CHIN. PHYS. LETT. Vol. 29, No. 4 (2012) 043201

Fluorescence and Auger Decay Properties of the Core-Excited F-Like Ions from Ne to Kr *

WANG Xiang-Li(王向丽)[1], DONG Chen-Zhong(董晨钟)[1**], SU Mao-Gen(苏茂根)[1], KOIKE Fumihiro[2]

[1]*Key Laboratory of Atomic and Molecular Physics & Functional Materials of Gansu Province, College of Physics and Electronic Engineering, Northwest Normal University, Lanzhou 730070*
[2]*Physics Laboratory, School of Medicine, Kitasato University, 1-15-1, Kitasato 252-0374, Japan*

(Received 27 December 2011)

We systematically study the decay properties of the K-shell excited F-like ions with $10 \leq Z \leq 36$ based on the multiconfiguration Dirac–Fock method. The Breit interaction, the QED corrections and the nuclear finite mass effects are also considered as perturbation. Auger transition rates, radiative, Auger and natural widths, as well as fluorescence and Auger yields for K-shell excited F-like ions are presented. It is shown by means of concrete figures that the decay properties change significantly with the increase of the atomic number Z; the Auger rate is overtaken at $Z = 30$ by the radiative decay rate. Several fitting formulae for the radiative and Auger widths and the fluorescence yields have been evaluated which is expected to be useful in plasma analysis and plasma modeling.

PACS: 32.80.Hd, 32.70.Jz DOI: 10.1088/0256-307X/29/4/043201

Atomic ions with K-shell vacancies are important productions in collisionally ionized and x-ray photoionized plasmas. They are unstable and therefore may decay either radiatively by emitting photons or non-radiatively by emitting Auger electrons.[1] For K-shell excited F-like ions, the following competing decay processes can occur,

$$1s2s^22p^6 \rightarrow \begin{cases} 1s^22s^22p^5(^2P) + \hbar\omega & A_r \\ 1s^22p^6(^1S) + e^- \; KL_1L_1 & \\ 1s^22s2p^5(^{1,3}P) + e^- \; KL_1L_{2,3} & A_a \\ 1s^22s^22p^4(^3P,^1D,^1S) + e^- \; KL_{2,3}L_{2,3} & \end{cases}$$

The radiative transitions may therefore lead to a spin-orbit doublet in the ground state ions, and the non-radiative Auger transition may end up with two vacancies in L-shell leading ten sub-levels. During the past decades, quite a few experimental and theoretical researches have been carried out on the emission lines of K-shell excited F-like ions. On the experimental side, transitions in F-like Fe XVIII were observed in tokamak spectra by Hill *et al.*,[2] in solar flare spectra by Seely *et al.*[3] and firstly in a controlled laboratory environment by Decaux *et al.*[4] Faenov *et al.*[5] measured the wavelengths of satellites due to transitions in Be-, B-, C-, N-, O- and F-like ions for elements Mg, Al, Si, P and S in a CO_2 laser produced plasma. The spectra from Ar plasmas produced with a plasma focus discharge have been observed between 3.8 Å and 4.2 Å by Biémont *et al.*,[6] in which two of the transitions of F-like argon ions have been identified. On the theoretical side, Fan *et al.*[7] reported and discussed the transition wavelengths, absorption oscillator strengths, transition probability and line strengths of F-like Cr atomic ions in the framework of relativistic configuration interaction (RCI) formalism using the multiconfiguration Dirac–Fock (MCDF) wavefunctions. Gorczyca *et al.*[1] have investigated the accuracy of the $1s$ vacancy fluorescence database obtained by Kaastra and Mewe[8] by means of atomic physics calculations and the subsequent scaling along Beryllium and Fluorine isoelectronic sequence. Behar *et al.*[9] calculated the wavelengths and oscillator strengths of the $1s$–np inner shell absorption lines in Li-like to F-like ions of Ne, Mg, Al, Si, S, Ar, Ca, and Fe, by using the Hebrew University Lawrence Livermore Atomic Code (HULLAC). We have thus a good amount of both experimental and theoretical values on the decay properties of the K-shell excited F-like ions. However, the data are still limited for the purpose of, for example, plasma diagnostics, and it is worth producing systematic and complete data sets on the dynamical processes of those ions. To diagnose and model the various plasmas, we need good theoretical models with accurate and complete set of atomic data, such as the energy levels and the rates of competing radiative and Auger decays.

