A FIRST EXPERIMENTAL VALUE FOR THE B_{1u} C-H STRETCH MODE IN BENZENE

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We investigate the vibrational properties of the benzene dimer in the C-H stretch region around 3 μm using Infrared Ion dip spectroscopy. Beside the well known IR active E_{1u} fundamental mode and other known combination bands, two "dimer bands" are observed that have been previously observed by others, however not yet been satisfactory assigned. IR spectra are also measured for isotopically mixed dimers C_6H_6 - C_6D_6. The IR spectra of those species depend on the ionization wavelength, showing that the two benzene rings are symmetrically in-equivalent. Based on the IR spectra, as well as on computations, we assign one of the "dimer bands" as the B_{1u} C-H stretch mode of the benzene monomer for which so far no experimental value exists. This mode is not IR allowed in the benzene monomer, however gains intensity in the reduced symmetry of the dimer. Experimental spectra and theoretical calculations will be presented.