VIBRONIC AND CATION SPECTROSCOPYOF ROTAMERS OF 4-CHLORO-3-FLUOROPHENOL

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We applied the two-color resonant two-photon ionization and mass-analyzed threshold ionization techniques to record the vibrationally resolved spectra of the ^{35}Cl and ^{37}Cl isotopologuesof the selected rotamers of 4-chloro-3-fluorophenol in the electronically excited S_1 and cationic ground D_0 states. The band origins of the $S_1 \leftarrow S_0$electronic transition (E_1's) and the adiabatic ionization energies (IEs) of the cis and trans rotamersof 4-chloro-3-fluorophenolare determined to be 35 233 ± 2 and 35 405 ± 2 cm^{-1}; 69 334 ± 5 and 69 460 ± 5 cm^{-1}respectively.The general features of the vibronic and cationspectra the two isotopologues are nearly identical. Most of the observed active vibrations result from in-plane ring deformation and substituent-sensitive motions. Theseexperimental data show that the frequency difference of therotamers and isotopologues somewhat depends on the nature, vibrational pattern, location and relative orientation of the substituents.