In this Letter, the decay properties of the K-shell excited Fluorine isoelectronic sequence from Ne^+ to Kr^{27+} are studied based on the MCDF packages GRASP92[10] and RATIP,[11] which have been described in detail elsewhere.[10–12] We have calculated the Auger transition rates and Auger widths Γ_A (the sum of all the Auger decay rates) of K-shell excited F-like ions throughout the atomic species with $10 \leq Z \leq 36$; the results are listed in Tables 1 and 2. For the radiative properties, we have already reported the transition rates of the individual species.[18] Here we compare the radiative properties with the nonradiative decay properties systematically for all the species of $Z = 10$ through 36, as shown in Table 2 too. In Table 1, the atomic number Z are shown in the first column, the second column lists the Auger rates of

*Supported by the National Natural Science Foundation of China under Grant Nos 91126007, 10964010 and 11064012.
**Corresponding author. Email: dongcz@nwnu.edu.cn
© 2012 Chinese Physical Society and IOP Publishing Ltd

the KL_1L_1 decay channel, the level-to-level Auger rates and the total Auger rates Σ of the $KL_1L_{2,3}$ and $KL_{2,3}L_{2,3}$ decay channels are listed in the 3–7 columns and the 8–13 columns, respectively. Meanwhile, the Γ_A and radiative width Γ_R (the sum of all the radiative decay rates) are listed in four columns of Table 2, which together with the natural width Γ (the sum of all the radiative and Auger decay rates) are also shown in Fig. 1.

Table 1. Calculated Auger rates (in $10^{13}\,s^{-1}$) of the K-shell excited Fluorine isoelectronic sequence from Ne to Kr with FAC for the three Auger decay channels KL_1L_1, $KL_1L_{2,3}$ and $KL_{2,3}L_{2,3}$.

