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“Application of binary-encounter-Bethe method to electron-impact ionization cross section calculations for biologically relevant molecules”

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APPLICATION OF BINARY-ENCOUNTER-BETHE
METHOD TO ELECTRON-IMPACT IONIZATION
CROSS SECTION CALCULATIONS FOR
BIOLOGICALLY RELEVANT MOLECULES

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Abstract. Electron-impact cross sections for platinum chemotherapeutic compounds, purine and pyrimidine molecules calculated using binary-encounter-Bethe model are presented as examples of possible applications of that method.

1. INTRODUCTION

It is well established now, than low- and intermediate-energy electron interactions should be taken into account in the studies of the processes induced within biological material by primary ionizing radiation [1].

One of the most important process which occurs in electron scattering from molecules is the electron-impact ionization. The maximum of efficiency of that process generally is located between 70-100 eV for large number of molecular target. The threshold for ionization process for polyatomic molecules is usually located within 7-11 eV energy range. Thus it is evident that the above energy ranges coincide with typical energies of the secondary electrons in biological media. The objective of that contribution is to show applicability of the binary-encounter method to electron-impact ionization cross section evaluation for biologically relevant targets and to present selected recent and new results.

2. THEORETICAL METHOD

Due to the binary-encounter-Bethe method (BEB) [2,3] the electron-impact ionization cross section of a given molecular orbital can be calculated according to:

\[ \sigma^{\text{BEB}} = \frac{S}{t + u + 1} \left[ \ln t \left( 1 - \frac{1}{t^2} \right) + 1 - \frac{1}{t} \ln t \right], \]

where \( u = U/B \), \( t = T/B \), \( S = 4\pi a_0^2 N R^2 / B^2 \), \( a_0 = 0.5292 \text{ Å} \), \( R = 13.61 \text{ eV} \), and \( T \) is the energy of impinging electron. The total cross section for electron-impact
ionization can be obtained as a sum of ionization cross sections calculated for all molecular orbitals:

\[ \sigma_{\text{ION}}^{\text{XON}} = \sum_{i} n_{\text{MO}} \sigma_{i}^{\text{BEB}} \]

(2)

Where \( n_{\text{MO}} \) is the number of the given molecular orbital. It is extremely important that in the BEB method there is no free parameter. All quantities have well defined physical meaning and can be quite precisely evaluated. The electron binding energy, \( B \), kinetic energy of the given orbital, \( U \), and orbital occupation number, \( N \), should be calculated for the ground state of the geometrically optimized molecules. Such calculations can be performed with quantum chemistry computer codes like GAUSSIAN [4] using appropriate basis set. In our works we have performed calculations at the Hartree-Fock level with, if it is possible, Gaussian basis set. Obtained that way, ionization energies are not precise enough and are usually higher more than 1 eV from experimental ones. For this reason we have usually performed also outer valence Green function (OVGF) calculations of ionization potentials [5] using the GAUSSIAN code.

3. METHOD APPLICABILITY AND SELECTED RESULTS

In Figure 1 total electron-impact ionization cross sections calculated for tetrahydrofuran (C₄H₈O) molecules [6] is compared with experimental results [7].

![Figure 1](image)

**Figure 1.** Comparison of total electron-impact ionization cross sections calculated [6] and measured [7] for tetrahydrofuran molecule.

The agreement between results of calculations with experimental data is quite satisfactory, especially for energies higher than 200 eV.
Having in hands such promising proof of the applicability of the BEB method we have applied that approach in the calculations of ionization cross sections for targets for which, due to its nature, measurements in the absolute scale can be extremely difficult. In Figure 2 we have compared ionization cross sections for cisplatin, carboplatin and oxaliplatin [8,9] molecules. These compounds are popular anticancer drugs, which can induce damage to tumors via their interactions with DNA. The most striking feature of ionization total cross sections for these compound is the fact that the value of the ionization cross section peak for cisplatin is about 1.9 and 1.8 times lower than those for oxaliplatin and carboplatin, respectively.

![Figure 2](image)

**Figure 2.** Comparison of total electron-impact ionization cross section calculated for platinum based chemotherapeutic compounds: cisplatin [8], carboplatin [9] and oxaliplatin [9].

In Figure 3 we have presented results of our recent calculations of electron-impact ionization cross section for pyrimidine and purine molecules. Purine molecule is one of the most occurring nitrogen-containing heterocyclic molecule and it is a base compound of guanine and adenine. Pyrimidine molecule can be regarded as base compound of cytosine, thymine and uracil. Calculations have been performed within 6-311 G basis set. The ionization threshold energies obtained with OVGF method are equal to 9.068 eV for purine and 9.151 eV for pyrimidine molecules. Ionization cross section for purine is much higher than those for pyrimidine in the whole studied energy range. For purine molecule cross section maximum of $17.53 \times 10^{-20}$ m$^2$ is located at 80 eV. Cross section maximum for pyrimidine of $12.47 \times 10^{-20}$ m$^2$ is peaked at 75 eV.
Figure 3. Electron-impact ionization cross sections calculated for purine and pyrimidine molecules.

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