Electron-Impact Ionization with Atoms at the Range ($E>E_i$ - 200) eV Incident Energy

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Abstract

A classical theory of inelastic atomic collisions is given. It is shown that inelastic scattering ionization interaction between charged particles (electrons) and atoms are due to the Coulomb interaction with atomic electrons and depend in a first approximation on their binding energy and momentum distribution. The effect of interaction between the charged particles depends on their velocity; hence, a description of collision processes based on Thompson and Rutherford formulas – describing the Coulomb scattering on particles at rest, to atomic collision- is bound to yield erroneous results if the velocity of the particle scattered on the atom becomes comparable to, or less than, the mean velocity of electrons in the atom. Our calculations of the ionization cross section are in a good agreement with the theoretical and experimental results of alkali atoms and fine for other atoms.

الملخص

تم تناول النظرية الكلاسيكية لحالة التصادم غير المرن في هذا البحث. وهي تظهر حالة تفاعل التأين بين كل من الجسيمات المشحونة (الألكترونات) والذرات نتيجة لتفاعل كولومب مع الألكترونات الذرية، وهي تعتمد في أول تقريب لها على كل من طاقة الترابط لتلك الألكترونات وتوزيع الزخم. إن التأثير بين الجسيمات المتفاعلة يعتمد على سرعة تلك الألكترونات، وحيث أن وصف عملية التصادم يستند الى صيغ كل من ثومسون ورذرفورد- وهي صيغ تصف استطارة كولومب من على الجسيمات عند الحالة السكونية، في التصادم الذري- التي تكون مقيدة بالحصول على نتائج متنوعة إذا كانت سرعة الجسيمات المستطارة من على الذرة قريبة أو أقل من معدل السرعة للألكترونات الذرية. حققت حساباتنا للمقاطع العرضية للتأين توافق جيد مع نتائج الحسابات والقياسات الأخرى لحالة الذرات القلوية وكان التوافق لابأس به لحالة الذرات الأخرى.

1. Introduction

Electron impact ionization is extensively used to generate positive ions for mass spectrometer. The ionization cross section is an important factor in quantitative interpretation, for example determination of the partial vapor pressure when a mass spectrometer is coupled with the Knudsen effusion method [1]. Separate more detailed information on the electron-impact ionization cross section is also important in electron transport for calculating the probability of emitting x-ray subsequent to inner-shell ionization and the accurate description of energy-loss straggling[2].

Reactions initiated by electron impact on atoms may be considered as Coulomb three-body problems in the independent particle model for the target. The Coulomb three-body problem is too difficult for a direct solution. It must be approached by interaction between experiment and theory. Approximations for certain aspects are justified and improved by comparison with experiment [3]. The theory of electron reactions on atoms can be formulate in terms of an optical potential [4], which contains the exact wave functions for ionized states. The effect of ionized states is important in calculating scattering to low-lying target states [5], but exact details of the model used are not critical. For calculating the ionization itself there is no approximation for the exact wave function as sophisticated as Close Coupling. The most complete calculation thus far has been factorized distorted wave impulse approximation, in which the electron interactions with target are represented by distorted waves calculated in the appropriate optical potential [6].

Among several sets of calculated ionization cross sections, four in particular [7-10], have been commonly employed in mass spectrometric studies at high temperatures. The first set was introduced by Otves & Stevenson [7], who drew attention to a theoretical result of Bethe that the ionization cross section of an atomic electron with quantum numbers (n,ℓ) is approximately proportional to the mean square radius of the electron shell (n,ℓ). Lotz [8] proposed an empirical formula, within the Bethe formalizm, with ionization cross section summation for the various accessible orbital. Whereas Mann [9,10] with equations similar to these of Bethe, the Born approximation and some additional assumption associated with its use at low energy, calculated the contribution of the electron (ℓ) to the total ionization cross section.

In the early 1990, Kim and his coworkers [11,12] developed a regorous method called Binary-Encountered-Bethe (BEB) model. In a wide range of energy from (0 to KeV), it successfully predicted the ionization cross sections as a function of electron impact energy for light (small) atoms. There are no adjustable or fitting parameters in the theory. The (BEB) model doesn't provide such as resonance in the continuum, vibrational and/or rotational excitations concomitant with ionization, multiple ionization, and dissociative ionization. It simply predicts the total ionization cross section as the sum of ionization cross sections for ejecting one electron from each of atom orbitals [13].

