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DIELECTRONIC RECOMBINATION CALCULATIONS FOR NEON AND SODIUM-LIKE SELENIUM

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Résumé - Nous présentons ici le spectre des raies satellites diélectroniques du sélénium sodiumoide (Se XXIV). Cette étude est approfondie par des calculs théoriques des 2 taux de recombinaison diélectronique impliquant le sélénium néonoide (Se XXV) : Se XXVI fluoroide - Se XXV et Se XXV - Se XXIV.

Les paramètres de Physique Atomique nécessaires à cette analyse sont alors les longueurs d'onde et forces d'oscillateur en absorption des différentes transitions mises en cause . Ils ont été calculés à l'aide du programme SUPERSTRUCTURE dans lequel ont été introduites 15 configurations : $1s^2\ 2s^2\ 2p^6\ 3l$; $1s^2\ 2s^2\ 2p^6$, $2p^5\ 3l$ et $2p^5\ 4l'$; $1s^2\ 2s^2\ 2p^5$ et $2p^4\ 3l$ (l = 0,1,2 et l' = 0,1,2,3). Les probabilités d'autoionisation, utilisées dans la détermination des raies satellites, sont issues du code AUTOLSJ.

Nous avons enfin tenté de comparer nos résultats avec ceux obtenus par les formules semi-empiriques de la littérature.

Abstract - We present here first the dielectronic satellite spectra of sodium-like selenium (Se XXIV) and we extend this analysis with theoretical calculations of recombination rate coefficients for fluorine Se XXVI to form neon-like Se XXV and Se XXV to form Se XXIV.

The atomic parameters required are : line wavelengths and oscillator strengths. They have been calculated with the program SUPERSTRUCTURE in which we introduced 15 configurations : $1s^2\ 2s^2\ 2p^6\ 3l$; $1s^2\ 2s^2\ 2p^6$, $1s^2\ 2s^2\ 2p^5\ 3l$, $1s^2\ 2s^2\ 2p^5\ 4l'$; $1s^2\ 2s^2\ 2p^5$, $1s^2\ 2s^2\ 2p^4\ 3l$ (l = 0,1,2 ; l' = 0,1,2,3). The autoionization probabilities, used in dielectronic satellite lines, derived from the outputs of the computer code AUTOLSJ.

For the dielectronic recombination rate coefficients, we use all the theoretical formulae available in litterature and try to compare the results obtained.

Dielectronic recombination : processes and rate coefficients

Dielectronic recombination involves a radiationless capture of a plasma free electron, usually into a high Rydberg nl-state, accompanied by the excitation of the recombining ion.

$$X^{+} + e \rightarrow X^{**} \quad (2)$$

X^{**} represents a doubly excited state (j,nl) of the recombined ion and X^{+} a single excited state i of the recombining ion.

Recombination is accomplished if, instead of autoionizing,

$$X^{**} \longrightarrow X^{+} + e \quad (1)$$

the electron returning to the continuum, the two-electron excited state undergoes a radiatively stabilizing transition to a singly excited state , which lies below the ionization threshold.

$$X^{**} \longrightarrow X^{*} + h\nu \quad (3)$$

This three-step process is schematically illustrated in Fig. 1. Generally, the initial state is assumed to be the ground state g of the recombining ion.

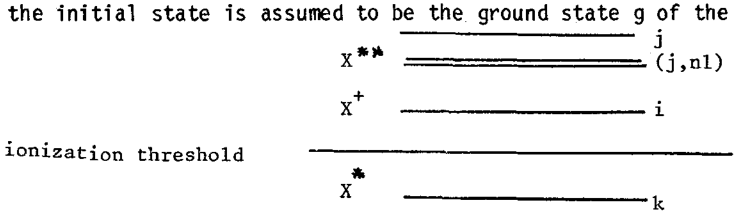


Fig.1. Three steps involved in the dielectronic recombination process.

Let α_d^{*} be the rate coefficient for dielectronic recombination ((2) and (3)), A_a and A_r, respectively, the autoionizing probability (1) and the total radiative transition probability for decay to bound states of the recombined ion (3), A being the sum of all radiative and autoionization rates from X^{**}.

Assuming a maxwellian distribution of electron velocity,

$$\alpha_d^{**} = (h^2 / 2\pi\, mkT_e)^{3/2} \omega^{**} / 2\omega^{+} \exp -E^{**} / kT_e \quad A_a A_r / A$$

where Te is the electron temperature, ω^{**} and ω^{+} the statistical weights of X^{**} and X^{+}, and E^{**} the energy of X^{**} relative to X^{+}.

