J. At. Mol. Sci.
doi: 10.4208/jams.013010.022010a

Vol. **1**, No. 2, pp. 134-142
May 2010

Theoretical study on the K_α transition properties of F-like ions

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Received 30 January 2010; Accepted (in revised version) 20 February 2010;
Available online 19 April 2010

Abstract. In a recent calculation on K_α transition properties of fluorine-like ions ($10 \leq Z \leq 79$) by Sur *et al*. [Phys. Rev. A 77 (2008) 052502], it was found that there is a crossover between $K_{\alpha 1}$ and $K_{\alpha 2}$ transition probabilities with increasing of atomic number Z. In order to examine this unusual behavior, a further theoretical study has been carried out by using multi-configuration Dirac-Fock (MCDF) method. In the calculation, Breit interaction, electron correlation and quantum electrodynamics (QED) effects have been included. The present study shows a contrary conclusion to the earlier theoretical results.

PACS: 32.30.Rj, 31.15.xr

Key words: F-like ions, K_α transition, Breit interaction, QED effect, MCDF method

1 Introduction

X-ray emission is a phenomenon resulting from the decay of atoms after bombardment by charged particles or electromagnetic radiation. The study of this phenomenon is very important for many fields. For example, the K-shell X-ray provides new ways in diagnostics on temperature, density, opacity, and charge distributions in plasmas [1]. Meanwhile, an accurate measurement of the relative intensities for K_α X-rays is of importance to test the relevant existing theories [2]. Furthermore, a precise determination of X-ray energies for transitions into ground state of a high-Z hydrogen-like ion is the most direct experimental approach for the investigation of the quantum electrodynamics (QED) effects in strong Coulomb field [3]. Of course, their importance in biomedical research as well as in X-ray astronomy is also pointed out [4–7]. F-like ions can give rise to K_α transition when there is a vacancy in K shell. Many studies have been done for F-like ions in both experimental observations and theoretical calculations [1, 8–19], but most of these works

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focused on spin-orbit intervals in the ground states. Therefore, it is necessary to perform a comprehensive theoretical research on F-like ions, including the ground-state fine structures, K_α transition energies and probabilities.

From a theoretical point of view, precise wavefunctions must be used for both the initial states and the final states to obtain accurate transition probabilities, but for a highly charged heavy ion with few electrons, relativistic and electron correlation effects must be treated, which poses a considerable challenge for obtaining an exact wavefunction [9]. So, in order to get more reliable information about the transition processes, large wavefunction expansions are often needed [20]. In ab initio calculations, these wavefunctions must include the most dominant physical effects, such as relativity, electron correlations, and relaxation within a common framework [21].

In this paper, we have calculated the doublet splitting of $1s^2 2s^2 2p^5\ ^2P_{3/2,1/2}$, and determined the contributions of both Breit interaction and QED effects to the transition energies from $1s2s^2 2p^6\ ^2S_{1/2}$ to $1s^2 2s^2 2p^5\ ^2P_{3/2,1/2}$ for F-like ions ($16 \leq Z \leq 92$). Much attention has been paid to the K_α transition probabilities. The fully relativistic multi-configuration Dirac-Fock (MCDF) method [22, 23] has been used to calculate exact wavefunctions, and the recently developed REOS99 program [24] has been used to compute transition energies and probabilities. The structure of this paper is as follows. In Section 2, we briefly introduce the method applied in the present calculations. The calculated results and discussion are given in Section 3. Also the conclusion is given in Section 4.

