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Theoretical study on decay of the 4d core-excited states of Cs III*

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In a recent XUV photoabsorption spectrum of Cs III ions by Cummings and O'Sullivan [2001 *J. Phys.* B **34** 199], rather large linewidths were found for the $4d^{9}5s^{2}5p^{6} - 4d^{10}5s^{2}5p^{5}$ transition which are quite in disagreement with corresponding quasi-relativistic multiconfiguration Hartree–Fock (MCHF) calculation. In the present work, a detailed multiconfiguration Dirac-Fock study has been carried out to explore this discrepancy. Owing to the detailed consideration of electron correlation effects, some 'forbidden' Auger decay channels, such as $4d^{10}5s^{2}5p^{3}5d$ and $4d^{10}5s^{0}5p^{6}$, would become 'open'. As a result, remarkable improvement of the linewidths has been obtained in our calculation. Furthermore, the theoretical Auger spectrum of the $4d^{9}5s^{2}5p^{6}$ core-excited states of Cs III ions is given in the present work.

Keywords: correlation effects, linewidth, Auger decay
PACC: 3120T, 3270F, 3280H

1. Introduction

A core-excited (ionized) state of atom (ion) is a state in which an electron from an inner-shell has been excited to an outer occupied or unoccupied shell. Such a core-excited state is at a high lying energy level that it is unstable and must decay to some lower states. In general, a core-excited state can decay through two decay channels: one is radiative decay channel by emission of photon, and the other is non-radiative process by emission of Auger electron. Core excited states can be obtained by the photo excitation (ionization) or atom, ion and electron collision with atoms or ions.[1] With the development of advanced facilities, such as synchrotron radiation technology, dual laser-produced plasma (DLP) method, ion storage ring and electron beam ion trap (EBIT), etc. it becomes possible to carry out more detailed and widespread study of properties of core-excited states.[2,3] However, due to the fact that a lot of possible transitions and subsequent cascading processes are involved in the decay of core-excited states, the final decay production is usually a mixture of ions in different ionization stages. As a result, the experimental detection and distinguishment of these states becomes very difficult. Theoretically, the study on non-radiative decay of core-excited states is always concerned about continuum states, while the properties of core-excited states are dependent on numerous transitions, hence, very complex. Meanwhile, for heavy elements, relativistic effect is so important that a systematical relativistic investigation is necessary.

Caesium is a medium Z alkali metal element. Recently many investigators have paid more attention to the properties of Cs ions in different ionization stages.[4−10] The ground state, low-lying excited states and some core-excited states have been studied experimentally and theoretically. Tauheed *et al*[4−7] observed the ground state and the low lying excited state as well as the pertinent radiative transition processes among those states of Cs IV, Cs V and Cs VI ions. They also performed some calculations by using quasi-relativistic configuration interaction (HFR+CI) method to identify the spectra obtained from the experiments. Aksela *et al*[8] and Mäntykenttä *et al*[9]

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made good use of synchrotron radiation technology to investigate the photoelectron spectra of the 4d, 5s and 5p core-excited states of Cs I; Cummings and O'Sullivan[10] observed the extreme ultra-violet (XUV) region of the photoabsorption spectra of Cs in different ionization stages up to Cs V by using the DLP method. They also identified the discrete structure of the 4*d* photoabsorption spectra by using the MCHF calculation. However, all the authors mentioned above have paid most attention only to the radiative processes of the Cs ions in different ionization stages and the Auger process of the neutral caesium. Meanwhile, most of the above theoretical results were obtained from the non-relativistic or quasi-relativistic theory. Obviously, further multi-configuration relativistic investigation into the radiative and the Auger processes will be helpful for understanding these systems.

