

## New Radiative Atomic Data

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**Abstract.** Large amount of new radiative atomic data for I) energy levels, II) oscillator strengths ( $f$ ), line strengths ( $S$ ), radiative transition probabilities ( $A$ ), III) photoionization cross sections ( $\sigma_{PI}$ ) - total and level-specific, and IV) unified total and level-specific electron-ion recombination rate coefficients,  $\alpha_R$ , including radiative and dielectronic recombination (RR and DR) are reported for various astrophysical applications. Most of the data are with fine structure. These data are not yet available from any databases. Photoionization and recombination data are self-consistent, using the same wave-function for both processes.

### 1. Introduction

Atomic parameters for radiative processes are obtained from ab initio quantum mechanical calculations using the close coupling approximation employing the R-matrix method, as developed under the OP (The Opacity Project 1995, 1996) and Iron Project (IP, Hummer et al. 1993, Berrington et al. 1995) and new theoretical developments for total electron-ion recombination using the unified method (Nahar and Pradhan 1992, 1994, Zhang et al. 1999), and large-scale theoretical spectroscopy calculations (Nahar and Pradhan 2000). Relativistic effects are included through the Breit-Pauli R-matrix (BPRM) method for most of the radiative data.

Compared to earlier results, such as those under the OP, present results include much more data in addition to  $\sigma_{PI}$  and  $f$ -values. Present calculations are more elaborate and extensive with the following important features:

i) wave-function expansions used for the new results are in general larger, i.e., they include more excited core states,  $E_t$ , yielding (1) more complete set of energy levels ( $E_\nu = E_t - z^2/\nu^2$ ), (2) larger sets of  $f$ ,  $S$ ,  $A$ -values for bound-bound transitions, (3) more Rydberg series of resonances in the cross sections belonging to the additional core states, (4) more accurate background cross sections at higher energies.

ii) observed energies, where available, are used for the core states which provide more accurate resonance positions determined from  $E_\nu = E_t - z^2/\nu^2$ .

iii) calculations are carried out using finer energy mesh.

### 2. Bound-Bound Transitions: $X^{+n} + h\nu \leftrightarrow X^{+n*}$

Present  $A$ ,  $f$ , and  $S$ -values are mainly for electric dipole (E1), i.e, dipole allowed and inter-combination ( $\Delta J = 0, \pm 1$ , parity change) transitions. However, forbidden transitions ( $\Delta J > 1$ ), e.g., electric quadrupole (E2), octupole (E3), magnetic dipole (M1), quadrupole (M2), are obtained for a number of ions.

One important advantage of BPRM method is that large number of bound-bound transitions can be considered. The spectroscopic identification of the computed levels and transitions are carried out with newly developed identification procedure based on quantum defect and channel contribution analysis. Each level is assigned with a spectroscopic notation,  $(C_t S_t L_t J_t \pi_t n l [K] s) J \pi$  where  $C$  denotes configuration and subscript  $t$  denotes target (or the core). The forbidden transition of type E2, E3, M1 and M2 are obtained through atomic structure calculations using updated version of SUPERSTRUCTURE (Eissner et al. 1974, Nahar et al 2003).

Data for Fe XVII (Nahar et al. 2003) is an example of new results. A total of 490 fine structure levels are obtained for this ion, compared to observed 52 levels. The calculated energies agree within 1% with the observed energies.  $A$ ,  $f$ , and  $S$ -values are obtained for over  $2.6 \times 10^4$  for allowed and inter-combination transitions; a comparison table of Fe XVII transitions is given below:

Table. Comparison of BPRM calculations for decay  $A^{E1}(j, 1)$  to the Fe XVII ground state  $C_1 T_1 = 2s^2 2p^6 1S_0$  with other work