The total dielectronic recombination rate coefficient is obtained on summing α_d^{**} over all contributing doubly excited states X^{**}:

$$\alpha_d = 1/2 \ (h^2 / 2\pi\, mkT_e)^{3/2} \sum_{**} f^{**} \exp -E^{**}/kT_e$$

f^{**} being the line factor of the state X^{**}.

As a result of numerical calculations, Burgess /1/ proposed a general formula for α_d :

$$\alpha_d = T_e^{-3/2} F_1(z) \sum_j f_{ij} F_2(z,j) \exp - \overline{E} / T_e$$

where, E_{ij} and f_{ij} being the excitation energy and oscillator strength of the $i \rightarrow j$ transition, z is the nuclear charge of the recombining ion, and :

$F_1(z) = 2.4\ 10^{-9}\ (z(z+1)^5 / z^2 + 13.4))^{1/2}$

$\overline{E} = E_{ij}/a$

$a = 1 + 0.015\ z^3 / (1+z)^2$

$x = E_{ij} / 13.6\ (1+z)$

$$F_2(z,j) = \begin{cases} x^{1/2} / (1 + 0.105\ x + 0.015\ x^2) & \text{if no change in principal quantum number is involved between } i \text{ and } j\ (\Delta n = 0) \\ 0.5\ x^{1/2} / (1 + 0.21\ x + 0.03\ x^2) & \text{for } \Delta n \neq 0 \text{ (Merts /2/)} \end{cases}$$

(E_{ij} and Te in ev ; α_d in $cm^3\ s^{-1}$)

Zhdanov /3/ proposed an other formula :

$$\alpha_d = 4.94\ 10^{-10}\ z^{7/6}\ T_e^{-3/2} \sum_j E_{ij}^{3/4}\ f_{ij}\ \exp(-E_{ij} / T_e)$$

for $\Delta n = 0$ and $\Delta n \neq 0$ transitions.

It's important to notice that all these semi-empirical formulae overestimate the dielectronic recombination rate coefficient ; they neglect reducer outer effects as collisional processes involving the final excited states, photoionization and density effects.

Atomic structure model and computer codes

To calculate dielectronic recombination for neonlike (Se XXV) and sodiumlike (Se XXIV) selenium, an atomic model of highly ionized selenium has been constructed. It includes 5 fluorinelike configurations : $1s^2\ 2s^2\ 2p^5$, $1s^2\ 2s\ 2p^6$ and $1s^2\ 2s^2\ 2p^4\ 3l$ (l = 0,1,2), 9 sodiumlike configurations : $1s^2\ 2s^2\ 2p^6\ 3l$ (l = 0,1,2)and $1s^2\ 2s^2\ 2p^5\ 3l\ 3l'$ (l = 0,1,2 ; l' = 0,1,2) for doubly excited states, and 17 neonlike configurations : $1s^2\ 2s^2\ 2p^6$, $1s^2\ 2s^2\ 2p^5\ 3l$ (l = 0,1,2), $1s^2\ 2s^2\ 2p^5\ 4l$ (l = 0,1,2,3) and $1s^2\ 2s\ 2p^6\ 3l$ (l = 0,1,2), $1s^2\ 2p^6\ 3l\ 3l'$ (l = 0,1,2 ; l' = 0,1,2) for autoionizing configurations.

The main atomic structure problem becomes then the determination of configuration interaction wavefunctions, from which can be deduced the different needed parameters : (E_{ij}, f_{ij}) and (f^{**}, E^{**}). The first part of these data are calculated in LSJ coupling using the SUPERSTRUCTURE code /4/ which derives from a relativistic modified Thomas-Fermi statistical potential approximation, where the different wave functions are considered as linear combinations of Slater determinants developped on a basis of monoelectronic orbitals s,p,d and f. The scaling parameters of the potential are obtained by a minimization procedure based upon the first four configurations of Se XXV :

$$\lambda_s = 1.1727 \quad , \lambda_p = 1.0873 \quad , \lambda_d = \lambda_f = 1.0963$$

Superstructure is also used for its relationship with the DISTORTED WAVES program /5/ which constructs the autoionizing states and with the code AUTOLSJ /6/ which determines the second part of the data.

