Investigation of the Synthesis of Water-Soluble 1,3,5-trihydroxy-2,4,6-trimethylsulfonic Acid Benzene, its complexes with Lanthanide Cations and Sulfonatoresorcin[4]arenes, and the Study of Gas Storage in Iodine Doped *p*- tert-Butylcalix[4]arenes

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ABSTRACT

The design of new calixarene derivatives based on supramolecular principles – the formation of molecules, ions, or complex ions with the weak non-covalent interactions to form a larger moiety with applicable properties compositioned by the starting material's attributes -- has attracted attention in many scientific fields.

Herein, the new synthesis method of 1,3,5-trihydroxy-2,4,6-trimethylenesulfonic acid benzene, **1** was studied. As a result, the new synthetic method was less complicated and required fewer steps than that of the previous work. This compound also presents a novel tautomeric conformational change using NMR spectroscopy. Furthermore, the lanthanide (Sm, Eu, La, Ho, and Nd) complexes of **1** are isostructural and the packing of the complexes is a bilayer structure arrangement with π-stacking between the benzene rings. In addition, the study investigated the formation of tetramethylsulfonatoresorcin[4]arenes, a diaza-18-crown-6, and LN(III) metal ions such as europium (Eu) holmium (Ho), and samarium (Sm) and their crystalline structures. The results show the various ways that these molecules can assemble into different supramolecular frameworks.

Hydrogen gas-storage properties of modified *p*-tert-butylcalix[4]arenes with doping by iodine molecules (I_2 doped TBC4) was studied. An evidence of hydrogen gas-sorption shows a good sign that I_2 doped TBC4 can possibly be developed for hydrogen gas storage in the future.