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The Effect of Isotopic Substitution on Quantum Proton Transfer Across Short Water Bridges in Biological Systems[1] JACOB BLAZEJEWSKI, CHASE SCHULTZ, JAMES MAZZUCA, Alma College — Many biological systems utilize water chains to transfer charge over long distances by means of an excess proton. This study examines how quantum effects impact these reactions in a small model system. The model consists of a water molecule situated between an imidazole donor and acceptor group, which simulate a fixed amino acid backbone. A one dimensional energy profile is evaluated using density functional theory at the 6-31G*/B3LYP level, which generates a barrier with a width of 0.6 Å and a height of 20.7 kcal/mol. Quantum transmission probability is evaluated by solving the time dependent Schrödinger equation on a grid. Isotopic effects are examined by performing calculations with both hydrogen and deuterium. The ratio of hydrogen over the deuterium shows a 130-fold increase in transmission probability at low temperatures. This indicates a substantial quantum tunneling effect. The study of higher dimensional systems as well as increasing the number of water molecules in the chain will be necessary to fully describe the proton transfer process.

[1]Alma College Provost's Office

Jacob Blazejewski
Alma College

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