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Electrons and positrons elastic collisions with pyrimidine and tetrahydrofuran

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HIGHLIGHTS

- Calculate ECS in nucleobases in low and high e^- and e^+ energies.
- Improves ECS at high energy in comparison to existing data or using the IAM-SCAR.
- Correct existing positron ECS cited in literature using IAM-SCAR model.
- Provide a compilation of ECS, EMFP, TECS and TMFP.

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ABSTRACT

The present study shows results of theoretical calculations for positrons and electrons elastic scattering from pyrimidine and tetrahydrofuran over a broad energy range. The work has been motivated by the fact that very few experimental data exist for most of the nucleobases in particular for positrons. Concerning the theoretical tool, we have made improvements on the method using the independent atom-screened additivity rule by calculating differential elastic cross sections and its integrals in a straightforward manner. Moreover, elastic scattering of electrons and positrons by atoms of the biomolecule was evaluated by means of relativistic (Dirac) partial wave analysis. Results concerning the total elastic cross sections (ECS) for electrons and positrons are shown and discussed in comparison to existing experimental and theoretical data. As central result, our electron ECS from pyrimidine and tetrahydrofuran are in good agreement with existing experimental data in the range 10 eV to 1 keV. Another important improvement concerns our data for positron; as it will be shown in the present study, our positron ECS can be considered as a correction of existing data in the literature using the independent atom screened additivity rule. Parameterization of our electron and positron total ECS, elastic mean free paths, first elastic transport cross sections and first elastic transport mean free paths are provided for pyrimidine and tetrahydrofuran in the energy range 10 eV to 100 keV.

1. Introduction

In the last decade, electron interactions with biomolecules have been a subject of a considerable interest in a wide variety of fields of study as well as Physics and Medicine, both theoretically and experimentally (Palihawadana et al., 2013; Ferraz et al., 2013). This is the result of present widespread use of ionizing radiation in medical practice for both imaging and therapy, throughout the world and understanding physicochemical phenomena in various environments (Nikjoo et al., 2016a). Positron interactions with biomolecules has also entered a new phase of research and they are being used in an increasing number of contemporary applications in technology and medicine (Ferraz et al., 2013). These include their use in the treatment of tumors and medical imaging via positron emission tomography (PET) (Anderson et al., 2014). Experimental studies in the case of positron scattering encounter similar problems plus some additional difficulties due to the significantly reduced incident positron fluxes (Sanz, 2014). From the theoretical point of view, despite the fact that no exchange effects are present, positron collisions are harder to model than the equivalent scattering of electrons. This is mainly due to the occurrence of positronium formation and the strong correlation-polarization interaction. This is reflected in the data available in the literature for positron collisions, which is much scarcer than in the electron case (Sanz, 2014).

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First experimental studies on the electron-scattering cross sections of DNA constituents were carried out mainly on tetrahydrofuran (THF), which is commonly used as substitute for deoxyribose composing the backbone of the DNA (Baek et al., 2014). With the ability of low-energy electrons to attach to DNA and induce single and double strand breakage, electron interactions with THF have received considerable attention from the electron scattering communities in recent years (Duque et al., 2015)and have been widely studied experimentally. Up to now only few cross sections for positron interactions with THF can be found in the literature.

THF is an organic compound. It is classified as a heterocyclic compound$(CH_2)_4O$, specifically cyclic ether with an exposed oxygen atom available for hydrogen bonding. This particularity in its structure makes it one of the most polar of the simple ethers and an interesting species to investigate from a more fundamental perspective (Chiari et al., 2013a).

Currently, there has also been great interest in studying other biological molecules, such as pyrimidine (PY) which is called heterocyclic compound, because it is made out of different kinds of atoms in the shape of a ring and it is also an aromatic organic planar compound (Katritzki and Pozharski, 2000).

PY(C4H4N2) with the composition is one of the three diazines, six membered heterocyclic with two atoms at positions 1 and 3 in the ring (Katritzki and Pozharski, 2000). Cytosine ($C_4H_5N_3O$), thymine ($C_5H_6N_2O_2$) and uracil ($C_4H_4N_2$) are all examples of pyrimidine; each with different chemical groups. It has also some interesting physicochemical properties that make it an appealing molecule to study from a fundamental perspective. These include a relatively large dipole polarizability and dipole moment, and electron charge cloud with a significant spatial extension (Palihawadana et al., 2011).

