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On the use of additivity rules to estimate electron production cross sections in proton-biomolecule collisions.

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Abstract. Additivity rules are employed to estimate electron production cross sections for proton collisions with nucleobases and amino acids, using as input experimental data for proton collisions with atoms and small molecules. Cross sections (total and single differential, in electron energy) are calculated for collision energies 10 keV$\leq E \leq$2 MeV. The results show that this simple procedure yields cross sections in good agreement with the available experimental and theoretical cross sections at high collision energies and it is able to reproduce the energy dependence of the total cross sections, including the presence of maxima at intermediate energies.

PACS. 34.50.Gb Electronic excitation and ionization of molecules – 87.53.-j Effects of ionizing radiation on biological systems

1 Introduction

Ion beam cancer therapy is based on the irradiation of the tumor by a beam of fast ions that causes the cell damage when collide with the biomolecules. The damage can be either direct, where the DNA strands are broken by ion impact, or indirect, where the DNA strands breaking is produced by secondary particle (ions, electrons of radicals) formed in ion collisions with other species. Therefore, the cross sections for different reactions in ion collisions with biomolecules are required in the simulation of ion tracks in the biological medium, needed to understand the mechanism of the biological damage and to evaluate the optimal dose. In this respect, microdosimetry simulations can be carried out using the GEANT4 Monte Carlo toolkit with the GEANT4-DNA physical models for the interactions of electrons, H, He, H^+, He^+ and He^{2+} with liquid water. The validity of these models has been assessed by comparison with experimental cross sections for collisions with water vapor in reference [1]. Moreover, the comparison of ion-track simulations with experimental results has been recently employed to gauge the accuracy of ionization cross sections for H^+, He^{2+} and He^+ collisions with N_2 and propane [2].

In this work we focus on the electron production (EP) processes in proton-molecule collisions. These reactions are of the form:

$$H^+ + M \rightarrow ne^- + H^{(1-m)+} + M^{(n+m)+}, \qquad (1)$$

where M is the target molecule, $m = 0, 1$ and $n \geq 1$. In practice, the most probable reactions are the single ionization ($m = 0$, $n = 1$), transfer ionization ($m = 1$, $n = 1$) and double ionization ($m = 0$, $n = 2$).

Cross sections for EP in proton collisions with nitrogenous bases have been calculated by Lekadir *et al.* [3], using a classical over barrier treatment (CTMC-COB); Champion *et al.* [4] used the first Born approximation; Galassi *et al.* [5] employed the first Born approximation with corrected boundary conditions (CB1) and the continuum distorted wave-eikonal initial state treatment (CDW-EIS) approximations. In general, the calculations are limited to high collision energies where the perturbative methods are appropriate and they are not able to reproduce the maximum of the total cross section. Ionization cross sections have been also evaluated [6] by applying a semiempirical method based on the dielectric formalism. A few experiments have reported total and differential cross sections for these collisions: Tabet *et al.* [7], Iriki *et al.* [8,9] and Itoh *et al.* [10].

Because of the need of data, several authors have suggested that cross sections for collisions with large molecules can be estimated by applying additivity rules (ARs), where the required cross sections are obtained by combining existing data for collisions with the atoms that constitute the molecular target. This idea was successfully applied by Toburen and Wilson [11] to estimate differential EP cross sections for $H^+ + H_2O$ collisions. A similar approach was employed by Nagy and Vegh [12] to estimate electron capture cross sections in proton-molecule collisions. The idea has been widely applied to electron-molecule collisions [13–15]. It must be noted that the methods of references [4,5] and [10] are based on a similar approach. These calculations start with a quantum chemistry calculation (CNDO in [4] and Hartree-Fock in references [5] and [10]) of the target molecular orbitals. Afterwards, the cross sections for ion-molecule collisions are expressed as linear combinations of the contributions of the atomic orbitals, weighted by their electron occupations, obtained by means of a Mulliken population analysis.

The aim of the present work is to study the applicability of the ARs by combining the available experimental for proton collisions with small molecules to obtain the values for the nucleobases. We have considered EP total cross sections (TCS) and single differential, in electron energy,

cross sections (SDCS). The paper is organized as follows: The results of applying the ARs are presented in section 2. We start by presenting in subsection 2.1 the TCS for collisions with relatively small molecules (H_2O, CH_4, CO_2 and NH_3). In subsection 2.2 we consider TCS for collisions with nitrogenous bases, and in subsection 2.3 the total cross sections for proton collisions with a few amino acids. In subsection 2.4, we present the SDCS for EP in proton collisions with nucleobases, evaluated by means of ARs. A brief summary is presented in section 3.

