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Shifts of Electronic *K*X-Rays in Muonic Atoms

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Energies of electronic *K*X-rays in muonic atoms were calculated for muons in various outer orbitals and for different numbers of electrons. Energy shifts were obtained with respect to characteristic X-rays belonging to nuclear charge $(Z-1)$ and their possible observation is discussed. The shifts in muonic Sn as an example amount to 19, 37, and 59 eV for the muon in $5g$, $6h$, and $7i$ states respectively. However, shifts due to the number of electrons present and the electron vacancy distribution in the *L*-shell are significantly larger. Accurate measurements of the *K*X-ray energies would therefore enable us to learn more about the electronic structure during the muonic cascade.

Introduction

Observations of energy shifts of electronic *K*X-rays in heavy muonic atoms have opened up new possibilities to study the electronic structure during the muonic cascade [1–3]. The shifts are attributed mainly to the screening of the nuclear charge by the muon. However, the number of electrons present and the vacancy distribution in the electron *L*-shell can have significant contributions to the shifts. Accurate measurements of the X-rays therefore would yield useful information on the complex interaction between the muon and the atomic electrons. Interpretation of measurements also requires accurate calculations of the detailed structure of the one-muon many-electrons atomic systems. It is the purpose of this study to make such accurate calculations for muonic atoms and to discuss them for Sn as an example.

After the initial capture of a muon by an atom into a Coulomb bound state of high n (probably around 20 or higher) the muon cascades down through the electron cloud into its $1s$ ground state, where it either decays or is absorbed by the nucleus. Rather little is known about the cascade process for $n>14$ when the muon is in the region of the electrons where muon electron interaction effects the cascade strongly. This region is also not easily accessible to experiment because the transitions here are predominantly converted which makes the observation of their X-rays a very difficult task. The cascade process from $n=14$ to the $1s$ state is better understood. It is essentially determined by the screened Coulomb potential of the nucleus and proceeds via Auger and radiation transitions [4, 5]. In the medium Z region one can roughly say that Auger processes dominate for $n>6$ and radiation processes dominate for $n<6$. Just before the Auger processes diminish and radiation processes take over, holes are expected to occur in the electron *K*-shell if the energy of muonic transition feeding this level n is greater than the binding energy of the *K*-electron and the transition has a significant Auger component. The energy of the electronic *K*X-rays emitted at this stage will depend on the atomic orbital in which the muon is present and on the vacancy distribution, i.e. electron depletion, especially in the *L*-shell. It will also depend strongly on the number of electrons present in the atom. The last two factors represent the greatest uncertainty in the estimation of the shifts because information about them is still lacking. The significance of electron depletion of mesic atoms for possible explanation of Auger electron spectra and the difference in mesic cascades in metals and insulators was first emphasized by Condo [6]. It is essential to understand the electron depletion problem in order to obtain accurate Auger transition rates, which in turn would allow us to estimate the intensities of

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electronic K X-rays. A detailed understanding of the electron depletion process may possibly have some relevance to the observed variations in kaonic, pionic, and muonic X-rays with nuclear charge Z [7]. Electron depletion in pionic atoms has recently been investigated by E. Bovet et al. [8] who have measured very accurately pionic transitions and then applied screening corrections due to possible electron configuration to interpret the experimental results.

Accurate measurements of electronic K X-rays would therefore enable us to learn something about the electronic structure with respect to these two factors during the muonic cascade. It is therefore worthwhile to calculate as accurately as possible the electronic K X-rays of muonic atoms and provide numbers which will help in the interpretation of experiments.

Method

The calculations are based on the relativistic self-consistent Dirac-Fock method. The details of the standard program which calculates averaged energies for electronic systems are described in [9-11]. In addition the QED-effects vacuum polarization and vacuum fluctuation were included in first order perturbation theory.

The K X-ray energies were obtained by taking the differences of total energies between initial and final states of the muon-electron atom. In this way the mutual screening of the muons and the electrons as well as the rearrangement of the electrons in the transition is included completely. The theoretical values of K X-ray energies obtained with the above method for Sn and In agree to within a few eV with the experimental values (Table 1). This comparison shows the necessity of including the Lambshift contribution (QED corrections) which amount to about 30 eV for Sn.

In this sophisticated program the presence of a muon was built-in by omitting all exchange integrals so that only the direct integrals in interaction with the electrons contribute [11]. When extra integrals are introduced one is able to couple the whole quantum mechanical system muon plus many-electrons to a state with good angular momentum J. This indicates that these are the most accurate calculations to date for muonic atoms. The relative positions of the expected X-ray transition in the presence of a muon and a number of electrons with respect to normal X-ray transitions will be accurate to within a few eV. In view of possible very accurate measurements it is therefore worthwhile to discuss the detailed structure of a quantum mechanical atomic system consisting of a number of several indistinguishable particles interacting with a single distinguishable particle. Such a comparison is not only of general interest but also essential in the interpretation of experimental data.

