

BERNSTEIN LECTURE



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4:00 PM

2033 Young Hall

“Extreme chemical reactivity in solution and in gas phase”

Acid-base equilibria drive most chemical reactions and are paramount for sustaining life processes. Stronger acids or bases are associated with a greater driving force, related to the greater Gibbs free energy of reaction. Unfortunately, the use of very strong acids or bases is limited because they are not compatible with the medium where the reaction takes place. For example, concentrated sulfuric acid reacts violently with most solvents. Fortunately, extreme acidity or basicity can be achieved by harnessing the energy of photons. A change of electronic configuration can bring about orders of magnitude greater acidity or basicity. This last statement will be illustrated by the characterization of the a super photobase. This compound (FR0-SB), with pK_a of 7 in the ground state has a pK_a^* of 21 in the excited state [*Angew. Chem. Int. Ed.* 57, 14742 (2018)]. Even more extreme reactivity can be achieved in the gas phase via strong laser field ionization. For example, alcohols under strong laser fields undergo exotic chemical processes involving making and breaking of multiple chemical bonds that result in the formation of H_3^+ , H_2O^+ , and H_3O^+ . The formation of H_3^+ , following strong-field photodissociation of methanol, is preceded by the formation of a neutral H_2 molecule that roams the parent ion and extract a proton [*Sci. Rep.* 7, 4703 (2017)]. Site-specific details and femtosecond time-resolved dynamics of H_3^+ formation for a series of alcohols have been obtained through a combination of time-resolved mass spectrometry, photoion-photoion coincidence measurements, and *ab initio* calculations [*Nat. Commun.* 9, 5186 (2018)]. The yield of these and related strong-field reactions has been recently found to be sensitive to the spectral phase of femtosecond laser pulses [*J. Chem. Phys.* 150, 044303 (2019)]. The existence of organic molecules and water in the universe is due in great part to the existence of H_3^+ , because, as a Brønsted–Lowry acid, H_3^+ donates protons to carbon and oxygen atoms as well as to more complex organic molecules. Our findings provide mechanistic and dynamic information about the chemistry of H_3^+ .