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SATELLITE LINES OF NEON-LIKE RESONANCE LINES, FOR $17 < Z < 48$

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Résumé

Les raies diélectroniques satellites des raies de résonance des ions néonoïdes, du type $1s^2 2s^2 2p^5 3d - 1s^2 2s^2 2p^6$, ont été observées dans des spectres produits par irradiation laser à Limeil, lors d'expériences Laser X, de plasmas collisionnels denses ($10^{20} < n_e < 10^{21} \text{ cm}^{-3}$, $T_e = 600 \text{ eV}$) de Cu, Ge, Se, Mo et Ag. Nous présentons ici les calculs théoriques des coefficients de taux de recombinaison diélectronique des ions néonoïdes vers les ions sodionoïdes. Les paramètres atomiques nécessaires à cette étude : énergies, longueurs d'onde, probabilités radiatives et d'autoionisation sont calculées à l'aide de deux codes : SUPERSTRUCTURE et AUTOLSJ.

Abstract

The dielectronic satellite lines of the neon-like resonance lines $1s^2 2s^2 2p^5 3d - 1s^2 2s^2 2p^6$ have been observed in the spectra obtained during the Limeil X-ray Laser experiments under collisional dense plasma conditions ($10^{20} < n_e < 10^{21} \text{ cm}^{-3}$, $T_e = 600 \text{ eV}$) for Cu, Ge, Se, Mo and Ag. We present here the theoretical calculations of dielectronic recombination rate coefficients for neon-like ions to form sodium-like ions. The atomic parameters required are energy levels, wavelengths, radiative and autoionization probabilities. The quantities are calculated with two coherent codes SUPERSTRUCTURE and AUTOLSJ.

Introduction

The X-ray spectra in the range of Ne-like resonance lines emitted from a soft X-ray Laser plasma is used to make a spectroscopic diagnostic of the plasma. By computing intensity ratios of Ne-like resonance and Na-like satellite lines, we are able to obtain plasma parameters (electronic density and temperature). This study implies the knowledge of the Z-dependence of different atomic parameters:

- * wavelengths (for the resonance and satellite lines)
- * autoionization and decay rates (of doubly excited states involved in the satellite lines)

or

- * corresponding line factors F_s^* :

$$F_s^* = g_s/g_i \cdot A_a A_r / (A_a + A_r) \quad (\text{see Figure 1}).$$

We used, to determine all these parameters, atomic structure and electron-ion computer codes:

- * SUPERSTRUCTURE
- and
- * AUTOLSJ.

The calculations, including relativistic effects in a fine structure scheme, have been done on a large selection of ions, from Ar to Ag.

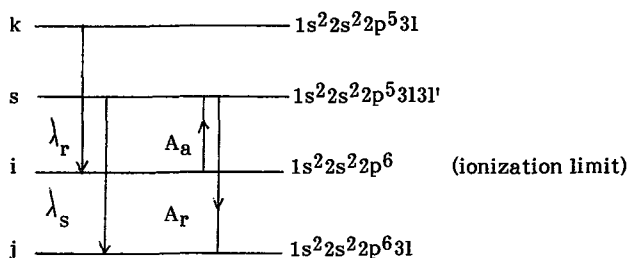


Figure 1 : Diagram of Ne- and Na-like ions, showing the resonance lines and associate satellite transitions.

Theoretical methods

The energy levels, wavelengths and decay rates are calculated using the SUPERSTRUCTURE computer code /1/. In a first step, this code constructs a set of non-relativistic wavefunctions of the 10-electron system by diagonalization of the non-relativistic Hamiltonian, using orbitals n_l calculated in a scaled Thomas-Fermi-Dirac potential, the scaling parameters λ_1 being obtained by a self-consistent energy minimization procedure of all the **terms** of the configurations $1s^2 2s^2 2p^6, 2p^5 3l$ ($l=s, p, d$) (see Figure 2). In a second step, the code diagonalizes on this basis the Breit-Pauli Hamiltonian, including relativistic corrections in configuration mixing, to determine all the **levels** of the following configuration sets:

- * $(1s^2 2s^2) 2p^6, 2p^5 3l, 2p^5 4l'; (1s^2 2s) 2p^6 3l, 2p^6 4l'$ ($l=s, p, d; l'=s, p, d, f$)
- * $(1s^2 2s^2) 2p^6 3l, 2p^5 3l 3l'$ ($l=s, p, d; l'=s, p, d$)

The autoionization probabilities and the line factors are calculated by using the AUTOLSJ code /2/, which needs as inputs, from SUPERSTRUCTURE :

- * the 'term coupling coefficients' for N and N+1 electronic systems ($N=10$),
- * the radiative de-excitation probabilities (A_r).

