UNIFIED AND SELF-CONSISTENT TREATMENT OF PHOTOIONIZATION AND RECOMBINATION:

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The bound-free transitions of photoionization and electron-ion recombination may proceed as:

i) Photoionization (PI) & Radiative Recombination (RR) (1-step):

$$\mathbf{X^{+Z} + h\nu \rightleftharpoons X^{+Z+1}} + \epsilon$$

ii) Autoionization (AI) & Dielectronic Recombination (DR) (2-steps):

$$\mathbf{e + X^{+Z} \rightleftharpoons (X^{+Z-1})^{**}} \rightleftharpoons \begin{cases} e + X^{+Z} & \text{AI} \\ X^{+Z-1} + h\nu & \text{DR} \end{cases}$$

The doubly excited autoionizing state [$(X^{+Z-1})^{**}$] introduces resonances

- **Radiative & Dielectronic Recombinations are inseparable in nature.**

THEORY

"Unified method for the total electron-ion recombination" (Nahar & Pradhan, PRL 1992, PRA 1994) in the ab initio close coupling approximation and R-matrix method.

• Advantages of the "Unified method":

• It subsumes both the Radiative Recombination & resonant Dielectronic Recombination

• It provides self-consistent set of photoionization cross sections, recombination cross sections and rate coefficients by using an identical wavefunction expansion for both the processes

• It provides "level-specific" recombination rate coefficients & photoionization cross sections for a large number of bound levels

Example: Ionization Fractions in Plasma in

i) Photoionization Equilibrium:

In photoionized nebulae, ionization equilibrium is attained through balancing the photoionization with the electron-ion recombination:

$$N(z)\int_{\nu_0}^{\infty}\frac{4\pi J_\nu}{h\nu}\sigma_{PI}(z,\nu)d\nu = N_e N(z+1)\alpha_{RC}(z,T_e)$$

J_ν = Photoionizing radiation flux, ν_o = Ionization potential of the ion
σ_{PI} = Ground state photoionization cross sections

(i) Coronal Equilibrium:

Electron-impact ionization is balanced by electron-ion recombination:

$$N(z-1)S(z-1) = N(z)\alpha_{RC}(z)$$

$S(z-1)$ = total electron impact ionization rate coefficient
α_{RC} = Unified recombination rate coefficient

Close-coupling (CC) R-matrix method

Total wavefunction expansion in the CC approximation:

$$\Psi_E(e+ion) = A\sum_{i}^{N}\chi_i(ion)\theta_i + \sum_j c_j\Phi_j(e+ion)$$

$\chi_i \longrightarrow$ target ion wavefunction, $\Phi_j \longrightarrow$ correlation functions of (e+ion)
$\theta_i \longrightarrow$ wavefunction of the interacting electron (continuum or bound)

- The complex resonant structures in collisional and radiative processes are included through channel couplings.

The Iron Project - The relativistic Hamiltonian in Breit-Pauli R-matrix (BPRM) approximation:

$$H_{N+1}^{\rm BP} = H_{N+1}^{NR} + H_{N+1}^{\rm mass} + H_{N+1}^{\rm Dar} + H_{N+1}^{\rm so},$$

where the non-relativisitc Hamiltonian is

$$H_{N+1}^{NR} = \sum_{i=1}^{N+1}\left\{-\nabla_i^2 - \frac{2Z}{r_i} + \sum_{j>i}^{N+1}\frac{2}{r_{ij}}\right\}.$$

Mass correction term $\rightarrow$ $H_{N+1}^{\rm mass} = -\frac{\alpha^2}{4}\sum_i p_i^4$, Darwin term $\rightarrow$ $H_{N+1}^{\rm Dar} = \frac{Z\alpha^2}{4}\sum_i \nabla^2(\frac{1}{r_i})$, Spin-orbit interaction term $\rightarrow$ $H_{N+1}^{\rm so} = Z\alpha^2\sum_i \frac{1}{r_i^3}\mathbf{l_i}.\mathbf{s_i}$
Spin-orbit term splits the LS terms into fine-structure levels

Solve Schordinger equation: $H_{N+1}^{BP}\mathit{\Psi} = E\mathit{\Psi}$

The channels introduce a set of coupled equations.

