QUASILINEAR EVIDENCE FOR THE EQUILIBRIUM STRUCTURE OF BeOH

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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, and laser induced fluorescence to observe the near UV rovibronic v'-0 bending progression of BeOH and BeOD. Rotationally resolved data have been obtained, which yield rotational constants of the ground and excited states, along with evidence of spin-rotation coupling. Theoretical collaboration with Per Jensen of Bergische Universitt Wuppertal revealed the need for the inclusion of large amplitude motion within the Hamiltonian operator to accurately simulate observed spectra. Inclusion of large amplitude motions indicates BeOH/OD is quasilinear in its ground state.

[a] A. Antic-Jovanovic, V. Bojovic, D. Pesic, *J. Chem. Phys.* **21**1988 (757)