TRIPLE-SINGLET MIXING in Si_3: 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 Si_3 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 assign to the breathing mode of the D_{3h}, equilateral triangle, Si_3 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 present of a static magnetic field. Magnetic fields are known to enhance the singlet-triple mixing[c]. Si_3 was produced using a supersonic pulsed discharge source (900 V, 20 μs, 6kΩ) with a 1% SiH_4 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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[b]N. 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).

[c]V. I. Makarov, I. V. Khmelinskii; *Advances in Chemical Phisics*, **Volume 118**, 45-98, (2001).