

## LIF SPECTROSCOPY OF A $^1\Sigma$ SPECIES CONTAINING Si: LINEAR SiOSi ?

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In our past SiCN investigation<sup>a</sup>, we found unknown bands with  $^1\Sigma - ^1\Sigma$  rotational structure in the laser induced fluorescence ( LIF ) excitation spectrum of SiCN. From the rotational constants, the spectral species may possibly be attributed to SiOSi. Although the most stable geometry of the ground electronic state is reported to be cyclic structure<sup>b</sup>, our CCSD(T) calculation with arg-cc-pCVTZ indicates the linear geometry,  $^1\Sigma_g^+$ , lying  $\sim 2,000\text{ cm}^{-1}$  above it. The potential energy surface calculated is very strange, and it indicates a barrier between the two geometries,  $\sim 10,000\text{ cm}^{-1}$  from the bottom. The dispersed fluorescence ( DF ) spectra from the single vibronic levels have fairly long progressions with very harmonic structure, but no hot-band structure. More precise computational works are underway, and we will discuss the assignment of the spectral species in this talk.

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<sup>a</sup>M. Fukushima and T. Ishiwata, J. Chem. Phys. 145, 124304 (2016).

<sup>b</sup>S. J. Paukstis, et al., J. Chem. Phys. A 106, 8435 (2002).