In recent years, a number of elaborate programs have been developed for calculating not only the level structures and wavefunctions[11−13] of medium and high Z atoms but also their excitation and decay properties[14−16] in quite detail. For complex atoms or ions with one or several open shells (as they occur rather often during the decay of inner-shell hole states), these codes are usually based on the multi-configuration Dirac–Fock (MCDF) method.[17] In particular, the GRASP92[12] and RATIP[14] packages have been applied successfully in the last few years to studying the photon emission and absorption of medium and high Z atoms[18−20] as well as the Auger decay of resonantly excited noble gases.[21−23]

In the present, we use these programs to analyse the discrepancy between the experimental and the theoretical linewidths of the $4d^9 5s^2 5p^6\ ^2D_{5/2}$ and $^2D_{3/2}$ core-excited states of Cs III. In Section 2, theoretical background and computational procedures are described. The results of radiative and Auger decay of the 4d core-excited states of Cs III ions are given in Sections 3.1 and 3.2, respectively. Furthermore, the linewidths of $^2D_{5/2}$ and $^2D_{3/2}$ core-excited levels of Cs III. are discussed in Section 3.3. Finally, the conclusion and brief summary of present work are provided in Section 4.

2. Computational procedures

In the present work, the relative Auger electron intensities and the linewidths of the 4d core-excited states are both calculated. The relative Auger electron intensity has been calculated by using a two-step model. In this model, the primary 4d photoabsorption of Cs III ions is assumed to take place independently of Auger decay of the 4d core-excited states. All of the states involved in the calculation are described within the MCDF theoretical framework. In this theory, the atomic state function (ASF) with given total angular momentum (J, M) and parity (P) is approximated by a linear combination of pure jj-coupled configuration state functions (CSFs) of the same symmetries as follows:

$$\alpha_i\,(PJM)\rangle\ = \sum_r c_{\gamma r}\,\Phi_r(PJM). \tag{1}$$

For all bound and reasonably well isolated resonance states in the continuum, the ASF can be generated by means of the GRASP92 program.[12]

For the photoabsorption process, the absorption oscillator strength can be obtained by[24]

$$f_{\rm ki} = \frac{\hbar\omega_{\rm ki}}{3(2j_{\rm k}+1)}\left|\left\langle\alpha_{\rm k}\,(PJM)\right|P^{(1)}\left|\,\alpha_{\rm i}\,(P'J'M')\right\rangle\right|^2, \tag{2}$$

where $\left|\alpha_{\rm k}\,(PJM)\right\rangle$ is the ASF for the ground state with an energy $E_{\rm k}$ which is coupled to the final core-excited state i with an energy $E_{\rm i}$ due to the coupling of the radiation field, $j_{\rm k}$ is the total angular momentum of the lower state k, $\omega_{\rm ki}$ is the frequency of the photon absorbed by the atom from the state k to the state i. For the study of the lower energy photoabsorption process in lower charged atoms/ions, it is certainly sufficient to take the dipole tensor operator $\mathrm{P}^{(1)}$ into account for the radiation field. For the photoabsorption cross-sections, the discrete features are assumed to have a Lorentzian profile and the resonant part of the cross-sections is calculated by using the formula

$$\sigma_{\rm ki}(Mb) = 109.7\frac{\Gamma_{\rm i} f_{\rm ki}}{2\pi(E_{\rm ki}-E)^2+\dfrac{\Gamma_{\rm i}^2}{4}}, \tag{3}$$

where $f_{\rm ki}$ and $E_{\rm ki}$ are the oscillator strength and transition energy (in eV) of photoabsorption process respectively, while $\Gamma_{\rm i}$ is the linewidths of the upper level i (in eV).

For non–radiative decay, the Auger decay rate from an initial state i to a final state f can be calculated from[25]

$$A_{\rm if}^a = \frac{2\pi}{\hbar}\left|\left\langle\alpha_{\rm f}\,(PJM)\,\right|\sum_{s<t}V_{st}\left|\,\alpha_{\rm i}\,(P'J'M')\right\rangle\right|^2, \tag{4}$$

where $\left|\alpha_{\rm i}\,(P'J'M')\right\rangle$ and $\left|\alpha_{\rm f}\,(PJM)\right\rangle$ represent the wavefunctions of the Auger initial and final states, re-

spectively, and V_{st} is the sum of Coulomb operator and Breit operator. For the generation of the final continuum states, the Dirac–Fock equation has to be solved also for a continuum electron with a given energy $\epsilon = E_{\rm i} - E_{\rm f}$, equivalent to the difference in energy between the initial and the final ionized states. Starting from the GRASP92 wavefunctions for the bound states, the Auger rate is calculated by means of the RATIP package which automatically generates and accounts for the coupling of the continuum spinors in the overall representation of the final state $\left|\alpha_{\rm f}(PJM)\right\rangle$.

