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EMPIRICAL COMPUTATION OF COLLISIONAL IONIZATION RATES OF ATOMS AND IONS BY ELECTRONS

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RESUMEN

Debido a la falta de información experimental sobre secciones de ionización por impacto de electrones para la mayoría de los átomos neutros e ionizados y a la dificultad teórica del cálculo de las mismas, es necesario emplear fórmulas empíricas para calcular estas secciones. Se propone una fórmula empírica de dos parámetros para este tipo de cálculos y se da una fórmula de interpolación para calcular uno de ellos cuando no se dispone de información experimental.

Se puede interpretar en forma sencilla la fórmula propuesta mediante la formulación clásica de Thomson para los procesos de ionización colisional.

ABSTRACT

A two-parameter empirical formula is proposed to compute the electron collisional ionization cross sections for atoms and ions. An interpolation formula is given to compute one of the parameters when experimental information is missing, and the corresponding ionization rate is computed.

Key words: ATOMIC PROCESSES.

The experimental cross sections for electron collisional ionization of atoms and ions, compiled by Kieffer and Dunn (1966) can be represented analytically by the formula

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

where I is the corresponding ionization energy, E is the energy of the incident electrons and E_m and σ_m are two free parameters that have to be chosen to fit the experimental points. The appropriate choice is to take σ_m as the maximum value of the experimental cross section and E_m as the energy for which the cross section is maximum.

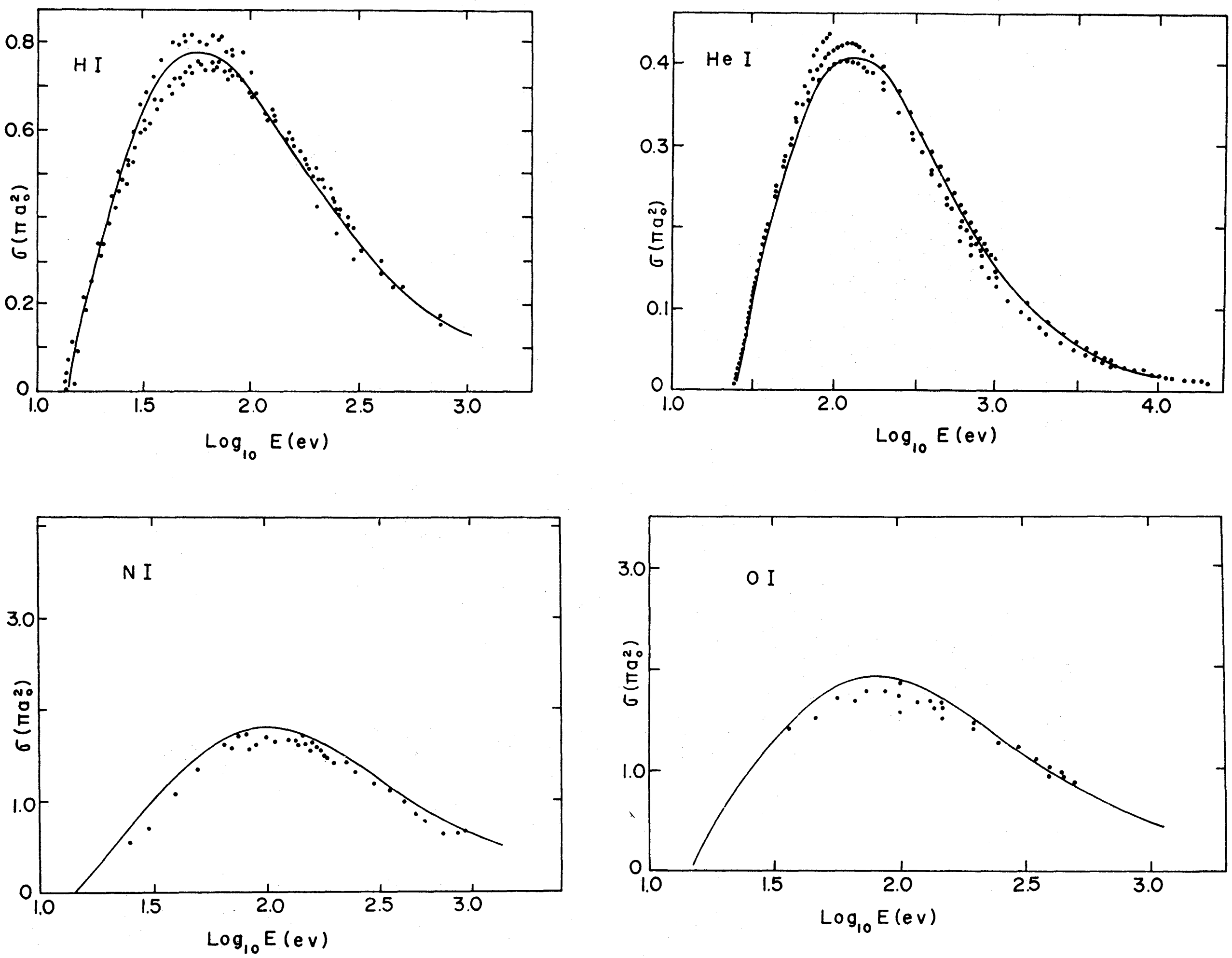
In Table 1 the values of these parameters corresponding to ions of astrophysical interest mentioned by Kieffer and Dunn are shown. In Figures 1 and 2 we compare the experimental values of the cross sections with those computed by the proposed method. For almost all the values of the incident electron's energy that have been measured, the computed values are within the experimental error given. If these curves are compared with those proposed by Lotz