2 Results

2.1 Total cross sections for H^+ collisions with small molecules.

In order to gauge the usefulness of different ARs, we have started by considering collisions with small molecules where experimental cross sections are available. In particular, for EP in collisions with H_2O, we have used, as an input, the experimental EP cross sections for H^+ collisions with H, H_2 and O_2 ($\sigma(H)$, $\sigma(H_2)$ and $\sigma(O_2)$, respectively) [16]. We have interpolated these cross sections and combined them through the ARs:

$$\sigma(H_2O) = \sigma(H_2) + \tfrac{1}{2}\sigma(O_2) \quad (2)$$

$$\sigma(H_2O) = 2\sigma(H) + \tfrac{1}{2}\sigma(O_2). \quad (3)$$

We have applied similar equations for collisions of protons with other molecules. Namely, for collisions with CO_2:

$$\sigma(CO_2) = \sigma(CO) + \tfrac{1}{2}\sigma(O_2) \quad (4)$$

$$\sigma(CO_2) = \sigma(CO) + \sigma(O), \quad (5)$$

where the data for collisions with atomic oxygen, $\sigma(O)$, have been taken from the calculation of Kirchner *et al.* [17]. For collisions with NH_3:

$$\sigma(NH_3) = \tfrac{1}{2}\sigma(N_2) + \tfrac{3}{2}\sigma(H_2) \quad (6)$$

$$\sigma(NH_3) = \tfrac{1}{2}\sigma(N_2) + 3\sigma(H), \quad (7)$$

and for collisions with CH_4:

$$\sigma(CH_4) = \sigma(CO) - \tfrac{1}{2}\sigma(O_2) + 2\sigma(H_2) \quad (8)$$

$$\sigma(CH_4) = \sigma(CO) - \tfrac{1}{2}\sigma(O_2) + 4\sigma(H). \quad (9)$$

$\sigma(N_2)$, $\sigma(H_2)$, $\sigma(H)$, $\sigma(CO)$ and $\sigma(O_2)$ in equations (4)–(9) are the interpolated experimental data of Rudd *et al.* [16]. We compare in Figure 1 the TCSs, calculated using the rules (2) – (9), with previous experimental and theoretical results. It is worth noting the general good agreement with the experimental results for the four collisions. For the particular case of $H^+ + H_2O$ collisions, equation (3), which employs cross sections from $H^+ + H$ collisions, yields cross sections closer to the experimental ones than those obtained with equation (2) that employs data for $H^+ + H_2$ collisions. For the other systems, the rules based on cross sections for collisions with diatomic molecules show a better agreement with the experiments than those that use data of collisions with atoms. This is probably due to the fact that the electron density near a given nucleus of the polyatomic molecules is more similar to that of the diatomic molecules than to the atomic electron density. In this respect, the ARs (6), (7) overestimate the total cross section for $H^+ + NH_3$, because they are based on data for collisions with N_2, and the electrons are released more easily from the π orbitals of N_2 than from the N-H σ bonds of NH_3. There is a general good agreement betwen our results and the CDW-EIS calculations of references [19,21] and [23] for energies above that of the maximum of the corresponding TCS, while these calculations underestimate the cross sections at low energies, as can be observed by comparison with the experimental data and the CTMC calculation [20] for $H^+ + H_2O$ collisions. As a conclusion of these comparisons, the additivity rules (2) – (9) are useful to estimate total cross sections for electron production in proton collisions with small molecules in a wide energy range, $10 \leq E \leq 1000$ keV.

2.2 Total cross sections for H^+ collisions with nucleobases.

In our approximation, the TCSs are obtained as linear combinations of the available experimental cross sections for collisions with small molecules. We have used the data of Rudd *et al.* [16] for proton collisions with CO, NH_3, H_2O, H_2 O_2, N_2 and CH_4. For instance, the cross section for EP in H^+ collisions with uracil is obtained by applying the equation:

$$\sigma(\text{Uracil}) = 4\sigma(CO) - \sigma(O_2) - \sigma(H_2) + 2\sigma(NH_3). \quad (10)$$

This expression is appropriate to describe the structure of the lactam tautomer (see Figure 2(a)). In particular, we have not employed the data for $H^+ + N_2$, because the electronic structure of this diatom is very different from that of the RR'NH groups contained in the molecule. Since experimental data for ethylene are not available, we have used the TCSs for collisions with CO and O_2 to simulate the cross section for collision with the C=C group: $\sigma(C=C) = 2\sigma(CO) - \sigma(O_2)$. Other tautomers of the molecule would be better described by employing alternative additivity expressions. In particular the aromatic tautomer (Figure 2(b)) contains OH groups, whose electronic structures are close to that of the water molecule, and we have recalculated the EP cross section by means of the additivity expression:

$$\sigma(\text{Uracil}) = 4\sigma(CO) - 2\sigma(O_2) + \sigma(N_2) + 2\sigma(H_2O) \quad (11)$$

