FIRST OBSERVATION OF THE $\tilde{B}\ ^1A_1$ 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 $\tilde{X}\ ^1A_1$, $\tilde{A}\ ^1B_1$, and $\tilde{a}\ ^3B_1$ states have been experimentally investigated. Recently, energetics and equilibrium structure of the next low-lying $\tilde{B}\ ^1A_1$ 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-v_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.

---

[a] Y. Yamaguchi, T. J. Van Huis, C. D. Sherrill, H. F. Schaefer III *Theor. Chem. Acc.* **97** 341 (1997).