AB INITIO R-MATRIX STUDY OF ELECTRON SCATTERING FROM TETRAHYDROFURAN

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In the last decade, low energy electron (LEE) scattering from biomolecules, and in particular from DNA constituents, has attracted considerable interest. It has been demonstrated [1] that not only primary high-energy radiation but also secondary LEEs can induce DNA damage. These electrons, produced by the ionizing radiation with energies below 20 eV, are the most abundant [2]. They can form resonant states when they scatter from DNA, which may lead to the fragmentation of the molecule via dissociative electron attachment (DEA). Indeed, DEA has been shown to be the main process of LEE induced DNA damage [3].

Tetrahydrofuran (THF), C_4H_8O, is of particular interest in the study of electron scattering on DNA, as it is the simplest model for the deoxyribose ring. Ptasińska et al. [4] recently showed that deoxyribose is extremely fragile compared to the nucleobases. Several experiments have been performed on this system (see [5] and references therein) both in gas and solid phase, but until now, no theoretical study was available.

In spite of the availability of several theoretical methods to treat low-energy electron-molecule collisions, processes involving DNA bases, sugars, etc. have hardly been treated. The size of these molecules (number of nuclei and electrons) presents an immense challenge to these methods that, until very recently, have been only applied to small molecules. Fortunately, this challenge is essentially computational.

We performed *ab-initio* calculations for electron collisions on THF within the fixed-nuclei approximation for incident electron energies up to 10 eV. For this purpose, we used the UK molecular R-matrix codes [6]. Of special interest were the lifetime and position of the resonant states that lead to DEA. THF is by far the biggest molecule ever treated with the R-matrix method. In addition, some of its low-lying electronic states have Rydberg character. This requires the use of diffuse basis sets and bigger R-matrix boxes (the standard box radius used in the calculations is 10 a_0).

Several target models using different basis sets and different state averaging procedures to generate natural orbitals were tested as the threshold for excitation is particularly sensitive to the diffuse character of the basis. Especial care was taken when testing the convergence of our results with the radius of the R-matrix box and the number of states included in the close-coupling expansion. No shape resonances were found for this system, but a few core-excited resonances were present in the energy region spanning the first 8 excited states.

Results for cross sections and resonance parameters will be discussed and analysed.

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