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ON COLLISIONAL IONIZATION RATE COEFFICIENTS

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RESUMEN

Se comparan las secciones rectas y las tasas de ionización colisional obtenidas por Cantó y Daltabuit (1974) con las publicadas por varios autores y se propone una corrección a la formulación empírica propuesta por ambos autores. La corrección muestra en general, un mejor ajuste a las secciones rectas experimentales que las obtenidas por otros autores. Además tiene la ventaja sobre la obtención de tasas de ionización colisional por otros métodos de que el cálculo es muy rápido y sencillo.

ABSTRACT

A correction to the two-parameter empirical formula for the collisional ionization cross-sections proposed by Cantó and Daltabuit (1974) is given. The computed cross-sections are in better agreement with the available experimental measurements than those obtained by other methods. The corresponding ionization rates have a simple analytical form. Our results are compared with those obtained by other authors.

Key words: **ATOMIC PROCESSES — PLASMAS.**

I. INTRODUCTION

There is a wide spectrum of problems in Plasma Physics and Astrophysics, where ionization by electron impact plays an important role. Beginning with Thomson in 1912 until nowadays, several theoretical and empirical attempts have been done to compute collisional ionization cross-sections and the corresponding ionization rates (Burgess 1964; Seaton 1964; Lotz 1966; Moores 1972). In the last 10 years, the experimental work has been improved and highly accurate data for some neutral, single ionized and double ionized atoms have been recently obtained. Based on this set of new experimental data, a comparison of the collisional ionization cross-sections near the threshold energies, computed with different methods has been performed by Burgess *et al.* (1977). The result of this comparison favours (on the average) the Exchange Classical Impact Parameter (ECIP) method described by Burgess (1964). However, in some particular cases, the semi-empirical formulation (SEF) given by Seaton (1964), or, the empirical formula due to Lotz (1966), or, the Coulomb-Born (C − B) approximation as given by Moores (1972), are in better agreement with the experimental cross-sections near the threshold energy (the important part for collisional ionization), than the ECIP values.

Cantó and Daltabuit (1974, hereinafter CD) have proposed an empirical formula to compute collisional ionization cross-sections. This formula fits very well the experimental data near the threshold energies. A small correction to the CD formulation is proposed in this paper, in order to predict the cross-section when experimental data is not available. With this correction, it is possible to introduce the effect of inner shell direct ionization with good results.

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II. RESULTS

a) Cross-sections

According to CD, the cross-sections can be obtained by the two parameter formula;