2 Theoretical method

In this study, wavefunctions have been generated by using the widely used relativistic atomic structure package GRASP92 [25], on the basis of the MCDF method in which an atomic state is approximated by a linear combination of configuration state functions (CSFs) with the same symmetry

$$|\Psi_\alpha(PJM)\rangle = \sum_{r=1}^{n_c} c_r(\alpha)|\gamma_\alpha(PJM)\rangle, \tag{1}$$

where n_c is the number of CSFs and $c_r(\alpha)$ denotes the representation of the atomic state in this basis. In a standard calculation, the CSFs are the antisymmetrized products of a common set of orthonormal orbitals which are optimized on the basis of the Dirac-Coulomb Hamiltonian. Further relativistic contributions to the representation $c_r(\alpha)$ of the atomic states due to (transverse) Breit interactions are added by diagonalizing the Dirac-Coulomb-Breit Hamiltonian matrix. And the dominant QED contributions to the transition energies have been included as a perturbation.

The Einstein spontaneous emission probability for transition from initial state β to final state α can be given by

$$A_{\alpha\beta} = \frac{2\pi}{2J_\beta + 1} \sum_{M_\alpha} \sum_{M_\beta} |M^{(L)}_{\alpha\beta}|^2, \tag{2}$$

where J_β is the total angular momentum of the state β, and $M_{\alpha\beta}$ is the transition matrix, the latter can be calculated by

$$\begin{aligned} M_{\alpha\beta}^{(L)} &= \langle \alpha(P_\alpha J_\alpha M_\alpha)|O^{(L)}|\beta(P_\beta J_\beta M_\beta\rangle) \\ &= \sum_{r,s} c_r(\alpha)c_s(\beta)\langle \gamma_r(P_\alpha J_\alpha M_\alpha)|O^{(L)}|\gamma_s(P_\beta J_\beta M_\beta\rangle), \end{aligned} \tag{3}$$

where $O^{(L)}$ is the tensor operator of radiation electromagnetic field with rank L. In calculations, the initial and final state wavefunctions are optimized through self-consistent field calculation with the extended optimal level (EOL) scheme, and the configuration interactions are considered by using the active space method in which electrons are excited from the occupied shells into unoccupied shells virtually.

3 Results and discussion

The ground state doublet splitting for the F-like ions are of considerable practical importance because of their use in the diagnostics of high temperature plasmas [26]. The results obtained in this paper are listed in Table 1. Besides, several experimental and theoretical results are also tabulated for comparison. In our calculations, both Breit interaction and QED effects are included. It can be seen from the table that the spin-orbit splitting along the fluorine isoelectronic sequence are larger and larger, especially for ions with high atomic number Z. This is attributed to the contributions of relativistic effect which is larger with increasing Z. Furthermore, it is obvious that the present calculations are in better agreement with both the experimental measurements [12, 19, 27] and the NIST results [28] than the computations of Sur *et al*. [9] .

It has been turned out by Dong *et al.* [29] that both Breit interaction and QED effects contribute much to the binding energies of the highly charged ions, especially for the few electrons system, and this will further influence the transition energies among different levels. In order to demonstrate their contributions to the transition energies of F-like ions, firstly, we calculate the transition energies including both Breit interaction and QED effects, then, we do it again without both corrections. Contributions of these two effects are obtained by subtracting the latter ones from the former and the results are presented in Fig.1.

It can be seen from Fig.1 that Breit interaction and QED effects have an obvious influence on $K_{\alpha 2}$ and $K_{\alpha 1}$ transition energies, and their contributions to $K_{\alpha 1}$ is greater than that to $K_{\alpha 2}$. The reason is that the actual electric field seen by valence electrons in $1s^2 2s^2 2p^5\ ^2P_{3/2}$ state is stronger than that in $1s^2 2s^2 2p^5\ ^2P_{1/2}$ state, which can be deduced from the discrepancies of transition energies between $K_{\alpha 2}$ and $K_{\alpha 1}$. In addition, with increasing of atomic number Z, their contributions are also going up. This change is made clear by considering the following fact: the electronic cloud of $1s^2 2s^2$ is shrunk very fast with increasing Z, and the electric field seen by valence is growing very fast with Z, so the high-order relativistic effects also become more important.