TABLE 1

PARAMETERS CHOSEN TO FIT THE COLLISIONAL IONIZATION CROSS SECTIONS

Ion	$I(eV)$	$\sigma_m\,(10^{-16}\,cm^2)$*	$E_m\,(eV)$*
HI	13.6	0.67	36
HeI	24.6	0.36	126
HeII	54.4	0.048	178
LiII	75.6	0.046	282
N I	14.5	1.57	100
N II	29.6	0.52	112
O I	13.6	1.60	79.5
NeI	21.6	0.83	170
NeII	41.1	0.32	200
NaII	47.3	0.27	250

* Taken from the experimental values of Kieffer and Dunn (1966).



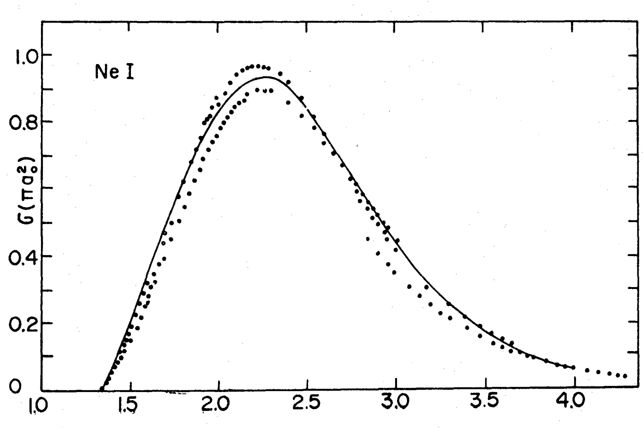
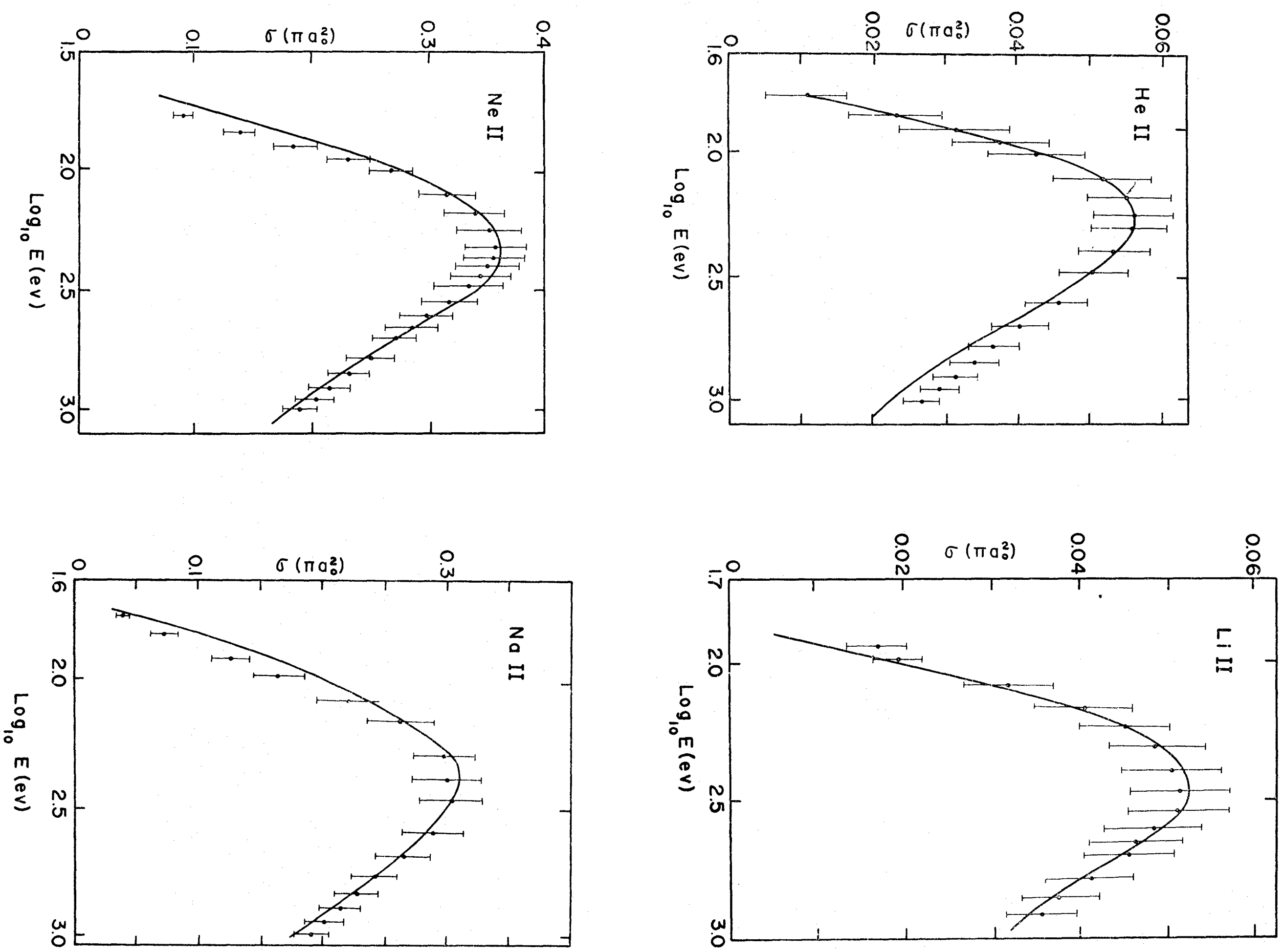