$C_j$	$T_j$	BPRM	$A(s^{-1})$ others
$2s^2 2p^5 3s$	$1P_1^o$	7.96(11) 8.28(11) <sup>a</sup> , 8.01(11) <sup>b</sup> , 7.75(11) <sup>c</sup> , 8.30(11) <sup>e</sup> , 9.40(11) <sup>‡</sup>	
$2s^2 2p^5 3s$	$3P_1^o$	9.35(11) 9.76(11) <sup>a</sup> , 9.44(11) <sup>b</sup> , 9.09(11) <sup>c</sup> , 9.34(11) <sup>e</sup> , 8.00(11) <sup>‡</sup>	
$2s^2 2p^5 3d$	$3P_1^o$	7.58(10) 9.19(10) <sup>a</sup> , 8.27(10) <sup>b</sup> , 7.77(10) <sup>c</sup> , 9.00(10) <sup>e</sup> , 8.89(10) <sup>‡</sup>	
$2s^2 2p^5 3d$	$3D_1^o$	5.93(12) 6.33(12) <sup>a</sup> , 5.68(12) <sup>b</sup> , 5.23(12) <sup>c</sup> , 6.01(12) <sup>e</sup> , 5.72(12) <sup>‡</sup>	
$2s^2 2p^5 3d$	$1P_1^o$	2.28(13) 2.24(13) <sup>a</sup> , 2.64(13) <sup>b</sup> , 2.44(13) <sup>c</sup> , 2.28(13) <sup>e</sup> , 2.52(13) <sup>‡</sup>	
$2s 2p^6 3p$	$3P_1^o$	4.03(11) 4.51(11) <sup>a</sup> , 3.66(11) <sup>b</sup> , 4.12(11) <sup>d</sup> , 3.40(11) <sup>e</sup> , 3.52(11) <sup>‡</sup>	
$2s 2p^6 3p$	$1P_1^o$	3.30(12) 3.34(12) <sup>a</sup> , 3.21(12) <sup>b</sup> , 3.29(12) <sup>d</sup> , 3.30(12) <sup>e</sup> , 3.25(12) <sup>‡</sup>	

a – Safronova et al 2001, b – Bhatia & Doschek 1992, c – Cornille et al 1994, d – present MCDF, e – NIST, ‡ – SS with *all* magnetic FS-components.

Following is the list of atoms and ions for which transition probabilities ( $f$ ,  $A$ ,  $S$ ) are available or calculations are in progress.

Fe ions: Fe I, Fe II, Fe III, Fe IV, Fe V, Fe XIII, Fe XVII, Fe XX, Fe XXI, Fe XXIII, Fe XXIV, Fe XXV

Ca ions: Ca VII, Ca XVIII

Ar ions: Ar V, Ar XIII, Ar XVI, Ar XVII

S ions: S II, S III, S XIV

Si ions: Si I, Si II, Si XII

Ne ions: Ne V, Ne VIII

O ions: O II, O III, O IV, O VI

C ions: C II, CII, C IV

Li-like: N V, O VI, F VII, Na IX, Mg X, Al XI, Ti XX, Cr XXII, Ni XXVI

He-like ions (elements as for Li-like)

### 3. Photoionization and Recombination: $X^+ + h\nu \leftrightarrow X^{++} + e$

The unified method for total electron-ion recombination developed by Nahar and Pradhan (1992, 1994) enables self-consistent sets of data for photoionization

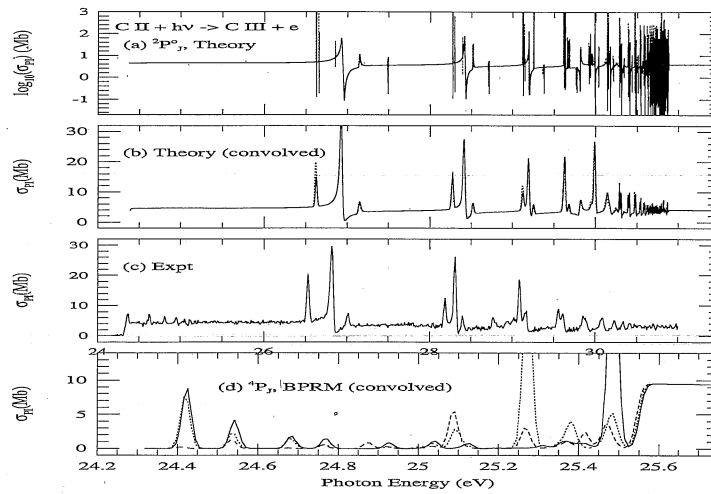


Figure 1. Comparison between theory - Nahar and experiment (Kjeldsen et al. 1999) of photoionization cross sections of C II

cross sections,  $\sigma_{PI}$ , and total recombination rate coefficients,  $\alpha_R(T)$  for atoms and ions.