We plot in Figure 3 the TCSs calculated using equations (10) and (11) together with the experimental data of reference [10]. At $E < 100$ keV we find small differences between both ARs, which indicates that there is also a small difference between cross sections for collisions with different tautomers. At high energies, the results from (10) show an excellent agreement with the experiments of reference [10], in accordance with the fact that the lactam

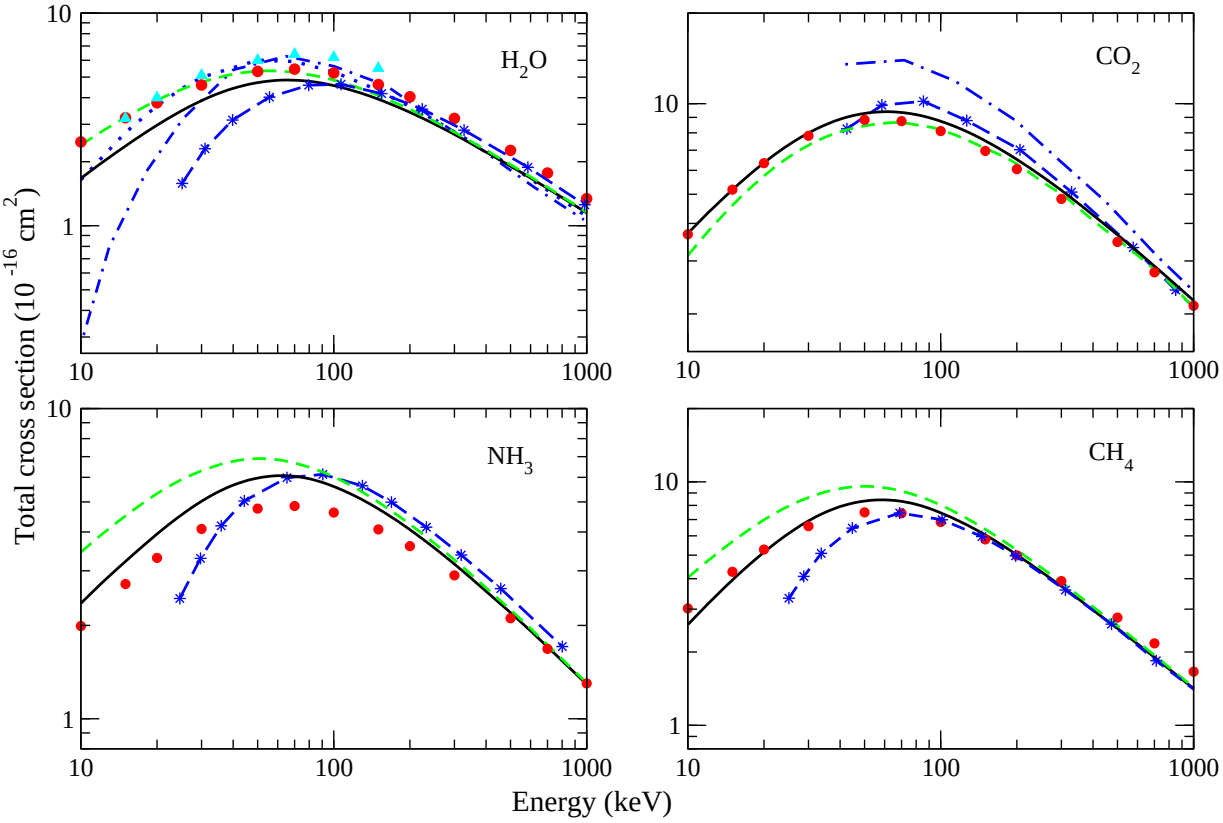

Fig. 1. Total cross section for electron production in proton collisions with H_2O, CO_2, NH_3 and CH_4, as functions of the collision energy. $H^+ + H_2O$ collisions: Additivity rules: full line equation (2), dashed line equation (3) . Experimental results: ▲,[18], ●, [16]. Theoretical results: (- - -), [19]; (· · ·), [20]; (⋆ - ⋆), [21]. $H^+ + CO_2$ collisions: Additivity rules: full line equation (4), dashed line equation (5). Experimental results: ●,[22]. Theoretical results: (⋆ - ⋆), [21]; (- · -); [23]. $H^+ + NH_3$ collisions: Additivity rules: full line equation (6), dashed line equation (7) Experimental results: ●,[22]. Theoretical results: (⋆ - ⋆), [21]. $H^+ + CH_4$ collisions: Additivity rules: full line (8), dashed line (9). Experimental results: ●,[22]. Theoretical results: (⋆ - ⋆), [21].

