S_1-S_0 VIBRONIC SPECTRA OF BENZENE CLUSTERS REVISITED: II. THE TRIMER

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As the second part of our recent reinvestigation on the electronic spectra of benzene clusters,[a] we present the trimer vibronic system studied by two-color (2C) resonance enhanced two-photon ionization (R2PI) and UV-UV holeburing experiments. This band system is observed only in the dimer-ion channel even with 2C-R2PI because of extensive fragmentation after photoionization, and thus it has been incorrectly assigned to an isomeric form of the dimer.[b] Detailed examination with mixed samples of C_6H_6 and C_6D_6 has revealed that the parent neutral has a single isomeric form for each isotopomer, $(C_6H_6)_m(C_6D_6)_n$ with $m + n = 3$. This observation confirms the equivalency in three benzene sites, which is consistent with the most stable cyclic form predicted by a NEMO calculation.[c] One of the intermolecular modes shows prominent Franck-Condon activity, implying a substantial conformational change via photoexcitation. Other details observed in the vibrionc spectra, *e.g.*, exitonic splitting, will also be discussed.

[a] T. Iimori and Y. Ohshima, *J. Chem. Phys.* **114**, 2867 (2001).
[b] W. Scherzer, O. Kratzschmar, H. L. Selzle, and E. W. Schlag, *Z. Naturforsch.* **47a**, 1248 (1992).
[c] O. Engkvist, P. Hobza, H. L. Selzle, and E. W. Schlag, *J. Chem. Phys.* **110**, 5758 (1999).