JET COOLED SPECTROSCOPY OF H_2DO^+ : ISOTOPE DEPENDENT TUNNELING DYNAMICS FROM H_3O^+ TO D_3O^+

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High-resolution infrared spectra of jet-cooled H_2DO^+ has been observed for the first time, sampling transitions in both the symmetric (ν_1) and antisymmetric (ν_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 H_3O^+, 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 HD_2O^+, undeuterated H_3O^+,[a] and fully deuterated D_3O^+,[b] these spectra of H_2DO^+ permit unprecedented analysis of structure, tunneling splittings and the ammonia-like inversion dynamics through the planar geometry.

[a] D. J. Liu and T. Oka, Phys. Rev. Lett. 54 (16), 1787 (1985).

[b] T. J. Sears, P. R. Bunker, P. B. Davies, S. A. Johnson, and V. Spirko, J. Chem. Phys. 83 (6), 2676 (1985).