ASSIGNMENT OF THE FIRST PHOTOELECTRON BAND OF FCH₂CHF (X²A) USING AB-ÎNÎTÎO QUANTUM MECHANICAL AND DENSITY FUNCTIONAL THEORY (B3LYP) COMPUTATIONAL CALCULATIONS

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VUV (He I) photoelectron spectra have been recorded for the reaction of atomic fluorine with 1,2 difluoroethane at different reaction times. A structured band associated with either CH₂CH₂F or FCH₂CHF as short-lived primary reaction product has been recorded at a mixing distance of 15 mm above the photon beam. The adiabatic and vertical ionization energies of this band were measured as (8.86 ± 0.04) eV and (9.36 ± 0.03) eV respectively. The average vibrational separation of (1070 ± 30) cm⁻¹ was observed in this band. Adiabatic and vertical ionization energies computed in this work for CH₂CH₂F (X²A) and FCH₂CHF (X²A) at MP2/6-311++G** and B3LYP/6-311++G** level of theory were compared with the corresponding experimental values and led to the assignment of the observed first photoelectron band to the ionization of FCH₂CHF (X²A). Mulliken population analysis and force constant calculations have also been carried out for CH₂CH₂F (X²A) and FCH₂CHF (X²A) and their singlet cationic states. The observed vibrational structure was then assigned to the excitation of C-F stretching mode in the ion.

References