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Rate Coefficients for the Electron-Impact Excitation, Ionization and Recombination of He-Like Ions, S XV, Ca XIX and Fe XXV, and Related Processes

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ABSTRACT: Data on the rate coefficients for the electron-impact excitation, ionization and recombination of S XV, Ca XIX and Fe XXV ions are reviewed to recommend a comprehensive set of values. Some related processes involved in the emission from the 1s2*l* states of those He-like ions and its satellite lines are also considered. All the rate coefficients recommended here are expressed in an analytic form of the electron temperature.

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1. INTRODUCTION

In 1991, a satellite was launched by ISAS to observe the solar X-rays. It was named YOHKOH. One of the instruments aboard YOHKOH, the Bragg crystal spectrometer (BCS), provides line spectra of the soft X-rays emitted from He-like ions, S XV, Ca, XIX and Fe XXV. To analyze those spectra, atomic data are needed for the electron collisions with those ions and related processes. The present report is a compilation of those atomic data.

The BCS spectrum shows the lines emitted from the fine structure levels of 1s2*l* configurations and their satellite lines. The upper levels, 1s2*l*, are produced by (i) direct excitation from the ground state $1s^2\ {}^1S$, (ii) cascading from the higher states, particularly those with 1s3*l*, and (iii) innershell ionization of Li-like ions, $1s^22s$. The satellite lines emitted from the Li-like ions are produced by (i) dielectronic recombination to the He-like ions in its ground state, and (ii) innershell excitation of Li-like ions. Furthermore the fraction of the specific ion is determined by the balance of the ionization and recombination. The latter includes both the radiative and the dielectronic processes. In the following sections, rate coefficients are presented for the collision processes listed above.

2. EXCITATION

2.1. Excitation of He-Like Ions

2.1.1. Data Sources

All the data sources considered here are given in Table 2.1. Three types of calculations have been reported on the excitation rate coefficients of S XV, Ca XIX, and Fe XXV. The most extensive calculation was done with the Coulomb-Born (CB) type approximation. Sampson et al. (1983) published their results for 20 He-like ions with nuclear charge Z in the range Z=4–74. Their calculation does not take into account resonance effects. Zhang and Sampson (1987) extended the calculation with including resonance effects. Vainshtein and Itikawa (1992) calculated the rate coefficients for 21 He-like ions with Z=6(2)46 with the approach very similar to, but completely independent of the method of Sampson's group.

Pradhan (1985) applied the distorted wave (DW) method to the calculation of the rate coefficient of Ca XIX and Fe XXV. In his calculation, he approximately considered the resonance

Table 2.1. Data sources on the rate coefficient for the electron-impact excitation of S XV, Ca XIX and Fe XXV. Sources are indicated by the symbols given in the footnotes and those for the recommended data are underlined.

transition	Fe XXV	Ca XIX	S XV
$1s^2 \rightarrow 1s2s,p$	P, S, V, Z	P, S, V, Z	Ke, N, S V, Z
$1s^2 \rightarrow 1s3s,p$	P, S, V	P, S, V	Ke, N, S, V
$1s^2 \rightarrow 1s3d$	S, V	S, V	N, S, V

Ke : Keenan et al. (1987)
N : Nakazaki et al. (1993)
P : Pradhan (1985)
S : Sampson et al. (1983)
V : Vainshtein and Itikawa (1992)
Z : Zhang and Sampson (1987)

effect. Nakazaki et al. (1993) obtained the cross section for S XV by using the R-matrix method (RM). They assumed the LS scheme for the angular-momentum coupling so that they report no data for the transitions among any fine-structure levels. Keenan et al. (1987) determined the excitation rate for the He-like ions with Z=9–25 by interpolating the theoretical results for Z=8, 12, 20, 26 (based on either the R-matrix or distorted wave method). The latter includes the calculation by Pradhan mentioned above.

It is worth mentioning here the calculation by Dubau and his collaborators, which is not listed in Table 2.1 but widely used in the analysis of observed X-ray spectra. On the basis of the distorted wave method, they made calculations of the effective rate coefficients for the emission of resonance and satellite lines of He-like ions. They published their results for Fe and Ca (Bely-Dubau et al., 1982a, b). Their rate coefficients include the cascade contribution, but no effects of resonance scattering. Later they estimated the resonance effect for the $1s^2\ ^1S$—$1s2s\ ^3S$ transition of Fe XXV (Faucher and Dubau, 1985). The result (without cascade) is very close to the corresponding value obtained by Zhang and Sampson (1987).

2.1.2. Recommended Data

(1) Selection of Data

The most accurate method of calculation available is the R-matrix method. It automatically includes resonance effects. For S XV, therefore, the calculation by Nakazaki et al. (1993) should be recommended as the best at present. Since no such calculations have been reported for Ca XIX and Fe XXV, Pradhan's calculation with the distorted wave approximation is selected. As the nuclear charge increases, the distorted wave method is getting more reliable, particularly once resonance effects are taken into account.

For the transitions $1s^2$–1s3s,1s3p of S XV, Nakazaki et al. found a large difference between their result and the corresponding value reported by Keenan et al. (1987). The latter authors obtained the rate by interpolating the results of calculations for some other members of the He-sequence, which includes Pradhan's DW calculation. In fact the temperature dependence of the rate coefficient for S XV of Keenan et al. resembles very much that for Ca XIX of Pradhan. Considering the discrepancy of the rate for S XV of Keenan et al. from that of Nakazaki et al., Pradhan's calculation for $1s^2$–1s3s,1s3p may include a large uncertainty. Until a more elaborate calculation becomes available for Ca XIX, a simple but well-founded claculation of Sampson et al. (1983) is recommended to be used for the $1s^2$–1s3s, 1s3p transitions of Ca XIX.

For the $1s^2$–1s3d transition of Ca XIX and Fe XXV, no results are available other than the CB type calculation. Here those of Sampson et al. (1983) are selected for use.

To see the reliability of the recommended data, examples of comparison of different calculations are shown in Fig. 2.1. The figure shows the effective collision strength (see below) for the excitation of 2 ^3S level of the He-like ions. For Fe XXV and Ca XIX, the calculations by Pradhan and by Zhang and Sampson include resonance effects. Other two calculations (Sampson et al. and Vainshtein and Itikawa) do not. For S XV, the resonance effects are taken into account in the calculations by Nakazaki et al. and by Zhang and Sampson. The values of Keenan et al. have been obtained from an interpolation of other He-like ions and, in this sense, include the resonance effects. It should be noted that this transition shows the largest disagreement among the different calculations considered here (except for the peculiar case of the excitation of n=3 states in Ca XIX and S XV, for which see the paper by Nakazaki et al. 1993).

