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Experimental and Theoretical Determination of the Structures and Molecular Vibrations of Benzocyclobutane in Its Ground and Excited Electronic States JAAN LAANE, ESTHER OCOLA, HEE WON SHIN, Texas A&M Univ, SUNGHWAN KIM, Hanyang University — The infrared and Raman spectra of vapor-phase and liquid-phase benzocyclobutane (BCB) have been recorded and assigned. The structure and molecular vibrations of BCB were also computed using theoretical calculations. The ring-puckering, ring-twisting, and ring-flapping vibrations were of particular interest as these reflect the rigidity of the bicyclic ring system. The fluorescence excitation spectra of jet-cooled BCB have also been recorded and together with its ultraviolet absorption spectra were used to assign the vibrational frequencies for this molecule in its $S_1(\pi,\pi^*)$ electronic excited state. Theoretical calculations were carried out to compute the structure of the molecule in its excited state and this was compared to that of the molecule in its electronic ground state as well as to the structures of five related molecules in their S_0 and $S_1(\pi,\pi^*)$ electronic states. In each case the decreased π bonding resulted in longer carbon-carbon bonds in the benzene ring in the electronic excited states. The vibrational frequencies in the electronic excited state were readily assigned and these were compared to the ground state and to the frequencies of similar molecules. The decreases in the frequencies of the out-of-plane skeletal modes also reflect the increased floppiness of these bicyclic molecules in their $S_1(\pi,\pi^*)$ excited state.

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