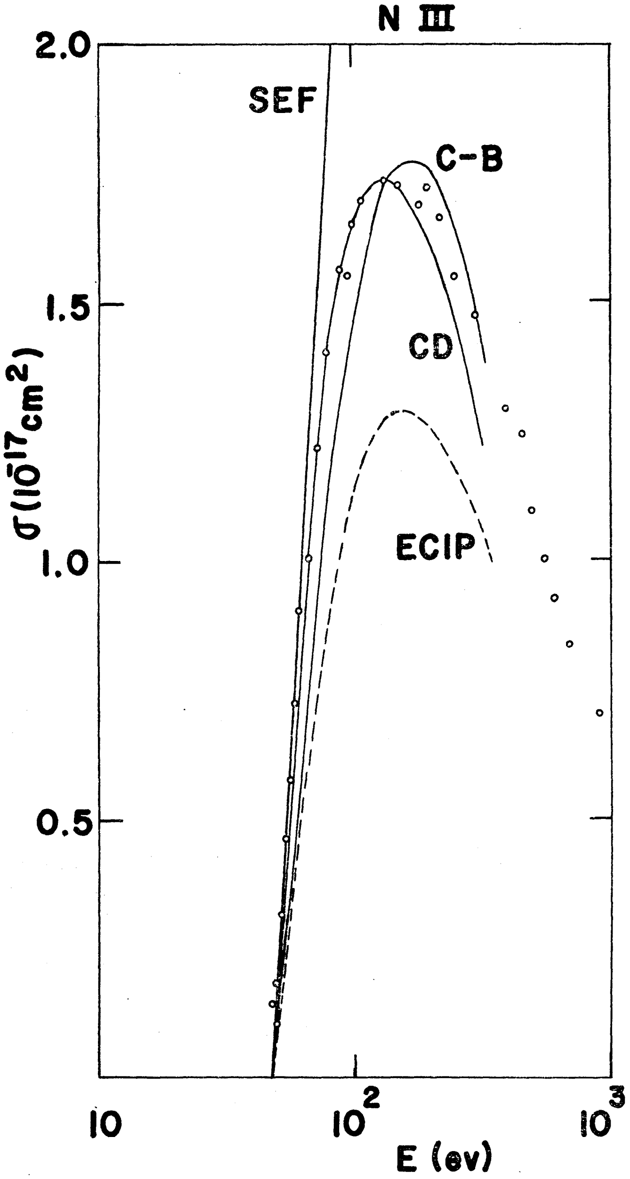

Fig. 1. Collisional ionization cross-sections for N III. The experimental points are those from Aitken, Harrison and Rundel (1971). Curves for SEF, C-B and ECIP have been taken from Burgess *et al.* (1977). Curve CD is obtained with equation (1).

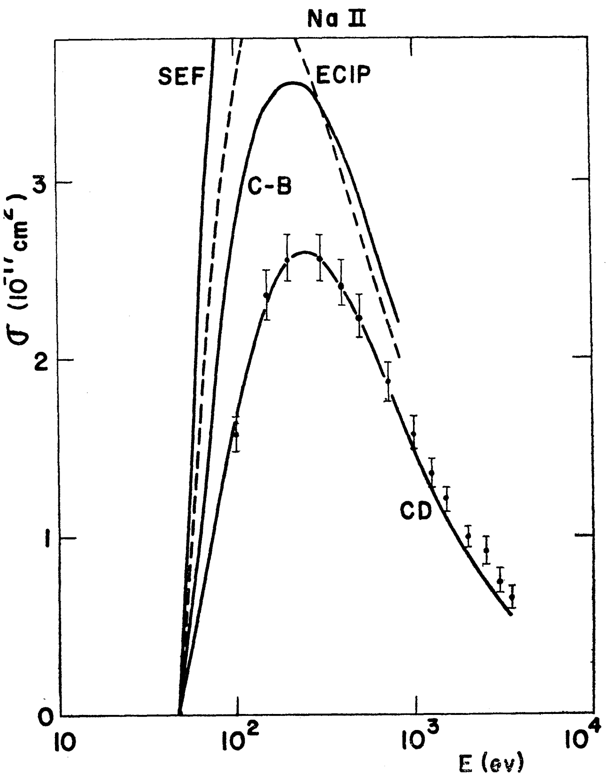

Fig. 2. Collisional ionization cross-sections for Na II. The experimental points are those from Peart and Dolder (1968). Curves labeled SEF, C-B and ECIP have been taken from Burgess *et al.* (1977). Curve CD is obtained with equation (1).

$$\sigma = \sigma_m \frac{4(E_m - I)\ (E - I)}{(E + E_m - 2I)^2}\,, \tag{1}$$

where I is the ionization energy for outer shell electrons, E is the energy of the incident electrons, σ_m the maximum value for the experimental cross-section, and E_m the energy for which the cross-section is maximum. A comparison of the cross-sections in the range of energies from the threshold up to E_m clearly favours the CD formulation over the other methods, as can be noticed in Figures 1-2 for the ions Na II and N III. In the case of equation (1), we are faced with the problem of choosing σ_m and E_m when experimental data is lacking. The interpolation formula for σ_m given by CD is wrong and they do not give any method to predict the value of E_m.

The available experimental data have been summarized in Table 1. According to these data, E_m and σ_m obey the relation;

$$\beta\sigma_m = 4.2 \times 10^{-14}\ N_e/I^2, \qquad (2)$$

where $\beta = E_m/I$ and N_e is the available number of electrons in the shell. The values for β range from 3 to 8 and, can be as high as 9 when autoionization is dominant (Ca II, Sr II). From Table 1 the following conclusions concerning β can de drawn:

1) For the isoelectronic sequences, β decreases with higher ionized species (for atoms with 2 to 20 electrons), reaching an apparent minimum for the double ionized atoms with $\beta = 3$ (except Mg III).
2) Neutral atoms from Li to Ne, show that β increases with atomic number (except for Nitrogen).
3) When inner shell direct ionization and autoionization become dominant β increases and for the case of inner shell ionization E_m sets to a value about 2.5 the inner shell ionization energy (I′).

