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Resonance formation in biological molecules¹

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Resonances (temporary anion states) can enhance non-dissociative electron-induced processes and be chemistry initiators by leading to the production of reactive species. They are also important in other processes like photo-detachment. Their theoretical identification and characterization is therefore crucial for the understanding of a number of electron-induced processes in biological systems. Electron-molecule scattering approaches have been successfully applied to resonance identification and characterization: shape resonances can be accurately described by a number of them both for small and larger, biological molecules. Core-excited resonances, that involve the electronic excitation of the target molecule, are harder to model accurately. However, both types of resonances (and vibrational Feshbach resonances) play an important role in biological processes like radiation induced damage and electron transfer reactions. Recent joint theoretical-experimental work [1,2] has confirmed the ability of R-matrix [3] method to accurately describe core-excited resonances in biologically relevant molecules. Biological processes occur in a condensed environment where molecules with a biological function are surrounded by water. Hydrated clusters are being investigated as systems that bridge the gap between the pure gas phase and the actual environment in which these collisions take place. Small clusters can be treated using the same ab initio methodology as isolated molecules. Using the R-matrix approach, simple calculations of electron scattering from pyridine-(H₂O)_n and thymine-(H₂O)_n with $n=1,2,3,5$ have been performed and the effects of microhydration analyzed. The results have been linked to recent experiments on microsolvated uracil and thymine [4]. [1] Regeta K, Allan M, Mašín Z and Gorfinkiel J D 2016 *J. Chem. Phys.* **144**, 024302. [2] Loupas A, Regeta K, Allan M and Gorfinkiel J D 2018 *J. Phys. Chem. A* **122**, 1146. [3] Tennyson J 2010 *Phys. Rep.* **491**, 29. [4] Gorfinkiel J D and Ptasinska S 2017 *J. Phys B.* **50**, 182001.

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