Anionic states of 5-cyanateuracil (5-OCNU) and 5-thiocyanateuracil (5-SCNU)

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Synopsis We present the calculated anion state spectra of the 5-cyanateuracil and 5-thiocyaniteouracil molecules in gas phase, as obtained from the integral cross section for the electron scattering of both systems. The calculations were performed using the Schwinger Multichannel method for the scattering amplitude. The anion states were given by the analysis of the resonances in the cross section signature.

The incidence of ionizing radiation in biological environment can lead to the formation of secondary species, in which low-energy electrons (LEEs) are the most abundant. Since the damaging properties of LEEs were first observed[1] the interactions between electrons with biomolecules have been widely studied both theoretically and experimentally.

Radiosensitizers are molecules that can enhance the damaging effects of LEEs to DNA in tumour cells therefore making cancer treatments more efficient. Using electronic structure technics for bound states, Bowen *et al.*[2] recently pointed 5-cyanateuracil (5-OCNU) and 5-thiocyanateouracil (5-SCNU) would be candidates for new radiosintesizers. When interacting with those molecules, LEEs could be trapped in vacant π^* orbitals and then be transferred to σ^* orbitals with significant probability on the C-X (X=OCN,SCN) bonds.

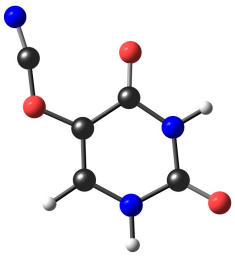

Figure 1: 5-OCNU in its planar geometry.

In the present work, we report a study on the anion spectra of 5-OCNU and 5-SCNU employing collisional techniques. We performed the calculations using the Schwinger Multichannel (SMC) method with pseudopotentials[3] for the integral cross sections in the static-exchange (SE) (Fig.1) and static-exchange plus polarizationn (SEP) aproximations.

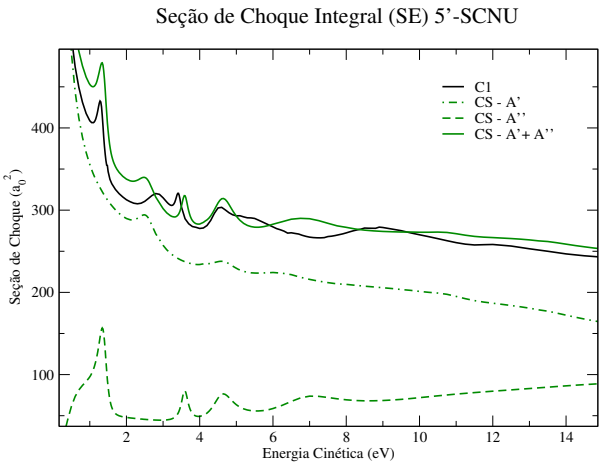

Figure 2: Integral cross section of 5-SCNU in the SE aproximation.

The anionic states of the systems are given by the analysis of the resonances in the cross section signature.

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References

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