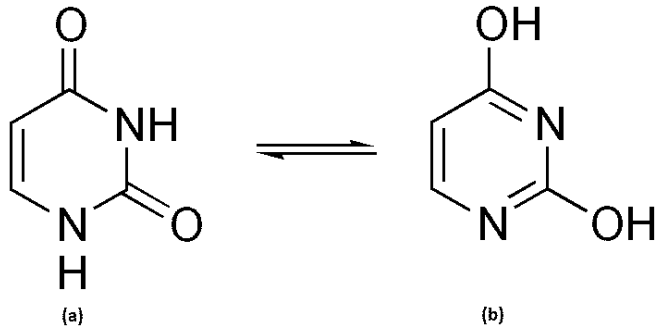

Fig. 2. Structures of two tautomers of the uracil. (a) Lactam. (b) Double lactim.

tautomer is the most stable and predominant in gas phase ([24] and references therein). There is also a good agreement between the values estimated from the AR (10) and the calculations of reference [10] in the range $E > 100$ keV, where those calculations were performed. The cross section reported by Tabet *et al.* [7] at $E = 80$ keV are almost one order of magnitude higher than those estimated using the ARs and it also overestimates the calculated values of references [3] and [10].

The TCSs for EP in proton collisions with the DNA bases have been calculated using the expressions:

$$\sigma(\text{Adenine}) = 5\sigma(\text{CO}) - \tfrac{5}{2}\sigma(\text{O}_2) - \tfrac{1}{2}\sigma(\text{H}_2) + \\ +2\sigma(\text{NH}_3) + \tfrac{3}{2}\sigma(\text{N}_2) \quad (12)$$

$$\sigma(\text{Cytosine}) = 4\sigma(\text{CO}) - \tfrac{3}{2}\sigma(\text{O}_2) + \sigma(\text{H}_2) + \\ +\sigma(\text{NH}_3) + \sigma(\text{N}_2) \quad (13)$$

$$\sigma(\text{Guanine}) = 5\sigma(\text{CO}) - 2\sigma(\text{O}_2) - 2\sigma(\text{H}_2) + \\ +3\sigma(\text{NH}_3) + \sigma(\text{N}_2) \quad (14)$$

$$\sigma(\text{Thymine}) = 4\sigma(\text{CO}) - \sigma(\text{O}_2) - 2\sigma(\text{H}_2) + \\ +2\sigma(\text{NH}_3) + \sigma(\text{CH}_4), \quad (15)$$

which are similar to the equation (10). The TCSs are shown in Figure 4, where one can note the excellent agreement of the results of equation (12) with the experimental

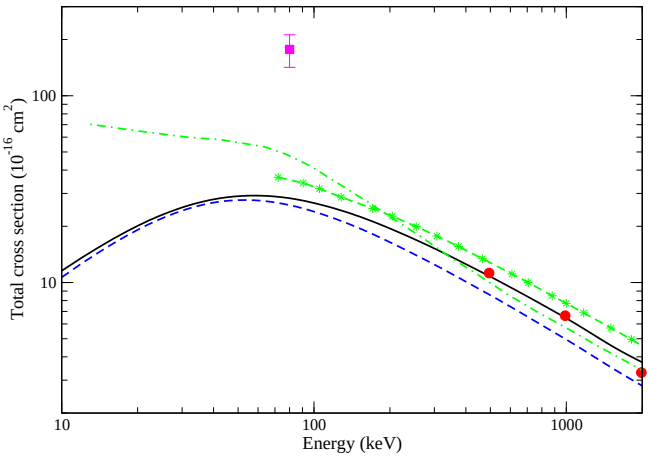

Fig. 3. Total cross section for electron production in proton collisions with uracil as a function of the collision energy. The full line is the present result, obtained by employing the expression (10), and the dashed line the result from the expression (11). Experimental values: ■,[7]; ●, [10]. Calculations: (- · - ·),[3]; (- ∗ - ∗),CB1 results reported in reference [10].

data of Iriki *et al.* [8] for H^+ + Adenine. The additivity rules lead to cross sections in very good agreement, for $E > 50$ keV, with the CDW-EIS calculations [5] for all bases, and a less satisfactory agreement with CB1 [4] and CTMC-COB calculations [3]. It must be noted that Champion *et al.* [25] have studied the validity of the these calculations for H^+ + Adenine, and they estimate that the CB1 method is useful for $E >$ 60-70 keV and the CTMC-COB for energies larger than 200-300 keV, which are the energy ranges where those calculations agree with the results of applying the additivity rules. At collision energies below those of the maxima of the total cross sections, the CDW-EIS cross sections decay very fast as E decreases. This behaviour might be a consequence of the limited validity of the perturbative treatments, because a similar behaviour is found for collisions with small molecules (see Figure 1), where the experimental data agree with the AR estimates at low energies. As in Figure 3, the cross sections of Tabet *et al.* [7] are higher than the calculated ones.

