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CALCULATION OF IMPURITY RADIATION FROM NON-CORONA-EQUILIBRIUM PLASMAS

S. Uchikawa, * H.R. Griem** and D. Düchs

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* Permanent address: Energy Research Laboratory,
Hitachi, Ltd.
1168 Moriyama-cho, Hitachi-shi,
Ibaraki-Ken 3/6 Japan

** Permanent address: University of Maryland, Dept. of Physics and Astronomy, College Park, Md. 20742, USA

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Abstract

The problem of the calculation of impurity line and continuum radiation losses in the absence of corona ionization-recombination equilibrium is considered and approximate rate coefficients for the important collision processes are listed for iron ions.

I. INTRODUCTION

Several calculations of radiation losses have been made for plasmas containing small admixtures of elements other than hydrogen or its isotopes. These calculations involve the assumption that the distribution of impurity ions over charge states is as in corona equilibrium, i.e., that collisional ionization by electrons is locally and instantaneously balanced by electron-ion recombination. This assumption is often questionable, both because transport, especially in the outer regions of a plasma, may be too fast for local corona equilibrium to hold, and because charge transfer from neutral hydrogen isotopes may effectively increase the electron-ion recombination rate. To obtain more realistic estimates of impurity radiation, rate equations must therefore be solved together with the impurity ion transport, and one must allow for neutral hydrogen-impurity ion collisions.

Some of the primary collision processes involve ions in excited states so that, strictly speaking, not only ground state ion densities should be considered in the combined transport and rate equations calculations. Since anything else is impractical, one must use suitably defined effective rate coefficients, e.g., for dielectronic recombination and for charge transfer. Essentially, these effective rate coefficients are sums of rate coefficients for primary processes which were multiplied with branching ratios for the final state in the chain of reactions to be a ground state. These branching ratios often depend on electron density, although this dependence should be weaker than suggested by some simple estimates (see comment in Sect. III following the formula for radiative recombination).

In the subsequent sections, we will consider the following processes: ionization by electron collisions, dielectronic and radiative recombination and charge transfer, excitation by electron collisions and, finally, recombination radiation and bremsstrahlung.

II. IONIZATION BY ELECTRON COLLISIONS

As is done in most calculations of impurity radiation, we use the ionization rate coefficient of Lotz[1] in its simplest form,

$$S_z = 6.7\times10^7 \sum_{i=1}^{N} \frac{a_i \xi_i}{T^{3/2}} \frac{E_1(I_{zi}/T)}{(I_{zi}/T)} \quad [cm^3 sec^{-1}] \tag{1}$$

I_{zi} ionization energy (eV) of the i-th subshell of ion Z.

T electron temperature (eV)

ξ_i number of equivalent electrons in i-th subshell

$E_1(x)$ exponential integral

For iron, $a_i \approx 4.5\times10^{-14}$. The ionization energies of the subshells were also calculated by Lotz.[2] We note that various experiments in transient plasmas[3,4] are consistent with these ionization rates to within a factor $\lesssim 2$ and that Eq. (1), which is generally considered to be an empirical formula, can actually be derived[5] by extrapolating the excitation formula of Sec. IV into the continuum. On the other hand, recent cross section measurements[6] for lithium-like ions show that at relatively high electron energies the ionization cross section may be enhanced by inner-shell excitation followed by auto-ionization. Inclusion of this ionization process is also suggested by consistency arguments, since it is, in a general sense but of course not in the sense of detailed balancing, the counterpart of dielectronic recombination. Following Jordan[7] we therefore add to Eq. (1)

$$\Delta S_z = 3.2\times10^{-6} f w_z^{-1} T_e^{-1/2} \exp(-w_z/T) \quad [cm^3 sec^{-1}] \tag{2}$$

where w_z is an estimate of the excitation energy of the auto-ionizing level, say, $I_{z2}-I_{z1}$, in terms of second and first ionization energies. The oscillator strength f is taken as $f \approx 0.7\xi_2$, where ξ_2 is the number of

electrons in the subshell next to the outer shell, provided $I_{z2}-I_{z1} > I_{z1}$ so that even the lowest excited state reached by inner-shell excitation lies in the continuum. In this case $w_z \approx I_{z2} - I_{z1}$. Otherwise, Jordan's suggestion is to use $w_z \approx I_{z1}$ with oscillator strengths reduced according to the following hydrogenic behavior:

Energy Ranges	f	W_z
$I_2-I_1 > I_1$	$0.70\xi_2$	I_2-I_1
$I_2-I_1<I_1$, $1.8(I_2-I_1)>I_1$	$0.13\xi_2$	I_1
$1.8(I_2-I_1)<I_1$, $2.4(I_2-I_1)>I_1$	$0.049\xi_2$	I_1
$2.4(I_2-I_1)<I_1$	$0.023\xi_2$	I_1

Depending on the level structure and temperature, ΔS_z is often comparable to and sometimes even larger than S_z.