- E $< 0 \longrightarrow$ Bound (e+ion) states Ψ_B
- E $\geq 0 \longrightarrow$ Continuum states Ψ_F

Bound-free Transition Matrix elements for photoionization and electron ion recombination:

$< \Psi_B || \mathbf{D} || \Psi_F >$

$\mathbf{D}$ → dipole operator in "length" and "velocity" forms:

$$\mathbf{D}_L = \sum_n r_n, \qquad \mathbf{D}_V = -2 \sum_2 \Delta_n,$$

n = number of electrons

The photoionization cross section (σ_{PI}) is proportional to the generalized line strength (S) defined as,

$$S = | < \Psi_j || \mathbf{D}_L || \Psi_i > |^2 = \left| \left\langle \Psi_f \right| \sum_{j=1}^{N+1} r_j \left| \Psi_i \right\rangle \right|^2 ,$$

The photoionization cross section is

$$\sigma_{PI} = \frac{4\pi}{3c} \frac{1}{g_i} \omega S,$$

ω → incident photon energy in Rydberg units

Recombination cross section, σ_{RC}, is related to σ_{PI} as,

$$\sigma_{RC} = \sigma_{PI} \frac{g_i}{g_j} \frac{h^2 \omega^2}{4\pi^2 m^2 c^2 v^2}.$$

The recombination rate coefficient, α_{RC}, is obtained as

$$\alpha_{RC}(T) = \int_0^\infty v f(v) \sigma_{RC} dv,$$

$f(v)$ = Maxwellian velocity distribution function

Total α_{RC} → Contributions from infinite number of recombined states

UNIFIED TREATMENT FOR TOTAL ELECTRON-ION RECOMBINATION

RR and DR are inseparable in nature although one may dominate the other

PREVIOUS WORKS: $\alpha_{RC} = \alpha_{RR} + \alpha_{DR}$

NEW METHOD: **A Unified Treatment for the total rate -** α_{RC}

- **Self-consistent treatment for photoionization & recombination using identical wavefunction expansion for both the processes**

- The treatment subsumes both the radiative and dielectronic recombinations in a unified manner.

- It considers infinite number of recombined states:

  i) Group (A) Low-n Bound States ($n \leq n_o \sim 10$):
σ_{PI} are obtained including autoionizing resonances

  ii) Group (B) High-n States ($n_o \geq n \leq \infty$):
These densely packed states are dominated by DR process. The radiation damping of highly excited states are considered through extension of Bell & Seaton theory for DR (1985, Nahar & Pradhan 1994).

- In close coupling approximation.

- Radiation damping of low-n resonances is important for H- and He-like ions

- Approximations:
i) Low-z Ions: Nonrelativistic LS coupling
ii) High-z Ions: Relativistic Breit-Pauli approximation with fine structure

SELF-CONSISTENT RESULTS FOR PHOTOIONIZATION AND ELECTRON RECOMBINATION

C: C I, C II, C III, C IV, C V, C VI
N: N I, N II, N II, N IV, N V, N VI, N VI, N VII
O: O I, O II, O III, O IV, O V, O VI, O VII, O VIII
F: F IV, F VII, F VIII, F IX
Ne: Ne V, Ne VIII, Ne IX, N X
Na: Na VI, Na IX, Na X, Na XI
Mg: Mg VII, Mg X, Mg XI, Mg XII
Al: Al VIII, Al XI, Al XII, Al XIIL
Si: Si I, Si II, Si IX, Si XII, Si XIII, Si XIV
S: S II, S III, S XI, S XIV, S XV, S XVI
Ar: Ar V, Ar XIII, Ar XVI, Ar XVII, Ar XVIII
Ca: Ca VII, Ca XV, Ca XVIII, Ca XIX, Ca XX
Ti: Ti XX, Ti XXI, Ti XXII
Cr: Cr XXII, Cr XXIII, Cr XXIV
Fe: Fe I, Fe II, Fe III, Fe IV, Fe V, Fe XIII, Fe XVII, Fe XXI, Fe XXIV, Fe XXV, Fe XXVI
Ni: Ni II, Ni XXVI, Ni XXVII, Ni XXVIII