The relative Auger intensity corresponding to the Auger decay from a core-excited state i to a final ionic state f of the Auger decay can be obtained as

$$I_{\rm if} = \sigma_{\rm ki} A^a_{\rm if} \Big/ \sum_n A^a_{n\rm f}. \tag{5}$$

As far as the broadening of a spectral line is concerned, it could be caused either by the apparatus and the other conditions in the experiments, or by the natural linewidths of transition, thus, by all the possible decay channels. According to the Heisenberg's principle of uncertainty, the natural linewidth of a given state is determined by the lifetime of this state. Theoretically, the lifetime is just the reciprocal of the sum of transition probability of all possible decay channels. So, it is needed to consider all possible decay channels, not only radiative but also Auger decay, in order to understand the natural width of a specific energy level.

As mentioned above, large discrepancies in the linewidth of the 4d core-excited state $4d^95s^25p^6$ between previous theoretical calculation and experimental observation were found.[10] The experimental results are one order larger than the theoretical results. Furthermore, only the $5s^25p^4$ and the $5s5p^5$ nonradiative decay channels were included as the main decay channels to interpret the experimental linewidth in the previous work. However, in fact, there exist more other decay channels, for example, the energetically forbidden state $5s^05p^6$ and other forbidden channel $5s^25p^35d$ which involve a three-electron change in Auger decay process. Figure 1 shows the low-lying level structures of Cs III and Cs IV ions. It can be seen from Fig.1 that the possible Auger decay channels are much more than radiative decay channels. The Auger decay can occur only if the discrete states of the next lower ionization stage are embedded within the core-excited state.

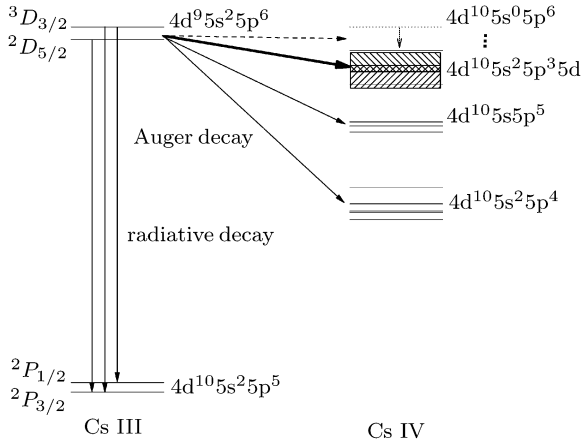


Fig.1. The energy level structures of Cs III and Cs IV ions.

In order to construct a correlation model for calculating the bound–state energies and wavefunctions, the $4d^{10}5s^25p^5$ and $4d^{10}5s^25p^4$ as well as $4d^{10}5s^15p^5$ are used as reference configurations for the final states of the radiative and Auger decay processes, respectively. From these reference configurations, then, the correlation models are determined, in which all the single and double excitations into $\{5s, 5p, 5d, 6s, 6p, 6d\}$ subshells are included within a rather systematic fashion. For the Auger initial states, we may wish to follow a similar correlation model to one applied to Auger final states. For an open 4d subshell, however, the number of CSFs increases very rapidly if single and double excitations are both included. Therefore, in order to keep the wavefunction expansion feasible, we just include $4d^{10}5s^25p^4$, $4d^{10}5s^15p^45d^1$, $4d^{10}5s^05p^6$, and $4d^{10}5s^25p^25d^2$ configurations and $4d^{10}5s^15p^5$ and $4d^{10}5s^25p^35d^1$ configurations for the even parity and odd parity configurations of the Auger final states respectively, which was fully successful in explaining the Auger electron spectrum of Xe I.[26] All the computations are based on the correlation model.