Δn ≠ 0 dielectronic recombination example : for neonlike selenium Se XXV to form sodiumlike Se XXIV

The neonlike target is determined by the ground state $1s^2\ 2s^2\ 2p^6$ and by 26 first excited states $2p^5\ 3l$. The doubly excited sodiumlike states $1s^2\ 2s^2\ 2p^5\ 3l\ 3l'$ lead to deexcitations to excited states $2p^6\ 3l$ (Fig. 2).

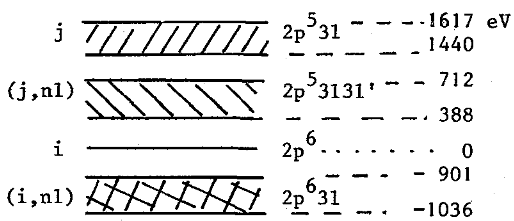


Fig.2. 206 levels and energies involved in the Δn ≠ 0 Se XXV dielectronic recombination

If we write : $\alpha_d = \sum_{n \geq n_0} \alpha_d(n)$

where n_0 is the smallest principal quantum number contributing to the process, AUTOLSJ allows us to calculate α_d(n = 3) for some electronic temperatures (noted * on Fig. 3).But, to follow the evolution versus time of a plasma, it may be attractive to express α_d(n = 3) as an explicit function of the temperature :$\bar{\alpha}_d$(n=3). Using average energies for each configuration, we find then :

$$\bar{\alpha}_d(n=3) = 1.65\ 10^{-10}\ T_e^{-3/2}\ F_3(\ T_e\ )$$

where :

$$F_3(\ T_e\ ) = 1313\exp(-667/T_e)+801\exp(-600/T_e)+9\exp(-509/T_e) +45\exp(-533/T_e)+54\exp(-462/T_e)$$

This averaged formula leads to relative errors never exceeding 0.1%. To consider the contribution of the upper quantum numbers, we assume a $1/n^3$ dependance of $\alpha_d(n)$, which gives :

$$\bar{\alpha}_d = 27\bar{\alpha}_d(n = 3)\sum_{n \geqslant n_0} 1/n^3 \quad = 3.433\ 10^{-10}\ T_e^{-3/2}\ F_3(\ T_e\ ) \quad (n_0=3)$$

We compare these results to semi-empirical calculations for a charge z = 24 (Fig. 3) to show the overestimation that these general formulae involve in α_d for $\Delta n \neq 0$ transitions : Merts' approximation (α_d^M) is accurate to 60% and Zhdanov's one (α_d^Z) to 20% in the range of 1 keV.

The photon emitted during the stabilization process (3) has an energy close to that of corresponding resonance line photon for a transition between the recombining state X^+ and an other excited state X^{++}. In this case, dielectronic recombination is responsible for the existence of satellite spectra lines on the long-wavelength side of the 3s - 2p and 3d - 2p Ne-like ion resonance lines, especially to $2p^6$ from $2p^5$ 3s ($^1P_1$ or $^3P_1$) and $2p^5$ 3d ($^3P_1$, $^3D_1$ or $^1P_1$) (Fig. 4).

Δn = 0 dielectronic recombination example : for fluorinelike Se XXVI to form neonlike Se XXV

In this case, α_d must be estimated by semi-empirical formulae (AUTOLSJ being unable to calculate correct line factors). We then assume that recombinations from the ground state $2p^5$ are able to restitute the total rate α_d

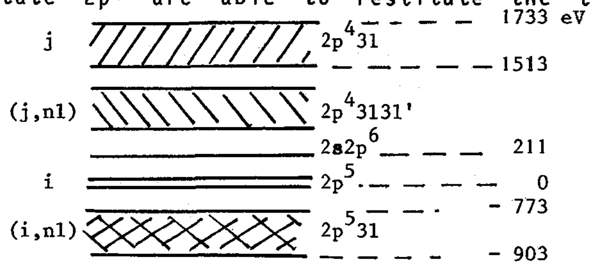


Fig.5. Levels and energies involved in Δ n = 0 Se XXVI dielectronic recombination.

