

TRIPLE-SINGLET MIXING in Si₃: the $1^3A_1'' - \tilde{a}^3A_2'$ TRANSITION^a

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The electronic spectrum of the triplet states of the D_{3h} isomer of Si₃ recorded using both mass selected REMPI and LIF spectroscopy was recently reported^b. In that same study the dispersed laser induced fluorescence (DLIF) spectra resulting from excitation of various bands in the visible range were recorded. The DLIF spectra exhibited a progression with a 505 cm⁻¹ spacing, which was assigned to the breathing mode of the D_{3h}, equilateral triangle, Si₃ molecule. In addition, and quite unexpectedly, the DLIF spectra exhibited a progression having a spacing of 173 cm⁻¹. This progression was tentatively assigned to transition involving the bending mode of the 1A_1 state of the C_{2v} isomer. A possible explanation for the observation of transitions in the singlet manifold is that upon laser excitation in the D_{3h} triplet manifold there is rapid intersystem crossing to the singlet manifold followed by fluorescence to the ground state of C_{2v} isomer. Here we address the issue of possible intersystem crossing by recording the excitation on DLIF spectra in the presence of a static magnetic field. Magnetic fields are known to enhance the singlet-triple mixing^c. Si₃ was produced using a supersonic pulsed discharge source (900 V, 20 μs, 6kΩ) with a 1% SiH₄ in argon mixture. Magnetic fields of approximately 500 and 950 Gauss were applied. We will report the interpretation of the magnetic field induced changes to the LIF and DLIF spectra and the implications for the singlet-triple mixing process.

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^bN. J. Reilly, X. Zhuang, V. Gupta, R. Nagarajan, R. C. Fortenberry, J. P. Maier, T. C. Steimle, J. F. Stanton, M. C. McCarthy; *J. Chem. Phys.*, **136**(19), 194307, (2004).

^cV. I. Makarov, I. V. Khmelinskii; *Advances in Chemical Physics*, **Volume 118**, 45-98, (2001).