Z	KL_1L_1	$KL_1L_{2,3}$					$KL_{2,3}L_{2,3}$					
	$^1S_0$	$^3P_2$	$^3P_1$	$^3P_0$	$^1P_1$	Σ	$^3P_2$	$^3P_1$	$^3P_0$	$^1S_0$	$^1D_2$	Σ
10	3.244	1.918	1.155	0.397	8.724	12.194	0.004	0.000	0.0001	1.885	23.500	25.389
11	4.794	2.113	1.282	0.445	10.060	13.900	0.012	0.000	0.0005	2.229	27.570	29.811
12	5.209	2.278	1.396	0.489	11.280	15.443	0.026	0.001	0.001	2.543	31.280	33.851
13	5.590	2.421	1.500	0.531	12.390	16.842	0.054	0.001	0.003	2.828	34.610	37.495
14	5.941	2.545	1.597	0.571	13.380	18.093	0.100	0.001	0.005	3.084	37.630	40.821
15	6.267	2.651	1.687	0.610	14.250	19.198	0.175	0.002	0.010	3.312	40.300	43.799
16	6.581	2.752	1.779	0.650	15.120	20.301	0.288	0.003	0.018	3.522	42.650	46.481
17	6.867	2.838	1.867	0.690	15.800	21.195	0.452	0.004	0.030	3.690	44.630	48.806
18	7.099	2.926	1.964	0.732	16.460	22.082	0.675	0.005	0.049	3.847	46.530	51.106
19	7.388	2.988	2.052	0.771	17.090	22.901	0.971	0.006	0.076	4.001	48.060	53.114
20	7.623	3.056	2.154	0.814	17.620	23.644	1.347	0.008	0.116	4.084	49.370	54.925
21	7.818	3.139	2.279	0.864	18.000	24.282	1.819	0.010	0.170	4.151	50.710	56.860
22	8.044	3.199	2.403	0.911	18.380	24.893	2.379	0.013	0.243	4.222	51.070	57.926
23	8.189	3.259	2.546	0.961	18.690	25.456	2.976	0.016	0.331	4.241	51.870	59.434
24	8.503	3.260	2.664	0.997	19.000	25.921	3.703	0.019	0.448	4.253	52.750	61.173
25	8.557	3.344	2.875	1.060	19.390	26.669	4.424	0.023	0.577	4.170	52.650	61.844
26	8.909	3.362	3.059	1.106	19.380	26.907	5.194	0.028	0.746	4.071	52.580	62.619
27	9.098	3.502	3.392	1.195	19.370	27.459	6.019	0.033	0.919	3.974	52.720	63.665
28	9.329	3.566	3.596	1.223	19.420	27.805	6.907	0.039	1.070	3.888	53.130	65.034
29	9.274	3.520	3.936	1.299	19.550	28.305	7.858	0.045	1.267	3.822	51.710	64.702
30	9.636	3.630	4.386	1.392	19.770	29.178	8.538	0.053	1.413	3.618	52.830	66.452
31	9.623	3.599	4.710	1.435	19.200	28.944	9.164	0.062	1.631	3.605	51.790	66.252
32	10.170	3.775	5.355	1.566	19.110	29.806	9.778	0.069	1.741	3.392	50.920	65.900
33	10.290	3.784	5.815	1.634	19.170	30.403	11.040	0.079	1.905	3.319	50.320	66.663
34	10.450	3.809	6.322	1.713	18.740	30.584	11.260	0.090	2.034	3.214	50.000	66.598
35	10.680	3.858	6.887	1.806	18.390	30.941	11.650	0.103	2.213	3.199	50.030	67.195
36	10.990	3.935	7.516	1.918	18.140	31.509	12.360	0.117	2.302	3.098	50.510	68.387

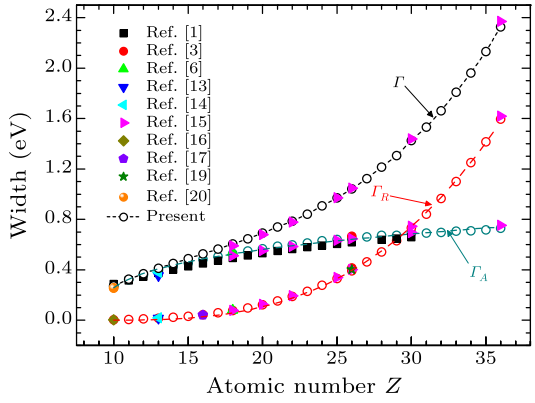


Fig. 1. Γ_A, Γ_R and Γ of the K-shell excited F-like ions with $10 \leq Z \leq 36$. Open circles: the present results; filled symbols: the results in literature.

In Table 1, one can find that the $KL_{2,3}L_{2,3}$ Auger decay is the predominant channel among the three Auger decay channels: KL_1L_1, $KL_1L_{2,3}$, and $KL_{2,3}L_{2,3}$ throughout the atomic numbers considered. Moreover, we find that the decays into $^1P_1$ final sublevels are predominant in the $KL_1L_{2,3}$ channel, and the decays into $^1D_2$ final sublevels are predominant in the $KL_{2,3}L_{2,3}$ channel, respectively. It can also be seen from Tables 1 and 2 that the Γ_A and all of the level-to-level Auger rates have a quite weak dependence on the atomic number Z. For example, the Γ_A can be well approximated by the fitting formula $\Gamma_A = 0.269(Z-9.139)^{0.307}$. Since the slater screening effect is considered here, the present fitting formula is different from the scale laws of $\sim Z^{0.7}$ obtained in Ref. [15]. For Γ_R, it can be seen from Fig. 1 that the present calculation compares well with the results by other authors, the change trends along the isoelectronic sequence exhibit a rapid increase as a function of atomic number Z, approximates by the fitting formula, $\Gamma_R = 8.854 \times 10^{-5}(Z-9.139)^{2.974}$. For Γ, it increases monotonically along the fluorine isoelectronic sequence as the radiative rates depend strongly on the atomic number Z, while the Auger rates have a much weaker dependence on it. Additionally, we find from Fig. 1 that the Γ_A are greater than Γ_R when atomic number Z is less than 29, but up to $Z = 30$, there is a crossover, i.e., the Γ_R becomes greater than Γ_A. This reflects that the Auger decay plays a prominent part when the atomic numbers Z are lower than 30, while the radiative transitions is more important for