As already mentioned for uracil, the ARs (13)-(15) correspond to the keto tautomers, which are the most stable forms for guanine and thymine. On the other hand, the most stable tautomer of cytosine is the amino-hidroxi tautomer [26], and accordingly, we have evaluated the TCS using the alternative expression:

$$\sigma(\text{Cytosine}) = 4\sigma(\text{CO}) - 2\sigma(\text{O}_2) + \sigma(\text{H}_2\text{O}) + \\ +\sigma(\text{NH}_3) + \sigma(\text{N}_2), \qquad (16)$$

which is similar to equation (11), and that leads to a TCS lower than that from equation (13) by about 6% (see Figure 4). The tautomers of adenine are obtained by H transfer between the four nitrogen atoms of the two rings of this molecule, which are all represented by the AR (12) within our approximation.

In order to estimate cross sections for collisions with large molecules it can be useful to scale the cross sections for small molecules. In this respect, Wilson and Toburen [27] pointed out that EP cross sections are roughly proportional to the number of *weakly bound* electrons. We have checked that the cross sections evaluated with the ARs (10), (12)-(15) fulfill this scale relationship. Specifically, the plots of the total cross sections as functions of E for the five nucleobases are parallel lines, and that the TCSs obtained from these ARs differ in less than 5% from the values scaled with the number of valence electrons near the maxima ($\approx$ 60 keV) of these cross sections.

2.3 Total cross sections for collisions with amino acids

As an additional application of the additivity rule method, we have evaluated the total cross sections for EP in H^+ collisions with some amino acids. We have considered some amino acids with molecular formulae $C_nH_mNH_2(OH)_lCO$ and applied the AR:

$$\sigma\ (\text{Aminoacid}) = \sigma(\text{CO}) + \sigma(\text{NH}_3) + l\sigma(\text{H}_2\text{O}) + \\ +n\sigma(\text{CH}_4) - \tfrac{1}{2}(l + 4n - m + 1)\sigma(\text{H}_2). \qquad (17)$$

In contrast to the situation for collisions with nucleobases, our TCSs (Figure 5) are the first results for this type of reactions and cannot be compared to experimental or theoretical results. Within our approximation, the TCSs for the isomers leucine and isoleucine are identical. One can note that the cross sections increase with the number of valence electrons, but a simple scale rule leads to errors of about 20% for the amino acids of Figure 5. A similar approach can be applied to other amino acids with more complex structures, with the exception of the amino acids containing sulphur (methionine, cysteine), because of the lack of experimental data for small sulphur-containing molecules.

2.4 Differential cross sections.

The experimental data for SDCS in proton collisions with atoms and small molecules have been reviewed by Rudd *et al.* [28]. These authors provide fittings of the measured cross sections by using the so-called Rudd's model [29]. In this work, we have used these parametrizations to build up the SDCS for collisions with the nitrogenous bases. Given the limited number of experimental data available, only a few additivity rules can be applied. In particular:

$$\sigma^\epsilon(\text{Base}) = a_1\sigma^\epsilon(\text{CO}_2) - a_2\sigma^\epsilon(\text{O}_2) \\ +a_3\sigma^\epsilon(\text{N}_2) + a_4\sigma^\epsilon(\text{H}_2), \qquad (18)$$

where σ^ϵ denotes the SDCS, $\mathrm{d}\sigma/\mathrm{d}\epsilon$, with ϵ the energy of the emitted electron, and the coefficients a_i are given in Table 1 and the calculated SDCSs are shown in Figure 6 for three collision energies.

The cross sections calculated using the ARs (18) are compared to the available theoretical and experimental

