

A MOLECULAR CAGE REPORTS ON ITS CONTENTS: THE INFRARED AND ULTRAVIOLET SPECTRA OF [2.2.2]BENZOCRYPTAND COMPLEXED WITH K^+ , Ba^{2+} , AND THE ION PAIR Ba^{2+} -ACETATE $^-$

CHIN LEE, *Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA*; CASEY DANIEL FOLEY, *Department of Chemistry, University of Missouri, Columbia, MO, USA*; KENDREW AU, *Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA*; EDWIN SIBERT, *Department of Chemistry, University of Wisconsin–Madison, Madison, WI, USA*; TIMOTHY S. ZWIER, *Combustion Research Facility, Sandia National Laboratories, Livermore, CA, USA*.

Cryptands are 3D molecular cages that initiated the field of supramolecular chemistry. They feature three ether bridges capped on either end by a tertiary amine, leading to a structure in which six oxygens and two nitrogens can bind to cations that fit inside the cage. We incorporate a phenyl ring in one of the ether bridges, forming [2.2.2]benzocryptand, in order to have an ultraviolet chromophore for our studies. Investigated complexes include benzocryptand with metal cations of potassium, barium and ion pair of barium-acetate. We will describe our results on the UV photofragment spectroscopy and IR-UV double resonance spectra that provide single-conformation IR spectra of the complexes under cryo-cooled conditions. In each case, there is a single dominant conformation of the complex. IR spectra in the alkyl CH stretch region are surprisingly sensitive to the ion in the cage, and to an anion binding to this caged cation.