SUPERSTRUCTURE calculates the different values of the required parameters (f_{ij} and E_{ij}, where i $\equiv$ $2p^5$ and j $\equiv$ $2p^4$ 3l) and the two rate coefficients are presented on Fig. 6. The Burgess' approximation (α_d^B) seems to be better than the Zhdanov's one (α_d^Z) and we choose it to represent this dielectronic process :

$$\bar{\alpha}_d = 1.634\ 10^{-6}\ T_e^{-3/2}\ (\ 0.275\exp(-1182/T_e)+7.50\exp(-1234/T_e))$$

Density effects : first approach

The effect of finite plasma density n_e consists of a modification of the recombination process since the recombined, but still excited, ion interacts with the surrounding plasma, and therefrom to a reduction of the rate coefficient. The procedure generally followed to include finite - electron density effect is to neglect levels having principal quantum numbers larger than the collision limit n_c: $n \leq n_c$ in the sum over **, capture to a level $n > n_c$ being considered to result in instantaneous ionization, which leads to the existence of a multiplying correction factor D :

$$D = \sum_{n=n_0}^{n_c} \alpha_d(n) \; / \; \sum_{n \geq n_0} \alpha_d(n)$$

Simple , but approximate , D formulae have been given by Post /7/

for $\Delta n = 0$ transitions $D = n_t / (n_t + 200)$

for $\Delta n \neq 0$ transitions $D = 0.0015((1+z)n_t)^2/(1+0.0015((1+z)n_t)^2)$

where $n_t^7 = 4.77\ 10^{18}\ z^6\ (Te\ 10^{-3})^{1/2} / n_e$, to modify Merts' or Burgess' approximation. Zhdanov tabulates some special values of D as a function of two parameters :

$x = 3.19\ 10^{-4}\ z^{1/3}\ E_{ij}\ (10^{17}\ Te^{1/2} / (zn_e))^{1/7}$

$v = (E_{ij} / 13.6)^{1/2}$

for $0.1 \leq v/z \leq 0.5$ and $1 \geq x \geq 0.07$, according to his formula.

One way of estimating the collision limit n_c is to consider the continuum lowering process for a Debye-Hückel plasma (if n_I represents the total ion density and Z^* the average charge of the plasma, the studied plasma is a Debye-Huckel plasma if :

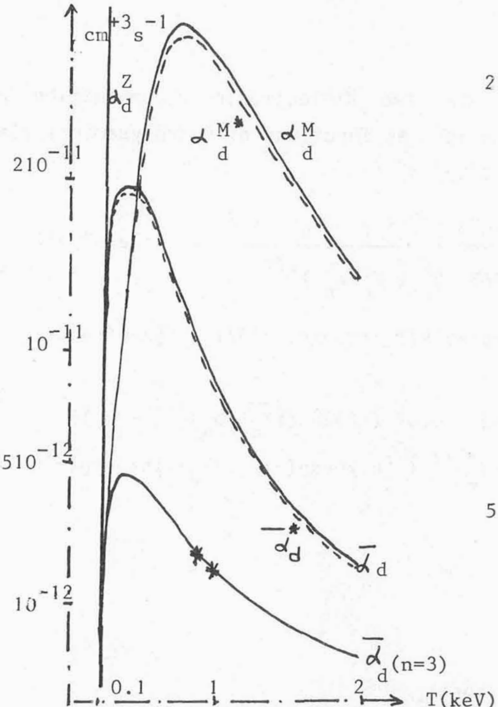
$$n_I \leq 8\ 10^{22}\ (Te / (10\ Z^{*2}))^3$$

n_c is defined by :

$$z / n_c^2 = 3\ a_0\ ((1 + (D/R)^3)^{2/3} - (D/R)^2) / R$$

where D is the plasma Debye length, a_0 the Bohr radius and R the plasma ion-sphere length : $1/D^2 = 108.8\,\pi a_0\,(1 + Z^*)\, n_e / Te$; $R^3 = 3 z / (4 \pi n_e)$

For a Debye-Hückel plasma presenting an average nuclear charge $Z^* = 25.65$ and an electron density $ne = 4\ 10^{20}\ cm^{-3}$, we remark that for $\Delta n \neq 0$ transitions, density effects do not play an important role in dielectronic recombination (Fig. 3 $D = \alpha_d^*/\alpha_d \sim 1$) unlike $\Delta n = 0$ transitions (Fig.6) where D can reach 2%.



