FIRST OBSERVATION OF THE $\tilde{B} ^1 A_1$ STATE OF SiH$_2$ AND SiD$_2$ RADICALS BY OODR SPECTROSCOPY

Y. MURAMOTO, H. ISHIKAWA and N. MIKAMI, Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan.

Silylene (SiH$_2$) is a silicon analogue of methylene (CH$_2$). The number of spectroscopic studies on SiH$_2$ is much smaller compared with that on CH$_2$ is small. Until now, only the $\tilde{X} ^1 A_1$, $\tilde{A} ^1 B_1$, and $\tilde{a} ^3 B_1$ states have been experimentally investigated. Recently, energetics and equilibrium structure of the next low-lying $\tilde{B} ^1 A_1$ state was studied by high-level calculations by Yamaguchi et al.$^a$ However, a corresponding electronic state has not yet been observed. In the course of our SEP spectroscopic study on highly excited vibrational levels of SiH$_2$, we have identified several bands that can be assigned as transitions to the $\tilde{B}$ state for the first time.

When a $J = 0$ rotational level of the $\tilde{A}$ state was used as an intermediate level of the OODR measurement, several vibronic bands of 1100 – 1200 cm$^{-1}$ interval were observed in the energy region of 28000 – 30100 cm$^{-1}$ above the $\tilde{X}$ state. Based on a rotational selection rule and a predicted bending vibrational frequency, we assigned these bands as an odd-$\nu_2$ progression. This means that the SiH$_2$ in the $\tilde{B}$ state behaves as a linear molecule. To confirm our assignment, it is necessary to observe OODR spectra via a $K_a = 1$ rotational level. To avoid a difficulty in measuring desired OODR transitions due to a predissociation in the $\tilde{A}$ state of SiH$_2$, an OODR spectroscopy of SiD$_2$ was also carried out. We have succeeded in measuring the OODR transitions to the $\tilde{B}$ state of SiD$_2$ and determined the value of $T_0$ of SiD$_2$ to be 27214.11 cm$^{-1}$. Our observation on SiD$_2$ confirmed the quasi-linear behavior in the $\tilde{B}$ state. Details of our observation will be presented in the paper.