It determines the bound-free transition matrix elements, in a Distorted Waves approximation, and calculates the recoupling coefficients, and, afterwards, the autoionization probabilities (A_a) and the line factors (F^*_s).

Application of the histogram-construction to the satellites of Ne-like resonance lines

On Figures 4 to 10, the histograms represent (solid lines) the line factors F^*_s of the dielectronic satellites:

- * $(1s^2 2s^2) 2p^5 3p 3d \longrightarrow 2p^6 3p$
- * $2p^5 3d^2 \longrightarrow 2p^6 3s, 3d$

normalized to their maximum (for each element) \bar{F}^*_s , reached at $\bar{\lambda}$ (see Figure 3), and (dashed lines) the position of the corresponding resonance lines versus wavelengths:

- * $(1s^2 2s^2) 2p^5 3l \longrightarrow 2p^6 1S_0$

key	upper 3l level	key	upper 3l level
3G	$3s \ ^1P_1$	3E	$3d \ ^3P_1$
3F	$3s \ ^3P_1$	3D	$3d \ ^3D_1$
		3C	$3d \ ^1P_1$

Comparisons, for Germanium ($Z=32$) and Selenium ($Z=34$), between theoretical histograms and experimental spectra obtained during the Limeil X-ray Laser program /3/ are presented on Figures 11 and 12. We can easily identify the 3-2 resonance lines and some important satellite lines, with approximate correct relative intensities.

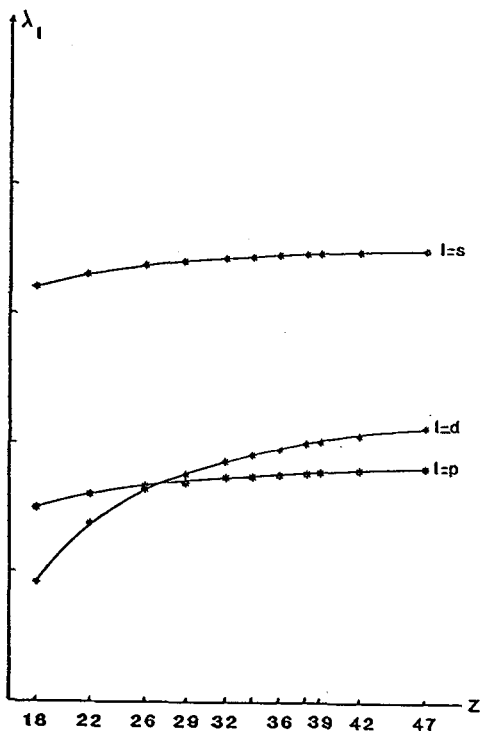


Figure 2 : Scaling parameters of a 10-electrons TFD potential versus nuclear charge.