TABLE 1

EXPERIMENTAL DATA

Ion	σ_m (10^{-16} cm²)	E_m (ev)	Ref.
H I	0.67	36	1
He II	0.05	178	1
He I	0.36	126	1
Li II	0.04	282	6
Li I	5.30	15	1
C II	0.55	78	3
N III	0.18	128	3
N II	0.52	112	1
O III	0.18	145	2
N I	1.57	100	1
O II	0.44	148	2
O I	1.6	80	1
Ne II	0.32	200	1
Ne I	0.86	170	1
Na II	0.26	250	6
Mg III	0.14	300	8
Na I	7.3	14	1
Mg II	0.51	40	5
Ar I	3.1	70	1
K II	0.99	100	6
K I*	8.2,7.7	10,32	1
Ca II†	1.75	100	7
Kr I	4.2	55	1
Rb II*	1.7,1.2	80,115	7
Rb I*	7.8,9	10,22	1
Sr II†	2.5	100	7
Xe I	5.7	40	1
Cs II*	1.7,2	70,100	7
Cs I*	10	15,30	1
Ba II*†	4.25	18,20	9
Tl II	1.7	100	4

* Double peaked due to inner shell direct ionization.

† Shows autoionization.

1) Kieffer and Dunn (1966). 2) Aitken and Harrison (1971).
3) Aitken *et al.* (1971). 4) Divine *et al.* (1976) 5) Martin *et al.* (1968). 6) Peart and Dolder (1968*a*,*b*). 7) Peart and Dolder (1975).
8) Peart, Martin and Dolder (1969). 9) Peart, Stevenson and Dolder (1973).

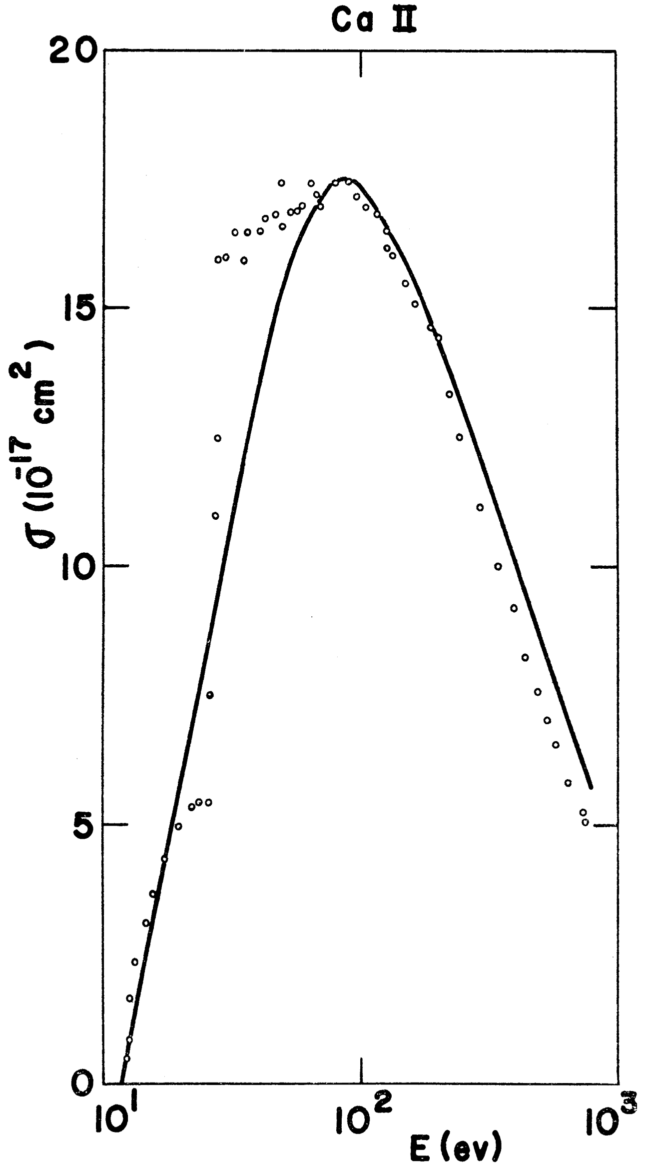

FIG 3. Collisional ionization cross-section for Ca II, using equation (2). The experimental points are those from Peart and Dolder (1975).

