LASER SPECTROSCOPY OF A HALOCARBOCATION: OBSERVATION OF THE ELECTRONIC SPECTRUM OF CH_2I^+

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We report the first observation of the gas-phase electronic spectrum of a simple halocarbocation, CH_2I^+. Fluorescence excitation and emission spectra were measured under jet-cooled conditions using a pulsed discharge source with CH_2I_2 as precursor. The spectral carrier was identified by: (1) comparison of experimentally derived ground state vibrational frequencies for various isotopomers with the predictions of Density Functional Theory (DFT) calculations, and (2) simulation of the observed rotational contour in our excitation spectra, which indicated an a-type transition, consistent with an excited state of A_1 symmetry. Calculations predict a triplet A_1 excited state with transition energy in the visible region, and the observed transition is therefore assigned as $^3A_1$-$^1A_1$, with band origin at 15180 cm^{-1}.