IS THE EQUILIBRIUM STRUCTURE OF BeOH LINEAR OR BENT?

KYLE J. MASCARITOLO, JEREMY M. MERRITT, and MICHAEL C. HEAVEN,
Department of Chemistry, Emory University, Atlanta, GA 30322.

The hydroxides of Ca, Sr, and Ba are known to be linear molecules, while MgOH is quasilinear. High-level ab initio calculations for BeOH predict a bent equilibrium structure with a bond angle of 140.9°, indicating a significant contribution of covalency to the bonding. However, experimental confirmation of the bent structure is lacking. IR and ESR spectra for matrix-isolated BeOH have been interpreted under the assumption of a linear equilibrium structure. Low resolution electronic spectra have been reported for gas phase BeOH and BeOD[a] but they have not been analyzed. In the present study we have used resonantly enhanced multiphoton ionization, with mass resolved ion detection, to observe the near UV electronic band systems of BeOH and $Be^{18}OH$. Rotationally resolved data have been obtained, which yield preliminary rotational constants. However, the resolution was not sufficient to show the asymmetry splttings that would be expected for a bent geometry. Experiments are now in progress to examine the rotational structure of BeOD, which should provide better constraints on the bond angle in both the ground and excited states. Results for both BeOH and BeOD will be reported.

[a] A. Antic-Jovanonvic, V. Bojovic, and D. Pesic *Spectrosc. Lett.* **21**(8),757-765 1988.