

CHEMISTRY DEPARTMENT

Seminar Series - Thursday, Jan 13



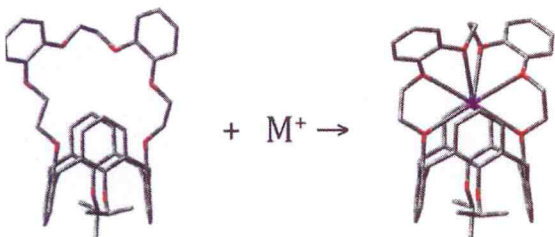
**DR. B. RAMU
RAMACHANDRAN**

**LOUISIANA TECH
UNIVERSITY**

Selective complexation of alkali metal ions using crown ethers derived from calix[4]arenes: A computational investigation of the structural and energetic factors

NCF Room 105

12:15 - 1:05 pm



The first part of this seminar will present a systematic analysis of the thermodynamics of alkali metal (i.e., Na^+ , K^+ , Rb^+ , and Cs^+) complexation by four calix[4]arene crown-6 ethers in the 1,3-alternate configuration. The calix-crown ethers are identical to, or closely related to, four molecules whose selectivity towards complexing Na^+ , K^+ , Rb^+ , and Cs^+ from aqueous solutions was studied experimentally by Casnati et al. in 2004. Our computational approach is able to qualitatively reproduce most of the experimental observations. Based on this success, we then use the computational approach to examine the structural and energetic factors that contribute to the observed selectivity. This suggests that the long-standing “conventional wisdom” in the field of calix-arene

Pizza lunch to follow - sponsored by LaTech - sign up required - see Chem Dept Secretary