Fitting of atomic data for astrophysical applications

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Abstract. We present (i) new analytic fits to the photoionization cross sections for the ground states of atoms and all ions of elements from H through Si, and S, Ar, Ca, and Fe; (ii) new analytic fits to the rates of radiative recombination towards H-like, He-like, Li-like and Na-like ions of all elements from H through Zn over a broad range of temperature; (iii) a compilation of wavelengths, statistical weights and oscillator strengths for 5904 permitted resonance spectral lines without wavelength restriction.

1. Analytic fits to the photoionization cross sections

Photoionization cross sections of atoms and ions are needed for many astrophysical applications. In earlier papers (Verner et al. 1993, Verner & Yakovlev 1995), we presented the Hartree-Dirac-Slater (HDS) calculations and analytic fits to the partial photoionization cross sections for all subshells nl of the ground states of all atoms and ions from H to Zn. Comparison with available experimental and theoretical data demonstrated high accuracy of the cross section fits for inner shells and far from the thresholds of outer shells. However, the theoretical HDS cross sections can be inaccurate near the thresholds of the outer shells, especially for neutral and low ionized species. The recent Opacity Project (OP) calculations (Seaton et al. 1992) based on the higher level methods such as the R-matrix method give more accurate low energy photoionization cross sections. In particular, the OP calculations reproduce many autoionization resonances near the ionization thresholds. For practical purpose, it is usually sufficient to use the photoionization cross sections smoothed over resonances (except some very wide resonances). Autoresonances could be important for calculating the photoionization rate produced by radiation in spectral lines whose positions coincide with the autoresonances. However, the OP theoretical energy levels deviate from experimental ones within 1–2% (Verner, Barthel, & Tytler 1994). This accuracy is clearly insufficient for astrophysical spectroscopy. Therefore, smoothing of the OP photoionization cross sections is preferable.

We have retrieved the ground state photoionization cross sections of atoms and all ions of the OP elements (H, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, S, Ar, Ca, Fe) from a database TOPbase 0.7 (Cunto et al. 1993), interpolated and smoothed them over resonances, and then fitted the smoothed cross sections by the fitting formula:

$$\sigma(E) = \sigma_0 \, F(y) \ \ \mathrm{Mb}, \qquad y = \sqrt{\left(\frac{E}{E_0} - y_0\right)^2 + y_1^2}, \tag{1}$$