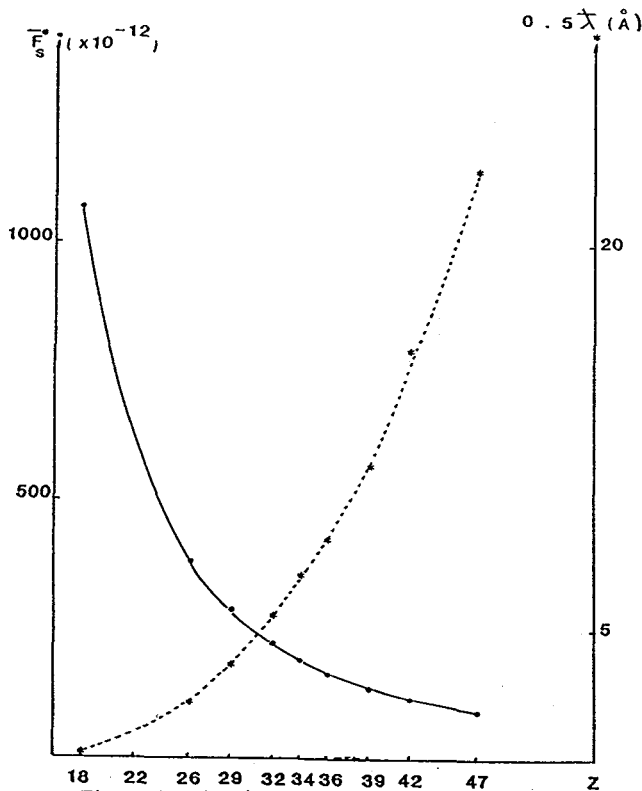


Figure 3 : Line factors and wavelengths of the strongest dielectronic satellite line ((1s²2s²2p⁵)3d² 2F_{7/2} - 2p3d 2D_{5/2}) versus nuclear charge.

Determination of the dielectronic recombination rate coefficients

All these calculations allow us to determine the dielectronic recombination rate coefficient $\alpha_d(j)$

- * from the Ne-like ground state $i=1s^2 2s^2 2p^6 1S_0$
- * to the Na-like ground state or one of the n=3 singly excited states $j=1s^2 2s^2 2p^6 3l$ (l=s,p,d)
- * via the chosen set of doubly excited states $s=1s^2 2s^2 2p^5 3l1'$ (l'=s,p,d)

which can be written, if T_e is the electronic temperature of the plasma (in eV) :

$$\alpha_d(j) = 1.65 \cdot 10^{-22} F^*(j) T_e^{-3/2} \exp(-E^*(j)/T_e) \quad (\text{see Figure 13})$$

The partial n=3 total dielectronic rate coefficient $\alpha_d^{tot} = \sum_{j=2p^6 3l} \alpha_d(j)$ is then approximated by :

$$\alpha_d^{tot} = A \exp(-Z^2/T_e) (T_e/Z^2)^{-3/2} \quad (\text{see Figure 14}).$$

References

/1/ W. Eissner, M. Jones, H. Nussbaumer *Comput. Phys. Comm.* **8**, 270 (1974)
 /2/ J. Dubau, M. Loulergue *J. Phys.* **B15**, 1007 (1981)
 /3/ O. Peyrusse and co-workers to be published in *J. of Appl. Physics*

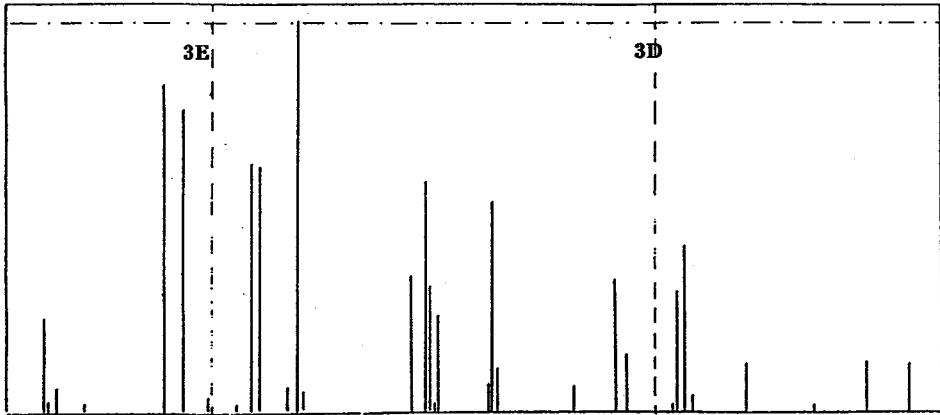


Figure 4 : Argon (Z=18)