Table 1: Spin-orbit splitting (eV) in the ground states of F-like ions

Z	Ion	Present	Ref. [9]	NIST [26]	Expt.
16	S^{7+}	1.25	1.72	1.25	1.25[a]
19	K^{10+}	2.92	3.43	2.92	2.91[a]
22	Ti^{13+}	5.89	6.44	5.85	5.85[a]
25	Mn^{16+}	10.70	11.29	10.60	10.64[a]
29	Cu^{20+}	20.72	21.78	20.93	20.93[b]
30	Zn^{21+}	24.18	25.29	24.41	24.42[b]
31	Ga^{22+}	28.05	29.24	28.32	28.32[b]
32	Ge^{23+}	32.28	33.65	32.67	32.66[b]
33	As^{24+}	37.20	38.55	37.53	37.53[b]
34	Se^{25+}	42.62	43.99	42.91	-
35	Br^{26+}	48.52	50.00	48.86	-
36	Kr^{27+}	54.90	-	55.35	55.37[c]
37	Rb^{28+}	62.11	-	62.53	-
38	Sr^{29+}	69.96	-	-	70.47[b]
39	Y^{30+}	78.55	-	-	79.01[b]
40	Zr^{31+}	88.01	-	-	-
41	Nb^{32+}	98.21	100.55	-	-
42	Mo^{33+}	109.30	111.82	109.89	-
43	Tc^{34+}	121.32	124.04	-	-
44	Ru^{35+}	134.48	-	-	-
45	Rh^{36+}	148.54	151.55	-	-
46	Pd^{37+}	163.72	-	-	-
47	Ag^{38+}	180.10	183.57	-	-
48	Cd^{39+}	197.71	201.45	-	-
49	In^{40+}	216.70	220.65	-	-
50	Sn^{41+}	237.03	241.27	-	-
51	Sb^{42+}	258.91	263.36	-	-
74	W^{65+}	1396.20	-	-	-
79	Au^{70+}	1892.12	1902.64	-	-
92	U^{83+}	3933.64	-	-	-

[a] As tabulated by Curtis and Ramanujam [27].

[b] Ref. [19] and references therein.

[c] Ref. [12].

Good wavefunctions are needed for getting reliable ground-state doublet separations, transition energies and probabilities. In the present calculations, we always use the agreement between the results in different gauges to confirm the accuracy of the wavefunctions. Table 2 lists the present E1 transition probabilities in both Babushkin and Coulomb gauges for F-like ions ($16 \leq Z \leq 92$). This table shows that the transition probabilities in

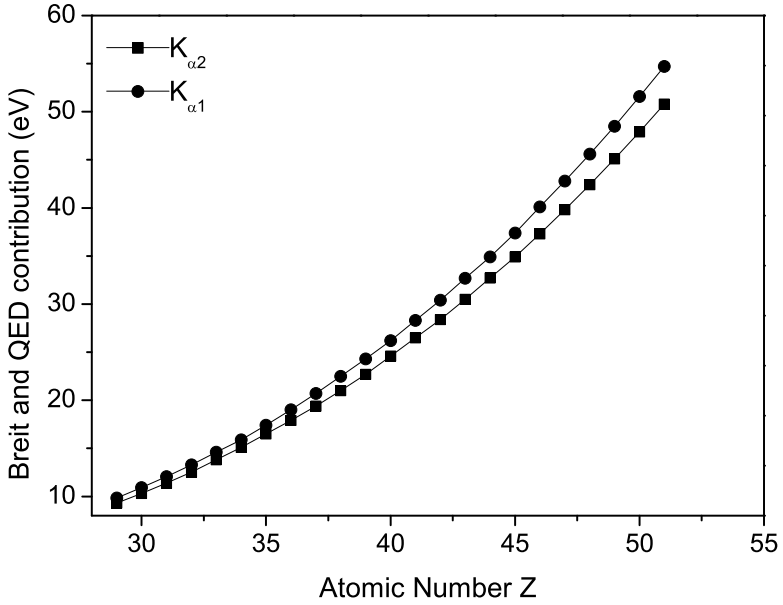

Figure 1: Contributions of both Breit interaction and QED effects to transition energies.

two gauges are in good agreement with each other, and the relative errors for $K_{\alpha 1}$ transition is less than 3% comparing to that of about 10% for $K_{\alpha 2}$ in most cases. It means that the present wavefunctions are accurate enough. Besides, it is noticeable that the wavefunctions corresponding to $K_{\alpha 1}$ transition is better than that for $K_{\alpha 2}$.

