S_2 - S_0 FLUORESCENCE, MOLECULAR STRUCTURE, AB INITIO CALCULATIONS, AND QUANTUM BEAT SPECTROSCOPY OF SILYLIDENE (H_2C=Si)

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Strong S_2 - S_0 fluorescence has been observed in LIF spectra of jet-cooled silylidene, H_2C=Si, produced by fragmentation of tetramethylsilane in a pulsed discharge jet. The experimental ground and excited state molecular structures have been obtained for the first time from rotational analyses of the 0_0^0 bands of H_2C=Si and D_2C=Si. These bands exhibit pronounced rotational level intensity anomalies indicative of nonradiative decay processes. Quantum beats are observed in the fluorescence decay of almost every rotational level in $v' = 0$ and in most of the higher vibrational levels. Fourier transforms of the beat patterns show line broadening and splittings at small magnetic fields of 10 - 70 Gauss. High quality ab initio studies have been done to locate the interacting electronic states and predict their vibrational frequencies and molecular structures.