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SEMI-EMPIRICAL CROSS SECTIONS AND RATE COEFFICIENTER FOR EXCITATION AND IONIZATION BY ELECTRON COLLISION AND PHOTOIONIZATION OF HELIUM T. FUJIMOTO

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Semi-empirical Cross Sections and Rate Coefficients for Excitation and Ionization by Electron Collision and Photoionization of Helium

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July 1978

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Experimental and theoretical data are reviewed on cross sections of transitions between various neutral helium states. Semi-empirical or empirical formulas are fitted to these cross sections. Analytical expressions are given for rate coefficients, i.e., for excitation, de-excitation, ionization, three-body recombination and radiative recombination.

INTRODUCTION

In the study of plasma spectroscopy, knowledge of cross sections for transitions of atoms and ions by electron collisions as well as of radiative transition probabilities is essential requirement in order to make a detailed analysis of ionization-recombination of the plasma and of the population density distribution of excited species in it. Helium is of particular interest from this point, since it is frequently used in gas discharge plasmas including gas lasers, in fusion research plasmas and so forth. It is also important in astrophysical plasmas. Therefore, it is of some value to compile these basic quantities for helium in a form which is convenient to be applied to these practical problems.

Radiative transition probabilities (1,2) between discrete levels of helium are well established. However, cross section data by electron collision, especially for excitation, were not sufficient until recent years, when such a large number of experimental and theoretical data have accumulated that one can make a reliable estimate of many cross sections.

In this report a brief review is made for cross sections of excitation and ionization by electron collisions and of photoionization for various neutral helium states. These cross sections are fitted by semi-empirical or empirical formulas, and finally transition rate coefficients are given in analytical forms for colliding electrons with the Maxwellian velocity distribution.

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1. EXCITATION

i) Optically allowed or dipole transition

For the transitions from $1^{1}S$ to $n^{1}P$ states (pricipal quantum number $n \ge 2$) there are several experimental⁽³⁻¹²⁾ and theoretical data.⁽¹³⁻¹⁵⁾ For transitions between excited states several theoretical calculations are available⁽¹³⁻²⁰⁾ as well as a recent experiment.⁽²¹⁾ Examples are shown in Figs. 1, 2 and 3.^{*}

* In Fig.14 of ref.15 the curve for the quartet contribution to $2^{3}S \rightarrow 2^{3}P$ excitation is understood to be multiplied by 10. This removes the inconsistency among refs. 13, 14 and 15.

For the excitation cross section from the state p to q the semi-empirical formula is given in the form

$$\sigma(U) = 4 \left(\frac{R}{\chi_{p,q}}\right)^2 f_{p,q} \pi a_0^2 Y(U), \qquad (1)$$

where $U \equiv E/\chi_{p,q}$ is the kinetic energy of the colliding electron in the threshold unit, $f_{p,q}$ is the absorption oscillator strength for the transition, R and a_0 are the Rydberg constant (13.6 eV) and the Bohr radius (0.529 Å), respectively. Various expressions for the shape factor Y(U) have been proposed by several authors. Here the one proposed by Johnson and Hinnov⁽²²⁾ is adopted:

$$Y(U) = U^{-1}[1 - \exp\{-t(U+1)\}]\ln(U+\delta), \qquad (2)$$

where

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$$t = \beta (f_{p,q} R/\chi_{p,q})^{-\gamma}.$$
 (3)

The parameters β , γ and δ are adjusted to give a best fit of the expression (1) - (3) to the existing data. Examples of this fitting are shown in Figs. 1, 2 and 3. The set of values of β , γ and δ thus determined are tabulated in Table 1. For other transitions than those given in the table, values of β , γ and δ are given as 0.5, 0.7 and 0.2, respectively, as recommended^{*} in ref.22.