Measurements of ionization cross section for electrons interact with atoms have been made for only a small fraction of the elements [14-19]. These cross sections are needed in thermodynamic studies with mass spectrometers to convert observed ion current to vapor pressures, and are used in other fields involving plasma physics. Until experimental cross sections are obtained theoretical values of the cross sections can be of considerable value [9].

2. Theory

If we consider the Coulomb interaction of the elementary particle with a complex system of charges in a state of dynamic equilibrium, this interaction with the individual elements of the system (electrons), which may lead to change of its internal energy; i.e. inelastic collision. Since the type of inelastic collision is specific by the change of energy and momentum of the electrons of scattering system, the problem will consist in calculating the cross section for definite collisions between the incident particle and the respective electrons of this system[20].

In the case of scattering on unoriented atoms and of the inelastic collision defined by a change of state of only one of the electrons of the atom, the calculating procedure will be comparatively simple [20]:

Denoting by $P_k(\upsilon_e, r)$ the probability that at a distance (*r*) from the nucleus an electron of a velocity (υ_e) belonging to the shell-*k* can be found, and by (σ) the cross section for a given change of dynamic variables of that electron, we can determine the cross section relating to the whole atom [20]:

$$\sigma^{atom} = \sum n_e^k \int_0^\infty \int_0^\infty P_k(\upsilon_e, r)\sigma[\upsilon_e, \upsilon_q(r)]4\pi r^2 dr d\upsilon_e \qquad \text{------------(1)}$$

Where (n_e^k) is the number of electrons in the shell-*k*, while the summation is extended over all shells of the atom, and $\upsilon_q(r)$ is the velocity of incident particle, which, in general, depends on the averaged potential of the whole system, and hence, is a function of the distance from the nucleus:

$$\upsilon_q(r) = \{(2/m_q)[E_q - \varphi(r)q]\}^{1/2} \qquad \text{---------------------------(2)}$$

While (E_q) is the kinetic energy of an incident particle with a charge (q) and a mass (m_q) outside the atom, and $\varphi(r)$ describes the averaged potential of the atom.

Assuming that between the kinetic energy of the electron and its distance from the nucleus there exists a unique relationship, which is to be expect from the laws of classical physics, the expression (1) may be rewriting as follows:

$$\sigma^{atom} = \sum_k n_e^k \int P_k(r)\sigma[\upsilon_e \upsilon_q(r)]4\pi r^2 dr \qquad \text{-------------------(3a)}$$

or in the alternative form:

$$\sigma^{atom} = \sum_k n_e^k \int f_k(\upsilon_e)\sigma[\upsilon_e, \upsilon_q(r)]d\upsilon_e \qquad \text{--------------------(3b)}$$

expressions (3a) and (3b) are equivalent if collisions of large energy exchange between the impinging particle and atomic electrons are considered; they are not equivalent for collisions of very small energy exchange, and then expression (3a) must be used. Neglecting the influence of the averaged field of the atom on the motion of bombarding particle, while putting $\varphi(r) = 0$ into (3b), we obtain

$$\sigma^{atom} = \sum_k n_e^k \int f_k(\upsilon_e)\sigma(\upsilon_e)d\upsilon_e \qquad \text{--------------------------(3c)}$$

on the basis of the theory of Coulomb collisions it is thus possible to deduce that the probability of the atomic electron having velocity (υ_e) decreases with increase of that velocity as the inverse third power of (υ_e). We must keep in mind, in the description that is slightly different from $(1/\upsilon_e^3)$ cannot be excluded.

