State-dependent Fragmentation of Protonated Uracil and Uridine Supporting Information for Publication

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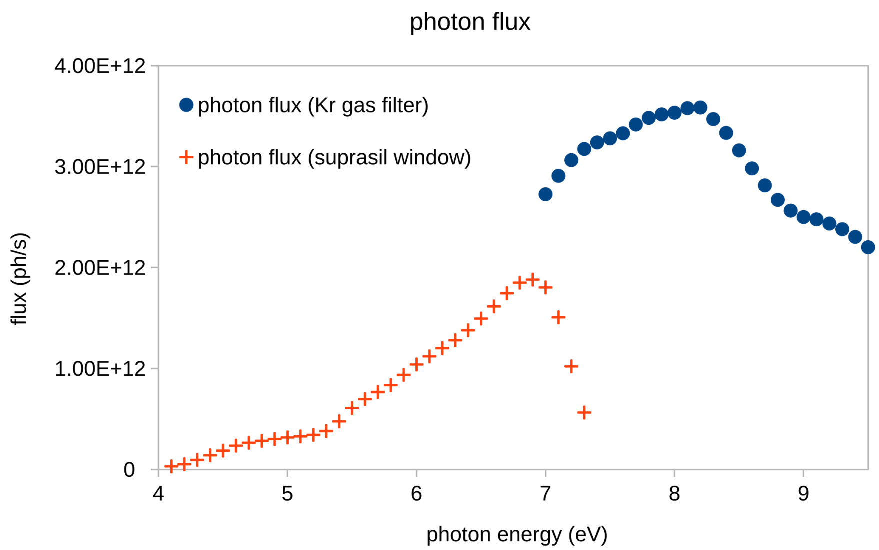

Figure 1: Photon flux of the beamline as a function of energy. Different strategies to block higher orders of the synchrotron light were used: In the low energy region, a suprasil window was used to block light above 7.2 eV, in the high energy region, krypton was used (1). The global factor between the two settings was accounted for by multiplying the fragment yields in the high-energy region by a constant factor of 1.9 (as determined from the overlap in the mass spectra, see main text).

(1) Nahon, L.; de Oliveira, N.; Garcia, G. A.; Gil, J.-F.; Pilette, B.; Marcouillé, O.; Lagarde, B.; Polack, F. DESIRS: a state-of-the-art VUV beamline featuring high resolution and variable polarization for spectroscopy and dichroism at SOLEIL. Journal of Synchrotron Radiation 2012, *19*, 508-520.