* In ref.22 these parameters are adjusted so that the calculated population density distribution for $n \ge 3$ excited states gives the best fit to the measured one in the lowpressure afterglow, resulting in the set of values, 0.5, 0.7 and 0.2 for β , γ and δ , respectively, for all the transitions. However, under this plasma condition the calculated population density distribution is insensitive to the magnitudes of the excitation and de-excitation rate coefficients for which $\chi_{p,q} >> kT_e$ holds, (k is the Boltzmann constant and T the electron temperature) i.e., for transitions starting from or ending to the lowest-lying states (n=1 and 2). Therefore, this set of values thus determined applies only to the transitions between high-Indeed, it is seen in Table 1 that various lying states. sets of parameter values should be employed for the transitions from n = 1 or 2.

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The excitation rate coefficient

$$C(p,q) = \int_{v_{th}}^{\infty} \sigma(v) v f(v) dv \qquad (4)$$

is derived for electrons with a Maxwellian velocity distribution, f(v), at temperature, T_e . In eq.(4) v_{th} denotes the velocity corresponding to the threshold energy. It is sometimes convenient to calculate the de-excitation rate coefficient F(q,p) first; then C(p,q) is given by

$$C(p,q) = \frac{g(q)}{g(p)} F(q,p) e^{-u}, \qquad (5)$$

where g(p) is the statistical weight of the state p and u $\equiv \chi_{p,q}/kT_e$. Now the de-excitation rate coefficient is given as

$$F(q,p) = K \frac{g(p)}{g(q)} \left[u^{-1} \left\{ ln(1+\delta) + exp\{(1+\delta)u\} [-Ei\{-(1+\delta)u\}] \right\} \right]$$

$$- \left[\beta(f_{p,q} R/\chi_{p,q})^{-\gamma} + u \right]^{-1} exp[-2\beta(f_{p,q} R/\chi_{p,q})^{-\gamma}]$$

$$\times \left\{ ln(1+\delta) + exp[(1+\delta)\{\beta(f_{p,q} R/\chi_{p,q})^{-\gamma} + u\}] \right\}$$

$$\times \left(-Ei[-((1+\delta)\{\beta(f_{p,q} R/\chi_{p,q})^{-\gamma} + u\}]) \right\}, \quad (6)$$

where

$$K = 4 \left(\frac{R}{kT_{e}}\right)^{2} f_{p,q} \sqrt{\pi} a_{o}^{2} \frac{2\sqrt{2}}{\sqrt{m}} \sqrt{kT_{e}}$$
$$= 2.19 \times 10^{-10} \left(\frac{R}{kT_{e}}\right)^{2} \sqrt{T_{e}} f_{p,q} \quad cm^{3}sec^{-1}, \qquad (7)$$

m is the electron mass and T_e is in the unit of degrees K. The exponential integral is defined as

$$Ei(-t) = -\int_{t}^{\infty} \frac{e^{-x}}{x} dx . \qquad (8)$$

When the electron temperature is so low that the argument t in eq.(8) is large (\gtrsim 10) one may employ an asymptotic formula⁽²³⁾

$$te^{t} \{-Ei(-t)\} \simeq \frac{t^{2} + 4.03640t + 1.15198}{t^{2} + 5.03637t + 4.19160}$$
 (9)

 ii) Optically forbidden transition without a spin change There are several experimental ^(3,5,9,10,21,24-33) and theoretical ^(13-20,34,35) cross section data for the low-lying states. Another semi-empirical formula ⁽²²⁾ is employed.

$$\sigma(U) = 4 \left(\frac{R}{\chi_{p,q}}\right) B \pi a_0^2 Y(U) , \qquad (10)$$

where the shape factor is

$$Y(U) = U^{-2} \{1 - \exp(-tU)\} (U - 1 + \delta)$$
 (11)

and

$$t = 1.6 \beta B^{-\gamma} \{ \left(\frac{r_0}{a_0} \right)^2 \frac{\chi_{p,q}}{4R} \}^{1-\gamma} .$$
 (12)