Gryzinski [20] rewrite an expression of paper [21], in a modified form of the ionization cross section:

$$\sigma_i = \frac{\sigma_o}{E^2} \times g\left(\frac{\varepsilon}{E};\frac{E_q}{E}\right) \quad \textbf{for} \quad m=m_q \text{ ----------------------(4)}$$

Where

$$g\left(\frac{\varepsilon}{E};\frac{E_q}{E}\right) = f_{\bar{\upsilon}}\left\{\frac{E}{\varepsilon} + \frac{2}{3}(1-\frac{E}{2\varepsilon})\ln\left[2.7 + \left(\frac{E_q - E}{\varepsilon}\right)^{1/2}\right]\right\}\left(1-\frac{E}{E_q}\right)^{1+\left(\frac{\varepsilon}{\varepsilon+E}\right)} \text{ ------(5)}$$

Where (E_q) is the energy of the incident particle, (E) is the binding energy of the orbital electron, and (ε) is the mean energy of the atomic electron and equal $(m\bar{\upsilon}_e^2/2)$.

To present a full picture, we also recall the velocity function

$$f_{\bar{\upsilon}} = \left(\frac{\bar{\upsilon}_e}{\upsilon_q}\right)^2 \left(\frac{\upsilon_q}{\upsilon_q^2 + \bar{\upsilon}_e^2}\right)^{3/2} \text{ -----------------------------(6)}$$

The magnitude $\sigma_o = \pi e^2 Z_q^2$ appearing in the above formulas has the value

$\sigma_o = Z_q^2 6.56\times10^{-14} eV^2 cm^2$ where (Z_q) is the charge of the bombarding particle in units of elementary charge (e).

The process of ionization by light particles (electrons) is described by formulas (4) and (5), which according to Gryzinski [20] rough assumption that $\varepsilon = E_{i,\ell}$, will assume a very simple form for each orbital-(ℓ) to obtain:

$$\sigma_{\ell}^{i} = \left(\frac{\sigma_o}{E_{i,\ell}^{2}}\right) g_{\ell}(x) \quad \text{-----------------------------------}(7)$$

&

$$g_{\ell}(x) = \frac{1}{x}\left(\frac{x-1}{x+1}\right)^{3/2} \times \left\{1 + \frac{2}{3}\left(1 - \frac{1}{2x}\right)\ln\left[2.7 + (x-1)^{1/2}\right]\right\} \quad \text{-----------------}(8)$$

Where by (x) the ratio of the kinetic energy of the bombarding electron to the binding (or ionization) of the electron in orbital-(ℓ), $(x = \frac{E_e}{E_{i,\ell}})$.

3. Results & Discussion

The electron-impact ionization cross section of atoms is one of the essential sets of data needed in a wide range of physics and its applications. The nature and the quantitative aspects of the collision process are determined, first and foremost, by occupation of the atomic levels with electrons, the mean velocities of electrons on these levels and obviously the spectrum of energy levels which otherwise defines the kind of inelastic process.

