Karla Claudio

Major: Chemical Engineering
University: Polytechnic University of Puerto Rico
Faculty Mentors: Dr. Timothy Glass and Dr. Jerry Atwood
Mentor Department: Chemistry
Funded by: Stevens' Chemistry Program

Host-guest complexes to molecular encapsulation of hydrogen

Karla Claudio, Tim Glass and Jerry Atwood

Science has always been about man learning from and attempting to mimic nature. In supramolecular chemistry this possibility is evident due to particularly interesting architectures of natural shell-like containers such as viruses and ferritin. One class of compounds studied for this purpose are calixarenes. Their typical cone structure allows them to sequester a variety of other molecules making it useful to form host-guest complexes or supramolecules. In such complexes, the host is a large molecule, in our case a calixarene, possessing a sizeable central cavity and the guest can be a monoatomic cation, a simple inorganic anion or a more sophisticated molecule such as a hormone, pheromone or neuro transmitter. In today's supramolecular chemistry field these compounds can be used for catalysis, biocatalysis, stabilization of reactive intermediates, drug transport, and the now emerging field of storage, processing and release of gases. The synthesis of this molecular capsule able to incorporate a guest begins with the methylation of the phenols present on the lower rim of calix[4]arene, an aldehyde was introduced along the upper ring followed by an oxidation to a carboxylic acid yielding tetracarboxycalix[4]arene. The tetrasubstituted calix[4]arene was crystallized from methanol and water to yield pale yellow crystals that were analyzed by X-ray. In this particular case, the objective was to incorporate gaseous hydrogen as the guest, which will be studied in due course. Further applications of this host-guest system could be the purification and storage of hydrogen for use in fuel cell. The nanoscale systems are a leading development strategy in many research areas. General advantages are the ability of saving time, space, costs, and materials for that reason supramolecular chemistry open a door to a new source of inspiration in the science world.