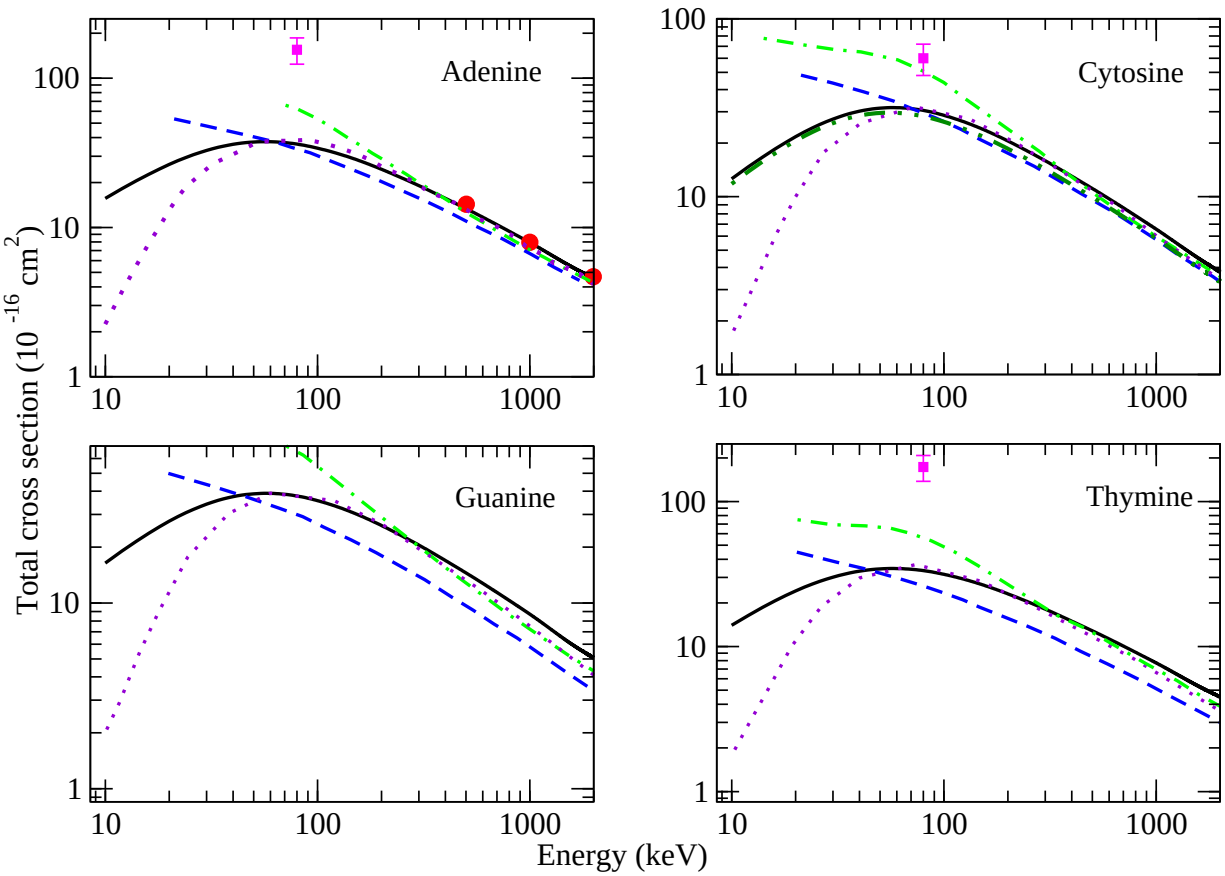

Fig. 4. Total cross section for electron production in proton collisions with DNA bases. The full lines are the results of applying the additivity rules (12)-(15). The dash-double-dotted line for cytosine is obtained by means of equation (16). Calculations: (- · - ·), [3]; (- - -), [4]; (· · ·), [5]. Experimental results: ■,[7]; ●, [8]

Table 1. Values of the coefficients a_i of equation (18).

Base	a_1	a_2	a_3	a_4
Uracil	4	-3	1	2
Adenine	5	-5/2	5/2	5/2
Cytosine	4	-7/2	3/2	5/2
Guanine	5	-9/2	5/2	5/2
Thymine	5	-4	1	3

data in Figure 7, where one can note the excellent agreement between our values and those from the CB1 calculations with some discrepancies with the CDW-EIS ones. The disagreement between CB1 and the experimental results at $\epsilon < 7$ eV was already pointed out by Itoh *et al.* [10], but it remains unexplained. A better agreement is found between the experimental values and the semiempirical calculation of reference [6]. The decrease of the experimental SDCS cross sections at $\epsilon < 7$ eV has not been observed in proton collisions with small molecules, in particular, the SDCS employed in equations (18) showed a smooth increase as ϵ decreases, which obviously makes impossible to obtain the shape of the experimental curves. The "humps" in the experimental curves might arise from interference effects between collisions with different atoms, not included in the ARs and that cannot be described by the calculations of references [5] and [10], where the SDCS are obtained by adding the cross sections for EP from all the atomic orbitals weighted by the electron populations on each target molecular orbital (see also the comment of reference [21] on this point).

