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RADIATIVE RECOMBINATION RATE COEFFICIENTS FOR BARE THROUGH F-LIKE ISOSEQUENCES OF Mg, Si, S, Ar, Ca, Fe, AND Ni

M. F. Gu[1]
Center for Space Research, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139
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ABSTRACT

We present distorted-wave calculations and analytic fits to the radiative recombination rate coefficients of bare to F-like isosequences of seven abundant astrophysical elements, including Mg, Si, S, Ar, Ca, Fe, and Ni. The fits are valid over a wide range of temperature, from 10^{-4} to 10^{4} eV. Extensive comparisons with existing data are made.

Subject headings: atomic data — atomic processes
On-line material: machine-readable table

1. INTRODUCTION

Radiative recombination rate coefficients are required in computing the ionization balance of plasmas departing from thermodynamic equilibrium, as is often the case in astrophysical environments. Although artificial, it is convenient in practice to separate recombination processes into the nonresonant radiative recombinations (RR) and resonant dielectronic recombinations (DR). In RR, a free electron is directly captured by the target, releasing its kinetic energy and the binding energy of the final bound state to the emitted photon. DR involves transitions from autoionizing states, which often dominates recombination rate coefficients at high temperatures for highly charged ions (Burgess 1964). Nevertheless, RR is an important contributor to the total recombination rate coefficients at least in some temperature ranges.

The commonly used set of RR rate coefficients in modern spectral modeling codes is due to the calculations and fits of Péquignot, Petitjean, & Boisson (1991) for C, N, O and Ne ions, and those of Shull & Van Steenberg (1982) for Mg, Si, Ar, Ca, Fe, and Ni ions. Data for K and L shell Fe ions have been revised by Arnaud & Raymond (1992), who based their revision on the photoionization cross sections of Clark, Cowan, & Bobrowicz (1986). The fitting formulae for these data are usually valid only in a restricted temperature range, and for many ions interpolations or extrapolations were used to derive the rate coefficients when detailed photoionization calculations are not available. Verner & Ferland (1996) presented RR rate coefficients of bare, H-like, He-like, and Ne-like ions for elements with $Z \leq 30$ in a wide temperature range, using the analytic fits to the photoionization cross sections of Verner et al. (1996) for the ground-state shells, and those of Clark et al. (1986) for the excited-state shells. (It is the recombining ion that we refer to when we speak of the recombination of a certain atomic ion.) The existing RR rate coefficients for these four isosequences are of higher quality than for other ions. In this paper, we present the results for bare to F-like isosequences of Mg, Si, Ar, Ca, Fe, and Ni ions using detailed photoionization cross sections calculated in a distorted-wave approximation, similar to the Dirac-Hartree-Slater model used in Verner et al. (1993).

[1] *Chandra* Fellow.

2. CALCULATIONS AND FITS

RR cross sections are obtained from the photoionization cross sections through the Milne relation. The photoionization cross sections for the $n \leq 10$ shells are calculated in the distorted-wave approximation, taking into account the electric dipole operators. The wave functions of bound and continuum orbitals are obtained by solving the single-electron Dirac equations with a spherical model potential, which is based on the self-consistent Dirac-Fork-Slater calculations. The computational procedure is similar to the fully relativistic distorted-wave method of Zhang (1998). The atomic code used in the computation is developed by the author, which has also been used to investigate atomic processes other than radiative recombination (Gu 2003). Photoionization cross sections are computed at six photoelectron energies of $E_e < 10E_{\rm th}$, where the $E_{\rm th}$ values are the ionization thresholds for corresponding shells. Cross sections at $E_e < 10E_{\rm th}$ are interpolated from these six points. For $E_e > 10E_{\rm th}$, we use a simplified version of the formula suggested by Verner et al. (1993),

$$\sigma_{\rm PI}(E_e) = \sigma_0 x^{-3.5-l+p/2}\left(\frac{1+b}{\sqrt{x}+b}\right)^{p}, \qquad (1)$$

where $x = (E_0 + E_e)/E_0$, l is the orbital angular momentum of the photoionized shell, and σ_0, E_0, p, and b are fit parameters. For the photoionization of a particular nl shell, we calculate the exact nonrelativistic cross sections of the hydrogenic ion with the residual nuclear charge and fit them with the above equation, fixing E_0 to be the binding energy of the orbital. We then match equation (1) to the calculated cross sections at two highest energy points to derive the parameters σ_0 and p, while holding E_0 and b fixed at the values obtained in the hydrogenic fit. The reason for using such a procedure is that the parameters E_0 and b are not very sensitive to the cross sections at $E_e < 10E_{\rm th}$. To derive them, one needs high-energy cross sections, which are less efficient to calculate in detail. However, we expect at least the energy dependence of the high-energy photoionization cross sections to follow that of the hydrogenic approximation as long as the relativistic effects are not too important, as is the case for the ions we consider in this work. Therefore, this extrapolation procedure preserves the correct nonrelativistic high-energy behavior of the photionization cross sections and matches them smoothly to the low-energy values calculated at $E_e < 10E_{\rm th}$.