Z greater than 30.

Table 2. Auger and Radiative widths (in eV) of the K-shell excited fluorine isoelectronic sequence with 10≤Z≤36. Γ_A: Auger width; Γ_R: radiative width.

Z	Γ_A		Γ_R (eV)	
	Present	Other theory	Present	Other theory
10	0.269	0.287[a]	0.004	0.004[g]
11	0.320	0.317[a]	0.007	
12	0.359	0.346[a]	0.011	
13	0.395	0.375[a]	0.016	0.017[b]
		0.354[b]		0.018 [c]
		0.379[c]		
14	0.427	0.402[a]	0.023	
15	0.456	0.427[a]	0.032	
16	0.483	0.451[a]	0.044	0.041[h]
17	0.506	0.474[a]	0.058	
18	0.529	0.494[a]	0.076	0.078[d]
		0.512[d]		0.080[e]
		0.538[e]		
19	0.550	0.514[a]	0.097	
20	0.568	0.532[a]	0.122	0.126[d]
		0.552[d]		
21	0.586	0.549[a]	0.153	
22	0.599	0.564[a]	0.188	0.193[d]
		0.585[d]		
23	0.613	0.579[a]	0.229	
24	0.630	0.592[a]	0.276	
25	0.640	0.605[a]	0.331	0.338[d]
		0.633[d]		
26	0.649	0.617[a]	0.393	0.401[d]
		0.645[d]		0.415[f]
		0.665 [f]		
27	0.660	0.628[a]	0.463	
28	0.673	0.639[a]	0.543	
29	0.674	0.649[a]	0.632	
30	0.694	0.659[a]	0.731	0.744[d]
		0.693[d]		
31	0.691		0.842	
32	0.698		0.965	
33	0.707		1.101	
34	0.709		1.251	
35	0.717		1.416	
36	0.731	0.752[d]	1.596	1.618[d]

[a]Ref. [1], [b]Ref. [13], [c]Ref. [14], [d]Ref. [15], [e]Ref. [6], [f]Ref. [3], [g]Ref. [16], [h]Ref. [17].

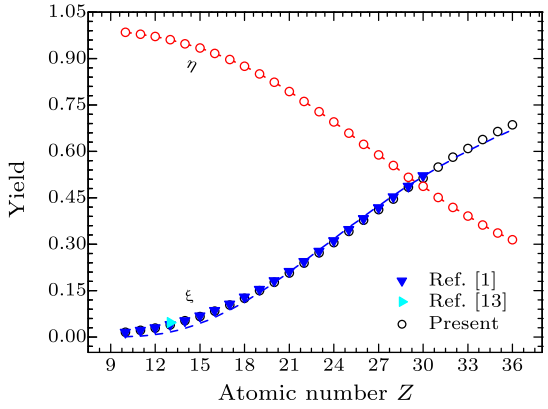


Fig. 2. Behavior of ξ and η of the K-shell excited F-like ions with 10≤ Z ≤36. Open circles: the present results; filled symbols: the results in literature.

