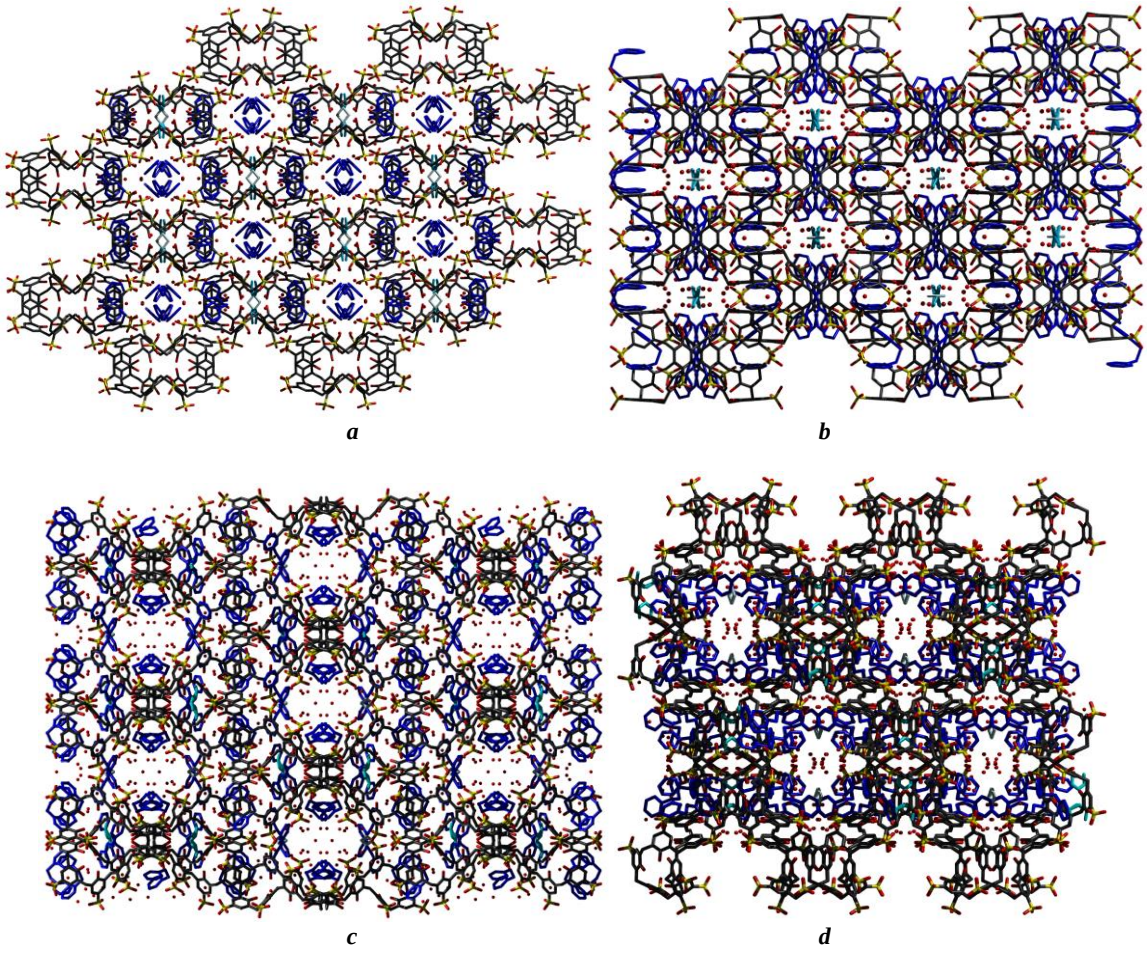
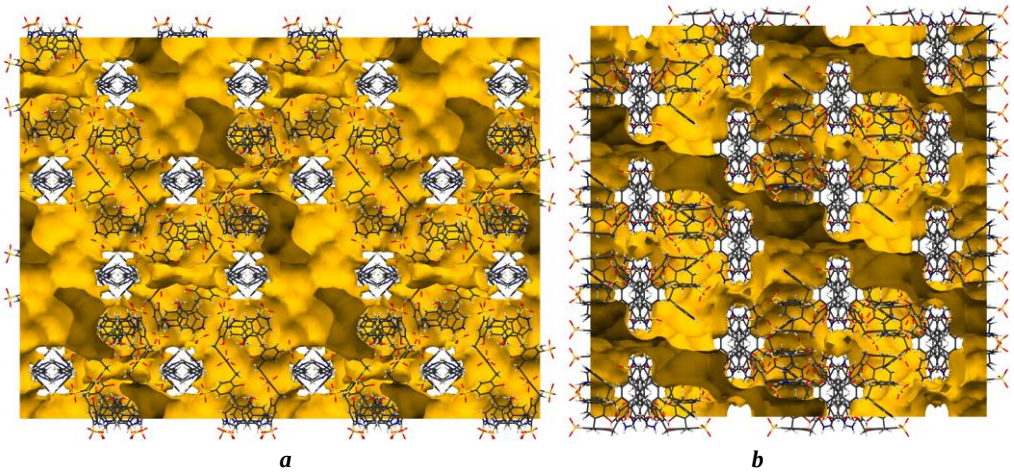
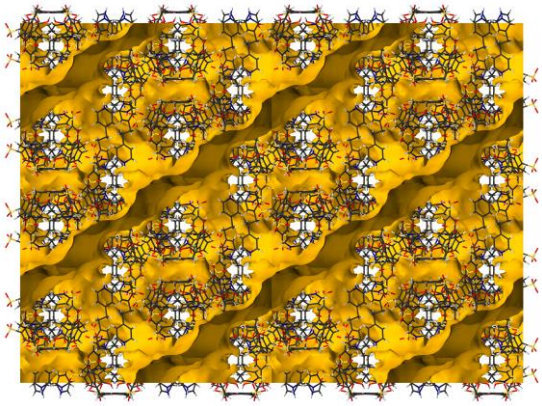
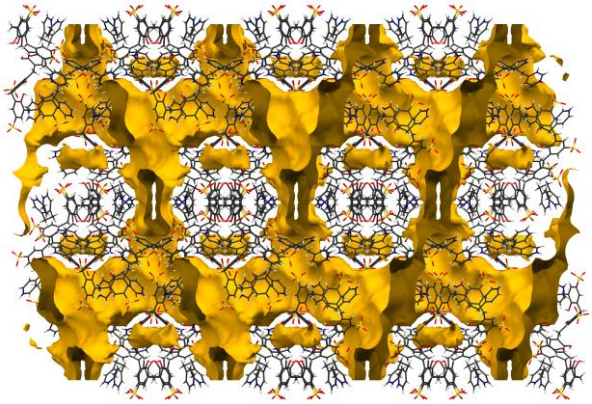


