

IDENTIFICATION OF A JAHN-TELLER ACTIVE GAS PHASE SILOXY FREE RADICAL (Cl_3SiO) BY LIF SPECTROSCOPY

TONY SMITH, *Ideal Vacuum Products LLC, Ideal Vacuum Products LLC, Albuquerque, NM, USA*; DENNIS CLOUTHIER, *Department of Chemistry, University of Kentucky, Lexington, KY, USA*.

A very strong LIF spectrum was observed in the 655 - 600 nm region from the products of an electric discharge through a dilute mixture of silicon tetrachloride and oxygen in argon. The same spectrum was obtained from a $\text{Cl}_3\text{Si-O-SiCl}_3$ precursor in argon. The LIF bands do not have resolved rotational structure, suggesting that the carrier of the spectrum is a heavy molecule. Emission spectra show substantial differences depending on which upper state vibronic level is probed, and these differences are readily understood if we assume that the spectrum is due to the Cl_3SiO free radical with a significant Jahn-Teller effect in the ground ^2E state. This conclusion is reinforced by our own ab initio calculations of the ground and excited state vibronic energy levels, band contours, chlorine isotope effects, and electronic excitation energies. Cl_3SiO is the first siloxy radical to be detected in the gas phase.