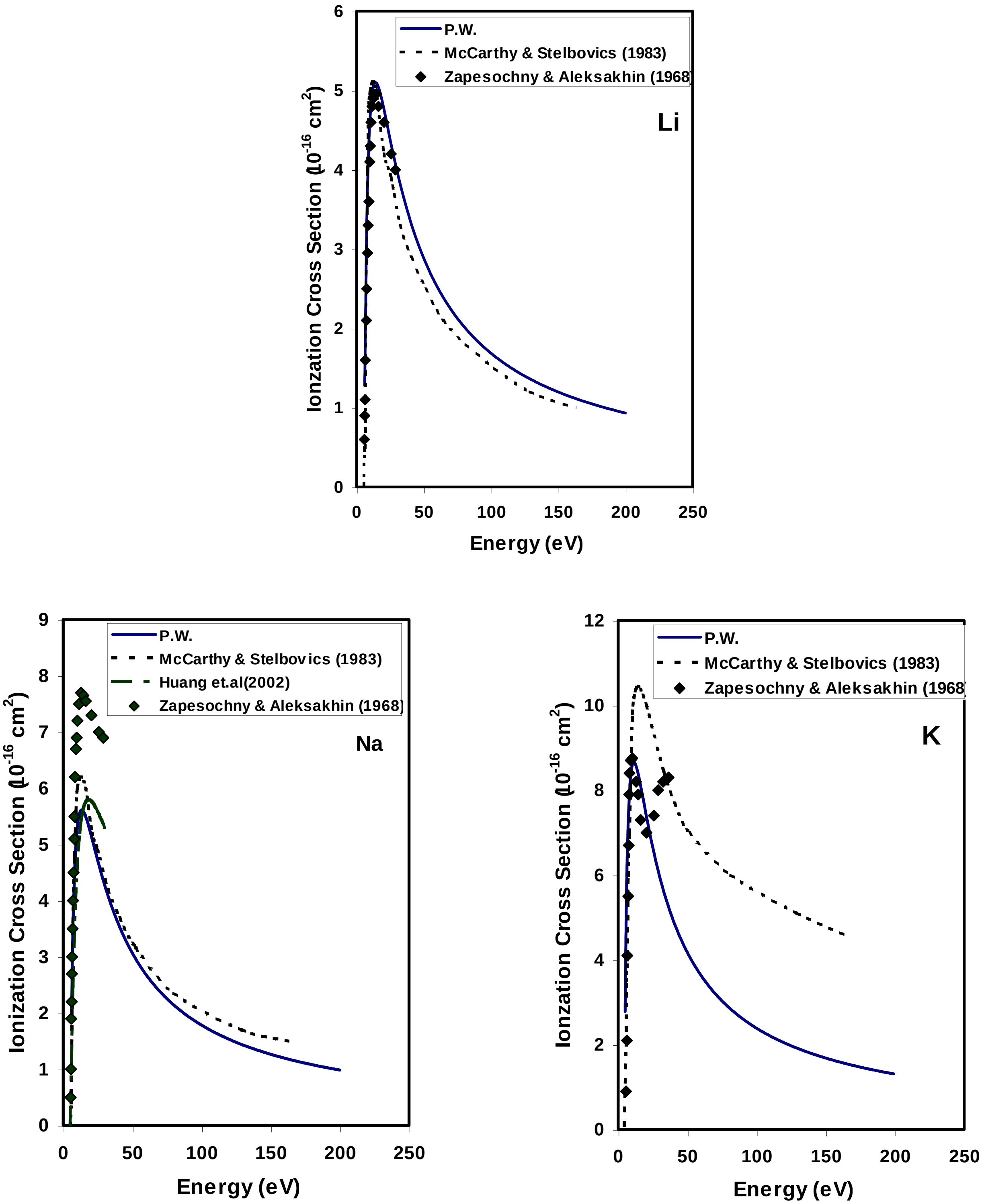
Our results of the ionization cross sections-mentioned by Present Work (P.W.)- for electron impact with neutral atom of various groups, starting with (Li, Na , & K)-atoms are generally in good agreement with the calculations of McCarthy & Stelbovics [3], Huang et al.[1] and the experimental measurements of Zapesochny & Aleksakhin [14] as shown in figure(1). Whereas, for (B, Al, Ga, & In)-atoms the agreement was good for some and fair for others, where some differences are noticeable at small incident energies (15-55) eV for (B & Al) atoms, while the results of (Ga & In) atoms was accepted. The comparison of this group made with the theoretical data of Moores [22], Margreiter et al.[23], and Lotz [8], and the measurements of Freund et al.[15], Patton et al.[16], and Shul et al.[17] as shown in figure(2). Finally, our data of the ionization cross section for (Ni, C, & N)-atoms shows in figure(3), where we compare it with the calculations of Arthurs & Moiseiwitsch [24] and Kim & Desclaux [25], and the

measurements of Smith & Kirkpatrick [19] and Brook et al.[18]. For Ni-atom the comparison was fine, whereas for (C & N) atoms, it was accepted from the side of the curve behaving, where it was the same but with no matching.