Figure 4. Packing of the complex **1**. Channels are filled by **BPE**, ethanol, methanol and water molecules. (a) view along [100] axis; (b) view along [010] axis; (c) view along [110] axis, (d) view along [101] axis.

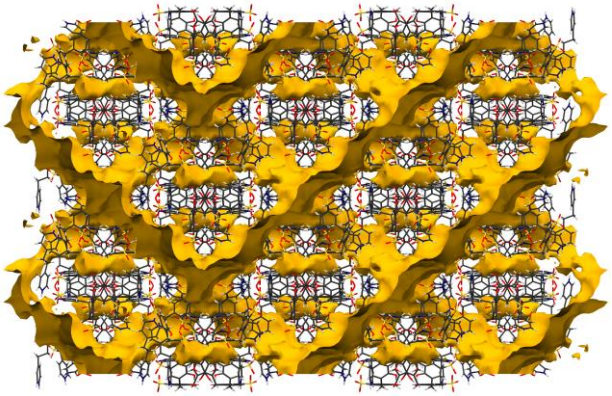




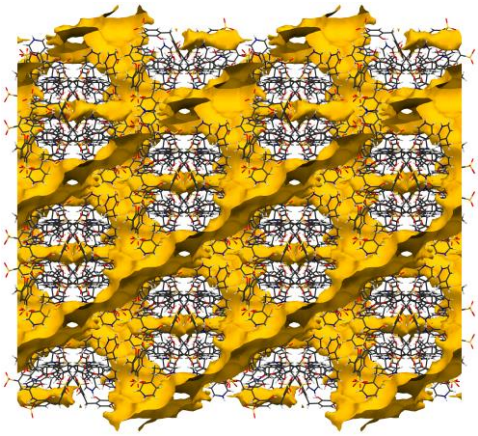
c



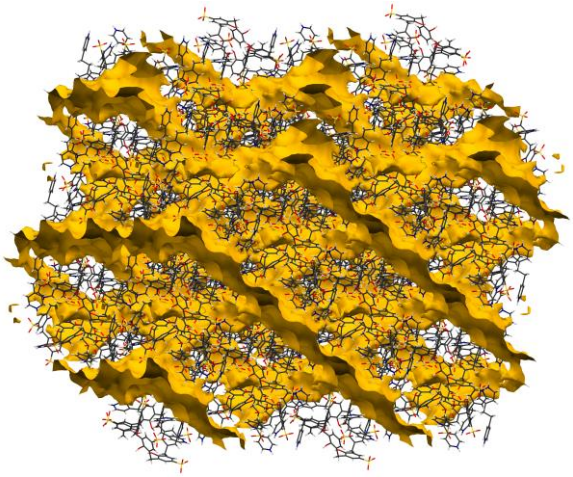
d



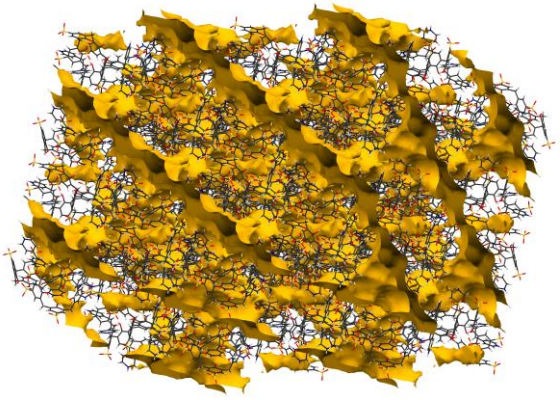
e



f



g



h

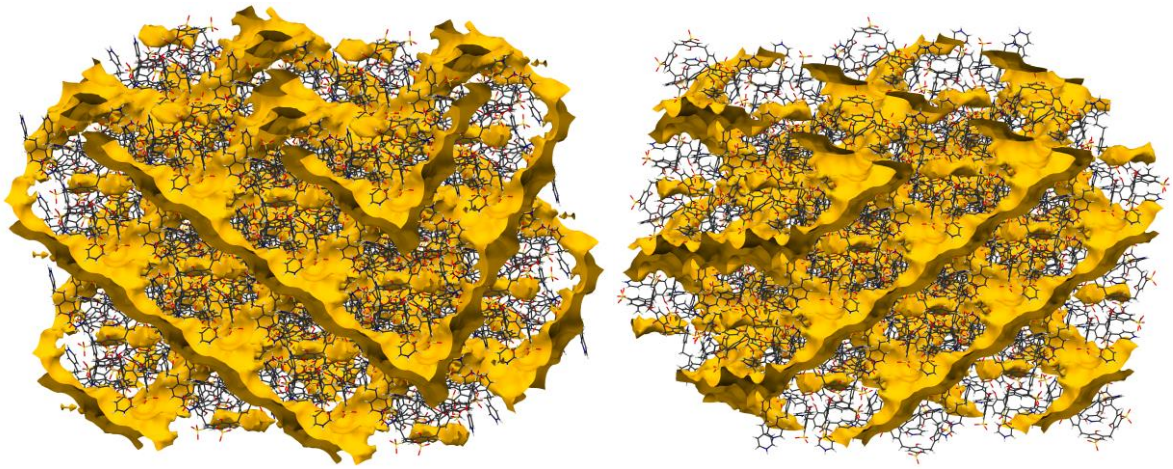