III. ELECTRON-ION RECOMBINATION AND CHARGE TRANSFER

For most ionization stages and temperatures of interest, dielectronic recombination is faster than radiative recombination by one or two orders of magnitude. Most notable exceptions are ions with vacancies in the K-shell, especially of course bare ions for which there is no dielectronic recombination. Since for these ions practically exact expressions are available for the radiative recombination coefficients, namely[8]

$$\alpha_z^r = 5.0\times10^{-14} z^4 \left(\frac{I_H}{T}\right)^{3/2} \left[\frac{1-\xi_z/2n_z^2}{n_z^3} \exp\left(\frac{z^2 I_H}{n_z^2 T}\right) E_1\left(\frac{z^2 I_H}{n_z^2 T}\right) + \sum_{n=n_z+1}^{\infty} \frac{1}{n^3} \exp\left(\frac{z^2 I_H}{n^2 T}\right) E_1\left(\frac{z^2 I_H}{n^2 T}\right)\right] \left[\mathrm{cm^3\,sec^{-1}}\right] , \qquad (3)$$

the major problem is to develop reasonably accurate expressions for dielectronic recombination. Before describing our procedure to do this, we note that in Eq. (3) we have used

- z - for the charge of the recombining ion
- I_H - for the ionization energy of hydrogen (13.59 eV)
- ξ_z - for the number of bound electrons in the outer main shell
- n_z - principal quantum number of electrons in this shell,

and that we have replaced the Gaunt factors by 1, thereby incurring errors of $\lesssim$20% for ξ_z=0. Also, in contrast to Ref. 8, we ignored the fact that radiative recombination into high n levels does not necessarily lead to an additional ion in the ground state because of further collisions competing with radiative stabilization. The estimate given in Ref. 8 for the highest principal quantum number to be used in the sum term is, however, generally too low because collision rates for $\Delta n = +1$ and $\Delta n = -1$ are about the same. This comment applies as well to corresponding truncations in dielectronic

recombination coefficients which are, however, much more critical. One would essentially have to deal with a diffusion problem in quantum number space, methods for which have been developed,[9,10] although the numerical accuracy of the high density corrections to recombination rates is questionable in view of the rather uncertain cross sections for ions in highly excited states.

As basis for our expressions for dielectronic recombination rates we used the general formula of Burgess[11]

$$\alpha_z^d = 7.6\times10^{-14}\ \frac{z^{1/2}(z+1)^{5/2}}{(z^2+13.6)^{1/2}}\ \sum_k f_k\ A(\gamma_k)\exp(-E_k/T)\ [\mathrm{cm}^3\mathrm{sec}^{-1}] \qquad (4)$$

but adjusted his coefficients $A(\gamma_k)$ to come closer to the more accurate calculations of Jacobs, Davis and Blaha[12] which, most importantly, also allow for a substantial reduction in recombination rates for some ions due to auto-ionization leading to excited states of the recombining ion of charge z. The coefficients of Burgess were

$$A(\gamma_k) = \gamma_k^{1/2}(1+0.105\gamma_k+0.015\gamma_k^2)^{-1} \qquad (5)$$

with $\gamma_k = \frac{E_k}{(z+1)I_H}\left[1+\frac{0.015\ z^3}{(z+1)^2}\right]$.

We kept this choice only if the excited state E_k of the recombining ion had the same principal quantum number as the ground states of the ion ($\Delta n = 0$ transitions). For other excited states, reached by $\Delta n = 1$ transitions, we multiplied $A(\gamma_k)$ by the following factors $C_z \leq 0.5$:

Ions	z	Transition	C_z
Fe II-VII	1-6	?	0.50
Fe VIII	7	3p→4s	0.35
Fe IX-XIV	8-13	3p→4d	0.35
Fe XV,XVI	14,15	3s→4p	0.35
Fe XVII	16	2p→3d	0.20
Fe XVIII-XXII	17-21	2p→3d	0.35
Fe XXIII-XXIV	22,23	2s→3p	0.50
Fe XXV,XXVI	24,25	1s→2p	0.50