Although relativistic computations are carried out traditionally within a $jj-$ coupled basis, we still denote the levels below in their $^{2S+1}L_J$ spectroscopic notation in order to facilitate the comparison with measurements. Furthermore, to indicate the mixing of the configuration state functions (CSFs) in the representation of the wavefunctions, the main components in $jj-$coupled basis are also displayed.

3. Results and discussions

3.1. Radiative decay process of 4d core-excited states

The only possible dipole in which the radiative transition of the core-excited state $4d^9 5s^2 5p^6$ is allowed should be the transition to the $5s^2 5p^5$ ground state of Cs III. All the 4 energy levels related to this transition are calculated and given in Table 1, together with the existing experimental results.[27] The main jj coupling components of the ASFs are also given in the table. It can be found that the calculations are in rather good agreement with measurements within just a minor deviation in a fine-structure splitting of about 2%. According to the main jj-components of the levels, it is an well-defined jj coupling pure state.

The transition energies, absorption oscillator strengths (gf) of the $4d^9 5s^2 5p^6 \rightarrow 4d^{10} 5s^2 5p^5$ radiative transition of Cs III are calculated by including the correlation and relaxation effects systematically and given in Table 2 together with the previous experimental and theoretical results. The calculations are in quite good agreement with existing data in transition energy and oscillator strength. It implies that the core-excited state $4d^9 5s^2 5p^6$ can be accurately described by using the present correlation model in our calculation.

Table 1. Levels and excitation energies (in cm^{-1}) of the $4d^{10} 5s^2 5p^5$ ground configuration and $4d^9 5s^2 5p^6$ core-excited configuration of Cs III.

Configuration	$^{2S+1}L_J$	E_{calc}	E_{exp}[27]	$jj-$components
$4d^{10} 5s^2 5p^5$	$^2P^o_{3/2}$	0	0	97% of $[(5p_{3/2})^3]_{3/2}$
	$^2P^o_{1/2}$	13726.3	13848.4	97% of $[(5p_{1/2})]_{1/2}$
$4d^9 5s^2 5p^6$	$^2D_{5/2}$	528519.1	529256.7	97% of $[(4d_{5/2})^5]_{5/2}$
	$^2D_{3/2}$	547220.5	543105.2	97% of $[(4d_{3/2})^3]_{3/2}$

Table 2. Energies and oscillator strengths (gf) of the $4d^9 5s^2 5p^6 \rightarrow 4d^{10} 5s^2 5p^5$ radiative transitions of Cs III.

Transition	This work		Previous calculation[10]		Experiment[10]
$i \rightarrow k$	E/eV	gf	E/eV	gf	E/eV
$^2D_{5/2} \rightarrow {}^2P_{3/2}$	65.52	0.548	65.54	0.5731	65.62
$^2D_{3/2} \rightarrow {}^2P_{1/2}$	66.14	0.342	66.06	0.3206	66.18
$^2D_{3/2} \rightarrow {}^2P_{3/2}$	67.85	0.057			

3.2. Auger decay process of the 4d core-excited states

If the correlation effects are neglected as considered in the previous work,[10] there are just two possible Auger decay channels, i.e. $4d^{10} 5s^2 5p^4$ and $4d^{10} 5s 5p^5$, from the 4d core-excited states. However, further configuration, such as the $5s^2 5p^3 5d$ which involves a three-electron change compared with the normal Auger decay process should also be the possible Auger final states due to the fact that sufficient correlation effects are taken into account. Given in Table 3 are the theoretical and experimental energy levels,[7,28] the main jj coupling components of these configurations, and the relative errors. A general agreement between our calculations and the previous measurements is obtained, however, the discrepancy is still large for the highly excited states. It is also found in Table 3 that the $5s 5p^5$ and $5s^2 5p^3 5d$ configurations are strongly mixed. The main jj components of the $4d^{10} 5s^2 5p^3 5d$ $(^2P)^3P^o_2$, $(^2D)^3P^o_1$, $(^2D)^3P^o_0$ and $(^2D)^1P^o_1$ states amount to just about 35%, 30%, 49%, 40% respectively. Hence, they cannot be described very well in the jj coupling notation.