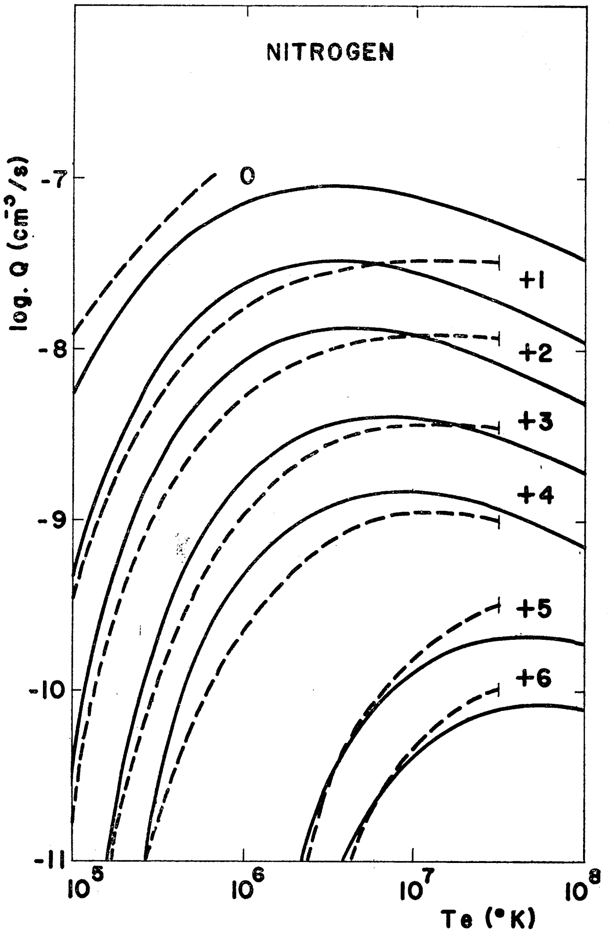

Fig. 4. Collisional ionization rates for Nitrogen; dashed curves show the ECIP values (Summers 1974*a*). Solid lines show the values obtained with equation (3).

With these experimental facts it is not possible to predict the value of β. However, reasonable values for β are: $\beta = 3$ for ionization stages higher than the double ionized one, $\beta = 2.5$ I′/I for inner shell direct ionization and $4 \leqslant \beta \leqslant 5$ for Be I, B I and C I.

It is important to point out that in obtaining equation (2), the data of those atoms and ions that show relevant contributions from inner shell direct ionization have been used. Atoms and ions that show great contributions from autoionization (Ca II, Sr II and Ba II) are not considered in this relation. Nevertheless, if N_e is taken as 5.35 for the case of Ca II, a good approximation to the cross-section is obtained, as can be seen in Figure 3. The expected accuracy for equation (2) is 20%.

b) *Ionization Rates*

In accordance to the former, the ionization rates are given by:

$$\langle\sigma v\rangle \equiv Q = 1.04 \times 10^{-7} N_e T_e^{1/2} I^{-2} \exp\left[-I/KT\right] g(\beta, Z), \qquad (3)$$

with

$$g(\beta, Z) = \frac{\gamma}{\beta}\left[1 + Z(\beta - 2) - Z(\gamma(\beta - 2) + 2\beta - 3) \exp(\gamma) E_1(\gamma)\right],$$

where T_e is the electron temperature, $Z = I/KT_e$, $\gamma = Z(\beta - 1)$ and $E_1(x)$ the exponential integral. Ionization rates obtained with equation (3) and the