For the lower ionization stages ($z \leq 7$), neither accurate calculations nor sufficient oscillator strengths were available. We therefore choose C_k to fit an even simpler formula[5] than that of Burgess, which can be obtained by extending the formula for excitation (Sec. IV) to below threshold energies and by using an estimate for the lowest state for the captured electron not to auto-ionize before stabilization can occur by a radiative transition of the excited electron. For the rest of the ions, our modified Burgess formula gives total recombination rates ($\alpha_z^r + \alpha_z^d$) agreeing with the values of Jacobs et al.[12] to within a factor of 2 or better, with our rates tending to be larger. (Fe IX and XXII, i.e., z=8 and 21, are notable exceptions.) This tendency may be due to an overestimate of the oscillator strengths f_k (see Sec. IV) used by us which are actually sums of oscillator strengths for a group of transitions characterized by a mean excitation energy E_k. (See Table I below for our set of f_k and E_k values.) However, it is also possible that the detailed calculations missed some contributions which we effectively included by estimating many of the oscillator strenghts from sum rules.

The reliability of our values for α_r^d is difficult to assess. For Fe IX, X and XI they are larger than recently measured values[3] in a dense ($N_e \gtrsim 10^{16} cm^{-3}$), transient plasma by factors up to $\sim$2, but then such factors could easily be explained by high density corrections. In any event, a factor of $\sim$3 uncertainty in the dielectronic rates should be expected. Furthermore, experimental evidence[3] would suggest that any such large deviation should be in the same direction as that for ionization rates.

Notwithstanding recent measurements[13] and calculations[14] of charge transfer cross sections from atoms of hydrogen or its isotopes to multiply ionized atoms, even less can be said about the accuracy of the corresponding rate coefficients. For the relative velocities of interest, including neutral

beam velocities, the cross sections appear to be of the order $z^2\pi a_o^2$, resulting in

$$\alpha_z^H \approx z^2\pi a_o^2 v_H = 0.88\times10^{-16} z^2 v_H [cm^3 sec^{-1}] , \qquad (6)$$

with $\alpha_z^H N_z N_H$ being the rate at which N_{z-1} increases if N_H neutral atoms $[cm^{-3}]$ with velocity v_H are present. Most of the charge transfer is into excited states so that removal of bound electrons from impurity ions by the inverse process should not be important.

IV. LINE RADIATION

In the present context, there is no need to predict the intensities of particular lines, e.g., for purposes of diagnostics. As for the calculation of dielectronic recombination rates, it is therefore sufficient to represent each ion by a small number of excited states with appropriate excitation cross sections as was done for oxygen ions[15] on the basis of measurements and calculations by optimizing the effective Gaunt factors $\bar{g}_k$ of Van Regemorter.[16] The specific power from line radiation is then

$$P_\ell^z = \frac{16\pi}{\alpha c}\left(\frac{\hbar}{m}\right)^2\left(\frac{\pi I_H}{3kT}\right)^{1/2} I_H \sum_k \bar{g}_k f_k \exp(-E_k/kT)\, N_z N_e \qquad (7)$$

$$\approx 2.5\ 10^{-24}\ T^{-1/2} \sum \bar{g}_k f_k \exp(-E_k/T)\, N_z N_e\ [\mathrm{W\ cm^{-3}}]\ .$$

Our choice has been $\bar{g}_k = 0.3$ for $\Delta n \neq 0$ transitions of $n \geq 2$ electrons and $\bar{g}_k = 1$ for all other transitions. With this choice we reproduce corona equilibrium calculations of total radiation losses reasonably well, in our opinion within common theoretical errors. This comparison is shown in Fig. 1. The set of excitation energies and oscillator strengths used is listed in Table I.

V. CONTINUUM RADIATION

As is now well established, impurity continuum radiation is comparable to or larger than line radiation only if most of the impurity ions are completely or almost completely stripped. It is therefore sufficient to use simple expressions which are reasonably accurate for bremsstrahlung and recombination radiation on bare ions and, to a lesser extent, on ions having a small number of bound electrons. Although for most of the ions in the latter class, radiation associated with dielectronic radiation is actually more important[17] than the continuum radiation included here, we can nevertheless neglect it because of the preponderance of line radiation for these ions.

