MILLIMETERWAVE AND FOURIER-TRANSFORM EMISSION SPECTRA OF THE BiS RADICAL

K. IZUMI, K. KAWAGUCHI, *Department of Chemistry, Okayama University, Okayama, Japan, 700-8530*; E. A. COHEN, *Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109-8099*; K. D. SETZER, and E. H. FINK, *Physikalische Chemie-Fachbereich C, Bergische Universität Wuppertal, D-42097 Wuppertal, Germany*.

The millimeterwave rotational spectrum of BiS in its $X_1\ ^2\Pi_{1/2}$ state was observed in the frequency range of 150-300 GHz. BiS was produced in a high-temperature oven by a discharge in a mixture of Bi vapor and CS2. A White-type multipath cell was used to enhance the absorption pathlength. Near infrared bands of the transition were measured by Fourier-transform emission spectroscopy in the 6400-7400 cm^{-1} region, where BiS was produced by reaction of bismuth and sulfur vapor and excited by collisional energy transfer from the metastable $a^1\Delta_g$ electronic state of O_2. A simultaneous analysis of millimeterwave and FT data was carried out to give rotational, fine and hyperfine constants for the $X_1\ ^2\Pi_{1/2}$ and $X_2\ ^2\Pi_{3/2}$ states. Ninety seven rotational $\Delta J = 1$ features from $J' = 23.5$ to 41.5 and 545 NIR features representing assignments of a wide range of J's were included in the fit. The hyperfine parameters are consistent with those of BiO[a] with slightly less unpaired electron density in the antibonding π orbital on the Bi atom. Examples of the spectra will be shown. The fitting procedure with SPCAT[b] and the resulting parameters will be discussed.

[a] E. A. Cohen, D. M. Goodridge, K. Kawaguchi, E. H. Fink, and K. D. Setzer, J. Mol. Spectrosc. 239 (2006) 16-23.
[b] H. M. Pickett, J. Mol. Spectrosc. 148 (1991) 271-377.