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Electron attachment to molecules of biological relevance

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Free electron attachment to biomolecules in the electron energy range from about 0 – 15 eV has been studied. The experiments have been carried out using a homebuilt crossed electron/neutral beams apparatus in combination with a quadrupole mass spectrometer described in detail in [1]. The electrons are monochromatized in a high resolution hemispherical electron monochromator with an energy resolution of about 110 meV in the present experiments. The biomolecules under study include thymine, alanine, glycolaldehydes, thymidine, uridine and uracil. In this presentation we want to focus on one particular experiment, where bond-selective H- ion abstraction by electron attachment to thymine has been studied [2]. This study has been performed using partially deuterated thymine to enable the measurement of electron attachment to certain bonds in the molecule. The results are particularly interesting as certain sites of the isolated molecules are not available (or even not present) when they are incorporated in the DNA structure. Therefore the present results can be used to evaluate the previously reported DEA to isolated undeuterated bases concerning their importance for real DNA environments. In particular the radiation damage due to (dissociative) anionic resonance states are assumed to be critical intermediates leading to DNA strand breaks. To support the experimental results we have also performed quantum chemical studies using the G2(MP2) method. In collaboration with Stephan Denifl, Sylwia Plasinska, Michael Probst, Paul Scheier, and Tilmann Maerk, Institut für Ionenphysik, Leopold-Franzens-Universität Innsbruck.

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[1] D.Muigg, G. Denifl, A. Stamatovic, T.D.Märk, *Chem. Phys.* 239 (1998) 409

[2] S. Ptasinska, S. Denifl, V. Grill, T.D. Märk, P. Scheier, S. Gohlke, M.A. Huels and E. Illenberger, Bond-Selective H⁻ Ion Abstraction from Thymine. *Angew. Chem. Int. Ed.* **44** (2005) 1647–1650