A DIFFUSION MONTE CARLO STUDY OF $H_5O_2^+$

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The protonated water dimer, $H_5O_2^+$, is an interesting case for vibrational study because it is the smallest aqueous proton transfer system. The potential energy surface has been extensively studied theoretically, and some reduced dimensionality calculations of the vibrational structure have recently appeared. The major difficulty in understanding this system lies in the strong coupling between anharmonic low frequency coordinates, among them motion of the central proton, which is associated with the most intense vibrational modes. In our study, the Diffusion Monte Carlo method is employed for a full-dimensional treatment of the system. Full-dimensional calculations are needed to benchmark the more approximate treatments of this molecule, and to provide a guide for the couplings that might be safely neglected. We have recently developed an improved trial wave function for $H_5O_2^+$ which, when employed as a guiding function for DMC, gives a very robust estimate of the zero-point energy of the $H_5O_2^+$ ion. Zero-point fluctuations in the ground-state are discussed with particular attention given to assessing the degree of coupling between several angular coordinates, torsions, and the central proton motion.