CHARACTERIZATION OF THE WATER DIMER DONOR TORSION VIBRATION BY FIR-VRT SPECTROSCOPY

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A quantitative description of the water dimer potential energy surface has been achieved through a collaborative effort between experiment and theory[a,b,c]. The major features of the surface are well established, but the details of the tunneling dynamics are more elusive. FIR-VRT spectroscopy is being used to characterize the water dimer because it probes the intermolecular vibrations and tunneling splittings which are the key to the detail of the energy surface.

The least energetic of the 6 intermolecular vibrations is the donor torsion. The most recently observed spectra for this motion are the lower fork K_a=1→0 transitions for $(D_2O)_2$ and $(H_2O)_2$ which lie essentially on top of each other around 1600 GHz. The $(D_2O)_2$ transition, coupled with previous data for this cluster, establishes the upper state acceptor switching splitting for J'=1 K_a=0 of the donor torsion as ~ 474 GHz. This AS splitting for $(H_2O)_2$ cannot be calculated because key transitions have not yet been observed, although they have been predicted by recent theoretical work[c]. Further experimentation is needed to completely characterize the donor torsion vibration.

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[a] L.B. Braly, et al. "Terahertz Laser Spectroscopy of the Water Dimer Intermolecular Vibrations. I.$(D_2O)_2$ II. $(H_2O)_2$" *J. Chem. Phys.* **112**, 10293 (2000).

[b] F.N. Keutsch, et al. "Complete Characterization of the $(D_2O)_2$ Ground State: High K_a Rotation-Tunneling Levels." Submitted 2000.

[c] G.C. Groenenboom, et al. "Water pair potential of near spectroscopic accuracy. II.Vibration-rotation-tunneling levels of the water dimer." *J. Chem. Phys.* **113**, 6702 (2000).