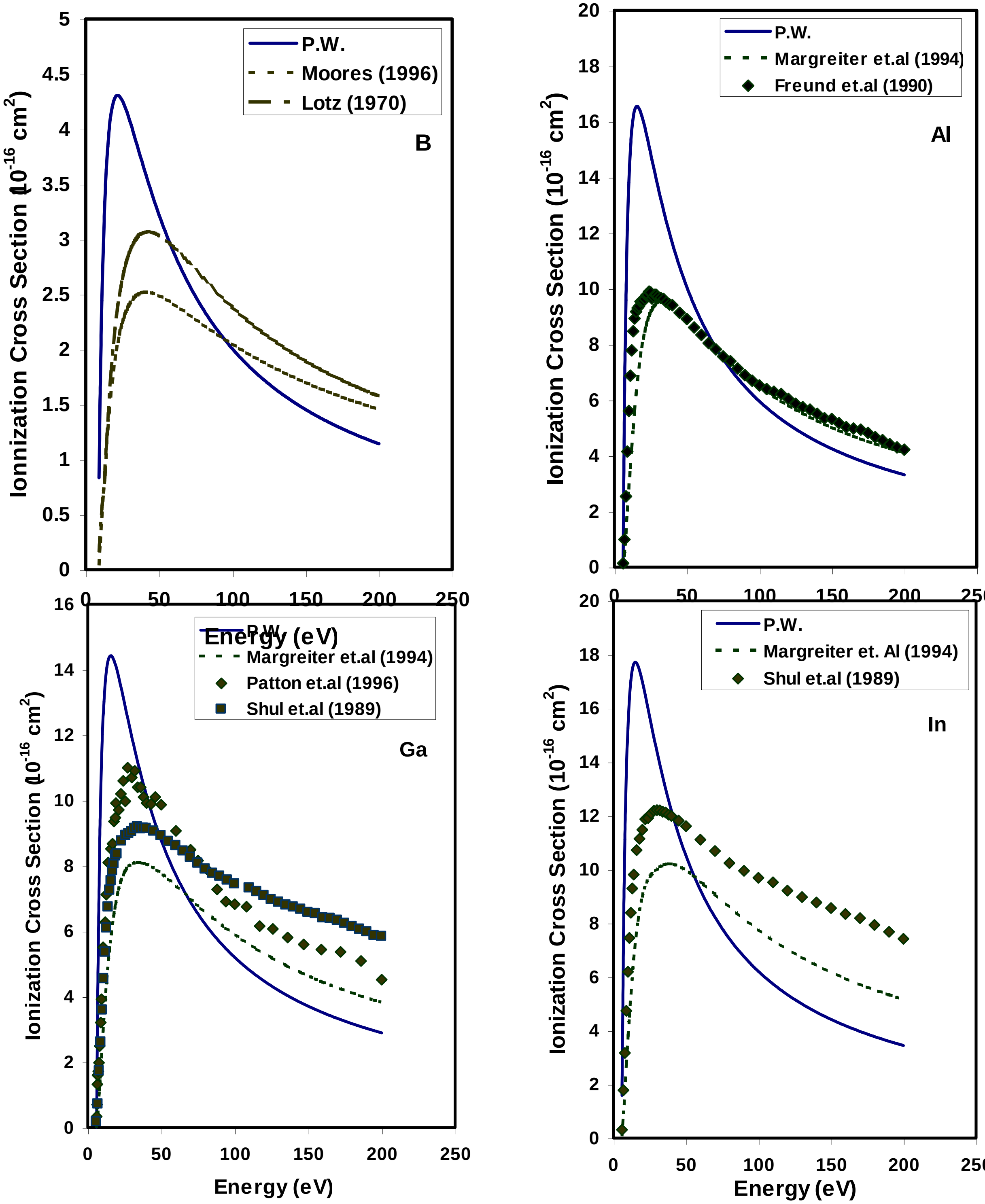
At the peak of the cross section, most of the contribution comes from the region where the scattered electron loses only sufficient energy to eject an electron from the atom. Each ion comes from that process has an intensity measured as a function of the energy of the ionizing electrons to establish the ionization efficiency and to determine the appearance energy, in particular, i.e., the minimum energy at which each ion is formed. We present in table(1) the ionization threshold energy for each atom we study it.

Table(1): Present (E_i) the ionization energy threshold, (Z) the atomic number . The mark (*) refers to Ref [26].

