Nuclear Quantum Dynamics of Malonaldehyde on an ab initio-derived Potential Energy Surface

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The rates of intramolecular proton transfer in malonaldehyde on an ab initio-inspired reactive electronic potential energy surface are estimated using Path-Integral Quantum Transition State theory and the Quantum Instanton approach. Estimates of the kinetic isotope effect using these approximate nuclear quantum dynamics procedures are in reasonable agreement. Using Centroid Molecular Dynamics, we also estimated the tunnel splitting. Improvements and extensions of this practical yet chemically accurate framework for the molecular dynamics simulation of reactive nuclear quantum dynamics are also discussed.