FIG. 1. Comparison of the experimental data for neutral atoms compiled by Kieffer and Dunn (1966) with the empirical calculation proposed. The solid line represents the computed values while the dots show the experimental values.



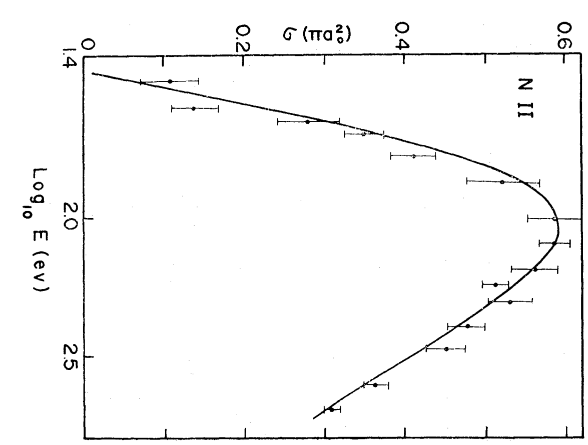


FIG. 2. Comparison of the experimental data for ions compiled by Kieffer and Dunn (1966) with the empirical calculation proposed. The solid line represents the computed values while the dots show the experimental values.

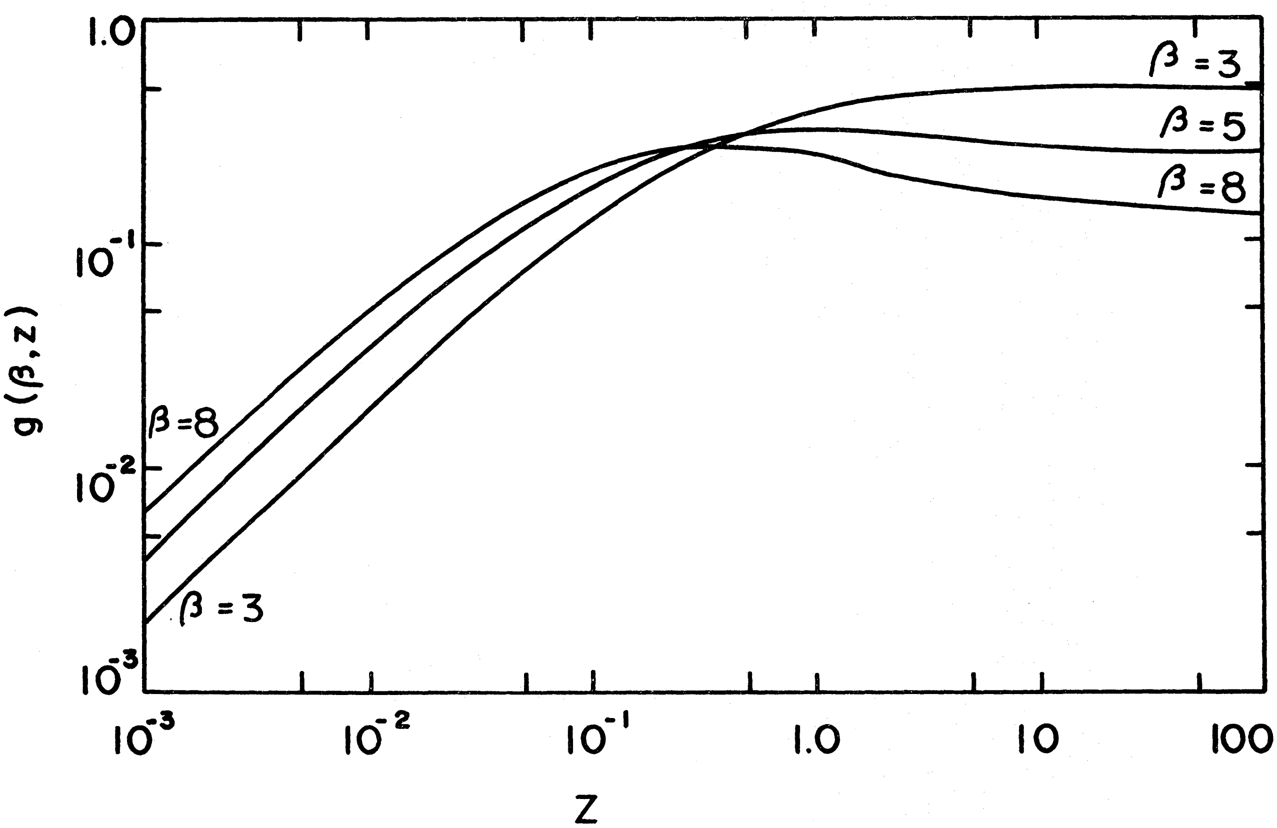


FIG. 3. Plot of $g(\beta, Z)$ as a function of Z for several values of β.

(1966) it can be seen that they differ by less than 10% for $I \leq E \leq 10I$. The discrepancy at high energies is due to the logarithmic behavicr of the cross section typical of this energy range (see for example Seaton 1962), which we have not taken into account.

The ionization coefficient corresponding to the cross section given by equation (1) is

$$< \sigma v > = \int_I^\infty \sigma(E)\ v(E)\ f(E)\ dE$$
$$= 16\ \sigma_m\ (KT\pi/2m_e)^{1/2} \exp(-I/KT)\ g\ (\beta, Z),$$

