Public Abstract

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Graduation Term:FS 2014

Department:Chemistry

Degree:PhD

Title:INVESTIGATION OF THE SYNTHESIS OF WATER-SOLUBLE 1,3,5-TRIHYDROXY-2,4,6-TRIMETHYLSULFONIC ACID BENZENE, ITS COMPLEXES WITH LANTHANIDE CATIONS AND SULFONATO-RESORCIN[4]ARENES, AND THE STUDY OF GAS STORAGE IN IODINE DOPED p-TERT-BUTYLCALIX[4]ARENES

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 ?-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 using single crystal X-ray crystallography. The results show the various ways that these molecules can assemble into different supramolecular frameworks. Different solvents result in drastically the different packing of these molecules resulting in the diverse range of packing motifs.
Hydrogen gas-storage properties of modified p-tert-butylcalix[4]arenes with doping by iodine molecules (I2 doped TBC4) was studied. The iodine-doped p-tert-butylcalix[4]arenes are structurally studied by using the 1H-NMR, 13C-NMR in liquid and solid-state 13C-NMR, and single crystal X-ray crystallography. The decomposition temperature was studied by thermogravimetric analysis. Iodine doped p-tert-butylcalix[4]arenes show an evidence of hydrogen gas-sorption which is a good sign that the new material, Iodine-doped - p-tert-butylcalix[4]arenes can possibly be developed for hydrogen gas storage in the future.

Notably, the weak non-covalent interactions that are often responsible for the formation of supramolecules are also responsible for reversible adsorption/desorption properties found in host-guest systems. Examples of guest species include gases, organic molecules, inorganic complexes, and metal ions. Therefore, this research is dedicated to exploring and designing new materials for sorption/desorption purposes, as they may
be useful in storage of fuel gases, for carrying/releasing drugs to the target parts of the body, or used as biological mimics.