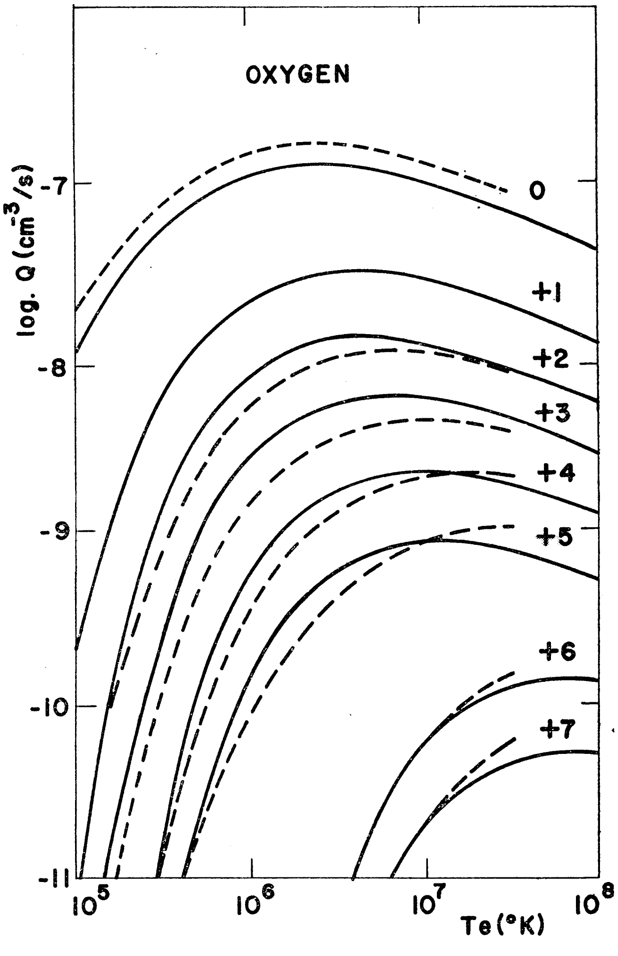

Fig. 5. Collisional ionization rates for Oxygen; dashed lines show the ECIP values (Summers 1974*b*). Solid lines show the values obtained with equation (3).

TABLE 2

COMPARISON OF IONIZATION RATES

Ion	KT/I	Q(ECIP)/ Q(exp.)	Q(this work)‡ (10^{-9}cm^3/S)	Q(this work)/ Q(exp.)
B IV*	0.77	1.25	0.2	0.83
C IV	2.33	0.85	1.7	1.12
C V*	0.55	1.00	0.06	0.75
N V	2.04	1.06	0.90	1.43
O V	1.23	1.06	0.90	1.28
O VI	1.45	0.89	0.40	1.14
Ne VII	0.96	0.76	0.30	1.03
Ar VIII	1.81	0.58	0.40	0.77
	1.01	0.85	0.23	1.15
Fe VIII†	0.73	1.17	0.32	1.07
Fe IX†	0.53	0.78	0.3	1.15
Fe X†	0.54	0.83	0.2	1.11
Average value (S. dev.)		0.92 (± 21%)		1.09(± 21%)

* Experimental error ± 25%.

† For Fe VIII, Fe IX and Fe X, we have used $N_e = 1.8$, 7.1 and 6 respectively

‡ We have used $\beta = 3$.

ECIP method, for Oxygen and Nitrogen are shown in Figures 4 and 5. As can be noticed from these figures, the ionization rates are very similar in the range of temperatures where the rates are increasing (the important part for collisional ionization), except for neutral atoms where a difference of a factor of two is noticeable due to charge transfer. The equilibrium ion abundances computed with both ionization rates do not show important differences.

Experimental measurements of the ionization rates for highly ionized atoms, have been obtainted with the *Plasma Spectroscopy Method.* Datla, Nugent and Griem (1976) have made a comparison of the best experimental results with the ECIP values. Their results are given in Table 2, where we have added the computations obtained with equation (3). The average values for the ECIP method and for our formulation for this restricted sample, are comparable. Nevertheless, taking into account the good results obtained with the cross-sections and the simplicity of our approximation we can conclude that our formulation for the ionization rates has two advantages over the ECIP method: *i*) for the cases where experimental data of σ_m and E_m are available, both the cross-section and the ionization rates computed with equations (1) and (3) are better and, *ii*) in general, the computations of the ionization rates with equation (3) are not time consuming.

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