Relations for impurity bremsstrahlung and recombination radiation corresponding to Eq. (3) for the radiative recombination rate coefficient are

$$P_c^z = \frac{32}{3}\frac{\alpha^2}{c}\left(\frac{\hbar}{m}\right)^2\left(\frac{\pi kT}{3I_H}\right)^{1/2} I_H \left[z^2 + 2z^4 \frac{I_H}{T}\left(\frac{1-\xi_z/2n_z^2}{n_z^3} + \sum_{n=n_z+1}^{\infty}\frac{1}{n^3}\right)\right] N_z N_e$$

$$\approx 1.5\times10^{-32} T^{1/2} [....] N_z N_e [\mathrm{W\ cm^{-3}}] \ , \qquad (8)$$

if T is in eV and the densities are per cm^3. This power density was added to the line power density, both summed over z with $\sum N_z = N_i$, in order to generate our curve in Fig. 1.

TABLE 1

Effective Excitation Energies and Oscillator Strengths

for Resonance Transitions of Iron Ions

z	Ion	Iso. Electronic Sequence	n_z	ξ_z	Δn	Type of Transition	E_k(ev)	f_k
0	Fe I	Fe	-	-	0		2.5	2.0
					1		5.0	3.0
1	Fe II	Mn	3	14	0		5.2	1.0
					1		10.0	3.0
2	Fe III	Cr	3	14	0		10.0	1.0
					1		15.0	3.0
3	Fe IV	V	3	13	0		18.0	1.5
					1		23.5	2.5
4	Fe V	Ti	3	12	0		32.0	2.0
					1		40.0	2.0
5	Fe VI	Sc	3	11	0		42.0	2.0
					1		60.0	1.5
6	Fe VII	Ca	3	10	0		56.4	3.0
					1		82.2	2.5
7	Fe VIII	K	3	9	0	$3p \rightarrow 3d$	64.4	3.0
					1	$3p \rightarrow 4s$	108.0	2.0
8	Fe IX	Ar	3	8	0	$3s \rightarrow 3p$	72.5	2.65
					1	$3p \rightarrow 4d$	149.5	2.0
9	Fe X	Cℓ	3	7	0	$3s \rightarrow 3p$	35.0	0.17
					0	$3p \rightarrow 3d$	71.0	2.5
					1	$3p \rightarrow 4d$	161.0	2.0
10	Fe XI	S	3	6	0	$3s \rightarrow 3p$	35.0	0.3
					0	$3p \rightarrow 3d$	68.0	2.0
					1	$3p \rightarrow 4d$	171.0	2.0
11	Fe XII	P	3	5	0	$3s \rightarrow 3p$	35.0	0.5
					0	$3p \rightarrow 3d$	64.0	2.0
					1	$3p \rightarrow 4d$	188.0	2.0
12	Fe XIII	Si	3	4	0	$3s \rightarrow 3p$	39.0	0.6
					0	$3p \rightarrow 3d$	62.0	1.0
					1	$3p \rightarrow 4d$	199.0	1.5

TABLE 1
(Continued)

z	Ion	Iso. Electronic Sequence	n_z	ξ_z	Δn	Type of Transition	E_k(ev)	f_k
13	Fe XIV	Aℓ	3	3	0	3s → 3p	42.0	0.7
					0	3p → 3d	59.0	0.5
					1	3p → 4d	210.0	1.0
14	Fe XV	Mg	3	2	0	3s → 3p	43.6	0.8
					1	3s → 4p	234.0	1.5
15	Fe XVI	Na	3	1	0	3s → 3p	36.0	0.4
					1	3s → 4p	246.0	1.0
16	Fe XVII	Ne	3	0	1	2p → 3d	814.0	3.7
17	Fe XVIII	F	2	7	0	2s → 2p	132.0	0.05
					1	2p → 3d	861.0	2.5
18	Fe XIX	O	2	6	0	2s → 2p	118.0	0.1
					1	2p → 3d	919.0	2.5
19	Fe XX	N	2	5	0	2s → 2p	98.0	0.12
					1	2p → 3d	966.0	2.0
20	Fe XXI	C	2	4	0	2s → 2p	105.0	0.15
					1	2p → 3d	1000.0	1.5
21	Fe XXII	B	2	3	0	2s → 2p	97.5	0.15
					1	2p → 3d	1054.0	1.0
22	Fe XXIII	Be	2	2	0	2s → 2p	93.0	0.15
					1	2s → 3p	1125.0	1.0
23	Fe XXIV	Li	2	1	0	2s → 2p	57.5	0.07
					1	2s → 3p	1167.0	0.8
24	Fe XXV	He	2	0	1	1s → 2p	6687.0	0.77
					1	1s → 3p	8000.0	0.30
25	Fe XXVI	H	1	1	1	1s → 2p	6892.0	0.42
					2	1s → 3p	8400.0	0.14

