THE ROTATIONAL SPECTRA OF THE $X_1\,^2\Pi_{1/2}$ and $X_2\,^2\Pi_{3/2}$ STATES OF BiO

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BiO has a $^2\Pi_r$ electronic ground state with a fine structure interval of ≈ 7087 cm^{-1} between the X_1 and X_2 states. In an extensive study of the BiO radical Shestakov, *et al.*[b] have determined spectroscopic constants for a total of nine of its electronic states. Their constants derived from the $X_2\,^2\Pi_{3/2} \rightarrow X_1\,^2\Pi_{1/2}$ bands provided an excellent basis for a further investigation by microwave spectroscopy at Nobeyama Radio Observatory. BiO was produced in a flow system by heating Bi to 1120 K in a Knudsen cell and reacting the resulting vapor with an approximately 1:1 mixture of O_2 and Ar in the presence of a dc discharge. A useful side effect of this method of production is the population of highly excited vibrational states of BiO. This is presumably due to collisional energy transfer from the metastable $a^1\Delta_g$ electronic state of O_2. As a result, transitions between vibrationally excited levels up to $v = 9$ in the $X_1\,^2\Pi_{1/2}$ electronic state and $v = 5$ in the $X_2\,^2\Pi_{3/2}$ state have been observed. Thus far, a total of 575 lines have been assigned and fitted using an effective Hamiltonian similar to that of Brown *et al.*[c] A merged fit of near infrared data for the $X_2 \rightarrow X_1$, 0–0 band[d] with the rotational data has resulted in the determination of a very precise set of parameters for that band. There is excellent agreement between the optical and microwave parameters for all levels for which rotational spectra have been obtained. In addition, all of the principal hyperfine parameters for both the X_1 and X_2 states have been determined as well as their vibrational dependence. Only the magnetic hyperfine constant, *d*, has sufficient effect on the optical spectra to have been measured previously. These will be compared to those of related compounds and atomic Bi.

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[b]O. Shestakov, R. Breidohr, H. Demes, K. D. Setzer and E. H. Fink *J. Mol. Spectrosc.* **190**, 28-77 (1998)

[c]J. M. Brown, E. A. Colbourn, J. K. G. Watson and F. D. Wayne, *J. Mol. Spectrosc.* **74**, 294-318 (1979)

[d]E. H. Fink, private communication.