Here r_0 is given by $a_0 n_p^* n_q^*$ with the effective principal quantum numbers of the states p and q, and B is the scale factor in the Born approximation, which is taken as one half of the interpolated value ^(36,37) to give the hydrogenic approximation. The adjustable parameters β , γ and δ are determined to give a reasonable fit of the cross section (10) to the existing data. Several examples of the cross sections are shown in Figs. 4 and 5. For all the transitions other than shown in Table 2, the parameter values are taken as 0.5, 0.7 and 0.2 for β , γ and δ , respectively. The de-excitation rate coefficient is given by

$$F(q,p) = K' \frac{g(p)}{g(q)} \left\{ \frac{1}{u} - \frac{e^{-t}}{t+u} - (1-\delta) \right\}$$

$$\times \left(-Ei(-u)e^{u} - [-Ei\{-(t+u)\}exp(t+u)] e^{-t} \right), \quad (13)$$

where

$$K' = 2.19 \times 10^{-10} \left(\frac{R}{kT_e}\right) u \sqrt{T_e} B cm^3 sec^{-1}$$
. (14)

iii) Excitation with a spin change

Data are not sufficient except for the transitions from the ground (3,5,9,11,12,17,24,28,29,31-33,38,39) and between the n = 2 states. (13-15,17) The cross sections from the ground state are approximated by a modified version of the formula of ref.40 as

$$\sigma(\mathbf{U}) = 4\pi a_0^2 \{ \mathbf{T} \, \mathbf{U}^{-9} + Q(-\mathbf{U}^{-5} + \mathbf{U}^{-3}) \}, \qquad (15)$$

where T and Q are adjustable parameters. Examples of fitting of eq.(15) to the existing data are shown in Figs. 6 and 7, and T and Q are given in Table 3. The de-excitation rate coefficient is given by

$$F(q,p) = K'' \frac{g(p)}{g(q)} \left(\Omega \left[\frac{4+u-u^2}{6} + \left\{ -\text{Ei}(-u) \right\} e^u u \left(\frac{u^2}{6} - 1 \right) \right] \right)$$

$$+ T \left[\frac{1}{7} \left(1 - \frac{u}{6} + \frac{u^2}{30} - \frac{u^3}{120} + \frac{u^4}{360} - \frac{u^5}{720} + \frac{u^6}{720} \right) - \frac{u^7}{5040} e^u \left\{ -\text{Ei}(-u) \right\} \right], \qquad (16)$$

where

$$K'' = 2.19 \times 10^{-10} u^2 \sqrt{T_e} cm^3 sec^{-1}$$
, (17)

For transitions between the n = 2 states there are several calculations.^(13-15,17) The following formula has been found to given a reasonable fit to these data;

$$\sigma(U) = 4\pi a_0^2 Q(\frac{U-1}{U^2}), \qquad (18)$$

where the scale factor Q is adjusted. An example is shown in Fig.8, and Q's determined are given in Table 4. The deexcitation rate coefficient is

$$F(q,p) = K''Q \frac{g(p)}{g(q)} [u - u^2 e^u \{-Ei(-u)\}].$$
(19)

2. IONIZATION

Experimental cross section are available only for transitions from the ground state $^{(41)}$ and $2^3s.^{(42,43)}$ The following formula $^{(40)}$ is fitted to these data;

$$(U) = 4\pi a_0^2 \left(\frac{R}{\chi_p}\right)^2 \eta \frac{U-1}{U^2} \ln(1.25 \beta U)$$
(20)

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where χ_p is the ionization potential of the state p, and U = E/χ_p . Here n and β are adjusted to give a reasonable fit to the existing data, and these are shown in Table 5. For other states n and β are given values of 0.66 and 1, respectively, to give a hydrogenic approximation. ⁽⁴⁰⁾ For the three-body recombination, i.e., the inverse process of ionization, the rate coefficient is calculated as

$$\alpha(p) = \frac{2h^3}{\pi^2 m^2} \pi a_0^2 \left(\frac{R}{\chi_p}\right)^2 \frac{g(p)}{\omega_i k T_e} \eta \frac{u}{1+u} \left[\frac{1}{20+u} + \ln\{1.25\beta(1+\frac{1}{u})\}\right]$$