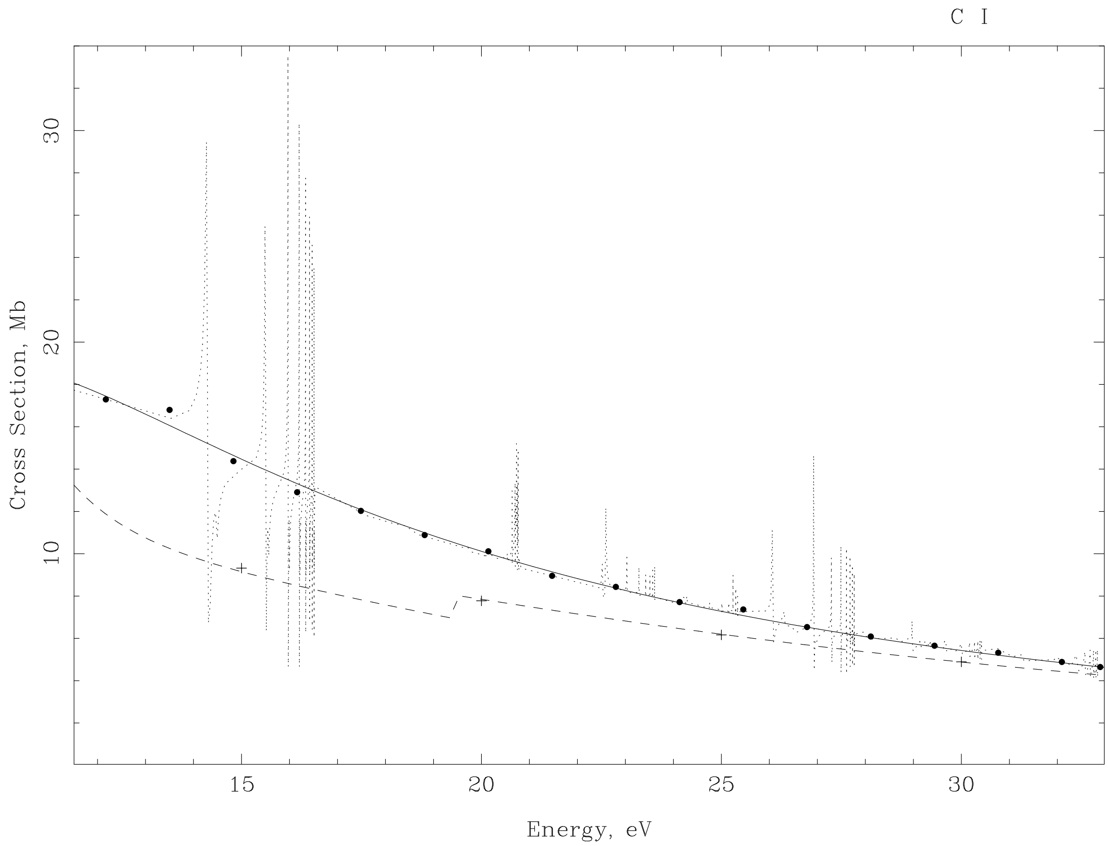

Figure 1. Total photoionization cross section of C I. Solid line: present fit; dashed line: fit from Verner & Yakovlev (1995); dotted line: Opacity Project data (Luo & Pradhan 1989); circles: Opacity Project data interpolated and smoothed over resonances; crosses: calculations from Reilman & Manson (1979).

$$F(y) = \left[(y-1)^2 + y_{\rm w}^2\right] y^{0.5P-5.5} \left(1 + \sqrt{y/y_{\rm a}}\right)^{-P}, \tag{2}$$

where E is photon energy in eV, and σ_0, E_0, $y_{\rm w}$, $y_{\rm a}$, P, y_0 and y_1 are the fit parameters. Our fits are valid in the energy range from the ionization threshold up to the first cross section jump due to inner shell photoionization. In combination with the earlier fits to the inner shell cross sections (Verner & Yakovlev 1995), we obtain the accurate and complete set of photoionization cross sections for calculating ionization balance in astrophysical plasmas. The fit parameters are to be published (Verner, Ferland, Korista, & Yakovlev 1995).

2. Analytic fits to the radiative recombination rates

For the most ionic species, the total recombination rates are dominated by dielectronic recombination. The exceptions are H-like ions which are not subject to dielectronic recombination at all, and He-like, Li-like and Na-like species which do not have low-lying autoionization states and therefore are not subject to low-temperature dielectronic recombination. For calculation of the ground level