- **Complete data for each ion include**

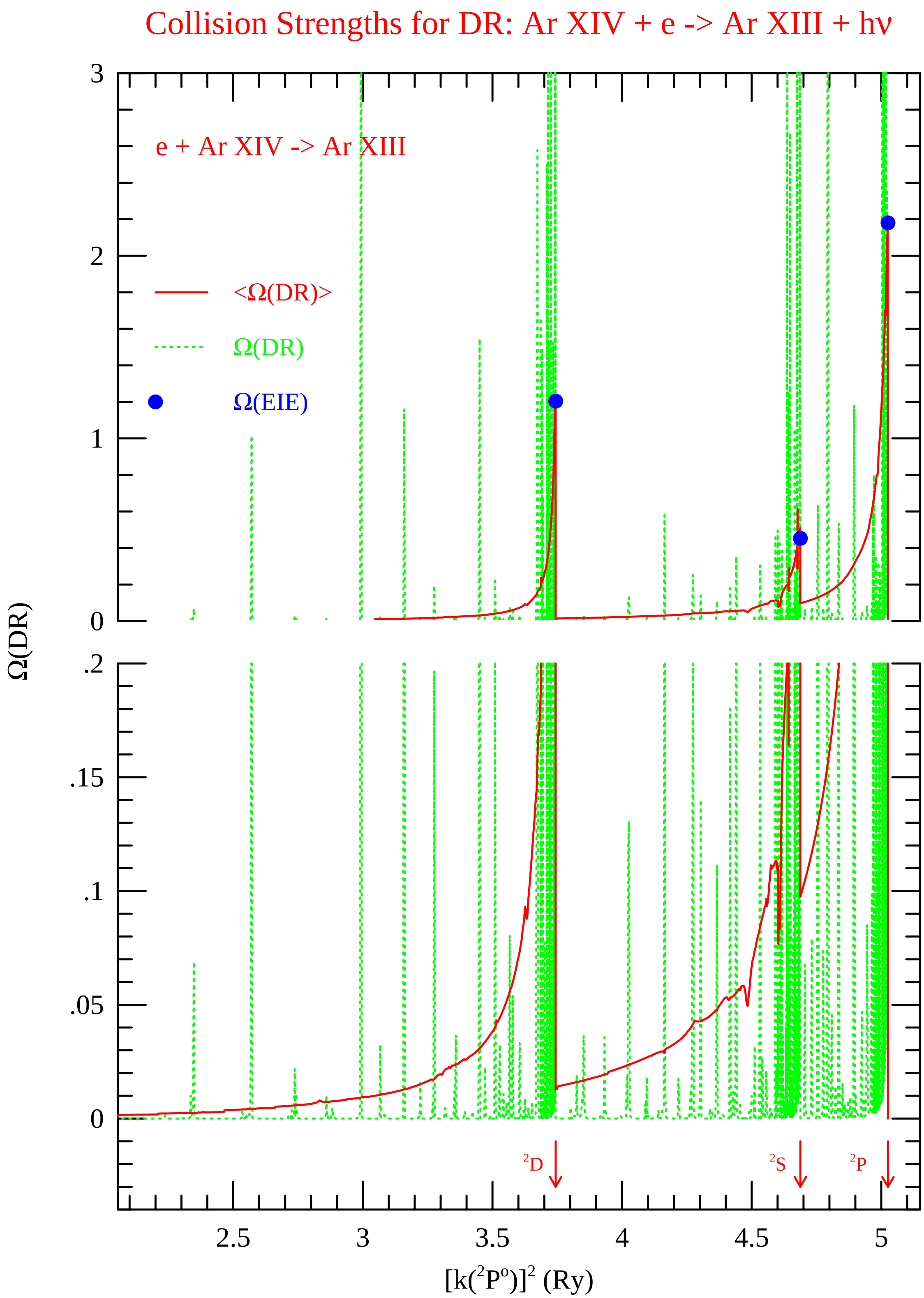
i) Total and level-specific photoionization cross sections (σ_{PI}),
ii) Total unified electron-ion recombination rate coefficients (α_{RC}),
iii) Level-specific $\alpha_{RC}(i)$ for hundreds of levels (with n $\leq$ 10),
iv) Total unified recombination cross sections for some ions,
v) Dielectronic satellite line strengths for He-like ions (in progress)

• Majority of the cross sections and rates are in LS coupling.
• However, fine structure effects are expected to be observed. Simple algebraic split of LS cross sections and rates into fine structure through statistical weight factor can be uncertain.
• We are carrying out calculations in relativistic BPRM approximations for ions, especially for highly charged ions.