= 4.58 × 10⁻²⁶ $\left(\frac{R}{\chi_p}\right)^2 \frac{g(p)}{\omega_i} \frac{\eta}{T_e} \frac{u}{1+u} \left[\frac{1}{20+u} + \ln\{1.25\beta(1+\frac{1}{u})\}\right]$
 $cm^6 sec^{-1}$, (21)

where h and ω_i are Planck's constant and the partition function of the ion (put equal to 2 except at very high temperature), and u is χ_p/kT_e . The ionization rate coefficient is given by the relation

$$S(p) = \alpha(p)/Z(p)$$
 cm³sec⁻¹, (22)

where

$$Z(p) = \frac{g(p)}{2\omega_{i}} \left(\frac{h^{2}}{2^{\pi}mkT_{e}}\right)^{3/2} e^{u} .$$
 (23)

3. PHOTOIONIZATION

For the ground⁽⁴⁴⁾ and the two metastable states⁽⁴⁵⁾ experimental data are available. Serveral theoretical calculations⁽⁴⁶⁻⁵⁰⁾ have been made for the n = 2 states. An example of these data is shown in Fig.9 for 2^3 S. For the n^{1,3}P (n = 3, 4

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and 5) states an experiment has been made ⁽⁵¹⁾ by the method of stepwise excitation and ionization with dye laser light, but the cross section data thus obtained correspond to those for ionization of aligned excited atoms by polarized photons instead of ordinary cross section for unpolarized photons. For the case of hydrogenic ions, on the other hand, there are several calculations of the photoionization cross sections $^{(52)}\sigma_{\rm p}(\nu)$ or the Gaunt factor $^{(53)}$ G(ν).

$$\sigma_{\rm p}(\nu) = \frac{2^6}{3\sqrt{3}} \frac{\pi^4 e^{10} m}{ch^6} \frac{1}{n_{\rm p}^5} \frac{1}{\nu^3} G_{\rm p}(\nu), \qquad (24)$$

where v is the frequency of the ionizing photons. In the case of helium this approximation should be valid for large azimuthal quantum number l. The experimental cross section data⁽⁵¹⁾ for $n^{1,3}P$, even though they are for l = 1, are converted into the cross sections for unpolarized photons by using the individual $l \neq l + 1$ and $l \neq l - 1$ cross sections in ref.52. Comparison of this and the hydrogenic cross sections $(n_p^5 \text{ in}$ eq.(24) is replaced by $n_p n_p^{*4}$) is shown in Fig.10 and a good agreement is seen especially for n^1P states.

Therefore, the hydrogenic Gaunt factor seems to be a reasonable approximation to these states and is applied to all the states except for 1^{1} S and $2^{1,3}$ S states. The Gaunt factor is found to be approximated well by

with

$$\log G_{p}(v) = \log g_{o} + a(t - t_{o}) + b(t - t_{o})^{2} \quad (25)$$

$$t = \log(\frac{hv}{R}).$$

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These coefficients are given in Table 6. In Fig.10 this approximation gives a small deviation compared to the widths of the lines. The radiative recombination coefficient is given as

$$\beta(p) = Lg(p)g_{0} \int_{1}^{\infty} x^{-1+a+b\log x} e^{-u(x-1)} dx$$
 (26)

with

$$L = \frac{2^{7}}{3\sqrt{3}} - \frac{\pi^{5} e^{10}}{m^{2} c^{3} h^{3}} \left(\frac{m}{2\pi k T_{e}}\right)^{3/2} \frac{1}{n_{p} n_{p}^{*4}}$$
$$= 8.15 \times 10^{-7} - \frac{1}{T_{e}^{3/2}} \frac{1}{n_{p} n_{p}^{*4}} - cm^{3} sec^{-1}, \quad (27)$$

and $u = \chi_p/kT_e$. Unfortunately eq.(26) does not lead to an analytical expression. Instead, for the states 1^1 S and $2^{1,3}$ S simple expressions are given corresponding to the approximate cross sections ($\sigma_v \propto v^{-2}$) in Fig.9.

$$\beta(1^{1}S) = 1.60 \times 10^{-11} g(1^{1}S) / \sqrt{T_{e}} cm^{3}sec^{-1}, (28a)$$

$$\beta(2^{1}, {}^{3}S) = 5.45 \times 10^{-13} g(2^{1}, {}^{3}S) / \sqrt{T_{e}} cm^{3}sec^{-1}. (28b)$$

