THE NEAR-INFRARED SPECTRUM OF HCBr REVISITED

ANDREW J. MARR and TREVOR J. SEARS, *Department of Chemistry, Brookhaven National Laboratory, Upton, NY 11973*.

High resolution measurements of many new bands in the $\tilde{\mathrm{A}}^1 A^{"} \leftarrow \tilde{\mathrm{X}}^1 A^{'}$ system of bromomethylene have been made by transient absorption spectroscopy using a frequency modulated tunable diode laser. In particular, the doubly excited bending hot band in DCBr, between 10300 and $10550\mathrm{cm}^{-1}$, has been completely rotationally assigned. Its rotational branches indicate that the upper level has rotational structure characteristic of a bent molecule, in contrast to most of those observed previously. The position of this band, together with the rotational assignment of several others in both HCBr and DCBr has led to a correction of the vibrational numbering for all previously observed bands involving bending vibrational excitation in the system. This reconciles an inconsistency noted previously.[a b] Definitive evidence for the position of the low-lying $\tilde{\mathrm{a}}^3 A^{"}$ state of HCBr remains elusive, but the position (approx. 2310 cm-1) of the (020) level in HCBr and its rotational structure do imply that it is perturbed and the triplet state seems the only likely candidate for the perturbing level.

Acknowledgement: This work was carried out at Brookhaven National Laboratory under contract DE-AC02-98CH10886 with the U. S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.

[a] S. Xu, K. A. Beran and M. D. Harmony, J. Phys. Chem., 98, 2742 (1996).

[b] A. J. Marr, S. W. North, T. J. Sears, L. Ruslen and R. W. Field, J. Mol. Spec. 188, 68 (1998).