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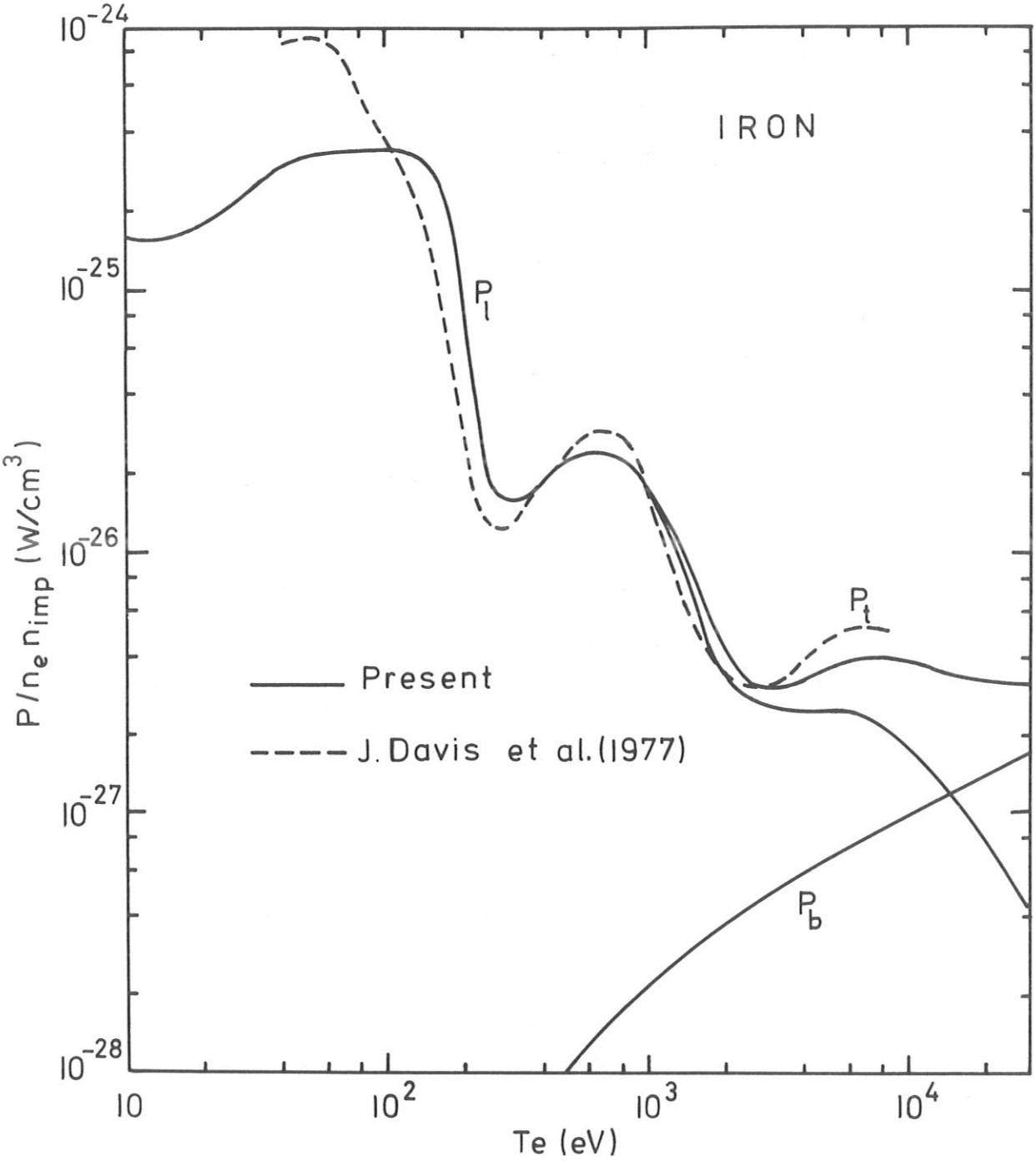

Figure 1 Radiation energy loss rate coefficients for iron at corona equilibrium; P_l : line radiation P_b bremsstrahlung, P_t : total radiative power.