4. DISCUSSION

For the excitation cross sections from the ground state the shape as well as the magnitude is well established for high energy region (U \geq 3) where the Born approximation is

valid. (See Figs. 1, 4, 6 and 7). Disagreements among the various data are typically 30% for excitation to the singlet states and a factor 2 for the triplet states. However, in the low-energy region near threshold substantial disagreements exist, as is seen in Figs. 4 and 7 as examples, by a factor of 2 for the singlet excitations and by an order in the case of triplet excitations. For the transitions between the excited states much less is known, and disagreements among the data are more severe, especially between the recent experiment⁽²¹⁾ and the theoretical calculations. (See Figs. 3 and 5). Fitting of the analytical expressions (1), (10), (15) and (18) is based primarily on the recent experimental data. The resulting cross sections lie within a spread of the data as seen in Figs. 1 ~ 8. For the transition of $\Delta n > 1$ between the high-lying states (n > 8), where hydrogenic approximation should be approximately valid, another semi-empirical formula⁽⁵⁴⁾ is available. Comparison of this and the sum of the cross sections (1) and (10) gives agreements within a factor of 2.

Instead of cross section itself excitation rate coefficient data are available for several transitions from experiment. (55-58) For the transition $2^3S \leftrightarrow 2^1S$ the theoretical cross section of refs. 13, 14 and 15 reproduces the excitation (56) and deexcitation (55) rate coefficients. Reference 57 gives experimental estimates of the rate coefficients for the several dipole transitions: $2^{1,3}S \leftrightarrow 2^{1,3}P$ and $3^{1,3}S \leftrightarrow 3^{1,3}P$. Excellent agreements are obtained between these values and the rate coefficient (5), giving a confidence in eq.(1). For several

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transitions between the n = 3 states ref.58 gives experimental rate coefficients, but those for the dipole transitions are smaller than eq.(5) by one to two orders of magnitude. The origin of this large discrepancy is not known.

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Table 1. β , γ , δ in eqs. (1), (2) and (3).

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b d	2 ¹ P	3 ¹ P	$\geq 4^{1}P$
l ¹ s	0.1, 0.3, 0.0	0.15, 0.2, 0.0	0.2, C.1, 0.0
2 ¹ s	0.8, 0.7, 0.0	0.1 , 0.7, 0.0	0.1, 0.7, 0.0

b ď	2 ³ P	3 ³ P	≥ 4 ³ P
2 ³ s	0.5, 0.2, 0.0	0.1, 0.1, 0.1	0.1, 0.1, 0.1

Table 2. β , γ , δ in eqs. (9), (10) and (11).

p	2 ¹ s	3 ¹ s	$\geq 4^1 s$
l ¹ s	1.0, 0.7, 0.15	0.1, 0.2, 0.07	0.3, 0.5, 0.02

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b ď	<u>></u> 3 ¹ s	≥ 3 ¹ D
2 ¹ s	0.3, 0.7, 0.2	0.3, 0.7, 0.2

b ď	≥ 3 ³ s	≥ 3 ³ D
2 ³ s	0.3, 0.7, 0.2	0.3, 0.7, 0.2

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Table

т, 2			0.0, 4.5(-2)/n ^{*3}
đ	1	I	≥ 4 ³ F
õ), 3.5(-3)	, 8.8(-2)/n ^{*3}
		0.0	0.0
<u>с</u> ,	I	33 ³ D	≥ 4 ³ D
т, 2	0, 4.5(-2)	0, 2.5(-2)	0, 7.5(-1)/n ^{*3}
-	0	0	0
<u>р</u> ,	2 ³ P	3 ³	- 4 ³ P
т, 2	1.07(-2) [*] , 3.13(-2)	0.0, 1.3(-2)	0.0, 2.75(-1)/n ^{*3}
Q	2 ³ S	33 33	- 4 ³ S

* 1.07(-2) is 1.07 × 10⁻².