Figure 5. Solvent accessible surface in complex **1**: (a) view along [100] axis; (b) view along [010] axis; (c) view along [001] axis; (d) view along [110] axis; (e) view along [011] axis; (f) view along [101] axis; (g) view along [111] axis; (h) view along [11-1] axis; (i) view along [-111] axis; (j) view along [1-11] axis.

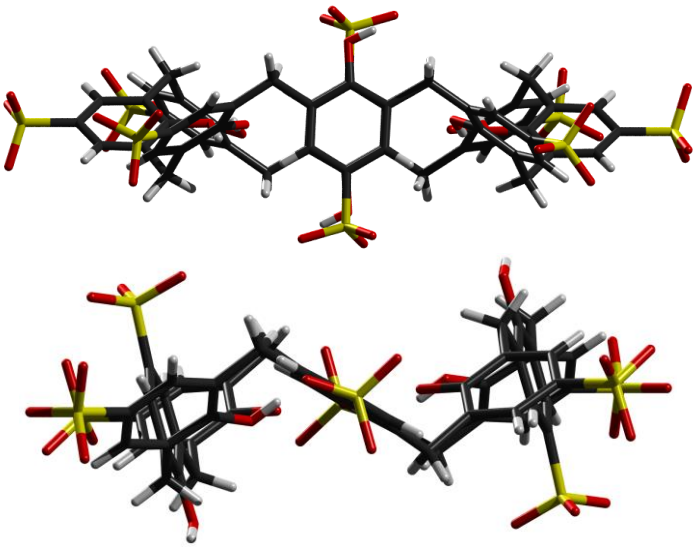


Figure 6. *para*-Sulphonato-calix[8]arene centrosymmetric conformation in complex **2**: side view.

