Low-energy electron collisions with uracil

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The mechanism for the lethal damage caused by any ionizing radiation on the living tissue is by far now quite well known [1]. It is the free secondary low-energy electrons produced by irradiation upon the cellular matter which causes the further damage by forming temporary anions or *resonances* with the cell molecules. In order to study such processes it is therefore important to identify and characterize these resonances in various constituent molecules of the cell.

With the aim of studying the resonant processes in nucleic acid bases and other constituent cell molecules, we are currently studying uracil molecule in the gas phase using *ab initio* theoretical methods. The theoretical method employed in this work is the *R*-matrix method. The UK polyatomic *R*-matrix code [2] is used in this study. Results have been obtained for eigenphases and total cross section by using various models and basis sets. The results show the existence of three low-lying shape resonances of π symmetry and apparently no resonance in σ symmetry. These results compare very well with those of Winstead and McKoy [3] obtained with Schwinger multichannel method. Our latest results on this problem will be presented at the conference.

References

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