Resonant excitation and capture by excited F II at low energies

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Resonant capture cross sections for the first excited state of the F II ion $(1s^22s2p^{5\,3}P)$ are calculated and the rate coefficients are evaluated at low energies involving excitation captures $(\Delta n = \Delta l = 0)$ to the singlet P state of the same configuration. The rates peak near the temperature kT=0.4 Ry, with the peak value of 2×10^{-12} cm³/sec. This is nearly 100 times larger than that for the ground states with intermultiplet excitations. The resonant contributions to the collisional excitation are also estimated. They are three orders of magnitude larger than the capture cross sections, mainly because of the smallness of the fluorescence yields of the resonance levels.

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In a recent paper [1], we reported the cross sections and rate coefficients for the dielectronic recombination (DR) by the singly charged F ions at very low energies. The multiplet excitation capture $(\Delta n = 0 \text{ and } \Delta l = 0)$ was found to be negligible compared with the directradiative-recombination (RR) cross sections, by as much as a factor of 10^3 . On the other hand, the intrashell excitation capture $(\Delta n = 0, \Delta l = 1)$ was large, with the peak rate near kT = 1 Ry of 7×10^{-12} cm³/sec.

The DR rates generated are used as input to the rate equations for plasma modeling. The rate equations contain in principle an infinite number of excited states and different charge states, and they are routinely truncated in some approximations before solving them. Depending on the number of states included in a given set of rate equations, the corresponding rate equations have to be adjusted to avoid double counting (that is, when the input rate coefficients have already been adjusted to take into account the effect of certain number of states, then the same states should not appear in the rate equations, and vice versa). Thus, the evaluation of the rates should in principle reflect this, but in practice this point has never been taken into consideration. In particular, the rates for the excited states which appear explicitly in the truncated rate equations have never been estimated properly. Although the excited-state population may be small in a locally thermalized plasma, the corresponding rates could be very large, enough to offset the Boltzmann factor. (For the F^+ plasma, kT = 1-3 Ry, where the F II ions are most abundant. The ionization energies of FI and FII in their ground states are 1.28 and 2.57 Ry, respectively.) This problem becomes more critical in a turbulent transient plasma, where the assumed local thermal equilibrium breaks down. Its effect on the rate coefficients is difficult to estimate; the very definition of the rate coefficient may have to be modified. With all the complications mentioned above, it is still of interest to make an estimate of the rates for the excited states. As suspected, the rates are generally very high, often two orders of

magnitude larger than that for the ground state [2].

In this paper we present the DR cross sections for the intermultiplet excitation from the first excited initial state of F II $(1s^22s^22p^{5\,3}P=i)$, which lies approximately 1.5 Ry above the ground-state configuration $1s^22s^22p^{4\,3}P=i_l$. The low-lying intermediate resonance states are a series of levels of the type $1s^22s^22p^{5\,1}Pnl=d_2$. The energy levels relevant to this transitions are given in Fig. 1. Thus we consider here the initial excitation from the triplet to the singlet, with the capture of the continuum electron to form the states d_2 ,

$$i + e_c \rightarrow d_2$$
,



FIG. 1. The energy level diagram for F I and F II, near the excited singlet and triplet core-state configuration $1s^22s2p^5nl$.

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e (Ry)	DR	RE			
		f_1	f_2	f_3	f_4
0.32	1.44[-20]	4.02[-17]	2.12[-17]	1.42[-18]	1.28[-17]
0.44	4.26[-20]	5.71[-18]	2.75[-18]	8.24[-18]	3.12[-16]
0.55	7.95[-21]	5.40[-18]	2.98[-18]	2.61[-19]	1.59[-18]
0.56	6.65[-21]	1.40[-21]	1.88[-18]	8.72[-20]	2.66[-19]
0.57	3.57[-20]	1.39[-18]	6.78[-19]	2.34[-18]	7.42[-17]
0.60	6.91[-21]	1.86[-18]	1.06[-18]	9.65[-20]	5.40[-19]
0.61	6.79[-21]	7.73[-22]	1.07[-18]	5.12[-20]	1.66[-19]
0.62	3.11[-20]	6.06[-19]	2.78[-19]	9.28[-19]	3.01[-17]
0.63	1.32[-20]	8.64[-19]	1.10[-18]	7.77[-20]	3.45[-19]
0.64	4.28[-20]	1.08[-18]	5.61[-19]	5.16[-19]	1.55[-17]
0.65	4.40[-20]	1.90[-19]	6.51[-19]	3.09[-19]	8.96[-18]
0.66	1.53[-19]	7.38[-19]	7.29 [-19]	4.78[-19]	1.42[-17]
0.67	1.27[-18]	3.90[-19]	4.86[-19]	3.01[-19]	9.30[-18]
Total	1.68[-18]	5.84[-17]	3.54[-17]	1.51[-17]	4.80[-16]

TABLE I. The DR and RE cross sections are given for the excited initial state *i* and the final excited states f_1 to $f_4 = i$, in units of cm². $\Delta e_c = 0.01$ Ry. Numbers in square brackets represent powers of 10.

where d_2 predominantly decay radiatively to $i_2nl = 1s^22s^22p^{4}$ Snl, but also very rapidly decay to the four available Auger channels $(i_1, i_2, i_3, \text{ and } i, \text{ to be defined later})$.

