

# Supramolecular Assembly of *p*-Sulfonatothiacalix[6]arene Yttrium Complex Supported by Hydrogen Bonding, $\pi-\pi$ Stacking, and S- $\pi$ Interactions

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Crystals of a yttrium complex composed from deprotonated *p*-sulfonatothiacalix[6]arene,  $[\{Y(H_2O)_8^{3+}\}_2\{p\text{-sulfonatothiacalix[6]arene}^{6-}\}] \cdot 16H_2O$  (**I**), were studied by single-crystal X-ray diffraction analysis. In the present crystal system of **I**, the thiacalixarene molecule maintains an 'up-down' double partial-cone conformation possessing two pseudo-thiacalix[3]arene cavities, which act as a 'molecular container' towards guest water molecules. Interestingly, the aquated yttrium center does not directly coordinate to the thiacalixarene sulfonate groups. In contrast, the aquated yttrium cations act as a connector to the thiacalixarene molecules to establish a one-dimensional hydrogen-bonded polymer by hydrogen bonding between the thiacalixarene molecules and the yttrium cations. The extended structure of the complex forms a supramolecular assembly via mutually supporting intermolecular  $\pi-\pi$  stacking, S- $\pi$  interactions, and hydrogen bonding between two differently oriented polymers.

**Key Words** : water-soluble thiacalixarenes, supramolecular assembly, crystal structure, rare-earth metals