Laser Induced Fluorescence Spectroscopy of the SiCN $A\ ^2\Delta - X\ ^2\Pi$ system: The spin-orbit constant of the $A\ ^2\Delta$ state

Masaru Fukushima and Takashi Ishiwata

Faculty of Information Sciences, Hiroshima City University,
Asa-Minami, Hiroshima 731-91294, Japan
fukushim@info.hiroshima-cu.ac.jp

We have measured the laser induced fluorescence spectrum of the $A\ ^2\Delta - X\ ^2\Pi$ transition of SiCN under the supersonic free jet expansion condition. The radicals were generated in the Ar jets, using the general laser ablation technique. We used a Si rod as the ablation target and the Si in the radical would be supplied from the Si ablated. The decomposition products from acetonitrile in the plasma generated by the ablation would be the source for CN. Our rotational analysis of the $A\ ^2\Delta$ $(00^00) - X\ ^2\Pi\ (00^00)$ vibronic bands gave the molecular constants; B' = 0.1933221(18), A' = 4.94483(18), B'' = 0.18490847(26), A'' = 140.82414(78), ν = 29,261.63989(81) in cm^{-1} [1]. The spin-orbit constant at the $A\ ^2\Delta$ state of SiCN is obtained as the positive value, while that of the CCN, which is isovalent with SiCN, is reported to be a negative value, -0.82 cm^{-1} [2]. The major electronic configuration of the $A\ ^2\Delta$ states is $\ldots\sigma^1\pi^2$, and thus the A constant should be 0 under single configuration approximation, because of the closed π molecular orbital. There are three possibilities for understanding the non-zero values of the A constant; (1) the spin-(other-orbit) interaction, (2) the second order spin-orbit interaction, and (3) configuration interaction with the higher electronic states. The negative A constants of diatomic hydride molecules consisting from relatively light atoms, such as CH and NH, can be understood as those affected by the spin-(other-orbit) interaction [3]. However the spin-(other-orbit) interaction decreases with increasing of the atomic number, and thus the interaction cannot understand the positive A constants of the molecules consisting from relatively heavy atoms, such as SiH [3]. On this paper, we discuss the major reason of the minus value of the A constant of the $A\ ^2\Delta$ state of SiCN.

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