POTENTIAL ENERGY CURVES OF THE $A\,^1\Sigma^+$ STATES OF AgH AND CuH

DOMINIQUE R.T. APPADOO, ALIREZA SHAYESTEH, PETER F. BERNATH AND ROBERT J. LE ROY,
Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

Some years ago Learner[a] recorded electronic spectra involving the $A\,^1\Sigma^+$ state of AgH, and found anomalous behaviour of the vibrational level spacings and B_v values which he attributed to the potential energy curve for this state having a "shelf". More recently, Witek *et al.*[b] reported *ab initio* results which supported Learner's assertion that the potential energy function for this state had an unusual shape, but found that rather than have a shelf, there was an abrupt stiffening of the bond for vibrational levels above $v \approx 4$. In order to clarify this situation, we have combined new and previously recorded visible $A-X$ spectra and high quality microwave and infrared data for $^{107/109}$AgH and $^{107/109}$AgD in a combined-isotopomer direct-potential-fit analysis which determines analytic potential energy and Born-Oppenheimer breakdown functions for this state. A similar approach is used to study the analogous $A\,^1\Sigma^+$ state of $^{63/65}$CuH and $^{63/65}$CuD.

[a] R.C.M. Learner, *Proc. Roy. Soc. (London)* **A 269**, 327 (1962).
[b] H.A. Witek, A. Viel and P.-O. Widmark, *J. Chem. Phys.* **116**. 8396 (2002).