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Dissociative Electron Attachment to Biomolecules.¹

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Dissociative electron attachment (DEA) to biomolecules plays an essential role in radiation damage initiated by high-energy radiation. A variety of biomolecular systems, including DNA, RNA, and proteins constituents have been the focus of a lot of the DEA experimental work over last two decades [1]. These studies showed rich fragmentation patterns formed via resonant electron capture into one of the metastable valence states of a molecule. However, resonance characterization still remains challenging in spite of a number of theoretical and experimental attempts. Therefore, our recent work focuses on targets, such as amides, that can be considered models for larger biologically relevant molecules, that are peptides. The choice of these simpler systems, containing amide bonds, was dictated by a possibility of performing high-level electronic structure calculations and a possibility of studying them in the gas phase. In this talk, we present our results of experimental and computational studies of the gas-phase DEA to three prototypical peptide molecules, formamide, N-methylformamide (NMF), and N,N-dimethylformamide (DMF). In addition to careful investigations of all fragments formed via DEA [2], our great focus has been on amide bond rupture. Interestingly, a double-resonant structure was observed at similar energies in the ion yields for all ions resulting from this C-N bond cleavage, such as NH₂⁻ for formamide, NHCH₃⁻ for NMF, and N(CH₃)₂⁻ for DMF. Several of possible mechanisms of electron attachment were considered computationally in order to characterize these peaks. Based on our calculations, these resonances can be assigned to core-excited dipole-supported resonances populated upon DEA [3]. Our results suggest that the formation of “spin-forbidden” dipole-supported resonances can be of a general implication of DEA to larger biological complexes, containing the amide bond. [1] J.D. Gorfinkiel, S. Ptasinska - Electron scattering from molecules and molecular aggregates of biological relevance. *Journal of Physics B: Atomic, Molecular, Optical Physics* (2017) 182001 [2] M.M. Dawley, S. Ptasinska - Dissociative electron attachment to gas-phase N-methylformamide, *International Journal of Mass Spectrometry* 365-366 (2014) 143-151 [3] Z. Li, M. Ryszka, M.M. Dawley, I. Carmichael, K. Bravaya, S. Ptasinska - Dipole-supported electronic resonances mediate electron-induced amide bond cleavage. *Physical Review Letters* (2019) in press

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