

JET COOLED SPECTROSCOPY OF  $\text{H}_2\text{DO}^+$  : ISOTOPE DEPENDENT TUNNELING DYNAMICS FROM  $\text{H}_3\text{O}^+$  TO  $\text{D}_3\text{O}^+$

FENG DONG, and DAVID J. NESBITT, *JILA, University of Colorado, Boulder, CO 80309*.

High-resolution infrared spectra of jet-cooled  $\text{H}_2\text{DO}^+$  has been observed for the first time, sampling transitions in both the symmetric ( $\nu_1$ ) and antisymmetric ( $\nu_3$ ) OH stretching bands. In addition to the structural information extracted, the tunneling splittings have also been obtained from the fractional populations in the lower and upper tunneling states. This ion represents the last to be observed in the sequential series of isotopically labeled  $\text{H}_3\text{O}^+$ , providing an unusually detailed view into large amplitude dynamics in this most fundamental molecular ion of acid-base chemistry. In conjunction other data on partially deuterated  $\text{HD}_2\text{O}^+$ , undeuterated  $\text{H}_3\text{O}^+$ ,<sup>a</sup> and fully deuterated  $\text{D}_3\text{O}^+$ ,<sup>b</sup> these spectra of  $\text{H}_2\text{DO}^+$  permit unprecedented analysis of structure, tunneling splittings and the ammonia-like inversion dynamics through the planar geometry.

---

<sup>a</sup>D. J. Liu and T. Oka, *Phys. Rev. Lett.* 54 (16), 1787 (1985).

<sup>b</sup>T. J. Sears, P. R. Bunker, P. B. Davies, S. A. Johnson, and V. Spirko, *J. Chem. Phys.* 83 (6), 2676 (1985).