

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

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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 C₄ symmetry, while C5A has at least two isomers; one isomer has C₅ 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.

^aT. Ebata, Y. Hodono, T. Ito and Y. Inokuchi, *J. Chem. Phys.* 126, 141101 (2007).