where $f(E)\ dE$ is the Maxwell Boltzmann distribution and

$$g(\beta, Z) = (\beta^2 - 3\beta + 2)Z^2 + (\beta - 1)Z - (\beta - 1)Z \exp[(\beta - 1)Z]E_1[(\beta - 1)Z] \times [(\beta^2 - 3\beta + 2)Z^2 + 2(\beta - 1)Z]$$

with

$$\beta = E_m/I, \qquad Z = I/KT$$

and

$$E_1(x) = \int_x^\infty [\exp(-t)/t]dt.$$

In Figure 3 a plot of g(β, Z) si shown.

Unfortunately, until now we only have experimental information about σ_m and E_m for some neutral atoms and some ions of charge +1. However, the proposed formula allows us to estimate with sufficient accuracy the values of the ionization rates if σ_m is known. Indeed, observe that, if $I/KT > 1$ we can consider that $g(\beta, Z) \simeq 0.3$ (corresponding to $\beta \simeq 4.5$), for any value of β within the observed range ($3 \leq \beta \leq 8$). For $I/KT < 0.1$ we can take $g(\beta, Z) \simeq (Z)^{0.77}$, which is a fit to the value corresponding to $\beta \simeq 5$. Since the majority of the experimental values of β are between 4 and 6, this approximation is reasonable. The error is estimated to be less than 30%.