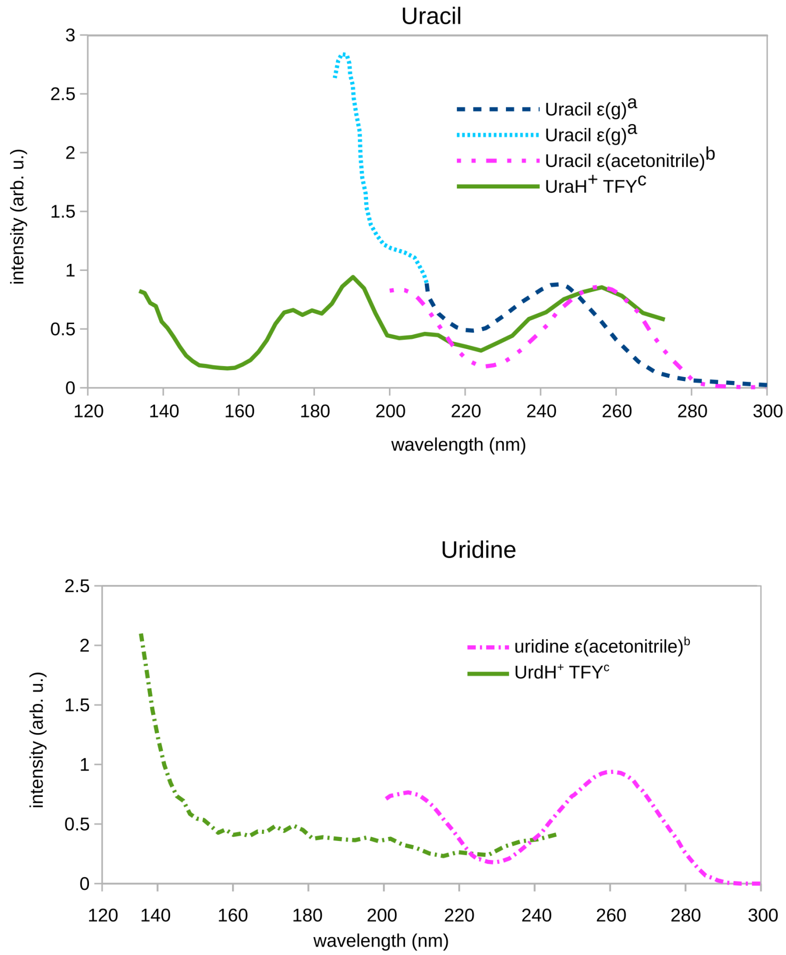

Figure 2: Top: Total fragment yield (TYF) of protonated uracil compared to extinction measurements in the gas phase (blue) and in acetonitrile solution (magenta). a: Ref. 2, b: Ref. 3, c: this work. For better comparison with the extinction measurements, all data are plotted as a function of wavelength.

(2) Clark, L. B.; Peschel, G. G.; Tinoco, I. Vapor Spectra and Heats of Vaporization of Some Purine and Pyrimidine Bases. The Journal of Physical Chemistry 1965, 69, 3615-3618.

(3) Kobayashi, T.; Kuramochi, H.; Suzuki, T.; Ichimura T. Triplet formation of 6-azauridine and singlet oxygen sensitization with UV light irradiation. Physical Chemistry Chemical Physics 2010, 12, 5140-5148

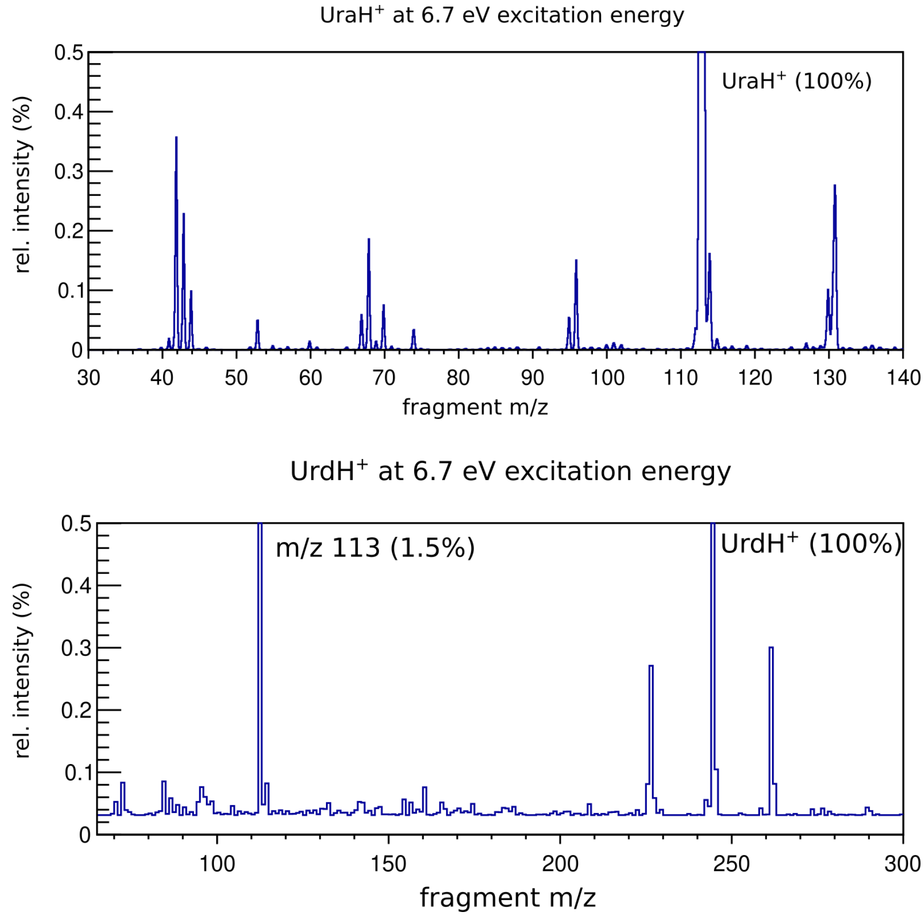

Figure 3: Fragment mass spectra of protonated uracil (top) and protonated uridine (bottom) after excitation with a photon energy of 6.7 eV (5s irradiation time). The intensity is normalized to the precursor. In both cases, the hydrated species (MH + 18 Da) can be seen at low abundance as well.