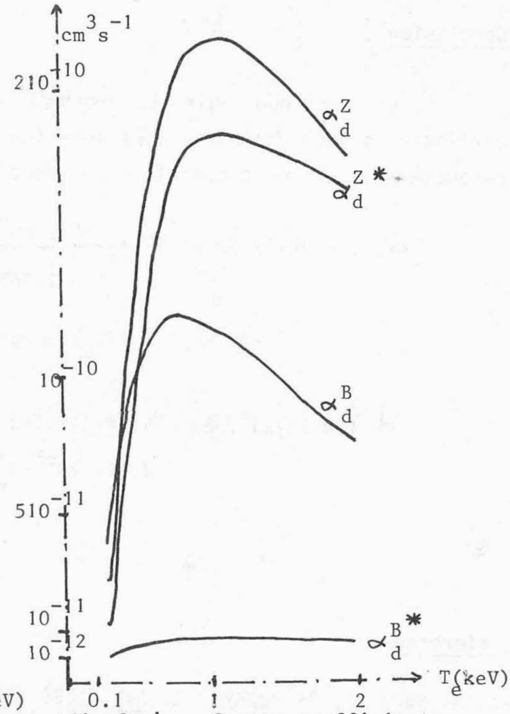


Fig.3. $\Delta n \neq 0$ rate coefficients

Fig.6. $\Delta n = 0$ rate coefficients

versus temperature, at $n_e = 4\ 10^{20}\ cm^{-3}$

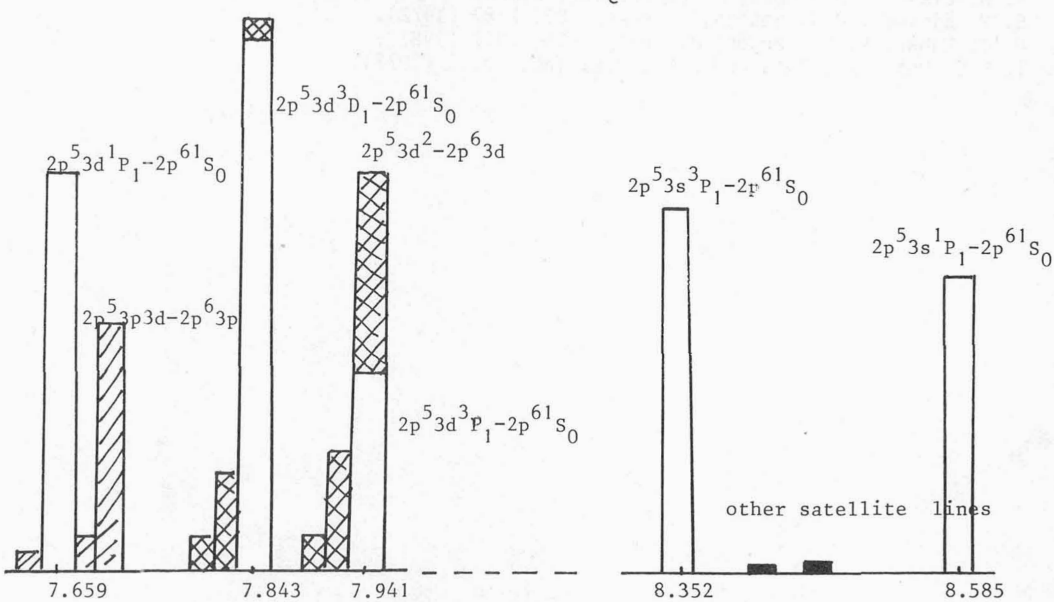


Fig.4. Resonance and unresolved satellite lines (versus wavelength (Å)) for $T_e = 1$ keV and $n_e = 2.4\ 10^{20}\ cm^{-3}$.

Conclusion

We are now able to express the two dielectronic recombination rate coefficients including Ne - like selenium ions as functions of hydrodynamical plasma parameters (electron temperature and density) :

$$\alpha_d \text{ (Se XXV / Se XXIV)} = \frac{6.052\ 10^{-3}\ T_e^{-3/2}\ (T_e/n_e^2)^{1/7}}{1 + 1.763\ 10^7\ (T_e/n_e^2)^{1/7}} \left(1313\exp(-667/T_e) + 801\exp(-600/T_e) + 9\exp(-509/T_e) + 45\exp(-533/T_e) + 54\exp(-462/T_e)\right)$$

$$\alpha_d \text{(Se XXVI) / Se XXV)} = \left(0.762 + 0.09\left(2528\left(\sqrt{T_e}/n_e\right)^{1/7} - 4\right)\right) \cdot 2.111\ 10^{-8}\ T_e^{-3/2}\left(56.70\exp(-1552/T_e) + 1644\exp(-1664/T_e)\right)$$

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