Table 3. Levels and excitation energies (in cm^{-1}) of the $4d^{10}5s^25p^4$, $4d^{10}5s5p^5$ and $4d^{10}5s^25s^25p^35d$ configurations of Cs IV.

Configuration	$^{2S+1}L_J$	E_{calc}	E_{exp}[7,28]	$jj-$components	relative error/%
$4d^{10}5s^25p^4$	$^3P_2$	0	0	90% of $[(5p_{3/2})^2]_2$ + 7% of $[(5p_{1/2})(5p_{3/2})^2]_2$	
	$^3P_0$	10194.6	9749.0	76% of $[(5p_{3/2})^2]_0$ + 21% of $[(5p_{3/2})^4]_0$	4.5
	$^3P_1$	12431.0	12901.7	97% of $[(5p_{1/2})(5p_{3/2})^3]_1$	3.6
	$^1D_2$	22834.1	20753.7	89% of $[(5p_{1/2})(5p_{3/2})^3]_2$ + 7% of $[(5p_{3/2})^2]_2$	10.0
	$^1S_0$	45257.9	43279.2	75% of $[(5p_{3/2})^4]_0$ + 20% of $[(5p_{3/2})^2]_0$	4.6
$4d^{10}5s5p^5$	$^3P^o_2$	114484.6	114307.7	78% of $[(5s_{1/2})(5p_{3/2})^3]_2$ + 6% of $[(5p_{3/2})^1(5d_{5/2})^1]_2$	0.2
	$^3P^o_1$	121635.0	121242.5	40% of $[(5s_{1/2})(5p_{1/2})]_1$ + 33% of $[(5p_{3/2})^1(5d_{5/2})^1]_1$	0.3
	$^3P^o_0$	127852.8	128086.3	74% of $[(5s_{1/2})(5p_{3/2})^3]_0$ + 9% of $[(5p_{3/2})^3(5d_{5/2})^1]_0$	0.2
	$^1P^o_1$	144049.9	141402.9	44% of $[(5s_{1/2})(5p_{3/2})^3]_1$ + 35% of $[(5p_{3/2})^3(5d_{5/2})^1]_1$	1.9
$4d^{10}5s^25p^35d$	$(^4S)\,^5D^o_2$	136574.67	136143.1	43% $\{[(5p^2_{1/2})(5P_{3/2})]_{3/2}5d_{3/2}\}_2$ + 31% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_2$	0.3
	$(^4S)\,^5D^o_0$	136877.55	136625.7	44% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{3/2}\}_0$ + 30% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_0$	0.2
	$(^4S)\,^5D^o_1$	136982.90	136868.6	43% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_1$ + 33% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{3/2}\}_1$	0.1
	$(^4S)\,^3D^o_2$	144991.53	142167.0	51% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{5/2}\}_2$ + 22% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{3/2}\}_2$	2.0
	$(^2D)\,^1P^o_1$	150882.22	141402.9	35% $\{[(5p^2_{1/2})(5p^2_{3/2})]_{3/2}5d_{5/2}\}_1$ + 26% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_1$	6.7
	$(^2D)\,^3F^o_2$	154676.94	150982.7	37% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_2$ + 33% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{3/2}\}_2$	2.4
	$(^2D)\,^1S^o_0$	154997.37	152832.1	40% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_0$ + 34% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{3/2}\}_0$	1.4
	$(^4S)\,^3D^o_1$	170672.25	148640.0	33% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{5/2}\}_1$ + 23% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{3/2}\}_1$	14.8
	$(^2P)\,^1D^o_2$	173690.03	166472.1	49% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{3/2}\}_2$ + 15% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_2$	4.3
	$(^2P)\,^3P^o_0$	175823.32	169843.8	34% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_0$ + 29% $\{[(5p^2_{1/2})(5p_{3/2})]_{3/2}5d_{3/2}\}_0$	3.5
	$(^2D)\,^3D^o_1$	177142.36	162425.9	25% $\{[(5p^2_{1/2})(5p^2_{3/2})]_{3/2}5d_{5/2}\}_1$ + 21% $[(5p^3_{3/2})(5d_{3/2})]_1$	9.1
	$(^2P)\,^3D^o_2$	177888.58	170401.9	37% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{5/2}\}_2$ + 31% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{5/2}\}_2$	4.4
	$(^2P)\,^3F^o_2$	183303.02	174718.7	35% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{3/2}\}_2$ + 23% $[(5p^3_{3/2})(5d_{3/2})]_2$	4.9
	$(^2P)\,^3P^o_2$	188548.46	179159.8	72% $[(5p^3_{3/2})(5d_{5/2})]_2$ + 11% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{5/2}\}_2$	5.2
	$(^2P)\,^3P^o_2$	195824.04	182511.0	35% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{3/2}\}_2$ + 19% $[(5s_{1/2})(5p^3_{3/2})]_2$	7.3
	$(^2D)\,^3S^o_1$	196642.69	179477.8	69% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{3/2}\}_1$ + 9 % $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_1$	9.6
	$(^2D)\,^3P^o_1$	202065.90	185913.9	30% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_1$ + 27% $[(5s_{1/2})(5p_{1/2})(5p^3_{3/2})]_1$	8.7
	$(^2P)\,^3D^o_2$	205494.10	187266.6	22% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{5/2}\}_2$ + 20% $\{[(5p_{1/2})(5p^2_{3/2})]_{3/2}5d_{5/2}\}_2$	9.7
	$(^2P)\,^3D^o_1$	207675.68	189391.7	46% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{3/2}\}_1$ + 15% $[5p^3_{3/2}5d_{5/2}]_1$	9.7
	$(^2D)\,^3P^o_0$	209047.39	192952.0	49% $[5p^3_{3/2}5d_{3/2}]_0$ + 23% $\{[(5s_{1/2})(5p_{1/2})]_0(5p^4_{3/2})\}_1$	8.3
	$(^2D)\,^1P^o_1$	212084.92	194685.9	40% $[(5p^3_{3/2})(5d_{3/2})]_1$ + 23% $\{[(5s_{1/2})(5p_{1/2})]_1 5p^4_{3/2}\}_1$	8.9
	$(^2D)\,^1D^o_2$	216643.41	197380.8	48% $[(5p^3_{3/2})(5d_{3/2})]_2$ + 26% $\{[(5p_{1/2})(5p^2_{3/2})]_{5/2}5d_{5/2}\}_2$	9.8
	$(^2P)\,^1P^o_1$	235052.94	213044.0[c]	56% $[5p^3_{3/2}5d_{5/2}]_1$ + 15% $\{[(5p_{1/2})(5p^2_{3/2})]_{1/2}5d_{3/2}\}_1$	10.3