(2) Analytical Fit

For the convenience of users, the present recommended data on the rate coefficient are fitted to an analytical form. To do that, the rate coefficient R_{ij} for the transition $i \rightarrow j$ is expressed in terms of the effective collision strengths γ_{ij} as a

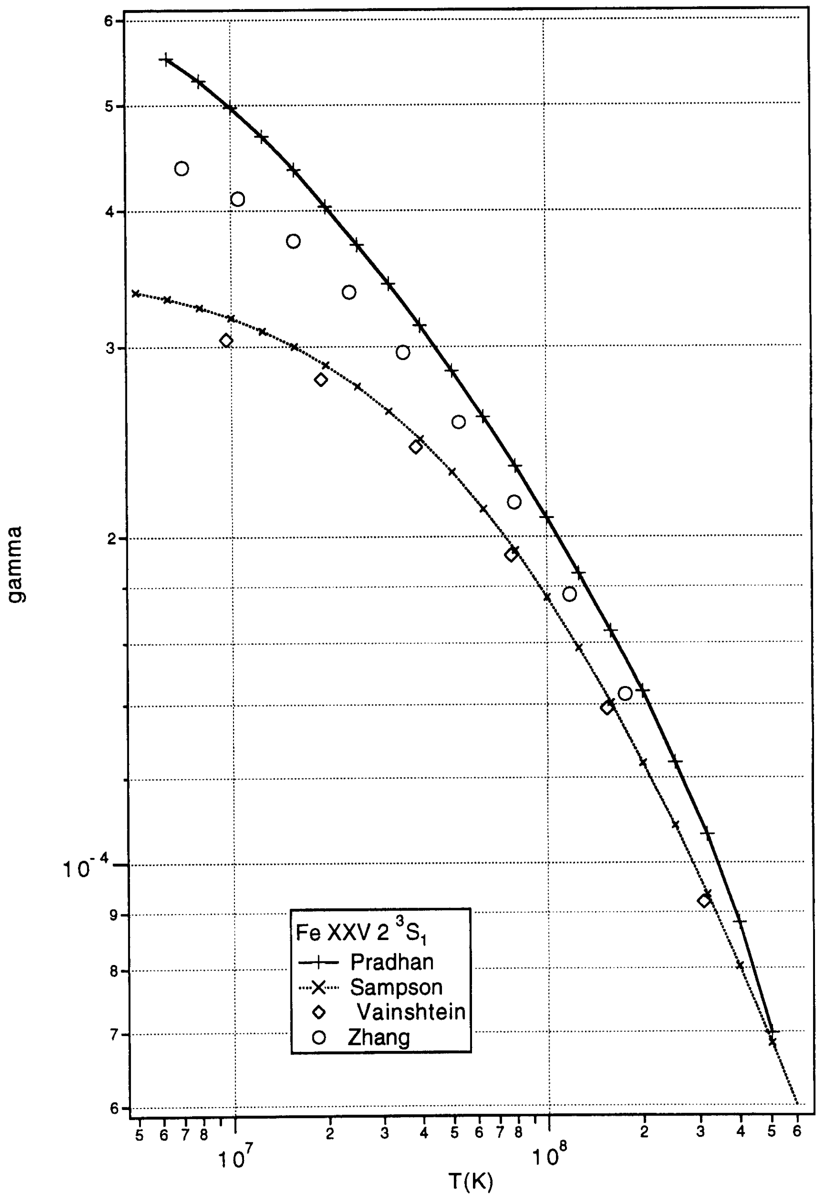

Fig. 2.1. Comparison of the effective collision strengths (γ_{ij}) for the transition $1\,^1S_0 \rightarrow 2\,^3S_1$ in (a) Fe XXV, (b) Ca XIX, and (c) S XV, calculated by Pradhan (1985), Sampson et al. (1983), Vainshtein and Itikawa (1992), Zhang and Sampson (1987), Keenan et al. (1987), and Nakazaki et al. (1993).

$$R_{ij}(T)\,[\text{in cm}^3\text{s}^{-1}] = \frac{8.629 \times 10^{-6}}{\sqrt{T}\,g_i} \exp\left(-\Delta E_{ij}/kT\right) \gamma_{ij}\,. \tag{2.1}$$

Here ΔE_{ij} is the transition energy, T is the electron temperature in K, and g_i is the statistical weight of the initial state. In the present paper, the effective collision strength is fitted to the form

$$\gamma_{ij} = y\left[(Ay^{-1} + C) + \frac{D}{2}(1-y) + e^y E_1(y)\left\{B - Cy + \frac{D}{2}y^2 + E\,y^{-1}\right\}\right]. \tag{2.2}$$

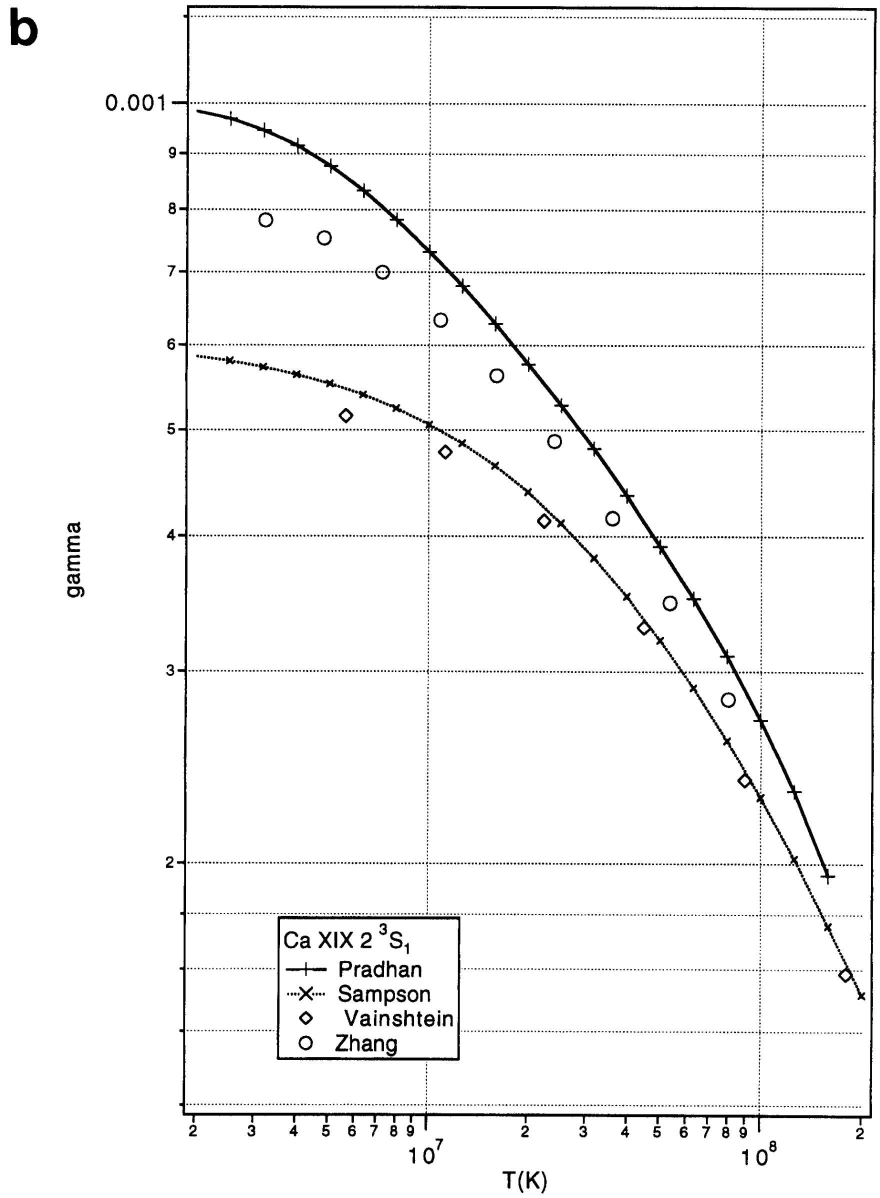

Fig. 2.1. (continued)

