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Electron Impact Ionization and Fragmentation of Bio-Relevant Molecules: Hydration Dependence

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Ionizing radiation penetrating biological tissue produces large numbers of low-energy secondary electrons which effectively induce damages in molecules. Here we discuss the influence of hydration on electron impact ionization of organic molecules, i.e. how water which is hydrogen bonded to the target molecule affects the reaction. As a model system we use tetrahydrofuran (THF, C_4H_8O) a five membered ring that is often regarded as the simplest surrogate for the sugar deoxyribose in the DNA backbone. Oxygen in THF is capable of one hydrogen-bonding link to water and forms reasonable simple THF-water dimers for which gas phase experiments and also electronic structure calculations are feasible. In contrast to the naive expectation that a water environment quenches THF fragmentation we find that water even catalyzes THF ring-break reactions. Compared to the THF monomer in the dimer the reaction barrier for the ring-break reaction is reduced by 3 eV and in hydrated THF ionization of the HOMO is sufficient to break the molecular ring. Qualitatively we can reproduce this observation by quantum chemical calculations. Furthermore, we were able to experimentally identify intermolecular Coulombic decay (ICD) in the THF-H_2O dimers [1]. In this energy transfer process an inner-valence electron-vacancy in the water molecule decays by ionizing the neighboring THF molecule. Therefore, ICD can produce rather severe damage in a biological system. These experiments were done at an impact energy of $E_0 = 67$ eV using a reaction microscope. For ionization of monomers and clusters produced in a supersonic jet two outgoing electrons were detected in coincidence with one or two ions. [1] X. Ren, E. Wang, A. D. Skitnevskaya, A. B. Trofimov, K. Gokhberg and A. Dorn, Nature Phys. **14**, 1062 (2018).