Figure 2 shows the fluorescence yields ξ (the ratio of Γ_R to Γ) and Auger yields η (the ratio of Γ_A to Γ) of the K-shell excited F-like ions with 10≤ Z ≤36. It is found that present calculations for ξ are in good agreement with the results of other authors. The yields also exhibit a rapid increase with the atomic number Z, and can be well approximated by the fitting formula $\xi = (1 + \frac{1}{5.711\times10^{-4}(Z-9.139)^{2.484}})^{-1}$.

In conclusion, the fluorescence and Auger decay properties of the K-shell excited F-like ions from Ne to Kr have been studied by using the MCDF method. Complete data sets of Auger transition rates, radiative, Auger and natural widths, as well as fluorescence and Auger yields are calculated. We find that the Auger and radiative widths of the F-like ions scales as $\sim(Z-9.139)^{0.307}$ and $(Z-9.139)^{2.974}$, respectively. The fluorescence yield can be well approximated by the fitting formula $\xi = (1+\frac{1}{5.711\times10^{-4}(Z-9.139)^{2.484}})^{-1}$. The validity of these formulae for higher Z atoms needs to be tested in the future as only atoms with Z up to 36 are considered at present. Meanwhile, it can be concluded that the Auger decay is the leading process when the atomic number Z is lower than 30, while the radiative transitions overtake the nonradiative transitions when Z exceeds 30.

References

[1] Gorczyca T W, Kodituwakku C N, Korista K T, Zatsarinny O, Badnell N R, Behar E, Chen M H and Savin D W 2003 *Astrophys. J.* **592** 636

[2] Hill K W, Goeleret S von, Bitter M, Campbell L, Cowan R D, Fraenkel B, Greenberger A, Horton R, Hovey J, Roney W, Sauthoff N R and Stodiek W 1979 *Phys. Rev.* A **19** 1770

[3] Seely J F, Feldman U and Safronova U I 1986 *Astrophys. J.* **304** 838

[4] Decaux V, Beiersdorfer P, Osterheld A, Chen M and Kahn S M 1995 *Astrophys. J.* **443** 464

[5] Faenov A Ya, Pikuz S A and Shlyaptseva A S 1994 *Phys. Scr.* **49** 41

[6] Biémont E, Quinet P, Faenov A Ya, Skobelev I, Nilsen J, Romanova V M, Scholz M, Karpinski L and Szydlowski A 2000 *Phys. Scr.* **61** 555

[7] Fan J Z 2009 *Phys. Scr.* **79** 025304

[8] Kaastra J S and Mewe R 1993 *Astron. Astrophys. Suppl. Ser.* **97** 443

[9] Behar E and Netzer H 2002 *Astrophys. J.* **570** 165

[10] Parpia F A, Fischer C Froese and Grant I P 1996 *Comput. Phys. Commun.* **94** 249

[11] Fritzsche S 2001 *J. Electron Spectrosc. Relat. Phenom.* **114-116** 1155

[12] Zhang D H, Dong C Z and KOIKE F 2006 *Chin. Phys. Lett.* **23** 2059

[13] Wang P, MacFarlane J J and Moses G A 1993 *Phys. Rev.* E **48** 3934

[14] Farnoux F C 1987 *J. Phys. Colloq.* **48** C9-199

[15] Chen M H, Crasemann B, Karim Kh R and Mark H 1981 *Phys. Rev.* A **24** 1845

[16] Omar G and Hahn Y 1991 *Phys. Rev.* A **43** 4695

[17] Fan Q, Liao Z J, Yang J H and Zhang J P 2009 *Phys. Scr.* **79** 015301

[18] Wang X L, Wan J J, Wang Y J and Dong C Z 2010 *J. At. Mol. Sci.* **1** 134

[19] Moribayashi K, Kagawa T and KIM D E 2006 *J. Plasma Fusion Res. Ser.* **7** 233

[20] Palmeri P, Quinet P, Mendoza C, Bautista M A, GarcÍa J and Kallman T R 2008 *Astrophys. J. Suppl. Ser.* **177** 408