Here $y = \Delta E_{ij} / (kT)$ and E_1 is the exponential integral

$$E_1(y) = \int_y^\infty \frac{e^{-t}}{t} dt \,. \tag{2.3}$$

The present form of γ_{ij} (i.e., Eq. (2.2)) is based on an analytical expression of the collision strength in the form

$$\Omega_{ij} = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X \tag{2.4}$$

with $X = E/\Delta E_{ij}$ and the formula,

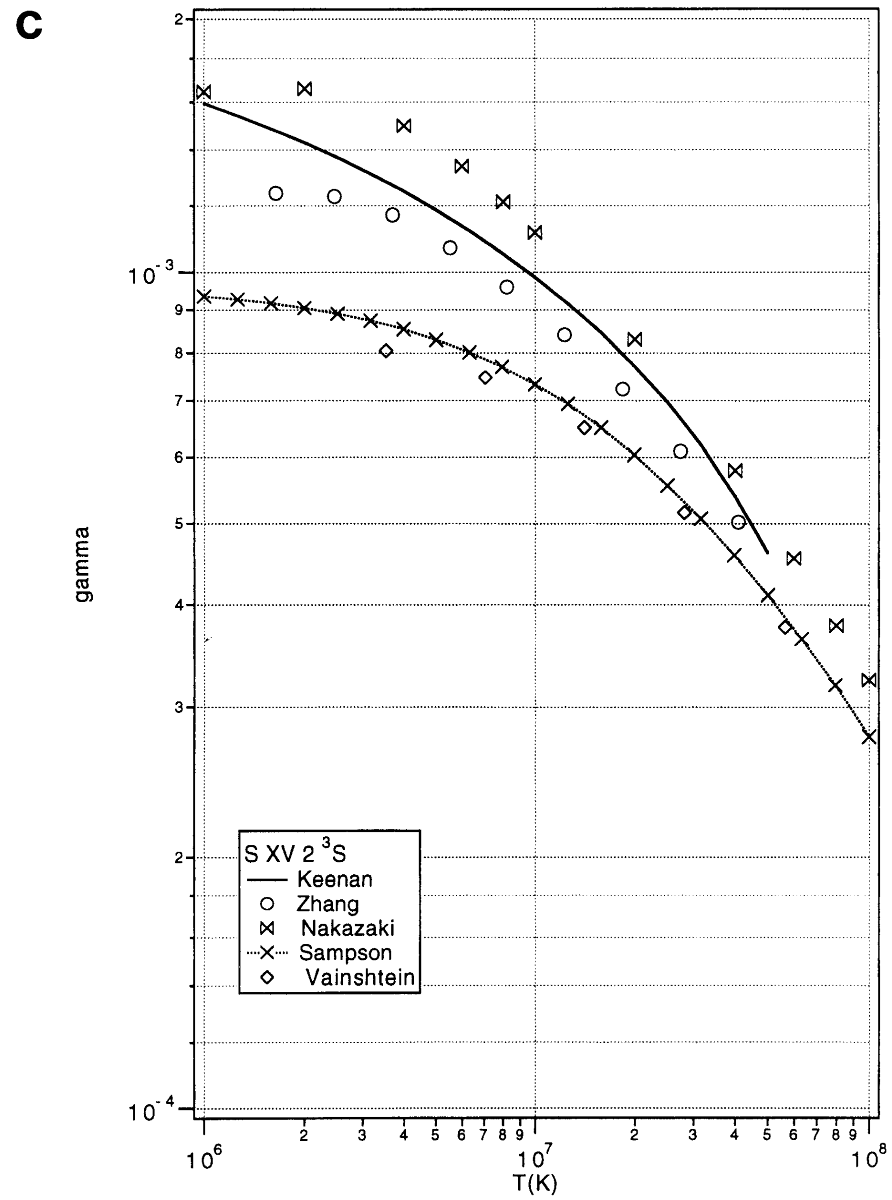

Fig. 2.1. (continued)

$$\gamma_{ij} = y\, e^{y} \int_{1}^{\infty} \Omega_{ij}\, e^{-yX}\, dX\,. \tag{2.5}$$

Tables 2.2–2.4 show the fit parameters A, B, C, D, E for the present recommended data on the effective collision strenth. For the $1s^2$–1s2s,1s2p transitions of Ca XIX and Fe XXV, Kato and Nakazaki (1989) already fitted the result of Pradhan's calculation to the above form. For those processes, no fitting procedure is repeated here and the result of Kato and Nakazaki is reproduced in the tables.

(3) Accuracy of the Recommended Data

It is very difficult to assess the accuracy of theoretical values without any comparison to experiment. The following accuracy rating is based on experience and serves only as a rough guide.

Table 2.2. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact excitation of Fe XXV. These parameters should be used in the temperature range: 5×10^6–6×10^8 K

Transition	ΔE (eV)	A	B	C	D	E
$1\ ^1S \rightarrow$						
$2\ ^3S_1$	6650	−4.11–5	6.25–4	−1.13–3	1.21–3	0
$2\ ^3P_0$	6670	−7.87–6	8.78–5	1.22–4	7.41–5	0
$2\ ^3P_1$	6680	1.66–3	−5.09–3	7.74–3	−3.56–3	0
$2\ ^3P_2$	6690	−4.46–5	4.79–4	4.81–4	4.63–4	0
$2\ ^1S_0$	6670	1.59–3	−1.53–3	7.48–4	0	−7.20–5
$2\ ^1P_1$	6710	7.22–4	−4.34–4	2.28–3	0	5.72–3
$3\ ^3S_1$	7874	−8.90726–6	7.40806–5	6.35525–5	−4.90841–5	0
$3\ ^3P_0$	7881	−2.03719–6	8.8801–6	8.2304–5	−3.64711–5	0
$3\ ^3P_1$	7882	3.07893–4	−8.70067–4	1.34064–3	−6.05388–4	0
$3\ ^3P_2$	7887	−1.70358–5	1.00534–4	3.0288–4	−1.08607–4	0
$3\ ^1S_0$	7882	1.22669–4	1.47829–4	−1.5502–4	0	5.7949–5
$3\ ^1P_1$	7891	9.3337–4	−1.08299–3	5.58628–4	0	7.14994–4
$3\ ^3D_1$	7893	1.38966–4	−2.51907–4	1.87066–4	−4.68834–5	0
$3\ ^3D_2$	7891	2.42042–7	−3.75331–6	2.21084–5	6.99675–6	0
$3\ ^2D_3$	7891	6.64819–5	−1.23403–4	1.08484–4	−1.62579–5	0
$3\ ^1D_2$	7893	5.64764–7	−8.75772–6	5.15861–5	1.63257–5	0

Table 2.3. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact excitation of Ca XIX. These parameters should be used in the temperature range: 2×10^6–2×10^8 K

Transition	ΔE (eV)	A	B	C	D	E
$1\ ^1S \rightarrow$						
$2\ ^3S_1$	3870	−2.49–5	4.05–4	−1.13–4	8.08–4	0
$2\ ^3P_0$	3890	−3.48–8	−3.44–5	6.92–4	−2.04–4	0
$2\ ^3P_1$	3890	6.45–4	−8.06–4	1.40–3	1.46–4	0
$2\ ^3P_2$	3890	−4.53–7	−1.66–4	3.41–3	−9.82–4	0
$2\ ^1S_0$	3890	2.87–3	−3.43–3	1.95–3	0	−1.97–4
$2\ ^1P_1$	3910	1.06–3	−7.09–5	3.06–3	0	1.04–2
$3\ ^3S_1$	4574	−2.55404–6	4.72669–5	2.18639–4	−9.88216–5	0
$3\ ^3P_0$	4580	3.08775–7	−7.24054–6	1.47114–4	−3.87383–5	0
$3\ ^3P_1$	4581	3.27829–5	−8.46766–5	5.2277–4	−1.5685–4	5.16363–5
$3\ ^3P_2$	4582	1.5435–6	−3.6194–5	7.35396–4	−1.93645–4	0
$3\ ^1S_0$	4580	4.57326–4	−2.47349–4	7.08187–6	1.49628–5	0
$3\ ^1P_1$	4587	1.05633–3	−2.10754–3	3.14182–3	−1.46319–3	1.7107–3
$3\ ^3D_1$	7752	2.56062–4	−4.62977–4	3.36859–4	−8.89341–5	0
$3\ ^3D_2$	7750	4.04459–7	−6.27189–6	3.69437–5	1.16918–5	0
$3\ ^3D_3$	7750	8.42666–5	−1.58572–4	1.51678–4	−1.60014–5	0
$3\ ^1D_2$	7751	9.43737–7	−1.46344–5	8.6202–5	2.72808–5	0

The R-matrix calculation of the S XV has an uncertainty less than 10–20%. Pradhan's DW method should be reliable with 20–30%. The CB-type calculation of Sampson et al. probably has an accuracy of 30%, except in the region of lower temperature. In the low-temperature region, particularly for forbidden transitions, a resonance process plays a significant role, which is not considered in the calculation by Sampson et al. (see Fig. 2.1).