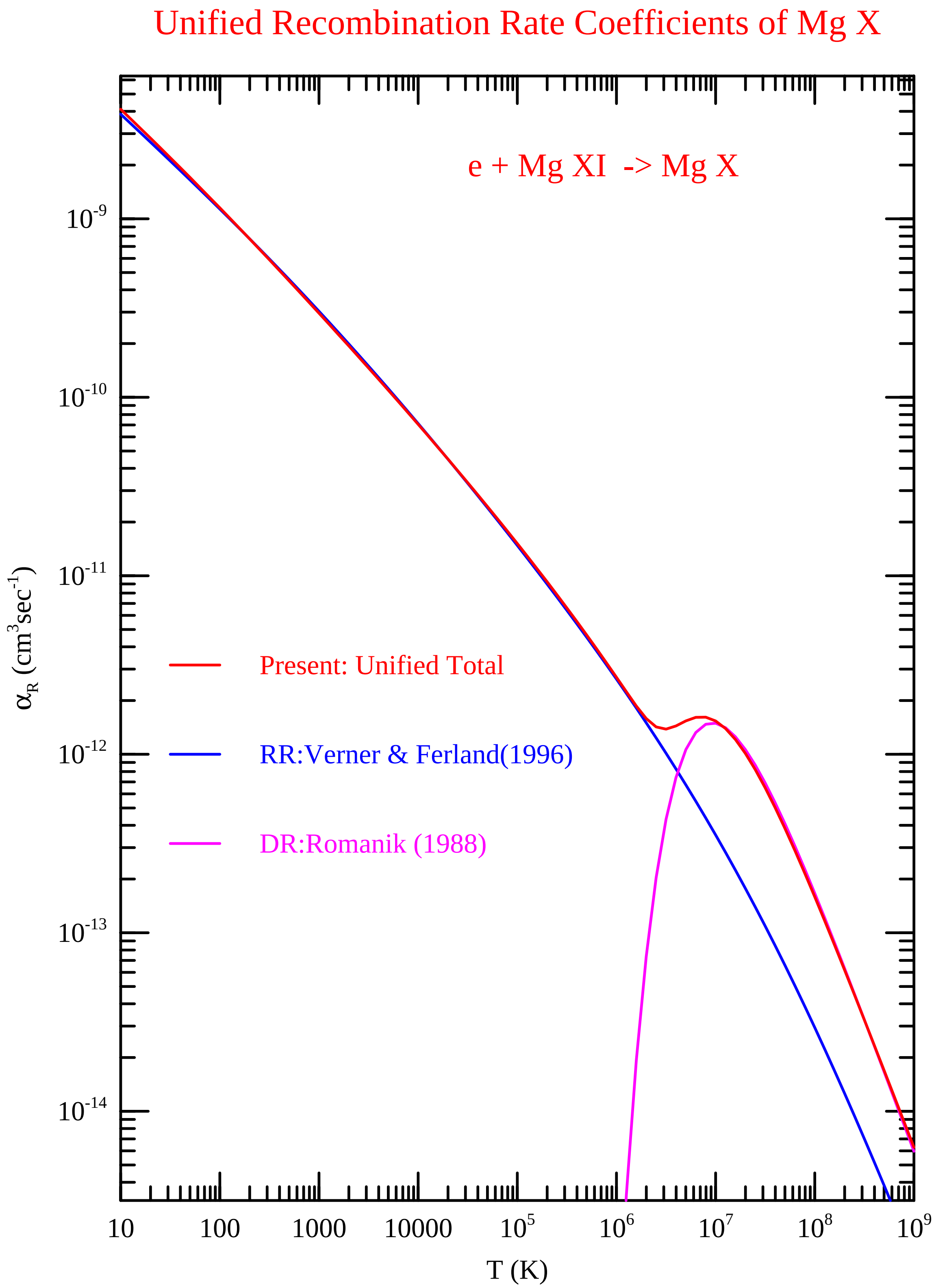
Data Accessibility - Ohio State University:

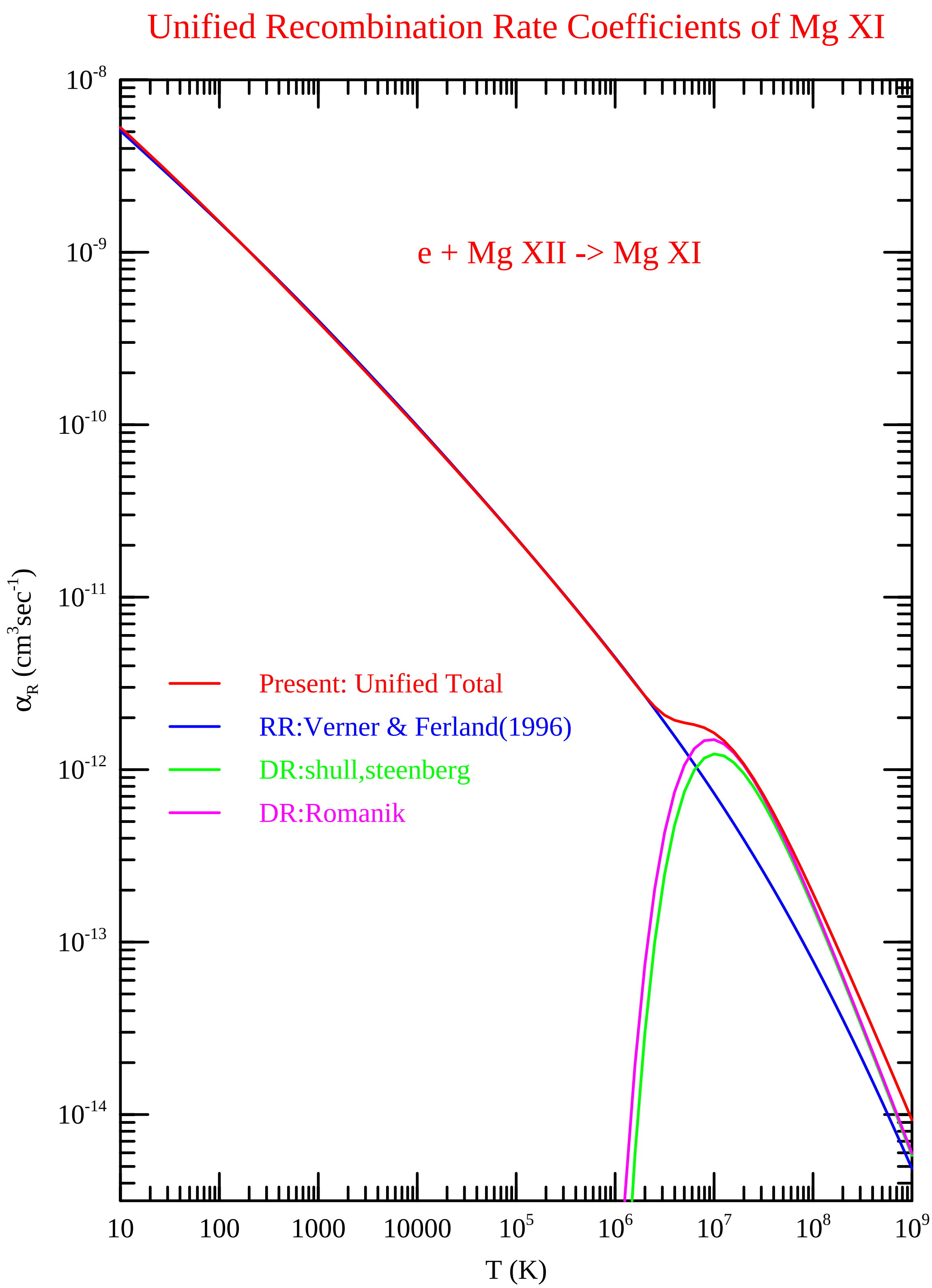
1. Anonymous ftp: ftp.astronomy.ohio-state.edu
2. Email: nahar@astronomy.ohio-state.edu

