AN UPDATED LOOK AT THE INFRARED SPECTRUM OF FULVENALLENE AND FULVENALLENYL

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The closed shell species fulvenallene (C_7H_6) and the fulvenallenyl radical (C_7H_5) are produced via thermal decomposition of phthalide ($C_8H_6O_2$) in a continuous-wave SiC pyrolysis furnace. Prompt pick-up and solvation of these species in helium droplets allows for the measurement of well-resolved infrared spectra in the CH stretching region. VPT2+K simulations based on a hybrid CCSD(T) force field with quadratic (cubic and quartic) force constants computed using the ANO1 (ANO0) basis set are used to predict anharmonic frequencies for both species. The 3300 cm^{-1}region of the spectrum contains the acetylenic stretch of fulvenallenyl which serves as a sensitive marker for the extent of delocalization between the conjugated propargyl and cyclopentadienyl subunits of the radical. This delocalization is explored with spin density calculations at the B3LYP/aug-cc-pVTZ and ROHF-CCSD(T)/ANO1 levels of theory.