Meanwhile, we also present a comparison between our calculations and Sur's relativistic coupled-cluster (RCC) results [9] of K_α transition probabilities for F-like ions in Table 3. It is found that the discrepancies in both results are larger. In our computations, probabilities for $K_{\alpha 1}$ transition are always greater than those for $K_{\alpha 2}$, but in Ref. [9], the probabilities for $K_{\alpha 2}$ transition are greater than $K_{\alpha 1}$ when atomic number Z less than 41, but up to Z=42, there is a crossover, i.e., $K_{\alpha 1}$ becomes greater than $K_{\alpha 2}$. It is obvious that our results are agreement with the results in Ref. [10] and Ref. [11] better than the results in Ref. [9]. In order to verify the reliability of the present results, we also calculated the K_α transition probabilities by using the Flexible Atomic Code (FAC) [30], the results are shown in Table 3 too. It is clear that the results calculated by using GRASP92 and FAC codes give a good consistency and there is not any crossover. Besides, it is very important that the probabilities for $K_{\alpha 2}$ transition have a good agreement among GRASP92, FAC and RCC results. For $K_{\alpha 1}$ transition, RCC results are smaller than GRASP92 and FAC results. Considering the agreement of different gauges, we have obtained that the wavefunctions corresponding to $K_{\alpha 1}$ transition are better than those of $K_{\alpha 2}$ in our calculations, so we guess that maybe there is some confusions for the transition probabilities

Table 2: Transition probabilities (s^{-1}) for F-like ions with different gauges

Z	Ion	$K_{\alpha 2}$		$K_{\alpha 1}$	
		B	C	B	C
16	S^{7+}	2.27(13)	2.19(13)	4.56(13)	4.33(13)
19	K^{10+}	4.96(13)	4.86(13)	1.00(14)	9.61(13)
22	Ti^{13+}	9.51(13)	9.46(13)	1.92(14)	1.86(14)
25	Mn^{16+}	1.66(14)	1.67(14)	3.38(14)	3.28(14)
29	Cu^{20+}	3.14(14)	3.21(14)	6.43(14)	6.27(14)
30	Zn^{21+}	3.62(14)	3.72(14)	7.44(14)	7.26(14)
31	Ga^{22+}	4.16(14)	4.29(14)	8.56(14)	8.36(14)
32	Ge^{23+}	4.75(14)	4.93(14)	9.81(14)	9.59(14)
33	As^{24+}	5.41(14)	5.63(14)	1.12(15)	1.09(15)
34	Se^{25+}	6.12(14)	6.40(14)	1.27(15)	1.24(15)
35	Br^{26+}	6.91(14)	7.25(14)	1.44(15)	1.40(15)
36	Kr^{27+}	7.76(14)	8.19(14)	1.62(15)	1.58(15)
37	Rb^{28+}	8.69(14)	9.21(14)	1.82(15)	1.78(15)
38	Sr^{29+}	9.70(14)	1.03(15)	2.03(15)	1.99(15)
39	Y^{30+}	1.08(15)	1.15(15)	2.27(15)	2.22(15)
40	Zr^{31+}	1.20(15)	1.29(15)	2.52(15)	2.47(15)
41	Nb^{32+}	1.32(15)	1.43(15)	2.80(15)	2.74(15)
42	Mo^{33+}	1.46(15)	1.58(15)	3.10(15)	3.03(15)
43	Tc^{34+}	1.60(15)	1.75(15)	3.42(15)	3.34(15)
44	Ru^{35+}	1.76(15)	1.93(15)	3.76(15)	3.68(15)
45	Rh^{36+}	1.93(15)	2.12(15)	4.13(15)	4.04(15)
46	Pd^{37+}	2.10(15)	2.33(15)	4.52(15)	4.42(15)
47	Ag^{38+}	2.29(15)	2.55(15)	4.94(15)	4.83(15)
48	Cd^{39+}	2.49(15)	2.79(15)	5.40(15)	5.27(15)
49	In^{40+}	2.70(15)	3.05(15)	5.88(15)	5.74(15)
50	Sn^{41+}	2.92(15)	3.32(15)	6.39(15)	6.24(15)
51	Sb^{42+}	3.16(15)	3.61(15)	6.93(15)	6.77(15)
74	W^{65+}	1.26(16)	1.73(16)	3.14(16)	3.03(16)
79	Au^{70+}	1.58(16)	2.28(16)	4.06(16)	3.91(16)
92	U^{83+}	2.55(16)	4.31(16)	7.31(16)	6.97(16)