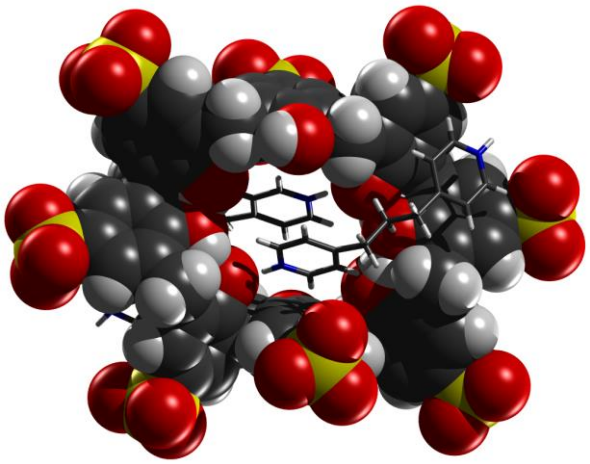


Figure 7. Host-guest inclusion, **C8S** anion with cavity occupied by two **BPP** cations.

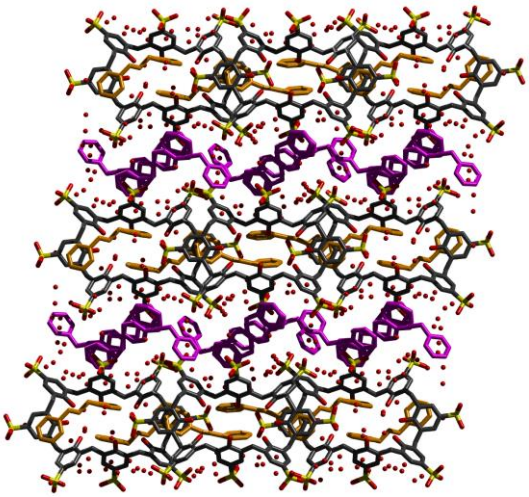


Figure 8. Packing of the complex **2**; **BPP** cations included into **C8S** cavities are marked in orange, the rest of the **BPP** cations in violet, water molecules are displayed as red balls ; (a) view along [100] axis.

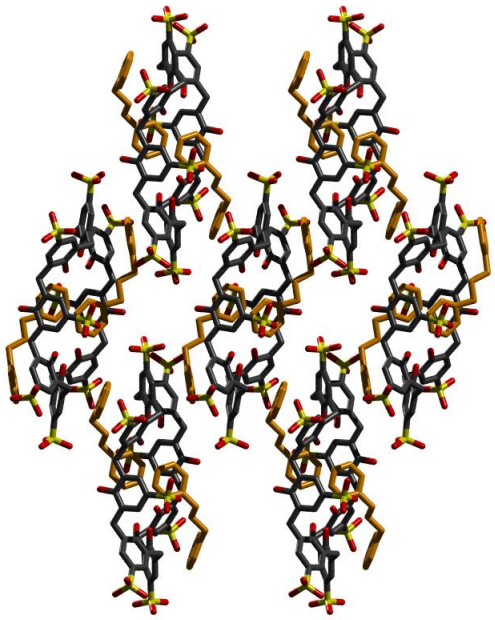


Figure 9. Arrangement of **C8S** anions and included **BPP** cations in first layer, view along [010] axis. Water molecules are omitted for clarity.

Single-crystal X-ray diffraction – disorder treatment

C8S-BPE complex (1): The ethanol, methanol and BPE (with 0.25 occupancy) molecules were modeled using DFIX command in order to retain the correct distances between atoms.

DANG were used to correct angle C6 C7 H1A in calixarene molecule.

The distances of sulphonate groups were modeled using SADI command in order to equal them/ retain the correct distances between atoms.

All BPE molecules were modeled using SIMU and DELU commands in order to change the direction of the anisotropic displacement parameters and to restrain the motion of atoms perpendicular to a planar group. The components of the displacement parameters in the direction of the bond are restrained to be equal.

C8S-BPE complex (1): The distances of sulphonate groups were modeled using SADI command in order to equal them/ retain the correct distances between atoms.

The BPP and water molecules were modeled using DFIX and DANG commands in order to retain the correct geometry.

The BPP rings were modeled using FLAT commands in order to restrain atoms to be coplanar.

Water oxygen atoms were modeled using ISOR command in order to prevent atoms from becoming 'non-positive-definite'.

All BPP molecules were modeled using SIMU and DELU commands in order to change the direction of the anisotropic displacement parameters and to restrain the motion of atoms perpendicular to a planar group. The components of the displacement parameters in the direction of the bond are restrained to be equal.