We expect this method to be more accurate for highly charged ions than for low-ionization states.

RR cross sections for $n > 10$ shells are estimated using the semiclassical Kramers formula

$$\sigma_{\rm RR}(E_e) = 2.10 \times 10^{-22}\ {\rm cm}^2 \frac{z^4 E_{\rm H}^2}{n E_e (z^2 E_{\rm H} + n^2 E_e)}\ , \quad (2)$$

where z is the residual charge of the ion and $E_{\rm H}$ is the Rydberg energy. Contributions up to $n = 10,000$ are taken into account. Using the asymptotic expansion method of Seaton (1959), we estimate that RR due to $n > 10,000$ states contribute only 6% of the total rate coefficients at a temperature of 10^{-4} eV for $z = 26$, and less for smaller z or at higher temperatures.

The Maxwellian averaged rate coefficients are computed using the total RR cross sections in the temperature range 10^{-4}–10^4 eV. The results are fitted with the formula proposed by Verner & Ferland (1996),

$$\alpha(T) = a\left[\sqrt{T/T_0}\left(1+\sqrt{T/T_0}\right)^{1-b}\left(1+\sqrt{T/T_1}\right)^{1+b}1\right]^{-1}\ , \quad (3)$$

where a, b, T_0, and T_1 are fit parameters. We find that this formula reproduces the calculated rate coefficients to within 5% in the entire temperature range for all ions considered in this work, except for F-like Mg, O-like Mg, and F-like Si, which are the three lowest-ionized species. For these three ions, we use a modified version of equation (3) by replacing b with $b + b_1 \exp(-T_2/T)$, where b_1 and T_2 are two additional fit parameters. With such generalizations, the formula reproduces the rate coefficients to within 5% for all ions. The DW approximation of photoionization cross