c: calculated results from Ref.[7].

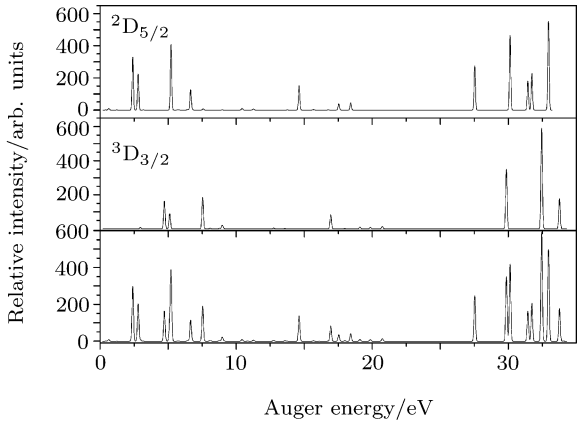


Fig.2. Theoretical Auger decay spectrum of the 4d core-excited states of Cs III.

According to the wavefunction expansions from the previous subsections, we therefore calculate the Auger energies and rates. The theoretical Auger spectra are given in Fig.2. Each discrete line is assumed to have a Gaussian profile with an FWHM of 0.12 eV. It can be found from the figure that the strongest peaks always occur in high Auger electron energy regions. As for the low Auger electron energy, it usually remains unobserved and often becomes dissolved into the background because of the set-up of the experiments. Up to now, to our best knowledge, no experiments have been carried out yet to determine the energies and/or intensities of the various Auger spectra from the 4d core-excited states of Cs III. Here, some relevant measurements are expected to identify the theoretical prediction. It will also be helpful for investigating the correlation effects on the Auger decay process.

