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On the Rate and Mechanism of Proton Transfer Reactions in Proteins¹ AIHUA XIE, YUNXING LI, EDWARD MANDA, BEINING NIE, WOUTER HOFF, Oklahoma State University, RICHARD MARTIN, Los Alamos National Lab — One of the fundamental processes in molecular biology is proton transfer reactions in proteins. Proton transfer is essential for the biological functions of proteins responsible in bioenergetics, biological signaling, and enzymatic catalysis. The mechanism of proton transfer is of great interests in order to understand the structural basis of biological functions. Despite of extensive experimental and computational efforts, it remains elusive what causes a proton to move from the proton donor to the proton acceptor. We will report a proof of concept study regarding a general mechanism of internal proton transfer reactions in proteins. Density functional theory, B3LYP/6-311+G(2d,p), is employed in this study. The results of our study provide deep insights into the structural basis to the rate and mechanism of proton transfer reactions in proteins, such as bacteriorhodopsin and green fluorescence protein.

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