TABLE 1
Fit Parameters for Radiative Recombination Rate Coefficients

Ion[a]	Z[a]	N[a]	a (10^{-10} cm^3 s^{-1})	b	T_0 (eV)	T_1 (eV)	b_1	T_2 (eV)
Ni XXIX	28	0	1.622E+02	7.924E−01	6.448E−03	3.170E+04	...	...
Ni XXVIII	28	1	1.380E+02	7.752E−01	7.031E−03	1.814E+04	...	...
Ni XXVII	28	2	1.307E+02	7.622E−01	6.108E−03	7.270E+03	...	...
Ni XXVI	28	3	1.320E+02	7.672E−01	5.143E−03	6.018E+03	...	...
Ni XXV	28	4	1.306E+02	7.703E−01	4.471E−03	5.036E+03	...	...
Ni XXIV	28	5	1.187E+02	7.668E−01	4.508E−03	4.852E+03	...	...
Ni XXIII	28	6	1.045E+02	7.608E−01	4.796E−03	4.683E+03	...	...
Ni XXII	28	7	8.981E+01	7.526E−01	5.271E−03	4.554E+03	...	...
Ni XXI	28	8	7.616E+01	7.428E−01	5.871E−03	4.409E+03	...	...
Ni XX	28	9	6.346E+01	7.306E−01	6.655E−03	4.210E+03	...	...
Fe XXVII	26	0	1.438E+02	7.911E−01	6.050E−03	2.816E+04	...	...
Fe XXVI	26	1	1.206E+02	7.730E−01	6.701E−03	1.627E+04	...	...
Fe XXV	26	2	1.140E+02	7.598E−01	5.760E−03	6.428E+03	...	...
Fe XXIV	26	3	1.153E+02	7.656E−01	4.784E−03	5.286E+03	...	...
Fe XXIII	26	4	1.142E+02	7.692E−01	4.096E−03	4.400E+03	...	...
Fe XXII	26	5	1.031E+02	7.658E−01	4.116E−03	4.254E+03	...	...
Fe XXI	26	6	8.931E+01	7.592E−01	4.440E−03	4.153E+03	...	...
Fe XX	26	7	7.534E+01	7.500E−01	4.966E−03	4.083E+03	...	...
Fe XIX	26	8	6.252E+01	7.389E−01	5.639E−03	4.014E+03	...	...
Fe XVIII	26	9	5.039E+01	7.244E−01	6.646E−03	3.899E+03	...	...
Ca XXI	20	0	9.351E+01	7.863E−01	4.843E−03	1.828E+04	...	...
Ca XX	20	1	7.368E+01	7.651E−01	5.760E−03	1.103E+04	...	...
Ca XIX	20	2	6.783E+01	7.499E−01	4.917E−03	4.212E+03	...	...
Ca XVIII	20	3	6.919E+01	7.590E−01	3.811E−03	3.376E+03	...	...
Ca XVII	20	4	6.844E+01	7.648E−01	3.089E−03	2.766E+03	...	...
Ca XVI	20	5	5.986E+01	7.615E−01	3.075E−03	2.726E+03	...	...
Ca XV	20	6	4.857E+01	7.526E−01	3.477E−03	2.772E+03	...	...
Ca XIV	20	7	3.743E+01	7.384E−01	4.223E−03	2.889E+03	...	...
Ca XIII	20	8	2.828E+01	7.215E−01	5.165E−03	3.052E+03	...	...
Ca XII	20	9	2.003E+01	6.960E−01	6.849E−03	3.323E+03	...	...
Ar XIX	18	0	7.835E+01	7.844E−01	4.459E−03	1.528E+04	...	...
Ar XVIII	18	1	6.018E+01	7.618E−01	5.441E−03	9.417E+03	...	...
Ar XVII	18	2	5.422E+01	7.452E−01	4.702E−03	3.580E+03	...	...
Ar XVI	18	3	5.522E+01	7.557E−01	3.560E−03	2.844E+03	...	...
Ar XV	18	4	5.449E+01	7.626E−01	2.815E−03	2.311E+03	...	...
Ar XIV	18	5	4.726E+01	7.598E−01	2.745E−03	2.294E+03	...	...
Ar XIII	18	6	3.716E+01	7.498E−01	3.158E−03	2.386E+03	...	...
Ar XII	18	7	2.738E+01	7.331E−01	3.972E−03	2.569E+03	...	...
Ar XI	18	8	1.976E+01	7.129E−01	4.989E−03	2.842E+03	...	...
Ar X	18	9	1.317E+01	6.813E−01	6.877E−03	3.339E+03	...	...
S XVII	16	0	6.429E+01	7.824E−01	4.064E−03	1.245E+04	...	...
S XVI	16	1	4.753E+01	7.579E−01	5.178E−03	7.902E+03	...	...
S XV	16	2	4.173E+01	7.393E−01	4.532E−03	3.000E+03	...	...

TABLE 1—*Continued*

Ion[a]	Z[a]	N[a]	a (10^{-10} cm^3 s^{-1})	b	T_0 (eV)	T_1 (eV)	b_1	T_2 (eV)
S XIV	16	3	4.266E+01	7.520E−01	3.292E−03	2.351E+03	...	...
S XIII	16	4	4.177E+01	7.599E−01	2.544E−03	1.898E+03	...	...
S XII	16	5	3.559E+01	7.577E−01	2.438E−03	1.912E+03	...	...
S XI	16	6	2.695E+01	7.464E−01	2.847E−03	2.040E+03	...	...
S X	16	7	1.729E+01	7.192E−01	4.337E−03	2.626E+03	...	...
S IX	16	8	1.296E+01	7.025E−01	4.654E−03	2.734E+03	...	...
S VIII	16	9	8.221E+00	6.645E−01	6.275E−03	3.606E+03	...	...
Si XV	14	0	5.130E+01	7.802E−01	3.665E−03	9.832E+03	...	...
Si XIV	14	1	3.625E+01	7.534E−01	4.901E−03	6.471E+03	...	...
Si XIII	14	2	3.048E+01	7.316E−01	4.435E−03	2.474E+03	...	...
Si XII	14	3	3.118E+01	7.471E−01	3.073E−03	1.906E+03	...	...
Si XI	14	4	3.016E+01	7.563E−01	2.309E−03	1.531E+03	...	...
Si X	14	5	2.556E+01	7.559E−01	2.080E−03	1.566E+03	...	...
Si IX	14	6	1.856E+01	7.434E−01	2.426E−03	1.731E+03	...	...
Si VIII	14	7	1.217E+01	7.186E−01	3.207E−03	2.131E+03	...	...
Si VII	14	8	8.021E+00	6.894E−01	3.847E−03	2.899E+03	...	...
Si VI	14	9	4.156E+00	6.323E−01	6.301E−03	2.072E+03	6.492E−02	1.063E+02
Mg XIII	12	0	3.959E+01	7.778E−01	3.243E−03	7.437E+03	...	...
Mg XII	12	1	2.616E+01	7.478E−01	4.678E−03	5.144E+03	...	...
Mg XI	12	2	2.082E+01	7.213E−01	4.392E−03	2.008E+03	...	...
Mg X	12	3	2.148E+01	7.415E−01	2.805E−03	1.503E+03	...	...
Mg IX	12	4	2.038E+01	7.524E−01	2.026E−03	1.207E+03	...	...
Mg VIII	12	5	1.705E+01	7.543E−01	1.681E−03	1.267E+03	...	...
Mg VII	12	6	1.165E+01	7.390E−01	1.946E−03	1.513E+03	...	...
Mg VI	12	7	5.314E+00	6.838E−01	4.443E−03	1.256E+03	5.602E−02	6.008E+01
Mg V	12	8	4.878E+00	7.060E−01	1.768E−03	1.024E+03	8.149E−02	5.967E+01
Mg IV	12	9	2.001E+00	6.339E−01	2.693E−03	1.071E+03	1.464E−01	4.992E+01