Finally it should be noted that the fit parameters shown in the tables cannot be used outside the temperature range indicated.

2.2 Innershell Excitation of Li-Like Ions

Here we consider the innershell excitation of Li-like ions: $1s^22s$–$1s2s2p$. This process

Table 2.4. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact excitation of S XV. These parameters should be used in the temperature range: 1×10^6–1×10^8 K

Transition	ΔE (eV)	A	B	C	D	E
$1\ ^1S \rightarrow$						
$2\ ^3S$	2430	2.46531–4	−1.99636–3	5.50332–3	−1.92783–3	0
$2\ ^3P$	2448	7.48166–4	−7.99328–3	2.76154–2	−1.44272–2	0
$2\ ^1S$	2448	3.43502–3	−2.25596–3	9.19539–4	0	1.2675–5
$2\ ^1P$	2461	−5.27989–4	8.18631–3	−2.04588–73	0	1.77309–2
$3\ ^3S$	2876	2.4211–6	1.5534–4	−5.93873–5	2.24564–4	0
$3\ ^3P$	2880	1.73637–5	−1.80648–4	2.18762–3	−5.37472–4	0
$3\ ^1S$	2880	1.02987–3	−1.15677–3	5.07232–4	0	−1.23125–4
$3\ ^1P$	2884	1.87729–3	−1.8834–3	1.1474–3	0	2.66027–3
$3\ ^3D$	2883	−3.68693–5	4.93927–4	−1.37161–3	1.41811–3	0
$3\ ^1D$	2883	1.23625–3	−2.39968–3	1.33562–3	0	−3.02112–4

Table 2.5. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact innershell excitation of Fe XXIV

Transition	ΔE (eV)	A	B	C	D	E
D_1 [a]	6620	8.52745–6	−3.21294–5	7.62144–4	−2.88035–4	3.44262–5
D_2	6664	6.21771–4	−1.81848–3	4.31443–3	−2.10888–3	2.3602–3
D_3	6688	4.79403–4	−1.40376–3	3.48975–3	−1.68616–3	1.82026–3
E_1	6626	6.20576–5	−1.95351–4	1.78516–3	−7.09763–4	2.39529–4
E_2	6676	2.1411–3	−6.25147–3	1.38267–2	−6.88229–3	8.12446–3
E_3	6691	1.61378–5	−6.15897–5	1.51919–3	−5.73426–4	6.5375–5

[a] D_1 $1s^22s-1s2s2p\ ^4P_{1/2}$
D_2 $1s^22s-1s(2s2p\ ^3P)^2P_{1/2}$
D_3 $1s^22s-1s(2s2p\ ^1P)^2P_{1/2}$
E_1 $1s^22s-1s2s2p\ ^4P_{3/2}$
E_2 $1s^22s-1s(2s2p\ ^3P)^2P_{3/2}$
E_3 $1s^22s-1s(2s2p\ ^1P)^2P_{3/2}$

Table 2.6. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact innershell excitation of Ca XVIII

Transition	ΔE (eV)	A	B	C	D	E
D_1 [a]	3843	3.14264–6	−2.15597–5	1.23117–3	−4.56426–4	1.54674–5
D_2	3876	1.35229–3	−3.95089–3	8.98215–3	−4.43867–3	5.13202–3
D_3	3890	4.98984–4	−1.46568–3	4.08002–3	−1.92006–3	1.89591–3
E_1	3846	2.26019–5	−9.06415–5	2.55614–3	−9.61032–4	9.28148–5
E_2	3879	3.53893–3	−1.03318–2	2.27593–2	−1.13047–2	1.34283–2
E_3	3891	1.48007–4	−4.55876–4	3.27636–3	−1.3311–3	5.68405–4

[a] Same as Table 2.5.

contributes significantly to the emission of satellite lines of He-like ion. Using the distorted wave method, Bely-Dubau et al. (1982a,b) calculated the cross section for the innershell excitation and reported the rate coefficients for them. They published their result only for Ca and Fe. Sampson et al. (1985) reported their calculation based on the Coulomb-Born approximation for the ions with nuclear charge of 6–74.

A detailed comparison shows that the rate coefficients obtained by Bely-Dubau et al. and by

Table 2.7. Fit parameters for the effective collision strengths (see Eq(2.2)) recommended for the electron-impact innershell excitation of S XIV

Transition	ΔE (eV)	A	B	C	D	E
D_1 [a]	2413	3.24551–7	−2.04789–5	1.91183–3	−7.04963–4	6.8186–6
D_2	2439	2.34012–3	−6.83379–3	1.5232–2	−7.56626–3	8.88–3
D_3	2449	5.22106–4	−1.53987–3	4.8824–3	−2.2351–3	1.98556–3
E_1	2414	6.97831–6	−5.93906–5	3.85995–3	−1.42858–3	3.76401–5
E_2	2441	5.34681–3	−1.56086–2	3.42611–2	−1.70881–2	2.02878–2
E_3	2450	3.71623–4	−1.1212–3	5.93519–3	−2.49764–3	1.42047–3

[a] Same as Table 2.5.

Sampson et al. agree very well with each other. Here we adopt the result of Sampson et al., because they have the values for all the three ions considered here (i.e., S XIV, Ca XVIII and Fe XXIV). As in the case of the excitation of He-like ions, the relevant collision strength is fitted by the analytical form

$$\Omega = A + \frac{B}{X} + \frac{C}{X^2} + \frac{D}{X^3} + E \ln X \tag{2.6}$$

with $X = E/\Delta E_{ij}$. The fit parameters A–E are given in tables 2.5–2.7. From these parameters, the rate coefficients can be easily calculated in the manner given in the case of excitation of He-like ions (see Eqs. (2.1) and (2.2)).

3. IONIZATION

Here we consider ionization cross sections of the H-, He-, Li- and Be-like ions of S, Ca, and Fe.

3.1. Total Ionization Cross Section

No experimental data are available for the ions considered here. Arnaud and Rothenflug (1985) evaluated the ionization and recombination rate coefficients to give a set of recommended data for a number of ions of astrophysical interest. They presented those data in an analytical form with parameters. Arnaud and Raymond (1992) updated the data for Fe ions. A part of their data have been taken from the calculation of Younger (1981, 1982). They pointed out that the coefficients in Table 2 of Younger (1982) are given not in 10^{-14} cm^{2}eV^2 as stated but in $\pi a_0^2 Ry^2$. Those values have been cited in many places. For example, therefore, the corresponding data given by Pindzola et al. (1987) and Lennon et al. (1988) have to be multiplied by 1.626.