3 Summary

We have evaluated total and singly differential cross sections for electron production in proton collisions with nucleobases by employing additivity rules and experimental data for collisions with atoms and small molecules. We have shown that this simple procedure yields cross sections in very good agreement with theoretical (perturbative) results in the energy range where the methods are appropriate. At collision energies below those of the maxima of the electron production TCS, the estimated values cannot be compared to experimental values, but from the experience of similar estimates for small molecules, we think that the semiempirical values are more accurate

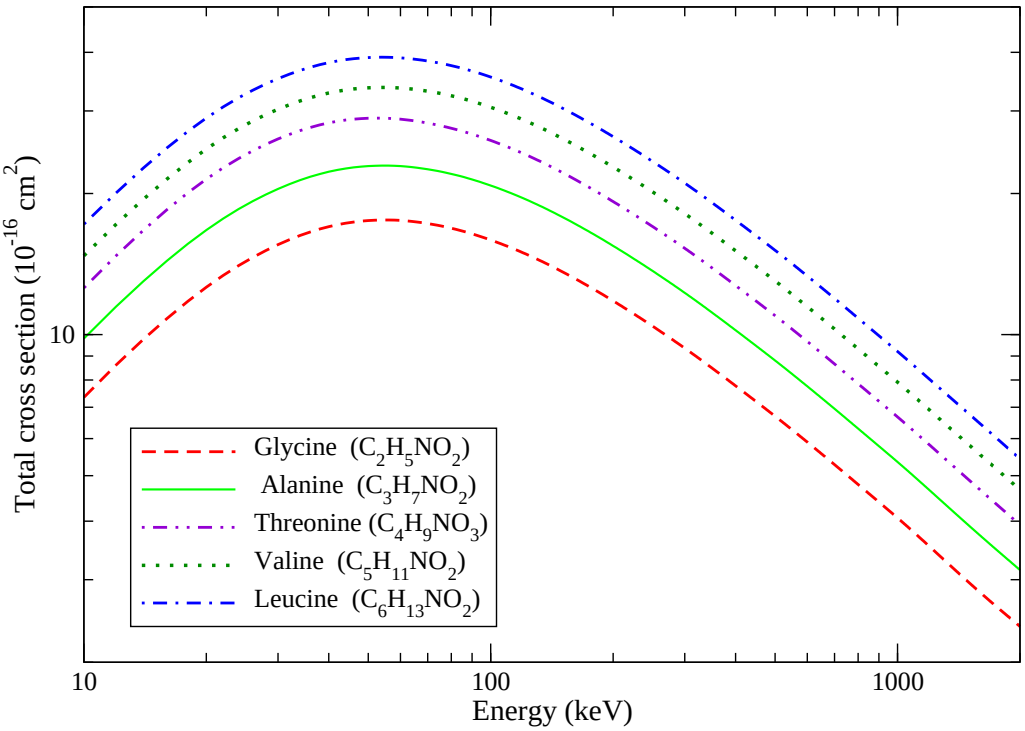

Fig. 5. Total cross section for electron production in proton collisions with several amino acids, as indicated in the figure.

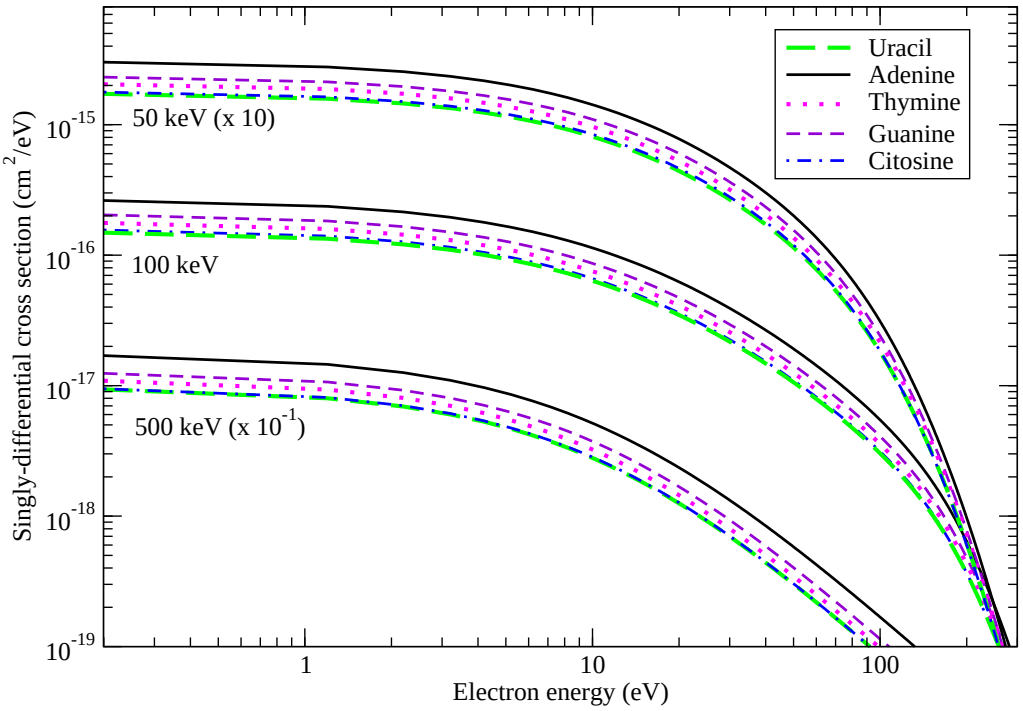

Fig. 6. Single differential cross sections for electron production as functions of the energy of the emitted electron, in proton collision with nucleobases