NOTE.—Table 1 is also available in machine-readable form in the electronic edition of the *Astrophysical Journal*.
[a] Refers to the recombining ion.

sections for such nearly neutral ions are most likely to contain significant uncertainties; the modification to the fitting formula needed may well be due to the inaccuracies in the calculated RR rate coefficients for these ions. Nevertheless, the recommended RR rate coefficients currently used in the most updated ionization balance calculations for these ions, e.g., that of Mazzotta et al. (1998), are derived from even more crude approximations, namely, the hydrogenic approximation and interpolation along the isosequences (Shull & Van Steenberg 1982). The present results should be at least as reliable as these early calculations even for such low-ionization species. Table 1 lists the fit parameters in detail.

In Figure 1, we compare the present RR rate coefficients of bare, He-like, C-like, and F-like Fe ions with previous results. For bare and He-like ions, the comparison is made with the work of Verner & Ferland (1996), and for C-like and F-like ions, the comparison is made with the data of Arnaud & Raymond (1992). It is seen that the present rate coefficients of bare and He-like ions agree with Verner & Ferland (1996) very well in the entire temperature range, except at the lowest temperatures (<0.01 eV), where the present results are ~10%–15% higher. Our results for bare ions agree with the asymptotic expansion of Seaton (1959) better than Verner & Ferland (1996). However, discrepancies at such low temperatures are of little practical importance. Similar good agreements are found for all bare, H-like, and He-like ions. For C-like and F-like Fe, the present results agree with those of Arnaud & Raymond (1992) at

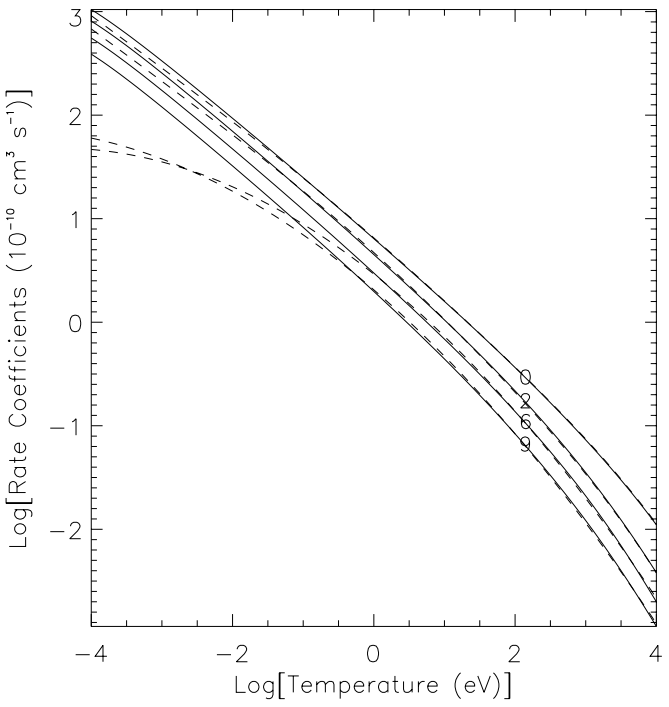

FIG. 1.—RR rate coefficients of bare, He-like, C-like, and F-like Fe ions. The solid lines are the present results. The number labeling each line indicates the number of electrons the recombining ion has. The dashed lines for bare and He-like ions are from Verner & Ferland (1996), and those for C-like and F-like ions are from Arnaud & Raymond (1992).