Examples of recombination rates and cross sections in the next few pages

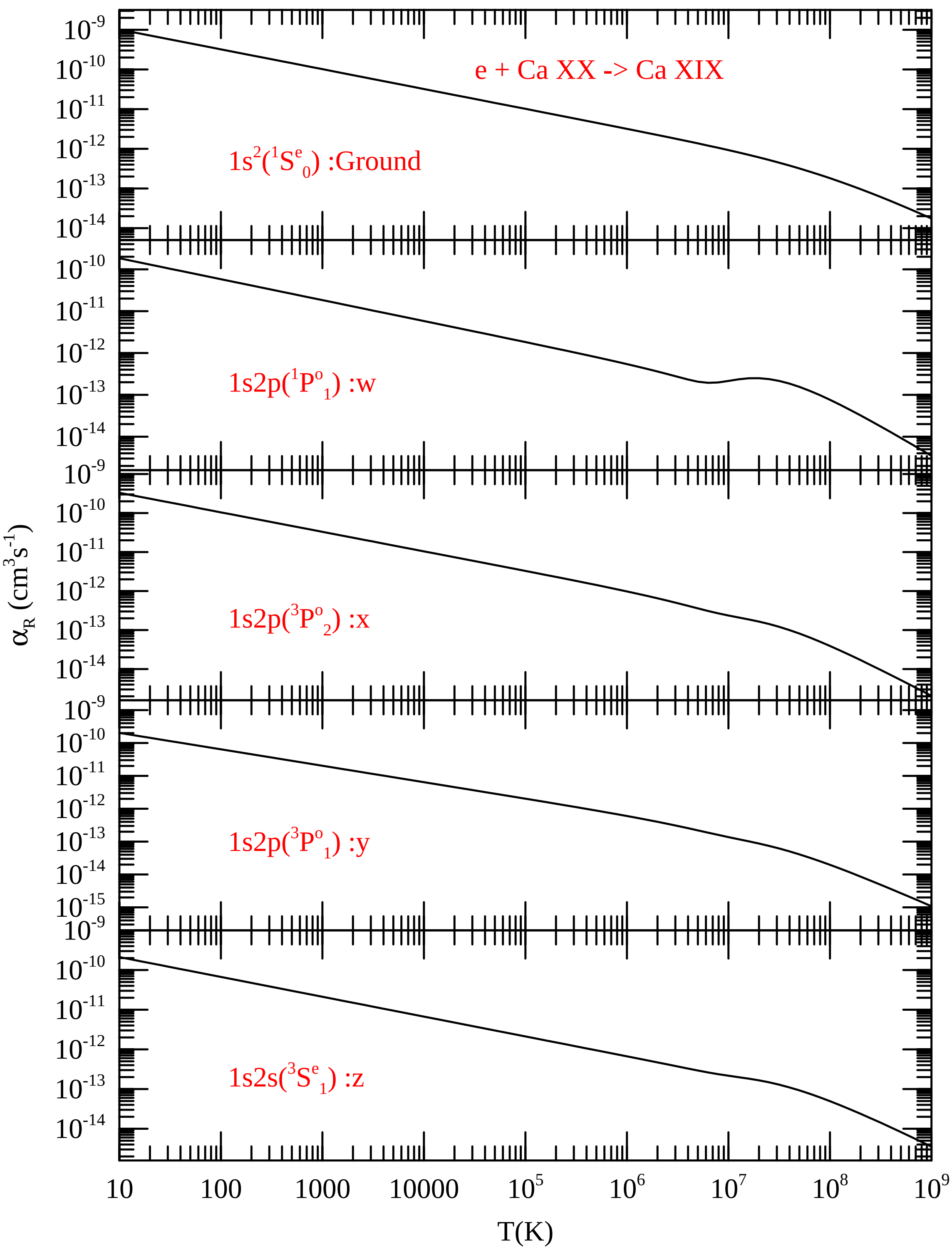


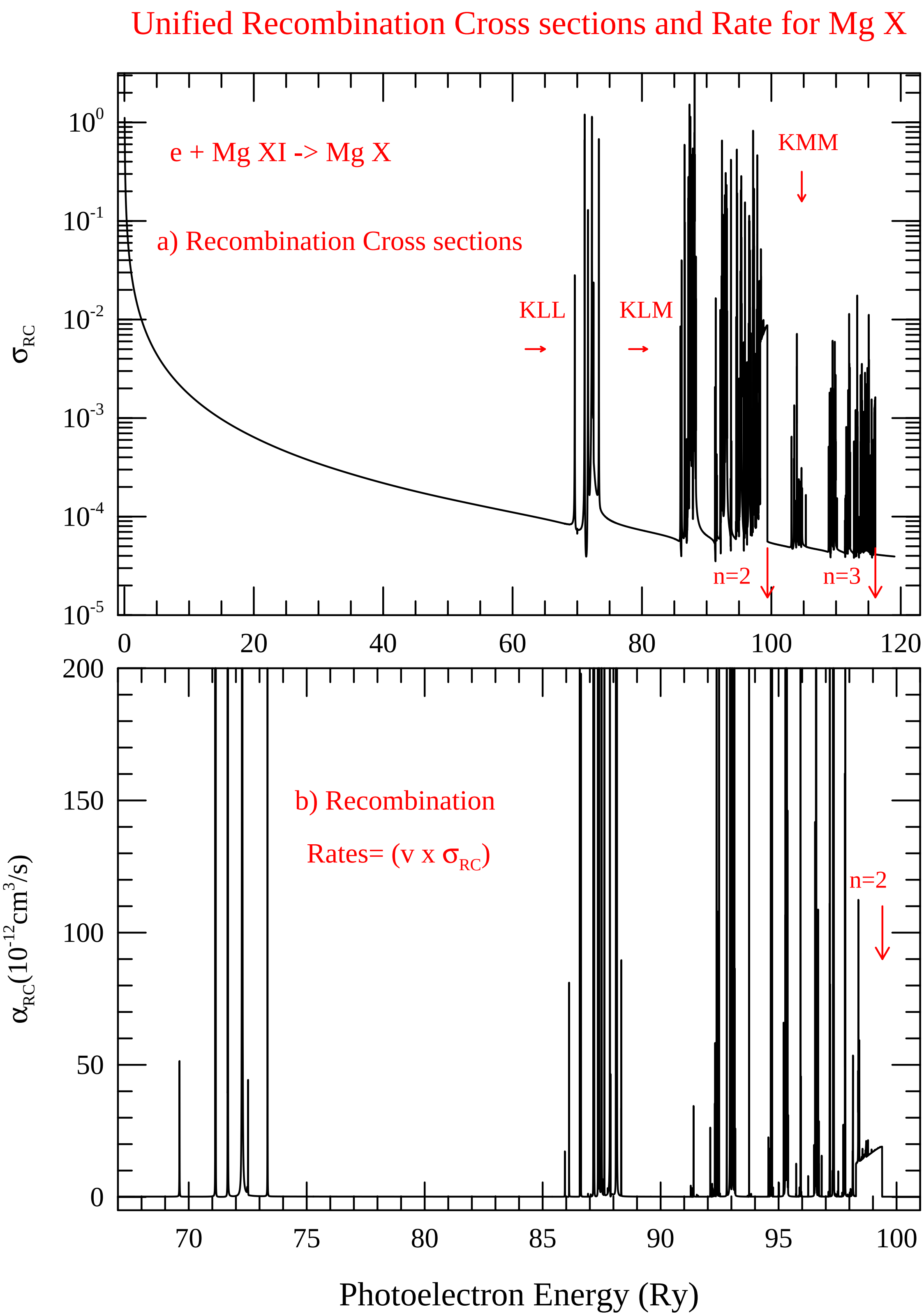
Collision Strengths for DR: Ar XIV + e -> Ar XIII + hν
e + Ar XIV -> Ar XIII
<Ω(DR)>
Ω(DR)
Ω(EIE)
Ω(DR)
0
1
2
3
0
.05
.1
.15
.2
2D
2S
2P
2.5
3
3.5
4
4.5
5
[k(2Po)]2 (Ry)


Unified Recombination Rate Coefficients of Mg X
e + Mg XI -> Mg X
Present: Unified Total
RR:Verner & Ferland(1996)
DR:Romanik (1988)
10^-9
10^-10
10^-11
10^-12
10^-13
10^-14
α_R (cm^3sec^-1)
10
100
1000
10000
10^5
10^6
10^7
10^8
10^9
T (K)


Unified Recombination Rate Coefficients of Mg XI
e + Mg XII -> Mg XI
Present: Unified Total
RR:Verner & Ferland(1996)
DR:shull,steenberg
DR:Romanik
α_R (cm^{3}sec^{-1})
T (K)
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10
100
1000
10000
10^5
10^6
10^7
10^8
10^9

Level-specific Recombination Rate Coefficients for Ca XIX




Unified Recombination Cross sections and Rate for Mg X
e + Mg XI -> Mg X
a) Recombination Cross sections
KLL
KLM
KMM
n=2
n=3
σ_{RC}
b) Recombination
Rates= (v x σ_{RC})
n=2
$\alpha_{RC}(10^{-12}cm^3/s)$
Photoelectron Energy (Ry)