$$3E=42.743 \text{ \AA} \quad 3D=42.180 \text{ \AA}$$

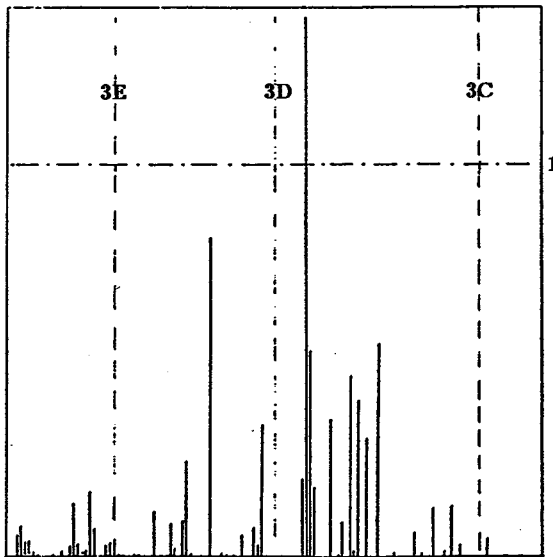


Figure 5 : Iron (Z=26)

$$3E=15.443 \text{ \AA} \quad 3D=15.243 \text{ \AA} \\ 3C=14.981 \text{ \AA}$$

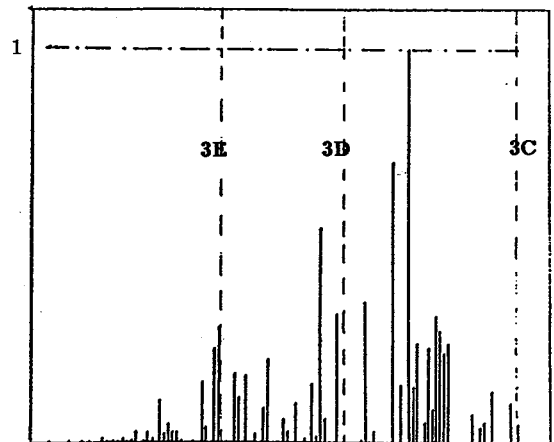


Figure 6 : Copper (Z=29)

$$3E=11.716 \text{ \AA} \quad 3D=11.566 \text{ \AA} \\ 3C=11.348 \text{ \AA}$$

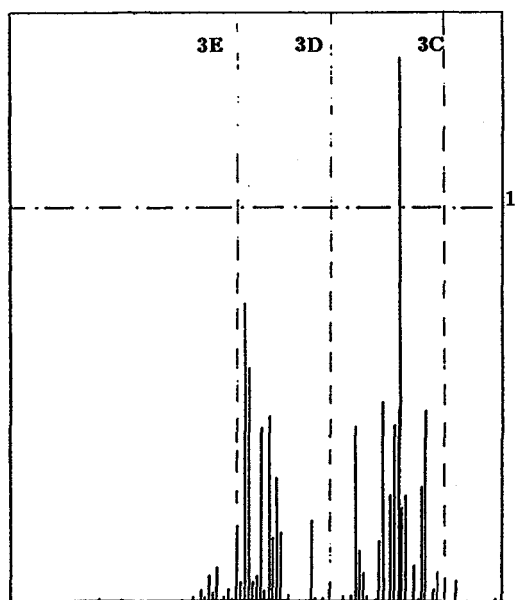


Figure 7 : Krypton (Z=36)

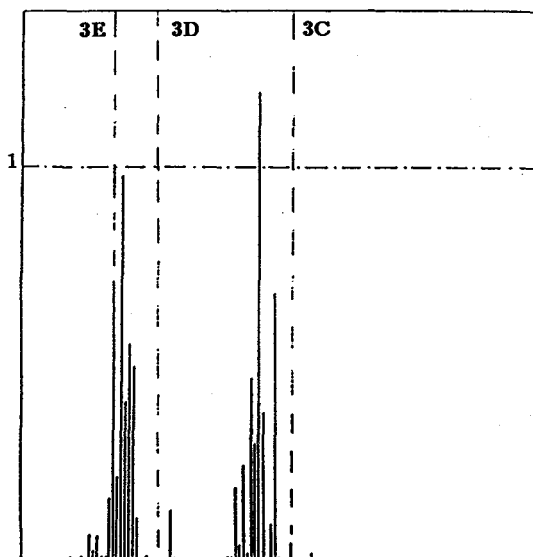


Figure 8 : Itrium (Z=39)

