ELECTRONIC SPECTRA OF CALIX[n]ARENE AND ITS VAN DER WAALS CLUSTERS IN SUPERSONIC JETS

T. EBATA, K. NISHIMOTO, N. HONTAMA AND Y. INOKUCHI, *Department of Chemistry, Graduate School of Science, Hiroshima University, Higashi-Hiroshima, 739-8526, Japan*.

Electronic structure and encapsulation of neutral guest molecules have been studied for Calix[4]arene (C4A)[a] and Calix[5]arene (C5A) in supersonic jets. By the measurements of UV-UV hole burning and IR-UV double resonance spectra, it was found that C4A has a single isomer with C_4 symmetry, while C5A has at least two isomers; one isomer has C_5 symmetry while the other isomer has the structure in which one of the phenol is inverted. The ability of the encapsulation has been studied by using rare gas, nitrogen, and methane as guest molecules. The electronic spectra suggest that the first guest molecule is encapsulated inside the cavity while the next molecules are bound outside.

[a] T. Ebata, Y. Hodono, T. Ito and Y. Inokuchi, J. Chem. Phys. 126, 141101 (2007).