S_1-S_0 VIBRONIC SPECTRA OF BENZENE CLUSTERS REVISITED: I. THE TETRAMER

T. IIMORI, and Y. OHSHIMA, *Department of Chemistry, Graduate School of Science, Kyoto University, Kitashirakawa-Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan*.

We revisit the vibronic band systems of benzene cluster isotopomers by mass-selective resonant two-photon ionization (R2PI) and ultraviolet-ultraviolet hole burning spectroscopies.[a] Hole burning spectra on the transitions previously assigned to the trimer[b] in the C_6H_6-localized 0_0^0 region show that there are five distinct isotopomers having C_6H_6 molecule(s). R2PI spectra which have similar band structure are recorded in the $(C_6D_6)_3^+$ mass channel as well. The results indicate that the transitions are due to the cluster larger than the trimer, and thus the mass assignments that have been accepted for a couple of decades must be corrected. The number of the isomers and observed splittings are discussed in terms of the tetramer that have the geometry with four equivalent sites belonging to S_4 point group, which is also consistent with a NEMO calculation[c] of its most stable structure.

[a] T. Iimori and Y. Ohshima, *J. Chem. Phys.* **114** 2867 (2001).
[b] J. B. Hopkins, D. E. Powers and R. E. Smalley, *J. Phys. Chem.* **84** 3739 (1981).
[c] O. Engkvist, P. Hobza, H. L. Selzle and E. W. Schlag, *J. Chem. Phys.* **110** 5758 (1999).