To calculate ECS for electron and positron scattering from biomolecules cited below, we have applied an independent atom model with a geometrical screening correction for each atom from the rest of the molecule by means of the screen corrected additivity rule procedure. In that case and to provide the elastic scattering of electrons and positron by atoms, we have used the relativistic (Dirac) partial wave analysis at incident energies between 10 eV and 100 keV. At low and intermediate energies (says less than 1 keV), the screening effect of all atoms contributing to the elastic collision is very strong; when the incident energy increases, the screening decreases and disappears completely at higher energies. At very high energy (greater than keV), the ECS can be easily evaluated by means of the additivity rule and the result rely on the accuracy of the atomic ECS. At very low energies, screening between atoms is important but other quantum effects should be considered. R-Matrix method (Burke, 2011) is more appropriate for few eV incident energies. Effects such rotational and vibrational excitations affect the differential ECS at very low energies; a useful approach known as ePOLYSCAT (Gianturco et al., 1994; Sanna and Gianturco, 1998) can be used to calculate the state-to-state rotationally elastic and inelastic differential cross section or alternatively POLYDCS (Gianturco and Lucchese, 2004) to calculate the differential elastic cross section (DECS) for polar molecules like PY. Rotational excitations cross sections decrease rapidly with increasing incident electron energy; At 100 eV incident electron energy, rotational excitation cross sections calculated in ref (Sanz et al., 2014) affect the electron DECS calculated from PY by 15% and drop to less than 5% at 150 eV. For polar molecules with important dipole moment, a first order corrective term to the DECS can be included in the model (Sanz et al., 2014, 2012) using the correction suggested by Dickinson (Dickinson, 1977). For energies greater than 60 eV, the dipole correction introduces small effect on the DECS in PY and THF in particular at medium and large scattering angles; the corresponding integral ECS are not truly affected. In Ref. Sanz et al. (2014), results concerning the DECS agree with experiment when rotational excitations and dipole correction are not included. In our theoretical model we calculate the ECS, rotational excitations and dipole correction are not considered.

The present study focuses on the effect of the screening between atoms of the biomolecule where atomic cross sections are calculated using Dirac partial wave Analysis. The validity of the present model will be discussed mainly at low and intermediate energy (above ~ 100 eV) where screening is important. Rotational excitations and dipole effect are neglected at these energies. At few keV incident energies, screening effect between atoms vanishes rapidly; consequently, our model reduces to a simple independent atomic model. In the following, details of the present study will be given in contrast of existing models using screening additivity rule and atomic cross section calculated from Schrödinger equation (Sanz, 2014; Blanco and García, 2004, 2007, 2009; Blanco et al., 2013; Fuss, 2013).

In the next section we review equations required to calculate positron and electron total ECS from PY and THF molecules; The resulting ECS are presented and compared to experimental and theoretical data available in the literature. Parameterization with simple analytic fitting expressions of our elastic and transport cross sections with their corresponding mean free paths are also provided; they can be used for Monte Carlo simulations of the transport of positrons and electrons in biomolecules. We end by concluding on the differences observed between the electron and positron elastic scattering.

2. . Theory and computation

In order to calculate ECS for electron and positron scattering from biomolecules cited bellow, we have used a corrected form of the independent atom method which reduces to the problem of collision with individual atoms by assuming that each atom of the molecule scatters independently. It must be noted that this treatment makes no use of molecular symmetry considerations but requires only data on atomic total cross sections and atomic positions in the biomolecule. This correction is described by an introduction of the screening effect of all atoms of the biomolecule. The method takes into account the geometry of the molecule (atomic and bond lengths) by using screening coefficients which adjust both the differential and integral cross sections, especially for lower energies and intermediate energies. This method has been extensively used in Refs. Sanz (2014), Blanco and García (2004, 2007, 2009), Blanco et al. (2013) and Fuss (2013) but as it will be shown in the following, our model differs in the derivation of the elastic differential cross section.

The additivity rule for a molecule composed of N atoms leads to the total ECS given as;

$$\sigma^{el} = \sigma_1^{el} + \sigma_2^{el} + ... + \sigma_N^{el} = \sum_{i=1,N} \sigma_i^{el} \tag{1}$$

where σ_i^{el} is the total ECS of each atom i of the molecule.

Introducing screening coefficients s_i to the additivity rule results in;

$$\sigma^{el} = s_1\sigma_1^{el} + s_2\sigma_2^{el} + ... + s_N\sigma_N^{el} = \sum_{i=1,N} s_i\sigma_i^{el} \tag{2}$$

which can be written as;

$$\int_0^\pi \frac{d\sigma^{el}}{d\theta}d\Omega = s_1\int_0^\pi \frac{d\sigma_1^{el}}{d\theta}d\Omega + s_2\int_0^\pi \frac{d\sigma_2^{el}}{d\theta}d\Omega + ... + s_N\int_0^\pi \frac{d\sigma_N^{el}}{d\theta}d\Omega \tag{3}$$

where $\Omega = 2\pi sin\theta d\theta$ with $\theta = [0 - \pi]$, the polar angle; Coefficients s_i depend only on the atomic total ECS, therefore;

$$\int_0^\pi \frac{d\sigma^{el}}{d\theta}d\Omega = \int_0^\pi (s_1\frac{d\sigma_1^{el}}{d\theta} + s_2\frac{d\sigma_2^{el}}{d\theta} + ... + s_N\frac{d\sigma_N^{el}}{d\theta})d\Omega \tag{4}$$

The differential ECS is given as

$$\frac{d\sigma^{el}}{d\theta} = s_1\frac{d\sigma_1^{el}}{d\theta} + s_2\frac{d\sigma_2^{el}}{d\theta} + ... + s_N\frac{d\sigma_N^{el}}{d\theta} \tag{5}$$

We have checked that the integral of the left side of Eq. (5) leads exactly to the value of the total ECS given in the left side of Eq. (2).