INVESTIGATION OF LARGE-AMPLITUDE MOTIONS OF H_5^+ AND THE DYNAMICS OF THE PROTON TRANSFER BETWEEN H_3^+ and H_2

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Protonated hydrogen dimer, or H_5^+, is the intermediate of the proton-transfer reaction between H_3^+ and H_2. The dynamics of this reaction has been postulated to play a significant role in the non-thermal H/D and ortho-/para- ratio in the interstellar clouds. As a weakly-bound, fluxional molecular ion, H_5^+ has a very rich vibrational spectrum. The large-amplitude vibrational motions of H_5^+ make theoretical studies interesting but challenging. This work aims at understanding how these large-amplitude motions are reflected in the dynamics of the proton transfer between H_3^+ and H_2, or between the deuterated analogues of these two species. The shared-proton stretch mode is closely related to the proton-transfer process and is thus of particular interest. Diffusion Monte Carlo calculations of minimum energy paths[a] are performed for the ground state and selected excited states, in order to explore how the vibrational energetics and wavefunctions evolve as H_5^+ dissociates into H_3^+ and H_2. The effects of deuteration on the structures and properties are also investigated.

[a] C. E. Hinkle and A. B. McCoy, J. Phys. Chem. Lett., 1, 562 (2010)