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Table 4. Q in eq. (17)

2 ¹ P	а. 5 С	5.0
2 ¹ S	7.0	27.5
b d	2 ³ S	23 ³ 7

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Table 5. η , β in eq.19

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1.0	2.5
.	
1.0	0.66
1 ¹ S	2 ³ S

f

Table 6. g_o, a, b in eq.(24) in hydrogenic approximation

ls	0.797, 0.293, - 0.220							
2s	0.935, 0.912, - 0.363	2p	0.857, - 0.091, - 0.	343				
3g	1.062, 0.986, - 0.271	3p	1.098, 0.561, - 0.	506 3đ	0.763, -	· 0.430, - 0.518		
4s	1.179, 1.000, - 0.210	4p	1.246, 0.797, - 0.	164 4d	1.131,	0.200, - 0.655	4f	0.603, - 0.785, - 0.665
5s	1.290, 0.940, - 0.116	δp	1.366, 0.864, - 0.	376 5d	1.352,	0.539, - 0.671	5£	1.037, - 0.133, - 0.825
6s	1.395, 0.915, - 0.081	6p	1.473, 0.880, - 0.	04 6d	1.511,	0.685, - 0.593	6f	1.336, 0.247, - 0.837
7s	1.449, 0.919, - 0.064	7P	1.556, 0.914, - 0.	:74 7d	1.578 <i>,</i>	0.819, - 0.558	7£	1.524, 0.476, - 0.769



Fig. 1 Excitation cross section for 1 ¹S → 2 ¹P. Experimental data; ------ : Jobe, ref. 4.
• : Moustafa Moussa, ref. 5. • : van Eck, ref. 6. • : Donaldson, ref. 8.
↓ : Hall, ref. 9. △ : Dillon, ref. 10. ↓ : Chutjian, ref. 11. ○ : Joyez, ref. 12.
Theoretical data; ------ : Vriens, ref. 8. ------ : Burke, ref. 13 and Berrington, ref. 14. ------ : Oberoi, ref. 15. Semi-empirical; ---- : eq. (1).





Fig. 3 Excitation cross section for 2 ³ S → 3 ³ P. Experimental data; §: Khakhaev, ref. 21. Theoretical data; ----- : Moiseivich, ref. 16. ----- : Ochkur, ref. 17. ----- : Vriens, ref. 18. ----- : Flannery, ref. 19. ---- : Flannery, ref. 20. Semi-empirical; ----- : eq. (1).



Electron energy (eV)

Fig. 4 ref. 24. • : Vriens, ref. 28. § : Rice, ref. 30. ----- : Brongersma, ref. 31. I Trajmar, ref. 32. ↓ : Hall, ref. 9. △ : Dillon, ref. 10. ○ : Joyez, ref. 12. Theoretical data; ----: Bell, ref. 35. Vriens, ref. 18. ----: van den Boss, ref. 34. ------ : Burke, ref. 13 and Berrington, ref. 14. ----- : Oberoi, ref. 15. Semi-empirical; —— : eq. (10).



Fig. 5 Excitation cross section for 2 ³ S → 3 ³ D. Experimental data; § : Khakhaev, ref. 21. Theoretical data; ----- : Moiseivitch, ref. 16. -----: Ochkur, ref. 17.
....: Vriens, ref. 18. ----: Flannery, ref. 19. ----: Flannery, ref. 20. Semi-empirical; ----: eq. (10).





 Fig. 7 Excitation cross section for 1 ¹ S → 2 ³ P. Experimental data; ----- : Jobe, ref. 4.

 ¹/₂ : Hall, ref. 9.
 ¹/₂ : Trajmar, ref. 32.
 ¹/₂ : Chutjian, ref. 11.
 ⁰ : Joyez, ref. 12.
 Theoretical data; ------: Ochkur, ref. 17. Semi-empirical; -----: eq. (15).





Fig. 9Photoionization cross section from 2 3 S. Experimental data; • : Stebbings, ref. 45.Theoretical data; ----- : Norcross, ref. 47. + : Bell, ref. 49. • : Jacobs, ref. 50.Approximation; ------ : $\sigma = 9.3 \times 10^{12} v^{-2} \text{ cm}^2$.