For highly charged ions,  $\sigma_{PI}$  and  $\alpha_R(T)$  are obtained for fine structure levels including relativistic effects; radiation damping is important for Li-like and He-like ions. For complex multi-electron systems, these quantities are obtained in LS coupling. Contrary to OP data in LS coupling, present results include much more data, including partial photoionization cross sections. Complete data sets include total and level specific photoionization cross sections and recombination rate coefficients for hundreds of levels (with  $n \leq 10$ ) for each ion.

Both the photoionization cross sections and unified recombination cross sections have been benchmarked with recent sophisticated experiments. Figure 1 shows comparison of C II  $\sigma_{PI}$  with the measurement by Kjeldsen et al (1999). Figure 2 presents total and level-specific  $\alpha_R(T)$  for Ni XXVI of interest to X-ray astrophysics.

Self-consistent sets of data for  $\sigma_{PI}$ , and unified recombination rate coefficients have been obtained or are in progress for over 50 ions:

Nickel: Ni II, Ni XXVI

Iron: Fe I, Fe II, Fe III, Fe IV, Fe V, Fe XIII, Fe XVII, Fe XXI, Fe XXIV, Fe XXV, Fe XXVI

Ca: Ca VII, Ca XV, Ca XVIII

Ar: Ar V, Ar XIII, Ar XVI

S: S II, S III, S XI, S XIV

Si: Si I, Si II, Si IX, Si XII

Oxygen: O I, O II, O III, O IV, O V, O VI, O VII, O VIII

Nitrogen: N I, N II, N II, N IV, N V, N VI, N VII

Carbon: C I, C II, C III, C IV, C V, C VI

C-like: F IV, Ne V, Na VI, Mg VII, Al VIII

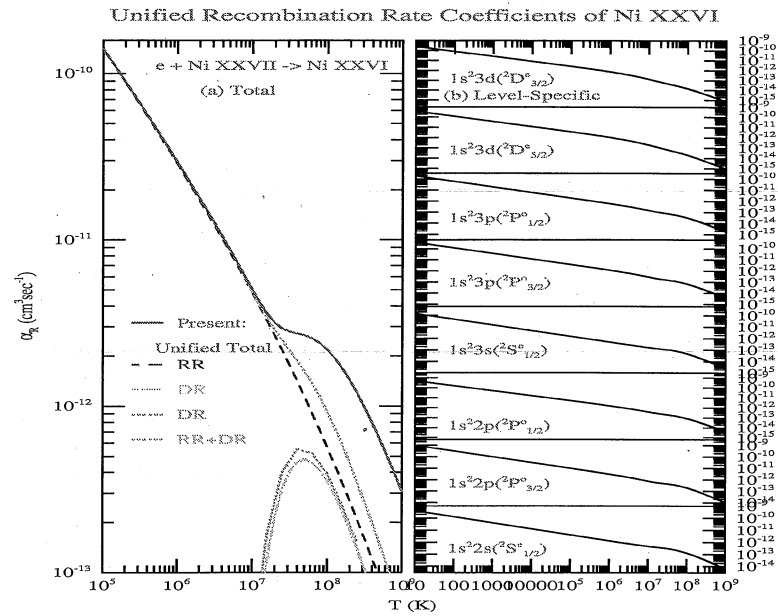


Figure 2. (a) Total unified recombination rate coefficient,  $\alpha_{RC}$ , and (b) level-specific recombination rate coefficients of Ni XXVI.

Li-like: Ti XX, Cr XXII and others  
 He-like (elements as for Li-like)

Data Accessibility - Ohio State University: (i) 1. Anonymous ftp: ftp.astronomy.ohio-state.edu, (ii) <http://www.astronomy.ohio-state.edu/~nahar>, (iii) Email: nahar.1@osu.edu

**Acknowledgments.** Supported partially by the U.S. NSF and NASA.

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