3E=6.927 Å 3D=6.842 Å
3C=6.666 Å

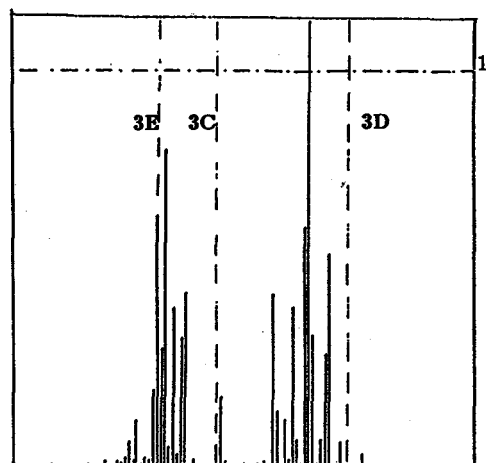


Figure 9 : Molybdenum (Z=42)

3E=4.823 Å 3C=4.765 Å
3D=4.602 Å

3E=5.735 Å 3D=5.664 Å
3C=5.496 Å

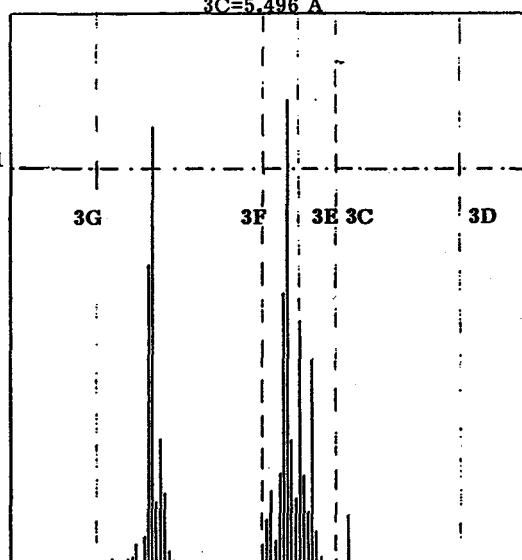


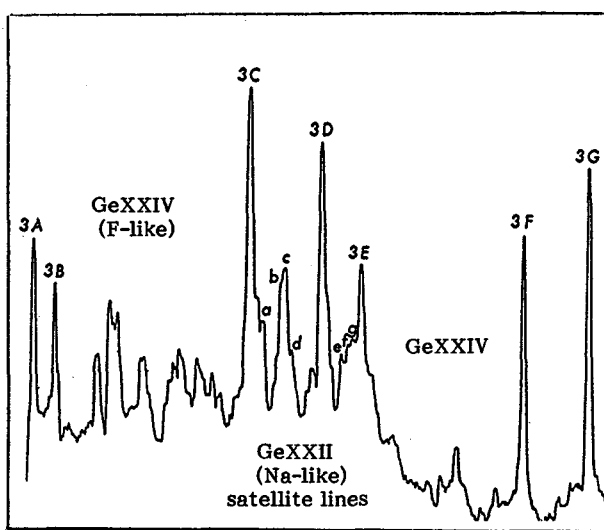
Figure 10 : Silver (Z=47)

3G=3.970 Å 3F=3.769 Å 3E=3.720 Å
3C=3.675 Å 3D=3.520 Å

Figure 11 : Germanium (Z=32)

Target :
500 Å Ge deposited on 500 Å CH

Laser :
non gaussian pulse
1 ns, $2 \times 10^{13} \text{ W/cm}^2$
 ω_0



a	$\sum F_s^* = 114.3$	$\lambda = 8.915 - 8.92$
b	=316.9	=8.96 - 8.97
c	=323.2	=8.98 - 8.985
d	=134.0	=9.00 - 9.10
e	=79.6	=9.13 - 9.14
f	=74.64	=9.15 - 9.16
g	=79.93	=9.165 - 9.175

(all the satellite lines are blended)
(F_s^* is in 10^{12} unit)