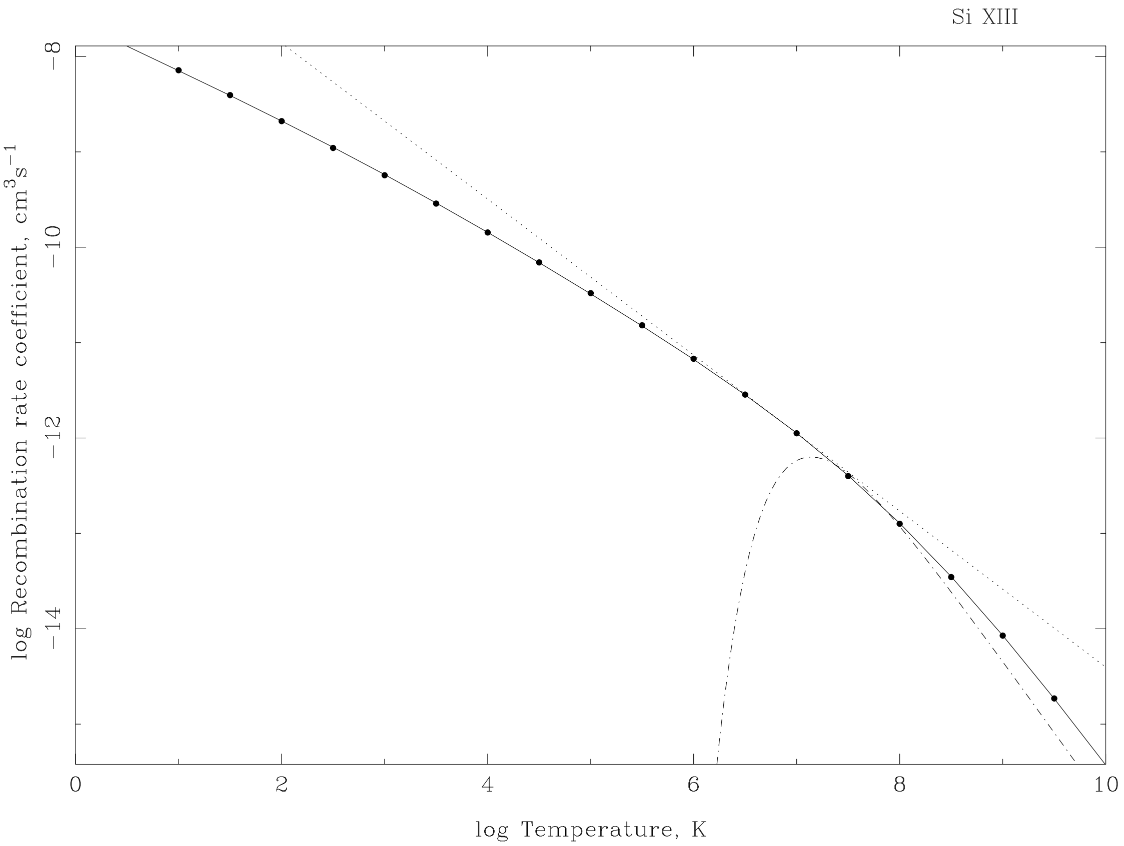

Figure 2. Radiative recombination rate coefficient of Si XIII vs. temperature. Circles: present calculations; solid line: present fit; dotted line: Arnaud & Rothenflug (1985); dash-dotted line: dielectronic recombination rate coefficient from Arnaud & Rothenflug (1985).

recombination rate coefficients for He-like, Li-like and Na-like ions, we used our new analytic fits to the photoionization cross sections which give the corrected threshold cross sections and near-threshold cross section behavior based on the OP data, and ensure accurate high energy cross sections by use of the fitting formula with the correct non-relativistic asymptote. For calculation of the rate coefficients to the excited levels with $n \leq 5$ of the five and more times ionized species, we used Clark, Cowan, & Bobrowicz (1986) fits to the partial photoionization cross sections. For calculation of the radiative recombination rates to the excited levels with $n \leq 10$ of the first four ionization states where Clark et al. fits are not valid, we used the Gould (1978) method of correction for incomplete shielding. We used the hydrogenic approximation for levels with $n > 10$ (four and less times ionized species) and for levels with $n > 5$ (five and more times ionized species). Careful integration of the Milne relation and use of the photoionization cross sections which are accurate as near the thresholds as at high energies ensure the high accuracy of the total radiative recombination rate coefficients in a wide range of temperature, from 3 K to 10^8 K. We fitted all the total rate coefficients obtained in the temperature range from 3 K to 10^{10} K using the formula

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

where a, b, T_0 and T_1 are the fitting parameters. Formula (3) ensures correct asymptotic behavior of the rate coefficients (Ferland et al. 1992) as at low as at high temperatures: $\alpha_\mathrm{r}(T) \propto T^{-0.5}$ at $T \ll T_0 \ll T_1$, and $\alpha_\mathrm{r}(T) \propto T^{-1.5}$ at $T \gg T_1 \gg T_0$. The average accuracy of fitting is better than 3% (maximum error is less than 6%) for all species. The fit parameters are to be published (Verner & Ferland 1995).

3. Atomic data for resonance spectral lines

In earlier paper (Verner et al. 1994) we presented a compilation of atomic data for absorption lines from the ground (zero energy) level at wavelengths greater than 228 Å. The radical improvement in spectral resolution and signal/noise provided by spectra from EUVE, DXS and ASCA in far-UV and X-ray bands has prompted to compile a set of atomic data for spectral lines without wavelength restrictions. Our new compilation, which is supposed to be the first part of the complete set of data for the X-ray and UV spectroscopy, includes accurate wavelengths, statistical weights and oscillator strengths for permitted resonance lines of all ions of the OP elements (see above). The OP data include oscillator strengths for all optically alloweded transitions between states with $n \leq 10$ and $l \leq 4$. We retrieved from the TOPbase (Cunto et al. 1993) the gf-values for all multiplets which involve the ground term. These 6018 resonance multiplets include 23505 lines. We calculated the f-values of all individual lines in multiplets based on LS-coupling rules. The TOPbase does not include the data for Fe I and Fe II. We obtained the f-values for 122 lines of 18 resonance multiplets of Fe I and Fe II from Fuhr, Martin, & Wiese (1988) and 212 lines of 18 resonance multiplets of Fe II from Nahar (1995). In the whole, our line database includes the f-values of 23839 lines of 6054 resonance multiplets. From them, 5904 lines have accurate wavelengths calculated from experimental energy levels. Our compilation of experimental energy levels is complete to August 1995. Work on a compilation of non-LS-type lines is in progress.

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