3.3. Linewidths

One of the main objectives of this work is to understand the rather large linewidths of about 120–130 meV for the decay of the core-excited $4d^9 5s^2 5p^6$ $^2D_{5/2}$ and $^2D_{3/2}$ levels as observed experimentally.[10] The decay channels as many as possible should be included for this purpose. However, due to the radiative decay probability of the 4d core-excited state is about 3 to 4 orders less than of Auger decay, only the Auger decay channels are taken into account in the calculation of the linewidths of core-excited states. The calculated linewidths of the 4d core-excited states are given in Table 4, and they are in excellent agreement with the previous experimental results.

Table 4. Natural linewidths (in meV) of the 4d core-excited states $4d^9 5s^2 5p^6$ of Cs III.

level	This work		Previous calculation[10]	Experiment[10]
$^2D_{5/2}$	66.79[a]	114.91	18.49	130
$^2D_{3/2}$	87.72[a]	128.67	18.48	120

a: only including the decay channels $4d^{10}5s^25p^4$ and $4d^{10}5s^15p^5$.

According to our calculations, the configuration interaction (CI) effects will reduce the Auger decay rate for a specific state. It is reasonable that the CI effects will lead to the redistribution of the effective interaction strength to different component configurations. Meanwhile, due to the CI effects, there are more opened Auger decay channels. So, these will also improve the total linewidths.

It is noticed that a further level at about 69 eV above the ground state of Cs III refers to the $4d^{10}5p^6$ $^1S_0$ state (in Figure 1) and appears just to be opened for the Auger process of the core-excited levels $^2D_{3/2}$ but closed for another level $^2D_{5/2}$ if sufficient correlation effects are taken into account in the present sophisticated correlation model. However, care must be taken if some vacancies occur in an inner shell, for these hole states often decay by very fast Coster–Kronig (CK) or even super-CK transitions. So, maybe this is also an important Auger decay channel. In fact, such a strong coupling to the electron continuum is known to be also able to cause a shift in the total energy. But we cannot deal well with those interactions between the continuum-discrete transitions even between the continuum-continuum transitions now. Such an additional correlation contribution due to the interaction with the continuum is—by the construction of the MCDF method—not included in any program for the bound–state wavefunctions but would require an additional principal-value integration over the full continuum. This is certainly beyond the scope of this work; however, it should give some contributions to the total linewidths. It also could be the reason of the discrepancy for $^2D_{5/2}$ that insufficient decay channels are taken into account. Therefore, another

measurement of the natural widths of the 4d emission lines not only results in an independent confirmation of the experiment but also may make impact on the further theoretical studies.

4. Summary and conclusion

A detailed theoretical study in the framework of the fully relativistic MCDF method has been carried out for the decay of the core-excited $4d^9 5s^2 5p^6\ ^2D_{5/2}$ and $^2D_{3/2}$ levels of Cs III. These two 4d core-excited states can decay by Auger or radiative transitions either to the levels of the $4d^{10} 5s^2 5p^4$ and $4d^{10} 5s5p^5$ configurations of Cs IV or, respectively, directly to the ground configuration $5s^2 5p^5$ of Cs III. By incorporating correlation effects in a rather systematic manner into the representation of the wavefunctions, the calculated linewidths are improved greatly compared with the previous quasi-relativistic computations. However, there still exists some discrepancy between the calculations and the previous measurements. For example. the linewidths of the higher level of 4d core-excited states $^2D_{3/2}$ is smaller than that of the lower states $^2D_{5/2}$ in experiment, but it is in contrast to our calculations. An independent re-measurement of these widths would be highly desirable to confirm the very fast decay of the 4d core-excited states. Meanwhile, theoretical Auger spectra are also given and expected to be further confirmed in experiment. This will be another way to investigate the decay dynamics of the 4d core-excited states of Cs III.

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