3C=8.885 Å 3D=9.079 Å
3E=9.196 Å

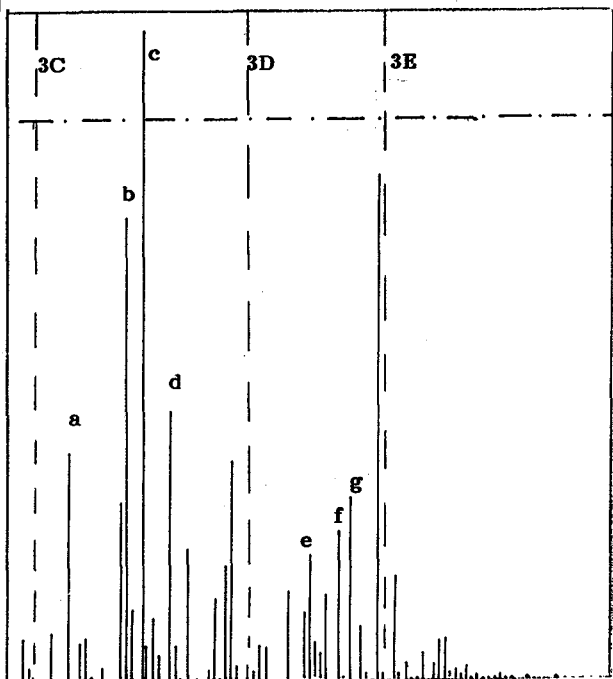
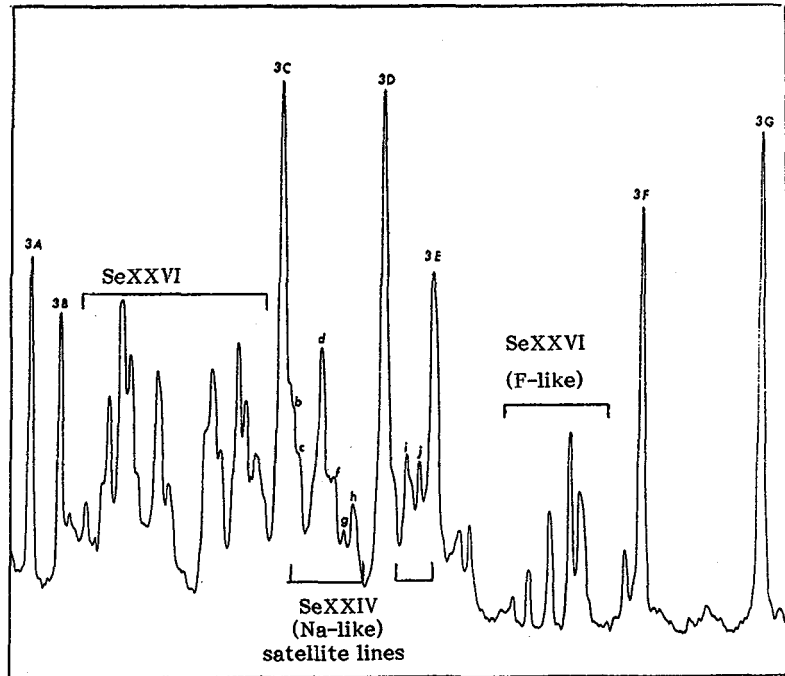


Figure 12 : Selenium (Z=34)

Target :
750 Å Se deposited on
1500 Å CH

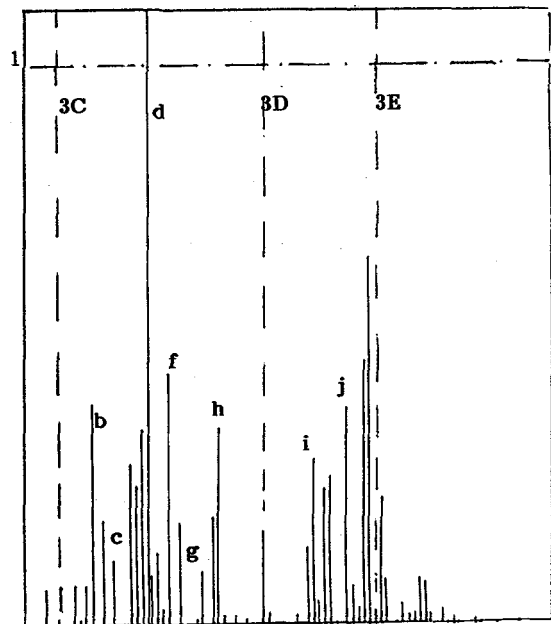
Laser :
gaussian pulse
600 ps, $2 \times 5 \times 10^{13} \text{ W/cm}^2$
 $2 \omega_0$