There are some recent calculations. Kao et al. (1992) calculated the ionization cross section of H-like ions with the relativistic distorted wave method. Their values are in good agreement with those by Younger (1982, with the correction mentioned above) and with the Lotz formula. Chen and Reed (1992) calculated the ionization cross section for Li-like ions in a similar manner, but with including autoionization. Badnell and Pindzola (1993) also presented cross sections including autoionization for Li- and Be-like ions. Their results for Li-like ions are smaller by about 20% than those of Chen and Reed. Since the energy range and the ion species of the above theoretical calculations are limited, here we adopt the data by Arnaud and Rothenflug (1985) for S- and Ca-ions, and Arnaud and Raymond (1992) for Fe ions.

Arnaud and Rothenflug (1985) fitted the direct ionization (DI) cross section (in cm^2) with the formula

Table 3.1. Fit parameters for the direct ionization (DI) rate coefficients (see eq.(3.2))

Ion	Shell	I_j(eV)	A_j	B_j	C_j	D_j (10^{-14} cm^{2}eV^2)
S XVI	1s	3493.0	12.8	−4.3	1.9	−10.5
S XV	1s2	3224.0	23.3	−7.6	4.0	−19.3
S XIV	2s	707.0	9.7	−2.8	1.4	− 6.4
	1s2	3075.0	22.8	−7.1	4.1	−18.0
S XIII	2s2	652.0	18.1	−4.4	2.7	−11.8
	1s2	3017.0	22.8	−7.1	4.1	−18.0
Ca XX	1s	5470.	12.9	−4.4	1.9	−10.5
Ca XIX	1s2	5129.0	24.0	−7.9	3.9	−19.6
Ca XVIII	2s	1157.0	9.5	−2.7	1.4	− 6.1
	1s2	4939.0	23.4	−7.4	4.1	−18.0
Ca XVII	2s2	1087.0	18.6	−4.6	2.7	−12.1
	1s2	4865.0	23.4	−7.4	4.1	−18.0
Fe XXVI	1s	9278	13.0	−4.5	1.9	−10.6
Fe XXV	1s2	8828.0	24.8	−8.4	3.8	−20.0
Fe XXIV	2s	2045.0	9.3	−2.6	1.4	− 5.8
	1s2	8580.0	24.1	−7.9	4.1	−18.0
Fe XXIII	2s2	1950.0	19.2	−5.3	2.7	−12.3
	1s2	8482.0	24.1	−7.9	4.1	−18.0

$$Q_{DI}(E)\,[\text{in cm}^2] = \sum_j \frac{1}{u_j I_j^2}\Big[A_j\Big(1-\frac{1}{u_j}\Big) + B_j\Big(1-\frac{1}{u_j}\Big)^2 + C_j \ln u_j + D_j \frac{\ln u_j}{u_j}\Big], \tag{3.1}$$

where $u_j = E / I_j$. Here E is the incident electron energy in eV and I_j is the ionization potential (in eV) of the j-th shell. The coefficients A_j to D_j (all in cm^{2}eV^2) are given in Table 3.1. The values of I_j are also given there. The rate coefficients (in cm^{3}s^{-1}) for the ionization is calculated by

$$C_{DI}(T_e)\,[\text{in cm}^3\text{s}^{-1}] = \frac{6.69\times10^7}{T_e^{3/2}} \sum_j \frac{e^{-x_j}}{x_j} F(x_j), \tag{3.2}$$

$$\begin{aligned} F(x_j) &= A_j[1 - x_j f_1(x_j)] \\ &+ B_j[1 + x_j - x_j(2 + x_j) f_1(x_j)] \\ &+ C_j f_1(x_j) + D_j x_j f_2(x_j), \end{aligned} \tag{3.3}$$

where T_e is the electron temperature in units of eV and

$$x_j = I_j / T_e$$

$$f_1(x) = e^x \int_1^\infty \frac{e^{-xt}}{t}\,dt$$

$$f_2(x) = e^x \int_1^\infty \frac{e^{-xt}}{t}\ln t\,dt\,.$$

For Li-like ions, excitation autoionization (EA) has a large contribution to the ionization for low Z elements. Arnaud and Raymond (1992) present the contribution for Fe XXIV expressed in the form

Table 3.2. Fit parameters for excitation autoionization (EA) rate coefficient for Li like ions (eq.(3.5))

Ion	Potential (eV)	A	B (10^{-16} cm^{2}eV)	C	D	E
S XIV	2428	1.10–1	1.17–2	−7.81–2	0.	1.44–1
Ca XVIII	3847	5.07–2	5.40–3	−3.61–2	0.	6.66–2
Fe XXIV	6592	1.64–2	1.76–3	−1.17–2	0.	2.16–2

$$Q_{EA}(E)\,[\text{in cm}^2] = \frac{1}{u\,I_{EA}}\,[A + B\,(1-\frac{1}{u}) + C\,(1-\frac{1}{u^2}) + D\,(1-\frac{1}{u^3}) + E\ln u], \tag{3.4}$$

where I_{EA} is the threshold energy (in eV) of the excitation process and $u = E/I_{EA}$. They estimated the coefficients A to E on the basis of the theoretical study by Sampson and Golden (1981). For S XIV and Ca XVIII, we rewrote the form given by Arnaud and Rothenflug (1985) into the form (3.4) to derive the coefficients. The coefficients for the process EA are summarized in Table 3.2. The rate coefficients for the EA is obtained from ($x = I_{EA} / T_e$)

$$C_{EA}(T_e)\,[\text{in cm}^3\text{s}^{-1}] = \frac{6.69\times10^7}{T_e^{1/2}}\,e^{-x}\,G(x), \tag{3.5}$$

$$G(x) = A + B\,[1 - x f_1(x)] + C\,[1 - x\,(1 - x f_1(x))] + D\,[1 - \frac{1}{2}(x - x^2 + x^3 f_1(x))] + E f_1(x). \tag{3.6}$$

The EA contribution becomes less significant as the nuclear charge increases. For Fe XXIV, it is less than 5%.

3.2 Innershell Ionization of Li-Like Ions

The process

$$1s^2 2s + e \rightarrow 1s2s\ {}^3S + 2e$$

is important in populating the metastable state of He-like ions. Sampson and Zhang (1988) calculated the rate coefficient of the process. It turns out that their result agrees with the Lotz formula within 5%. Here we give the latter, because it has a simple form to use.

The Lotz formula for the rate coefficient of the above process is given by

$$C_{II}(T_e)\,[\text{in cm}^3\text{s}^{-1}] = \frac{4.52\times10^{-6}}{T_e^{3/2}}\,\frac{1}{x}\int_x^\infty \frac{e^{-t}}{t}\,dt \tag{3.7}$$

with

$$x = I\,(1s)\,/\,T_e\,.$$

Here we have considered the statistical weight of the final level. The respective ionization potential $I\,(1s)$ for the Li-like ions of S, Ca, and Fe ions are 3138, 5019 and 8684 eV, respectively.

4. RECOMBINATION

Here we consider the recombination of H-, He-, Li-, and Be-like ions of S, Ca, and Fe to produce He-, Li-, Be-, and B-like ions of each element.

4.1. Radiative Recombination

The recommended data for S and Ca by Arnaud and Rothenflug (1985) and for Fe by Arnaud and Raymond (1992) are adopted here. They give the rate coefficient in the form

$$\alpha_{\rm rad}\,(T_e)\;[\text{in }\ \text{cm}^3\text{s}^{-1}] = A\;(1.16\;T_e)^{\gamma} \tag{4.1}$$

with

$$\gamma = -\alpha - \beta\,\text{Log}\,(1.16\;\;T_e)\;.$$

Numerical values of the coefficients A, α, β are given in Table 4.1.