[a] B and C denote transition probabilities in Babushkin and Coulomb gauges, respectively.

* a(b) denotes $a \times 10^b$.

of $K_{\alpha 1}$ transition in [9]. Maybe this problem need a further study in experiment.

In order to further understand the present large discrepancy, we take Cu^{20+}, Nb^{32+} and Sb^{42+} as examples, study the configuration interaction (CI) effect on the transition probabilities. The results are listed in Table 4. In column 3, the wavefunctions of tran-

Table 3: Comparisons of K_α transition probabilities (s^{-1}) for F-like ions

Z	Ion	Our results				Other results			
		GRASP92		FAC		RCC [9]		Others	
		$K_{\alpha 2}$	$K_{\alpha 1}$	$K_{\alpha 2}$	$K_{\alpha 1}$	$K_{\alpha 2}$	$K_{\alpha 1}$	$K_{\alpha 2}$	$K_{\alpha 1}$
16	S^{7+}	2.19(13)	4.33(13)	2.40(13)	4.78(13)	1.81(13)	6.66(12)	2.11(13)[a]	4.17(13)[a]
19	K^{10+}	4.86(13)	9.61(13)	5.21(13)	1.04(14)	4.26(13)	8.52(12)		
22	Ti^{13+}	9.46(13)	1.86(14)	9.97(13)	1.99(14)	1.01(14)	1.18(13)		
25	Mn^{16+}	1.67(14)	3.28(14)	1.74(14)	3.48(14)	1.78(14)	2.59(13)		
29	Cu^{20+}	3.21(14)	6.27(14)	3.31(14)	6.62(14)	2.99(14)	8.42(13)		
30	Zn^{21+}	3.72(14)	7.26(14)	3.83(14)	7.66(14)	3.47(14)	1.09(14)		
31	Ga^{22+}	4.29(14)	8.36(14)	4.40(14)	8.82(14)	4.08(14)	1.32(14)		
32	Ge^{23+}	4.93(14)	9.59(14)	5.04(14)	1.01(15)	4.66(14)	1.73(14)		
33	As^{24+}	5.63(14)	1.09(15)	5.75(14)	1.15(15)	5.55(14)	1.88(14)		
34	Se^{25+}	6.40(14)	1.24(15)	6.53(14)	1.31(15)	5.90(14)	2.29(14)		
35	Br^{26+}	7.25(14)	1.40(15)	7.39(14)	1.48(15)	6.58(14)	2.65(14)		
36	Kr^{27+}	8.19(14)	1.58(15)	8.33(14)	1.67(15)				
37	Rb^{28+}	9.21(14)	1.78(15)	9.35(14)	1.88(15)				
38	Sr^{29+}	1.03(15)	1.99(15)	1.05(15)	2.10(15)				
39	Y^{30+}	1.15(15)	2.22(15)	1.17(15)	2.35(15)				
40	Zr^{31+}	1.29(15)	2.47(15)	1.30(15)	2.61(15)				
41	Nb^{32+}	1.43(15)	2.74(15)	1.44(15)	2.90(15)	1.36(15)	1.33(15)		
42	Mo^{33+}	1.58(15)	3.03(15)	1.59(15)	3.21(15)	1.51(15)	1.53(15)		
43	Tc^{34+}	1.75(15)	3.34(15)	1.76(15)	3.55(15)	1.67(15)	1.69(15)		
44	Ru^{35+}	1.93(15)	3.68(15)	1.94(15)	3.91(15)				
45	Rh^{36+}	2.12(15)	4.04(15)	2.13(15)	4.30(15)	1.99(15)	2.03(15)		
46	Pd^{37+}	2.33(15)	4.42(15)	2.33(15)	4.71(15)				
47	Ag^{38+}	2.55(15)	4.83(15)	2.55(15)	5.16(15)	2.41(15)	2.46(15)		
48	Cd^{39+}	2.79(15)	5.27(15)	2.79(15)	5.64(15)	2.65(15)	2.71(15)		
49	In^{40+}	3.05(15)	5.74(15)	3.04(15)	6.15(15)	2.89(15)	3.02(15)		
50	Sn^{41+}	3.32(15)	6.24(15)	3.30(15)	6.70(15)	3.11(15)	3.27(15)		
51	Sb^{42+}	3.61(15)	6.77(15)	3.59(15)	7.28(15)	3.41(15)	3.78(15)		
74	W^{65+}	1.73(16)	3.03(16)	1.66(16)	3.47(16)				
79	Au^{70+}	2.28(16)	3.91(16)	2.16(16)	4.56(16)	2.16(16)	2.31(16)	1.59(16)[b]	3.42(16)[b]
92	U^{83+}	4.31(16)	6.97(16)	3.96(16)	8.65(16)				

