

Vacuum Ultraviolet Mass-Analyzed Threshold Ionization Spectroscopy of Tetrahydrofuran

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A vibrational spectrum of tetrahydrofuran (THF) cation in the gas phase was measured by one-photon vacuum ultraviolet mass analyzed threshold ionization (MATI) spectroscopy. The cation of a designated mass was detected with a time-of-flight mass spectrometer by pulsed field ionization of the molecule in the high Rydberg states delayed by a laser pulse scanning across the region of the vibrational spectrum. From the position of the 0-0 band in the zero field limit and the photoionization efficiency curve, the accurate first adiabatic ionization energy was measured, which is 9.4256 eV. The observed ionization energy was assigned as a result of the transition of the molecule with C_2 symmetries on both the ground S_0 and cationic ground D_0 states. Quantum chemical calculations for the molecule in the S_0 and D_0 states were performed and the peaks in the spectrum were successfully assigned employing the dipole selection rules between the S_0 - D_0 transition and Franck-Condon factors calculated by varying structural parameters, which determines the accurate molecular structure of the tetrahydrofuran cation.