Table 4.1. Fit parameters for radiative recombination rate coefficients (eq.(4.1))

Ion	A (cm^3s^{-1})	α	β	T (eV) range
S XIV	2.00–10	.806		5 –1400
S XV	2.91–10	.840		14 -3400
S XVI	4.30–10	.807		170–4300
Ca XVIII	4.61–10	.833		14 -3400
Ca XIX	5.62–10	.839		22 -5400
Ca XX	8.44–10	.819		270–5400
Fe XXIII	3.91–10	.523	6.15–2	8.6–8.6+3
Fe XXIV	4.33–10	.531	5.77–2	8.6–8.6+3
Fe XXV	4.77–10	.537	5.49–2	8.6–8.6+3
Fe XXVI	5.84–10	.546	4.02–2	8.6–8.6+3

4.2. Dielectronic Recombination

Arnaud and Rothenflug (1985) evaluated the dielectronic recombination (DR) coefficient for a number of ions to determine a set of best values. Arnaud and Raymond (1992) updated them for Fe ions.

Recently detailed calculations have been done for the DR coefficients by several authors. Karim and Bhalla (1988, 1989) calculated the DR coefficients for H- and He-like ions with using the Hartree-Fock-Slater model. Nilsen (1986a,b) obtained the data for H- and He-like ions with the Multi-Configuration-Dirac-Fock method. With the Coulomb-Born method for the autoionization probability and the experimental oscillator strengths for the radiative one, Romanik (1988) produced the data for He-, Li-, and Be-like ions. Based on the single configuration HF function (LS coupled) and the distorted-wave continuum, Roszman (1987) and McLaughlin and Hahn (1984) obtained the values for Li-like ions.

In Fig. 4.1, we compare the relevant rate coefficients for the DR process reported by the authors mentioned above. Generally, different theoretical data agree well with each other for H- and He-like ions. In particular, the data by Nilsen (1986b) and Romanik (1988) for He-like ions are in very good agreement. For Li-like ions, the values of Romanik (1988) agree with those of McLaughlin and Hahn (1984), except at 3 keV. The values of Roszman (1987) are always smaller than those of Romanik (1988) and McLaughlin and Hahn (1984) by about 60%.

Judging from the theoretical method used and the above comparison, we adopt here the data by Nilsen for H- and He-like ions and those by Romanik for Li- and Be-like ions. Nilsen presented

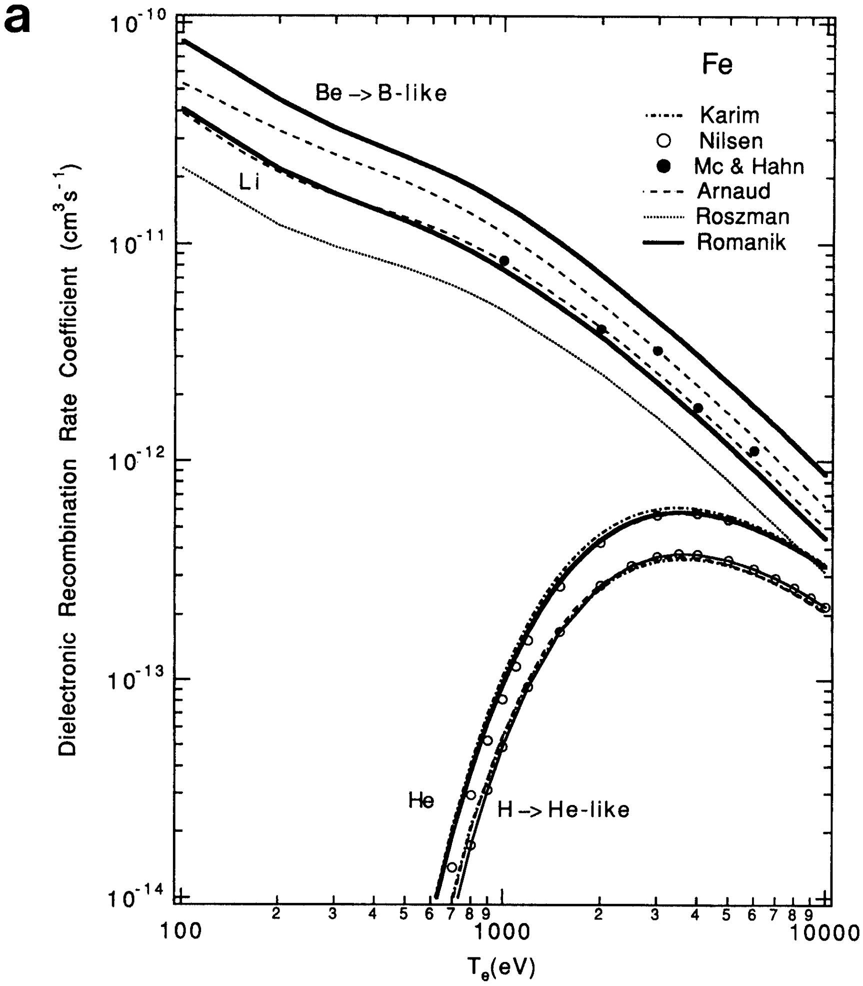

Fig. 4.1. Dielectronic recombination coefficients as a function of the electron temperature: (a) Fe ions, (b) Ca ions, and (c) S ions. Open circles: Nilsen (1986 a, b); solid lines: Romanik (1988); dot-dashed lines: Karim (1988, 1989); dashed lines: Arnaud and Raymond (1992); filled circles: McLaughlin (1984); dotted lines: Roszman (1987).

the rate coefficients in the form

$$\alpha_{DR}(T_e)\,[\text{in cm}^3\text{s}^{-1}] = \frac{4.4817}{X^{3/2}}\,\alpha_{\max}\,e^{-\frac{3}{2X}} \tag{4.2}$$

with

$$X = \frac{3}{2}\,\frac{T_e}{\Delta E}\,.$$

He tabulated the parameters $\alpha_{\max}$ and ΔE only for a limited number of elements. We have interpolated those values to obtain the data for S and Ca. Romanik (1988) proposed another form of $\alpha_{\rm DR}$, which is an extention of (4.2). That is

$$\alpha_{DR}(T_e)\,[\text{in cm}^3\text{s}^{-1}] = T_e^{-3/2}\,\sum_j A_j\,\exp\left(-\frac{\Delta E_j}{T_e}\right)\,. \tag{4.3}$$

To express his results, Romanik uses as many as 10 terms of A_j. We have refitted his values to the

