

## 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 CS<sub>2</sub>. 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<sup>-1</sup> 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<sub>2</sub>. 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<sup>a</sup> with slightly less unpaired electron density in the antibonding  $\pi$  orbital on the Bi atom. Examples of the spectra will be shown. The fitting procedure with SPCAT<sup>b</sup> and the resulting parameters will be discussed.

---

<sup>a</sup>E. A. Cohen, D. M. Goodridge, K. Kawaguchi, E. H. Fink, and K. D. Setzer, *J. Mol. Spectrosc.* 239 (2006) 16-23.

<sup>b</sup>H. M. Pickett, *J. Mol. Spectrosc.* 148 (1991) 271-377.