The excited states of the type $(1s^22s^22p^3nln'l')$ corresponding to the intershell excitations $(\Delta n \neq 0)$ are also populated in this energy region, but their contributions are found to be small due to strong cascade corrections.

The method of calculation employed here and the ap-



FIG. 2. The DR rate coefficients for the excited FII state $i=1s^22s^22p^{5\,3}P$ are given as functions of temperature kT (Ry). Also included for comparison are the radiative recombination rates (RR), and the DR rates for the ground-state configuration with $\Delta n = 0$ but $\Delta l = 0$ and 1.

proximations introduced are the same as in Ref. [1], to which we refer for the details. The DR cross sections are presented in Table I as functions of collision energy e_c , and the energy bin size $\Delta e_c = 0.01$ Ry. For each bin, there are on the average 10 to 20 LS-coupled states which contribute, so that the listing of the cross sections from the individual terms is too voluminous; the details of the data are available if needed. The rate coefficients are plotted in Fig. 2. The DR rates and the cross sections for the initial state *i* is very large, a factor of 100 larger than that for the ground states with multiplet excitation transitions. This is consistent with the earlier studies [2] of DR by the metastable states of the He-like C and O ions. In Table II we also show the l dependence of the cross sections; as expected, the l = 1 contribution dominates in DR. (As will be discussed, the l=0 intermediate states are important for resonant excitation processes.)

In addition to the DR cross sections, the resonantexcitation (RE) contribution to the total collisional excitation may also be estimated [3,4] simultaneously in the course of the DR calculation. In fact, all the components necessary in the evaluation of RE are already available once the DR cross sections are calculated; the total widths contain the complete information on all possible decay channels for each resonance state. Compared to

TABLE II. The *l* dependence of the resonant (DR) and (RE) cross sections for the intermediate states $d_2 = 1s^2 2s 2p^{51}P$ is shown. The initial stage of the excitation is from the initial state $i=1s^2 2s 2p^{53}P$. The cross-section sums are given in units of cm², with $\Delta e_c = 0.01$ Ry. Numbers in square brackets represent powers of 10.

		RE					
1	DR	f_1	${f}_2$	f_3	f_4		
0	2.43[-20]	4.99[-17]	2.26[-17]	1.91[-18]	1.56[-17]		
1	1.25[-18]	8.57[-18]	4.04[-18]	1.30[-17]	4.63[-16]		
2	1.80[-19]	3.48[-21]	4.77[-18]	2.27[-19]	7.28[-19]		
3	8.95[-22]	7.76[-25]	9.39[-22]	1.29[-23]	2.13[-24]		

the energy-averaged DR cross section

$$\sigma_{id}^{\text{DR}} = \frac{4\pi \mathcal{R}^2}{e_c \,\Delta e_c} \, V_a(i \to d) w(d) (\pi a_0^2) \,, \tag{1}$$

where V_a is the radiationless excitation-capture probability, and we have for RE,

$$\sigma_{id}^{\rm RE} = \frac{4\pi \mathcal{R}^2}{e_c \,\Delta e_c} \, V_a(i \to d) z(d) (\pi a_0^2) \,. \tag{2}$$

Here, \mathcal{R} is the Rydberg constant. Obviously the difference between the two expressions are in the partial Auger and fluorescence yields, defined by

$$w(d \to f) = A_r(d \to f) / \Gamma(d) , \qquad (3)$$

where A_r is the radiative transition probability, and

$$w(d) = \sum_{f} w(d \to f) \tag{4}$$

and

$$z(d \to f) = A_a(d \to f) / \Gamma(d) , \qquad (5)$$

where A_a is the Auger transition probablity. We have for the total widths

$$\Gamma(d) = \sum_{f} A_{r}(d \to f) + \sum_{f'} A_{a}(d \to f')$$
(6)

so that Γ contains all the partial widths needed to evaluate both the DR and RE cross sections.

The RE cross sections may be obtained for the initial state *i* and the final states *f*, where $f_1 = 1s^22s^22p^{43}P = i_1$,

 $f_2 = 1s^2 2s^2 2p^{4} D = i_2$, $f_3 = 1s^2 2s^2 2p^{4} S = i_3$, and $f_4 = i$. Note that the RE collisions to f_1 , f_2 and f_3 , are excorgic. The RE cross sections are tabulated in Table I, again using the energy bin of $\Delta e_c = 0.01$ Ry. They are very large, a factor of one thousand larger than the corresponding DR cross section. The last column involves $i \rightarrow d_2 \rightarrow i$, which describes the resonant elastic scattering for the state *i*. The dependence of the RE cross sections on the angular momentum *l* of the intermediate states d_2 is shown in Table II. Unlike in DR, the l=0 state contribution is important in RE.

As stressed above, the main ingredients in the DR and RE cross sections are contained fully in the total widths Γ , so that experimental testing of DR complements the study of RE and vice versa. This inter-relationship was emphasized earlier [3], and should be useful in the study of resonant collisions, especially when the available experimental data on RE and DR are limited. More importantly, the enhancement of the rates for the excited states requires a more careful treatment of the role of the excited states in the rate equations for plasma modeling [5]. A similar RE cross-section calculation for the ground state F II is in progress, where 30 different final states are possible [6].

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