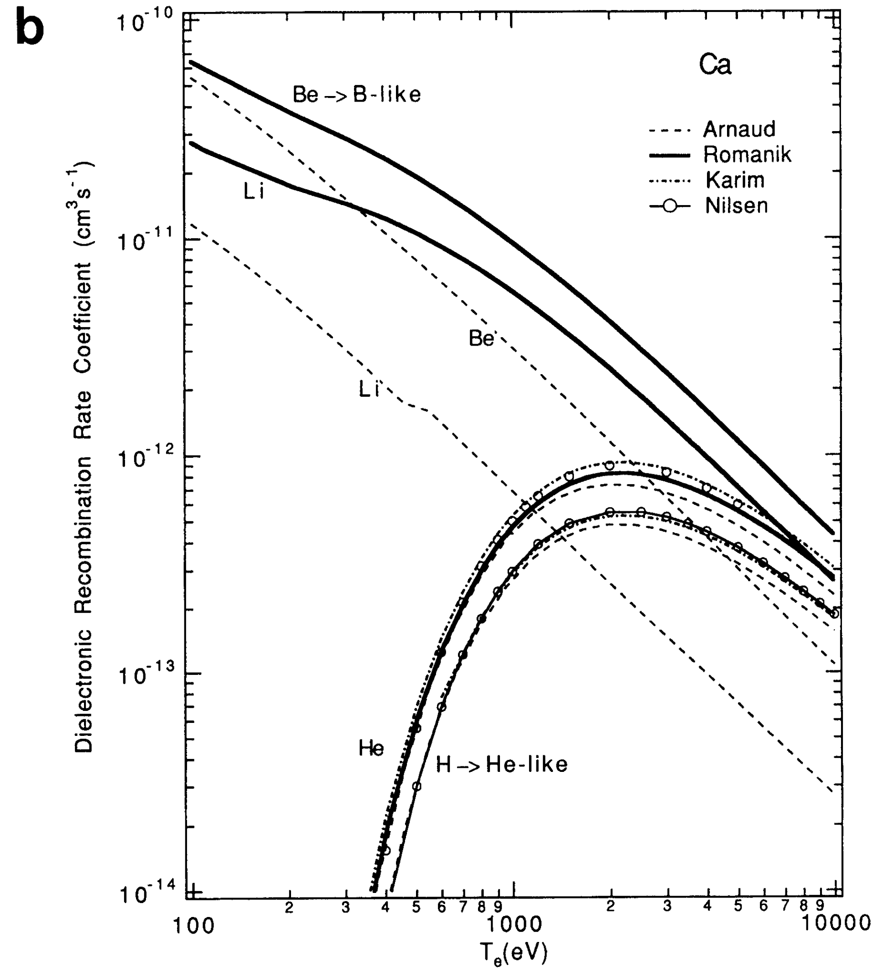

Fig. 4.1. (continued)

same form with fewer terms. The resulting values of the coefficients are tabulated in Table 4.2.

Figure 4.1 compares also the present recommended data (i.e., Nilsen's one for H- and He-like ions and Romanik's for Li- and Be-like ions) with the recommended values by Arnaud's group. There is a significant difference between the two sets of the recommended values for Li- and Be-like ions. For those ions of S and Ca, the discrepancy reaches a factor of 5 or more. This is caused by the fact that Arnaud and Rothenflug (1985) based their DR coefficients on rather old calculations.

4.3. Satellite Lines Through DR

The dielectronic satellite lines serve as an important diagnostic tool, from which, for instance, electron temperature can be deduced. The wavelengths and intensities of the satellite lines were calculated by Dubau et al. (1981) for He-like ions, Gabriel (1972), Bhalla et al. (1975), Bely-Dubau et al. (1979a,b) and Bely-Dubau et al. (1982a) for Li-like ions, Vainshtein and Safronova (1978, 1980) for He- and Li-like ions, Nilsen (1987) for He-like ions, Nilsen (1988) for Li-like ions, Chen (1986) for Li-like ions, and Chen and Craseman (1987) for Be-like ions. Cornille et al. (1988) calculated the lines of Be- to O-like ions due to the transitions $1s2s^k2p^m - 1s^22s^k2p^{m-1}$.

Here we recommend the satellite line data calculated with the MZ method by Vainshtein and Safronova and with the AUTOSLJ method by Dubau et al. Their calculation presents a

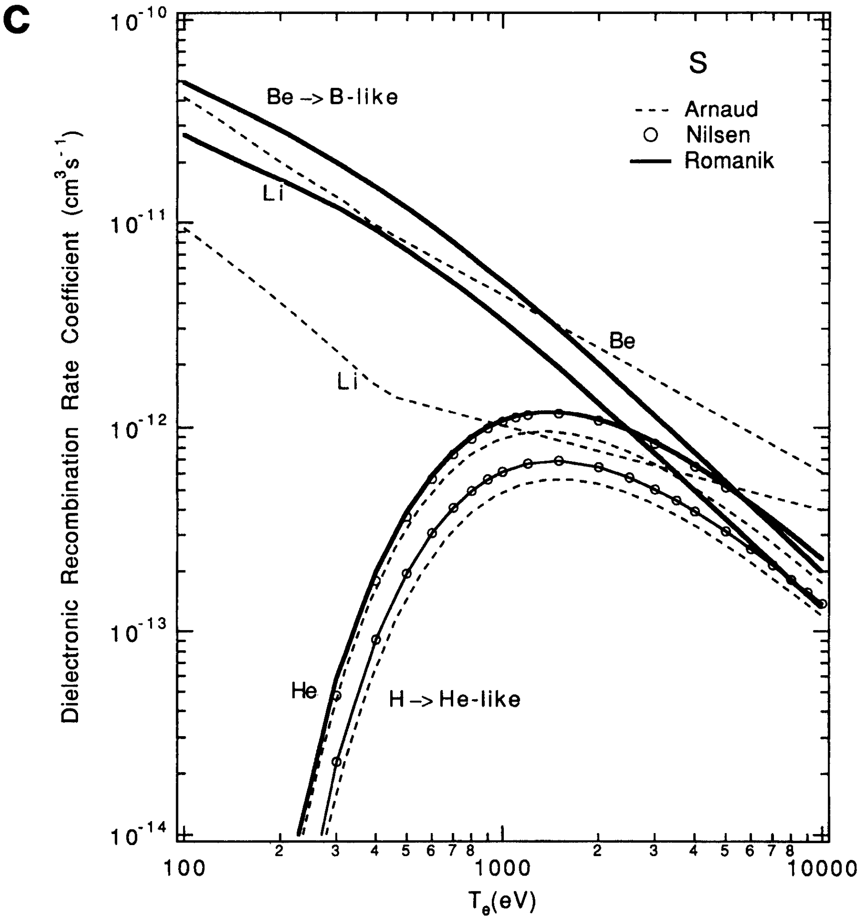

Fig. 4.1. (continued)

Table 4.2. Fit parameters for dielectronic recombination rate coefficients (eq.(4.3))

Ion	i	A_i ($cm^3s^{-1}eV^{1.5}$)	ΔE_i(eV)	Ref.
S XVI	1	1.704–7*	2183*	Nilsen
S XV	1	2.757–7*	2105*	Nilsen
S XIV	1	1.55–9	0.354	Romanik
	2	9.62–9	13.8	
	3	2.11–8	40.3	
	4	1.01–17	344	
S XIII	1	1.00–9	0.95	Romanik
	2	4.64–9	8.86	
	3	6.18–8	44.1	
	4	1.36–7	337	
Ca XX	1	2.589–7*	3326*	Nilsen
Ca XIX	1	4.025–7*	3239*	Nilsen
Ca XVIII	1	3.60–9	6.2	Romanik
	2	2.64–8	28.6	
	3	2.37–7	464	
Ca XVII	1	8.13–9	8.09	Romanik
	2	8.23–8	49.5	
	3	3.31–7	435	
Fe XXVI	1	3.75–7	5492	Nilsen
Fe XXV	1	5.63–7	5393	Nilsen
Fe XXIV	1	1.07–8	10.2	Ronamik
	2	4.72–8	44.4	
	3	3.93–7	726	
Fe XXIII	1	1.73–9	1.45	Romanik
	2	2.16–8	14.6	
	3	1.30–7	74.3	
	4	7.54–7	823	

