LASER SPECTROSCOPY OF THE JET-COOLED SICF FREE RADICAL

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The SiCF free radical has been detected through the $A^2\Sigma^+$ - $X^2\Pi$ band system in the 605 - 550 nm region. The radical was produced in an electric discharge through a dilute mixture of CF_3SiH_3 in high pressure argon and studied by laser induced fluorescence. The vibronic levels of the ground and excited states have been measured through LIF and emission spectroscopy and a Renner-Teller analysis has been undertaken for the ground $^2\Pi$ levels. The observed vibrational frequencies, partially resolved rotational band contours, Renner-Teller parameter, and electronic excitation energy are in accord with our predictions from high level ab initio (CCSD(T)/aug-cc-pVTZ) calculations. Theory shows that the radical has a silicon-carbon double bond in the ground state and a much shorter triple bond in the excited state. This is the third in the series of SiCX (X = H, Cl, and F) free radicals we have produced and studied in the gas phase.