Synthesis of Tribenzo-1,4,7-triazacyclononene "N3-CTV" (Cyclophane family) and Derivatives as Supramolecular Scaffolds

A toolbox of supramolecular derivatives useful for organic- and opto-electronic materials.

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Field
- Fine Chemicals
- Qualitative/Quantitative ion analysis
- Drug delivery vehicles & diagnostics
- Materials science
- Catalysis

Technology
- Supramolecule scaffold and derivatives that can be solubilized in water and tuned for host-guest specificity.

Key Features
- Conformationally flexible binding site
- Binding site modified by peripheral substituents
- Soluble in aqueous and non-aqueous solvents
- Attachment to solid support/resin systems

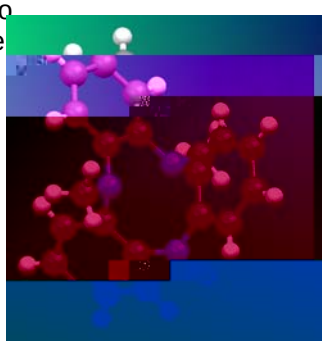
Key Benefits
- Patent contains broad coverage for composition of matter as well as for synthetic routes for parent compound and numerous derivatives.

Supramolecular compounds

Supramolecular chemistry involves the formation of complex molecular entities that have the capacity to participate in specific molecular recognition of guest molecules and finds commercial application over a wide range of analytical methodologies, materials science and medical diagnostics end uses. This results from their principal characteristic of being able to form non-covalent molecular complexes with a variety of ionic and non-ionic moieties in aqueous and non-aqueous solution. A commonly employed scaffold in supramolecular chemistry is the symmetric crown-shaped molecule cyclotriveratrylene (CTV) that is useful for its unique functionality and targeted capacity for guest-host recognition and binding stability. CTV has been studied extensively for its capability of binding a number of smaller organic and organometallic guests within its bowl-shaped cleft and has been used as a building block enabling the construction of more complex cryptophanes. The new N3-CTV derivatives employ three nitrogen atoms in the cyclononene core to dramatically enhance the versatility of CTV. General applications of N3-CTV include use as a transition-metal ligand, qualitative and quantitative analysis of metal and non-metallic ions in solution, encapsulation of drugs, environmental analysis, catalysis, magnetic resonance, medical diagnostic imaging and optoelectronic applications.

Synthesis of Tribenzo-1,4,7-triazacyclononene (N3-CTV) and derivatives

The inventors have claimed the composition of matter of the new supramolecular scaffold designated as N3-CTV and its derivatives and have developed a new, patented, synthetic route to the family of compounds. Derivatives may be easily prepared with enhanced water solubility over the commonly-employed CTV (cyclotriveratrylene). The binding site or cavity, containing 3 nitrogens in a 9-membered ring, can produce pH-dependent binding and conformational properties which can be important in modulating its binding properties. The derivative compounds lend themselves to attachment to solid substrates/resins via alkylation, ester or amide formation.



X-Ray crystal structure of N3-CTV

N3-CTV supramolecule and its derivatives provide enhanced functionality as a family of compounds

The popular supramolecular scaffold CTV (cyclotriveratrylene) is insoluble in water. Replacement of the three capping methylenes of CTV with nitrogen atoms significantly enhances water solubility and also provides manifold