[a] Ref. [11].

[b] Ref. [10].

* c(d) denotes $c \times 10^d$.

Table 4: Transition probabilities (s^{-1}) for F-like ions with different models

Ion	Transition	Model A	Model B
Cu^{20+}	$^2S_{1/2}-^2P_{1/2}$	3.25(14)	3.21(14)
	$^2S_{1/2}-^2P_{3/2}$	6.34(14)	6.27(14)
Nb^{32+}	$^2S_{1/2}-^2P_{1/2}$	1.44(15)	1.43(15)
	$^2S_{1/2}-^2P_{3/2}$	2.76(15)	2.74(15)
Sb^{42+}	$^2S_{1/2}-^2P_{1/2}$	3.63(15)	3.61(15)
	$^2S_{1/2}-^2P_{3/2}$	6.81(15)	6.77(15)

* a(b) denotes $a\times10^b$.

sition initial and final states are obtained by using single configuration approximation; in column 4, the wavefunctions are calculated by using multi-configuration approximation. We can find that the CI influences the results slightly and it is not large enough to change the transition probabilities greatly. We speculate that the differences between our calculations and Sur's results may not be caused by the correlation effects.

4 Conclusions

We have studied the K_α transition properties for F-like ions ($16\leq Z\leq 92$), including the ground-state doublet splitting, the contribution of both Breit interaction and QED effects to the energies of K_α transition, and the transition probabilities. For Spin-orbit splitting, the present results are in good agreement with both the experimental measurements and the NIST results, and they are increasing along the fluorine isoelectronic sequence just like the contributions of both Breit interaction and QED effects to the energies of K_α transition; For K_α transition probabilities, our MCDF and FAC results are in good consistency, but there is a big difference between the present results and the RCC results about a crossover. We find that it is not caused by the CI effect. It is necessary to carry out some high-accuracy experiments in the future.

Acknowledgments. This work has been supported by the National Natural Science Foundation of China under Grant Nos. 10774122, 10876028 and 10847007, the Specialized Research Fund for the Doctoral Program of Higher Education of China under Grant No. 20070736001, the Foundation of Center of Theoretical Nuclear Physics of National Laboratory of Heavy Ion Accelerrator of Lanzhou.

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