b	$\Sigma F_s^* = 165.6$	$\lambda = 7.686 - 7.69$
c	=67.9	=7.695 - 7.70
d	=215.5	=7.725 - 7.735
e	=80.5	=7.74 - 7.75
f	=172.9	=7.75 - 7.76
g	=38.6	=7.78 - 7.79
h	=198.3	=7.79 - 7.805
i	=157.8	=7.88 - 7.89
j	=164.3	=7.91 - 7.92

(all the satellite lines are blended)
(F_s^* is in 10^{12} unit)

3C=7.659 Å 3D=7.842 Å
3E=7.942 Å



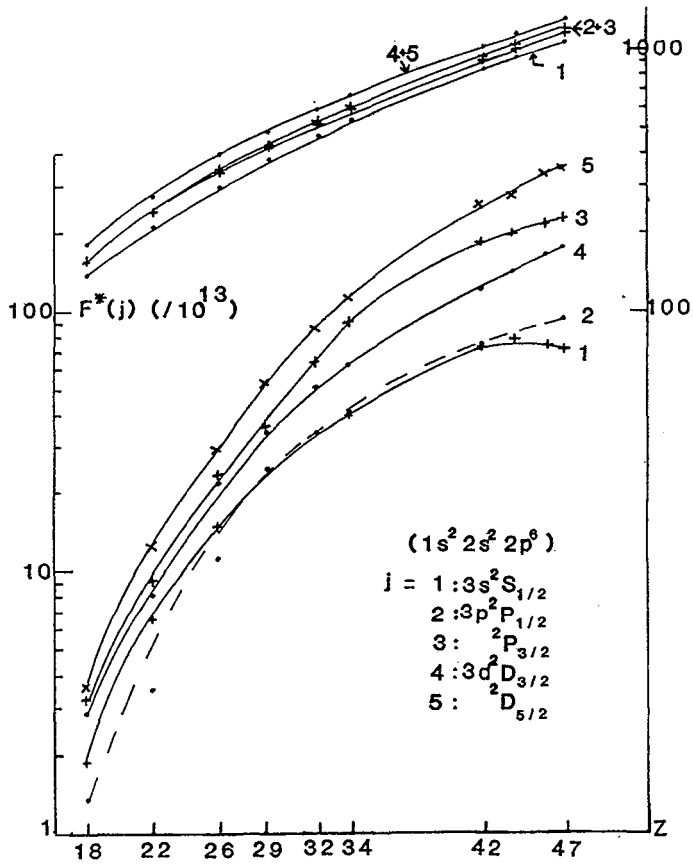


Figure 13 : Total line factors and averaged energies versus nuclear charge.

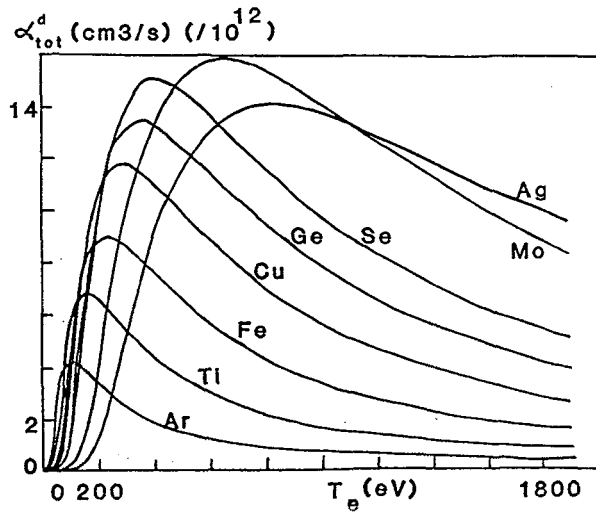


Figure 14 : Partial n=3 total dielectronic recombination rate coefficient versus electronic temperature for Na-like ions.