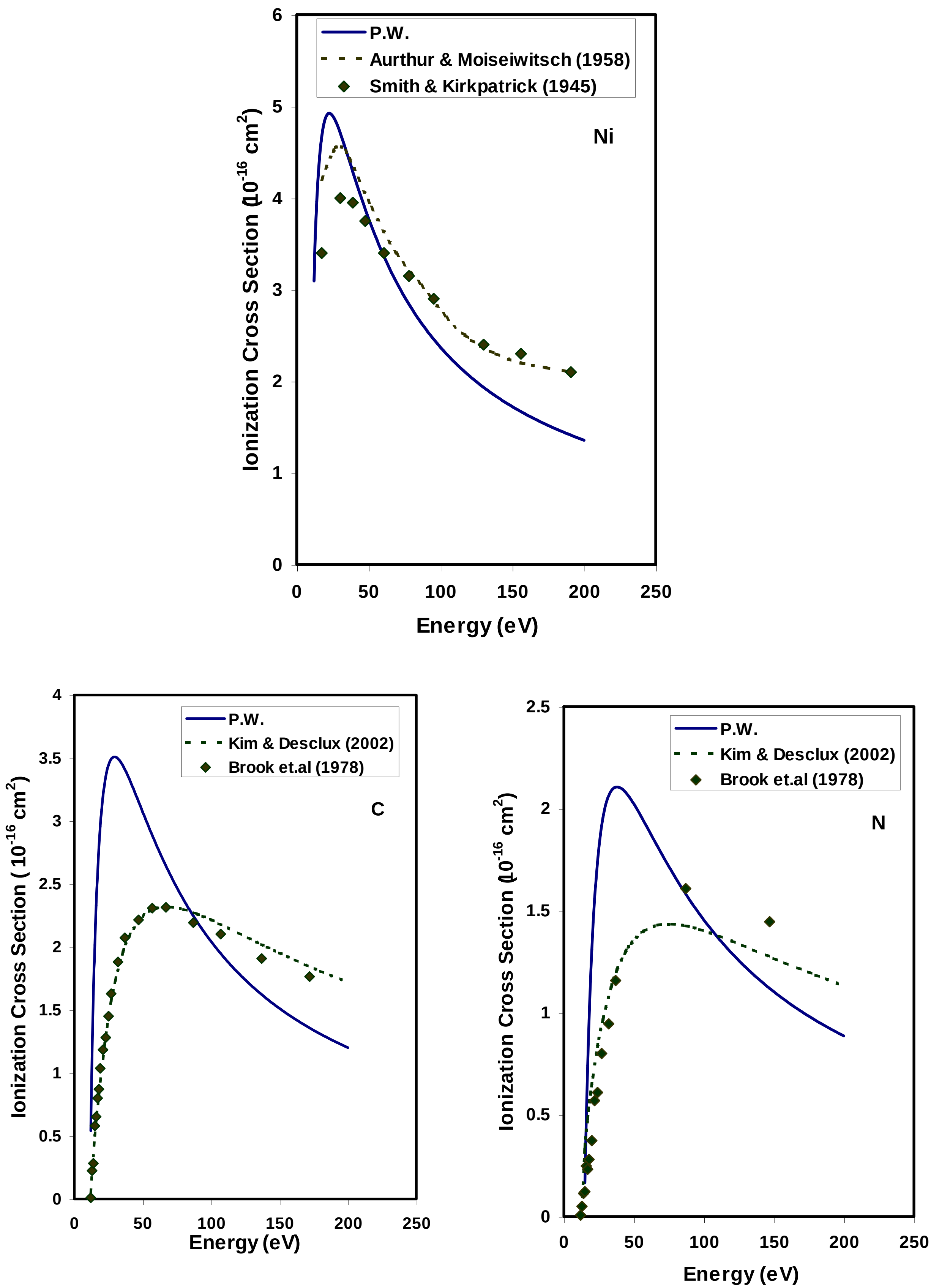
Element	**Atomic No.(Z)**	**E_i(eV)$^{(*)}$**
Li	3	5.391
B	5	8.298
C	6	11.259
N	7	14.532
Na	11	5.139
Al	13	5.986
K	19	4.34
Ni	28	8.675
Ga	31	5.998
In	49	5.786



Figure(1): The Ionization cross section for (Li, Na, & K)-atoms vs



Figure(2): The Ionization cross section for (B, Al, Ga, & In)-atoms vs



Figure(3): The Ionization cross section for (Ni, C, & N)-atoms vs Energy

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