RING PUCKERING POTENTIALS OF THREE FLUORINATED CYCLOPENTENES: C₅F₈, C₅HF₇, and C₅H₂F₆

E. A. ARSENAULT, B. E. LONG, WALLACE C. PRINGLE, Department of Chemistry, Wesleyan University, Middletown, CT, USA; YOON JEONG CHOI, S. A. COOKE, Natural and Social Science, Purchase College SUNY, Purchase, NY, USA; ESTHER J OCOLA, JAAN LAANE, Department of Chemistry, Texas A & M University, College Station, TX, USA.

A systematic study on the ring puckering potentials of three fluorinated cyclopentenes has been performed using Fourier transform microwave spectroscopy in tandem with quantum chemical calculations. Spectra between 8 GHz and 16 GHz have been measured for octafluorocyclopentene, 1H-heptafluorocyclopentene, and 1H,2H-hexafluorocyclopentene, where the hydrogens sequentially replace the fluorines on the sp² hybridized carbons. Rotational constants and centrifugal distortion constants have been determined for the parent species and all ¹³C isotopologues. In regards to the ring puckering, double minimum potential, both cross state and intra-state transitions were observed for all molecules except the 1H,2H-hexafluorocyclopentene. Experimental Coriolis coupling constants and ΔE₀₁ values will be presented and discussed. The ring puckering barrier heights for C₅F₈, C₅HF₇, and C₅H₂F₆, have been calculated to be 222 cm⁻¹, 302 cm⁻¹, and 367 cm⁻¹, respectively.