* Interpolated

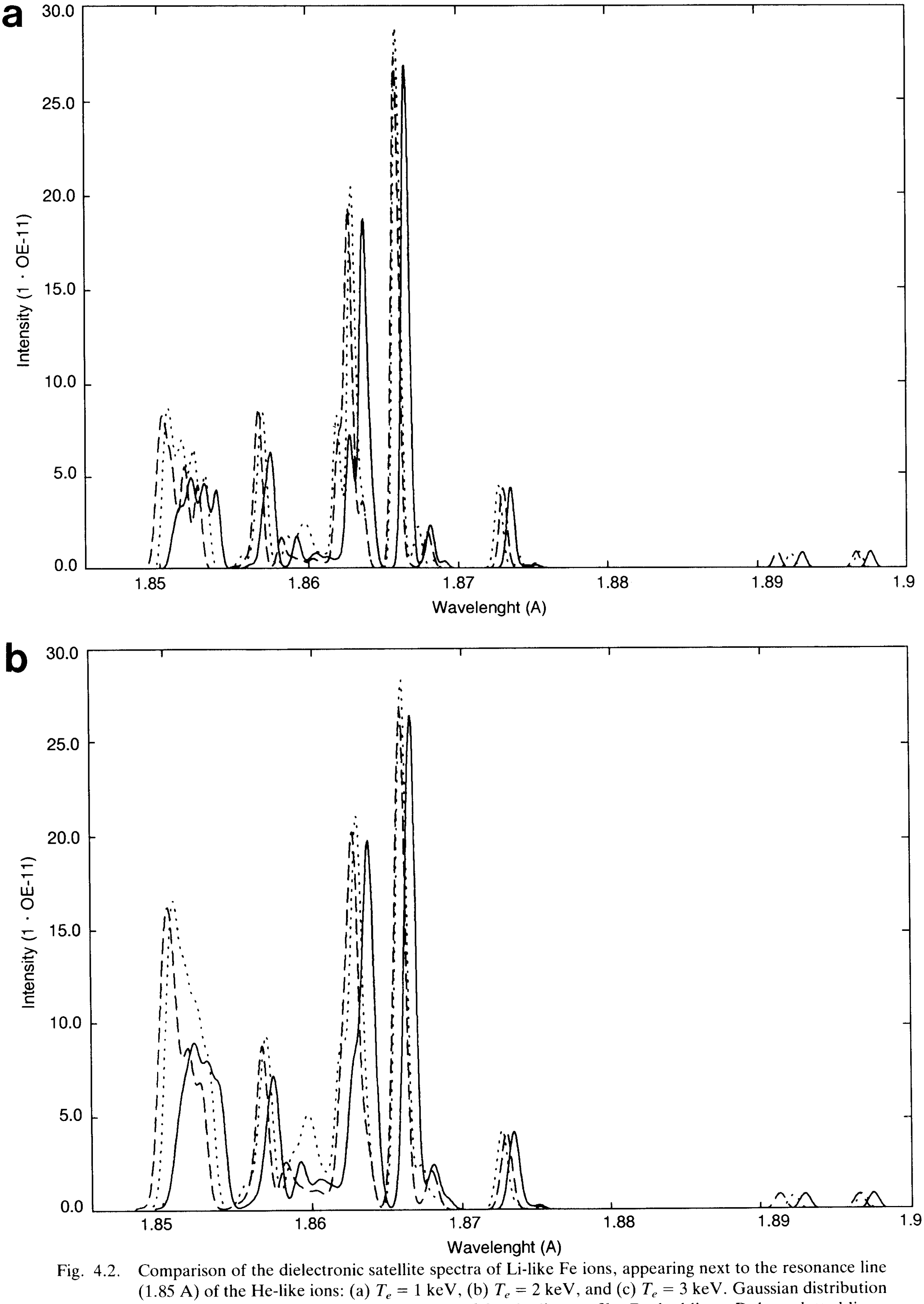

Fig. 4.2. Comparison of the dielectronic satellite spectra of Li-like Fe ions, appearing next to the resonance line (1.85 A) of the He-like ions: (a) $T_e = 1$ keV, (b) $T_e = 2$ keV, and (c) $T_e = 3$ keV. Gaussian distribution with the ion temperature ($T_i = T_e$) is assumed for the line profile. Dashed lines: Dubau; dotted lines: Safronova; solid lines: Nilsen (1988).

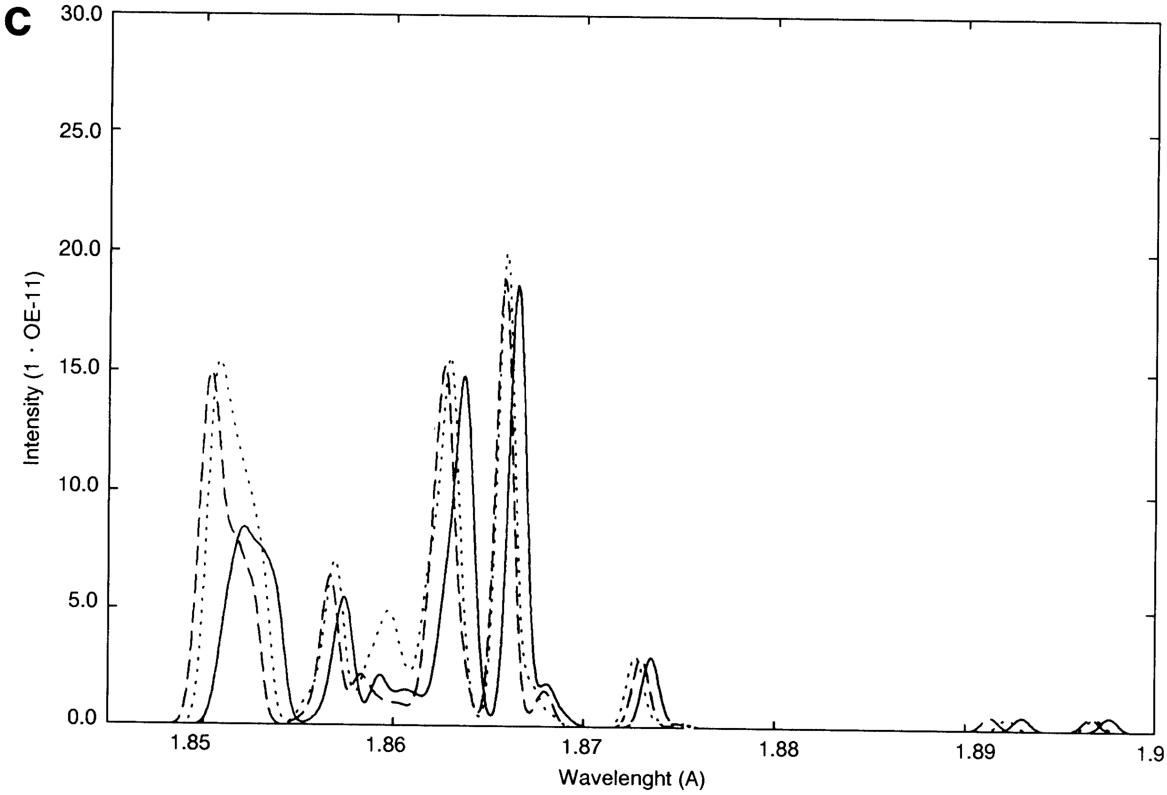

Fig. 4.2. (continued)

comprehensive set of data for all the ions (which will be published in a separate paper). For He-like ions, we calculate the total recombination rate coefficient by summing all the satellite line intensities of Safronova. The result is in good agreement with the coefficient reported by Nilsen. Figure 4.2 compares the satellite line spectra of Li-like ions produced on the basis of the data by Safronova, Dubau and Nilsen. There appear some quantitative differences. The temperature derived from these spectra, however, agrees with each other within 20%. For Be- to O-like ions of Fe, Cornille et al. (1988) made a detailed comparison of the two methods adopted here.

Two measurements of the satellite lines from laboratory plasmas have been reported for Fe ions. Decaux et al. (1991) measured the spectra of Fe XXV in a tokamak plasma. Beiersdorfer et al. (1992) observed satellite spectra of Fe XXIV in EBIT. Both the experimental spectra have been compared with theoretical results. Beiersdorfer et al. show that the theoretical spectra based on the Safronova data reproduce the experiment within the experimental uncertainty (20%), except for a few weak lines.

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