PROTON TUNNELING IN FORMIC ACID DIMER

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Formic Acid Dimer (FAD) is a model system for the types of hydrogen bonding structure found in large, biological systems, yet remains theortically tractable. Modeling of the dynamics and tunneling rates of the double proton transfer is an intriguing problem, which requires an accurate representation of the potential barrier. A good measure of the barrier are the tunneling splittings between pair states. Tunneling splitting of FAD for the ground state and with one quantum of CO stretch have recently been measured by Madeja and Havenith (J. Chem. Phys. **117**, 7162 (2002)). We model FAD by inlcuding three degrees of freedom (DOF) in a reaction surface, with all other DOF treated as a set of coupled harmonic oscillators whose frequencies vary across the reaction surface. We use a discrete variable representation to calculate the ground state splitting of 0.0023 cm^{-1} in good agreement with experimental results. Calculations with one quantum of CO stretch are on going.