Poster Presentations

[MS38-P10] Structural Diversity in Supramolecular Compounds of para-Sulfonato[6]calixarenes with Phenanthroline.

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Two crystalline complexes of para-sulfonato[6] calixarene with 1,10-phenanthroline were obtained and characterized by means of X-ray crystallography. One of the obtained complexes was crystalized from mixed water-tetrahydrofuran solvent. The second can be obtained from either methanol-water or water-ethanol mixtures. Molecules of calixarenes in both crystals adopt centrosymmetric classical up-down conformation, thus providing two identical binding sites which interact with phenanthroline molecules. 1:2 Host:guest stoichiometry is observed for both inclusion compounds. Two molecules of phenanthroline form a dimer with triplex π–π "face-to-face" interaction and are encapsulated in the cavity of two adjacent calixarenes. The inclusion complexes are also stabilized by host-guest C–H···π interactions. The complex molecules form parallel columns. The space between the columns are filled with water molecules and additional guest molecules. In one of the discussed structures one-dimensional channels filled by water molecules are observed. Similar polymeric capsules formed by *para*-sulfonatocalix[6]arene and 1,10-phenanthroline dimers were described by Liu [1].

[1] Liu, Y., Guo, D.S. & Chen K. (2007). *Cryst. Growth Des.* 7 (9), 1672–1675.

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