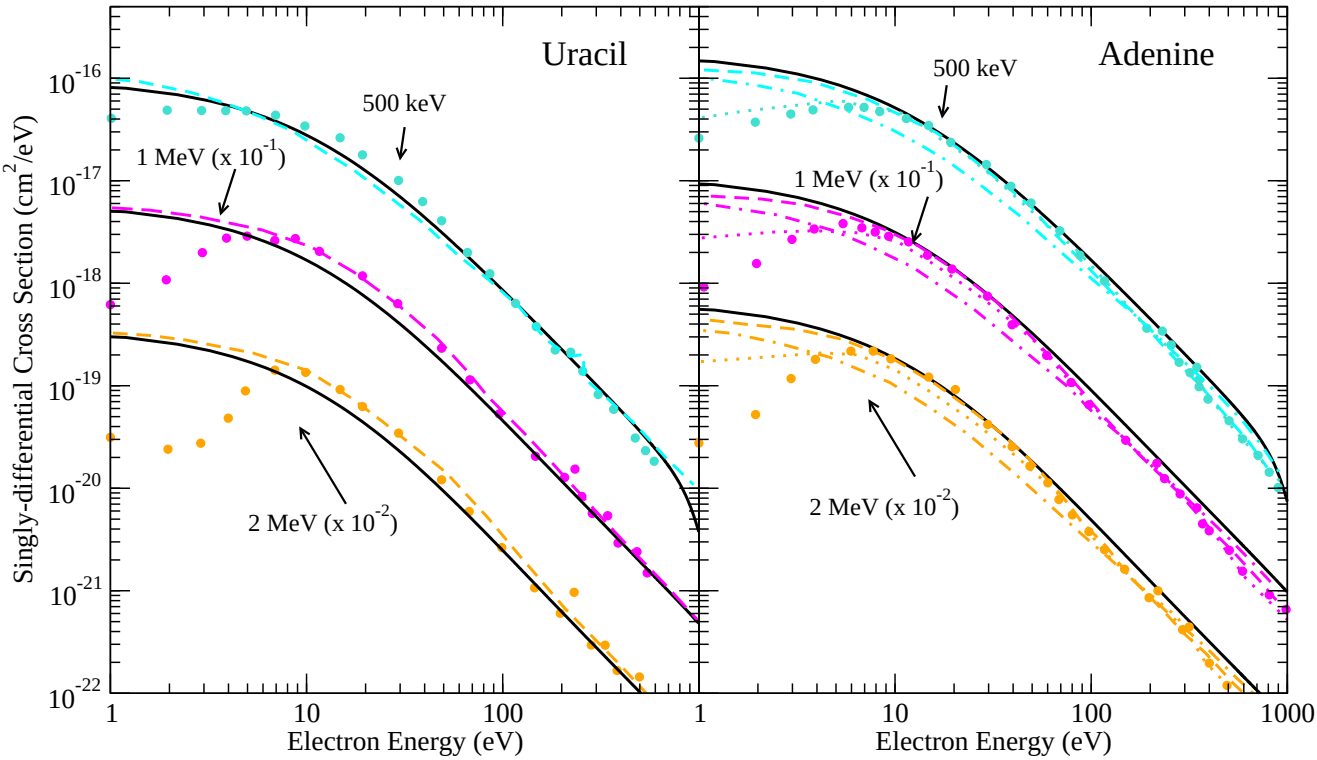

Fig. 7. Single differential cross section for electron production in proton collisions with uracil and adenine, as functions of the energy of the emitted electron. The full lines are the present results obtained by applying the AR (18). The dashed lines are the CB1 results of references [10](uracil) and [5] (adenine); the dashed-dotted lines in the right panel are the CDW-EIS results of reference [5], and the dotted lines the results of reference [6]. The circles are the experimental results of references [10], for H^+ + uracil, and [9] for H^+ + adenine.

than the theoretical calculations. In order to show the possible applications of the procedure, we have employed the same idea to estimate electron production cross sections for proton collisions with amino acids, which are of predictive value, given the lack of previous studies of these systems. Additional work is required to explain the two main discrepancies with the few available experiments. Namely, the overestimation of the TCSs by the experiments of reference [7] and the decrease of the experimental SDCSs at low electron energies in references [10,9]. In both cases, our results support the previous theoretical results [5,10], although the agreement might be a consequence of the fact that the computational methods evaluate the cross sections as weighted sums of atomic contributions, which is an approach related to the additivity rules.

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