To obtain the value of σ_m when experimental information is lacking, observe that, as is shown in Figure 4, we can write

$$\sigma_m(\text{cm}^2) = 7.24 \times 10^{-15}/[I(eV)]^{1.44},$$

for atoms or ions with more than two, but less than ten, electrons. We then have for these ions

$$< \sigma v > (\text{cm}^3\, s^{-1}) = (5.25 \times 10^{-9})\ (T(^\circ\text{K}))^{1/2}$$
$$\exp(-I/KT)/[I(eV)^{1.44}, \quad I/KT > 1$$

and

$$< \sigma v > (\text{cm}^3\, \text{s}^{-1}) = (2.35 \times 10^{-5})\ (T(^\circ K))^{-0.27}$$
$$/[I(eV)]^{0.67}, \quad I/KT < 0.1.$$

The first of these formulae coincides within 10% with that proposed by Cox and Tucker (1969) for the cases in which a comparison was made.

For the hydrogen and helium iso-electronic sequences the available experimental information does not allow the proposal of adequate interpolation formulae. But, if an interpolation with only two reference points is allowed, we can write

$$\sigma_m(\text{cm}^2) = 9.55 \times 10^{-15}/[I(eV)]^{1.90}$$

for the hydrogen iso-electronic sequence, and

$$\sigma_m(\text{cm}^2) = 1.44 \times 10^{-14}/[I(eV)]^{1.86}$$

for the helium iso-electronic sequence as is also shown in Figure 4.

A simple interpretation of the proposed formula to reproduce the experimental cross sections is based on the classical Thomson formulation of the collisional ionization process (see for instance Ochkur and Petrun'kin 1963 and Bely and van Regemorter 1970). This formulation is based on the integration of Rutherford's differential cross sections from the threshold energy I to the maximum energy that can be transferred, that is, the incident energy ξ. The cross section is then

$$\sigma = N_{eff} \int_I^\xi 4\pi\, a_0^2\, I_H^2 \frac{1}{\xi} \frac{d\varepsilon}{\varepsilon^2}$$

where N_{eff} is the effective number of bound electrons that participate in the process and I_H is the hydrogen ionization potential. If we assume that the incidence

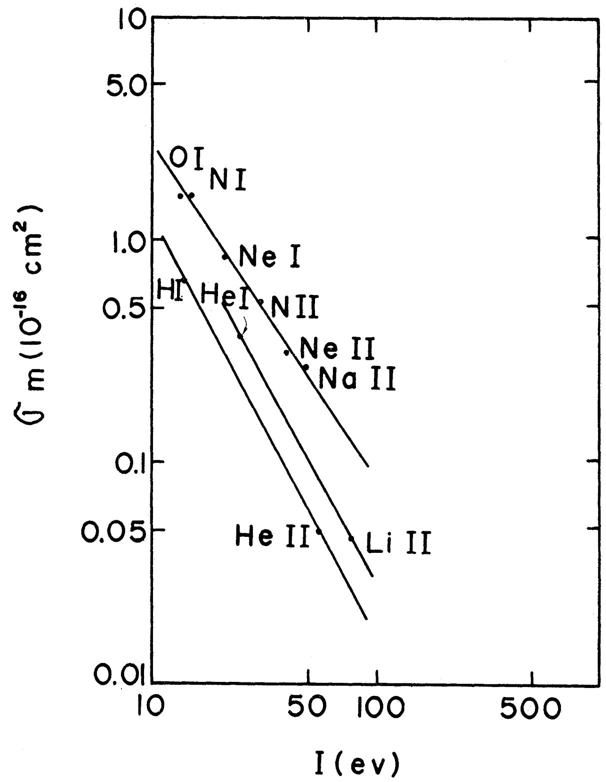


FIG. 4. Linear relations between log σ_m and log I that lead to the interpolation formulae proposed.

energy ξ near the point where the collision occurs is a linear function, $\xi = a + bE$, of the incidence energy at infinity E, such that $\xi(I) = I$, we obtain equation (1) with $a = (1 - b)I$, $b = I(E_m - I)$, $N_{eff} = \sigma_m I_2^2/\pi a_2^2 I_H^2$. This linear function represents, to first order, the combined effects of the ionic field and of the movement of the bound electrons.

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