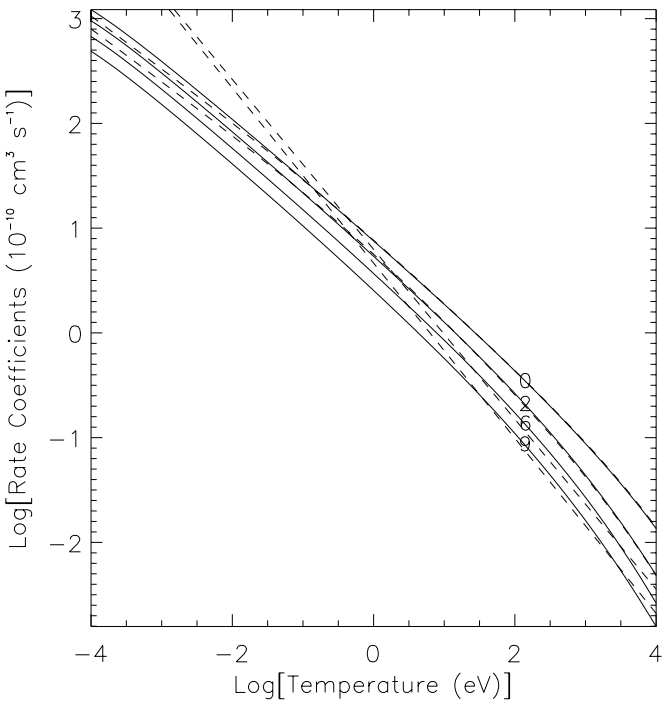

FIG. 2.—Same as Fig. 1, but for Ni ions. The dashed lines for bare and He-like ions are from Verner & Ferland (1996), and those for C-like and F-like ions are from Shull & Van Steenberg (1982).

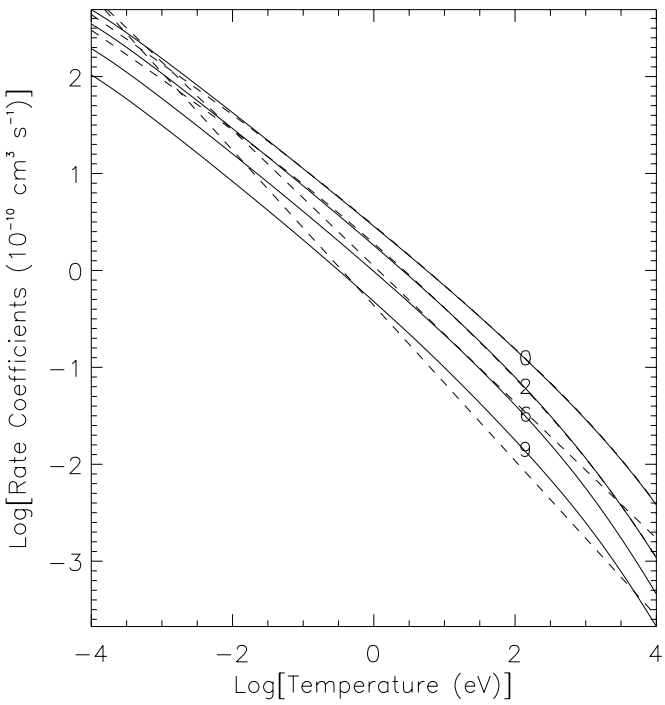

FIG. 3.—Same as Fig. 1, but for Ar ions. The dashed lines for bare and He-like ions are from Verner & Ferland (1996), and those for C-like and F-like ions are from Shull & Van Steenberg (1982).

temperatures above ~1 eV, for which the fitting formula of Arnaud & Raymond (1992) is valid. Our results should be more accurate at lower temperatures. The good agreement at high temperatures for these ions indicates that the extrapolation procedure for the high-energy photoionization cross sections used in this work is sufficiently accurate for the purpose of calculating total RR rate coefficients. In Figures 2 and 3, we make similar comparisons for Ni and Ar ions, respectively. For C-like and F-like ions, the comparison is made with the results of Shull & Van Steenberg (1982), which are widely used in spectral modeling codes. It is evident that the existing data for these ions are of poor quality. Similar discrepancies are found for all L shell ions of elements other than Fe.

In summary, we have presented RR rate coefficients of bare to F-like isosequences of seven abundant astrophysical elements, including Mg, Si, S, Ar, Ca, Fe, and Ni. The present results agree with existing data for bare, H-like, and He-like isosequences, and for Fe ions at temperatures for which the previous fits are valid. Significant discrepancies are found for other ions, and we believe that our results are of higher quality for these ions.

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