Table 1. Comparison of experimental and theoretical K X-ray energies for $Z=50$ (Tin) and $Z=49$ (Indium). Experimental values are from [13]

		Experiment (from Ref. 13) (eV)	Theory	
			(Lambshift included) (eV)	Lambshift contribution only (eV)
$Z=50$	$K_{\alpha 1}$	25,271.3	25,270.25	32.13
	$K_{\alpha 2}$	25,044.0	25,042.7	31.72
$Z=49$	$K_{\alpha 1}$	24,209.7	24,208.4	29.96
	$K_{\alpha 2}$	24,002.0	24,000.0	29.75

Table 2. Muonic transition energies, radiation and Auger components and rates of circular transitions for Sn. Values derived from [4]

Transition	Energy	R	A	P_R	P_A
$1s-2p$	3,448	100	3×10^{-5}	8.10×10^{17}	3.3×10^{11}
$2p-3d$	1,019	99.99	1×10^{-2}	8.36×10^{16}	9.48×10^{11}
$3d-4f$	344	99.75	0.25	1.78×10^{16}	5.84×10^{13}
$4f-5g$	159	97.56	2.44	5.50×10^{15}	1.95×10^{14}
$5g-6h$	86	80	20	2.12×10^{15}	4.63×10^{14}
$6h-7i$	52	53	47	9.58×10^{14}	1.06×10^{15}
$7i-8k$	34	22	78	4.82×10^{14}	1.5×10^{15}
$8k-9l$	23	13	87	2.63×10^{14}	1.0×10^{15}

R = Radiation component in %, A = Auger component in %, P_R = Radiation rate, P_A = Auger rate

Results and Discussion

We study here the electron K X-ray energy shifts in the muonic Sn atom as an example. The reason for choosing Sn ($Z=50$) is, that for Z-values in this region the K-electron Auger transition is energetically possible (for $\Delta n=1$ transitions) only after the muon has reached the $8k$-level. This is due to the fact that the binding energy of the K-electron for Sn is less than the $7i-8k$ muonic transition energy. The muonic transitions $7i-8k$, $6h-7i$, and $5g-6h$ are 78%, 47%, and 20% converted respectively [4] (see Table 2). We can therefore expect that most of the electronic K-shell holes will be generated by the above three muonic transitions. Since K X-ray emission rate for $K_{\alpha 1}$ and $K_{\alpha 2}$ is about [12] $8.9\cdot 10^{17}\,s^{-1}$ and the muonic transition rates for $7i-8k$, $6h-7i$, and $5g-6h$ transition [4] are all of the order of $2\cdot 10^{15}\,s^{-1}$, the majority of electronic K-shell holes

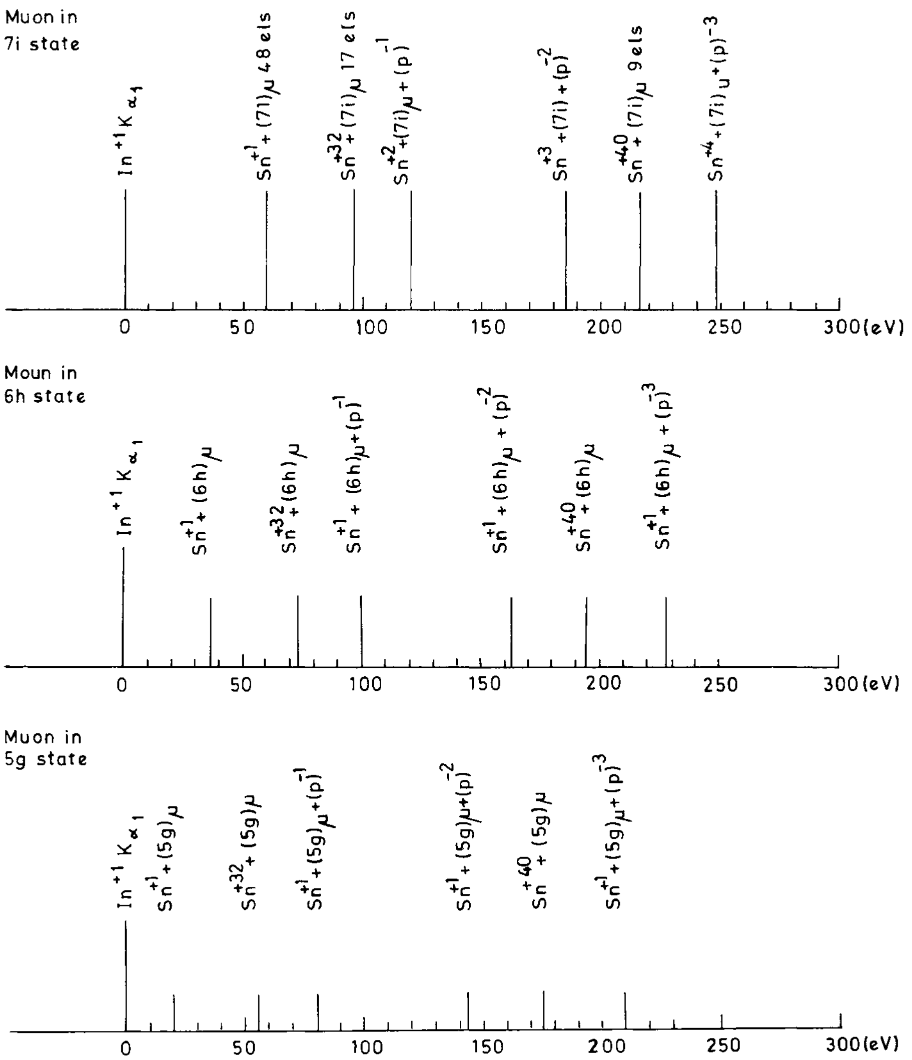

Fig. 1. $K_{\alpha 1}$ line position of Sn for different muonic states and different electron configurations relative to the characteristic In $K_{\alpha 1}$ line

generated by these transitions will decay while the muon is still in $7i$, $6h$, and $5g$ states respectively. Subsequent muonic transitions, i.e. $4f-5g$ to $1s-2p$, have higher transition rates but because these transitions are predominantly radiative, relatively few electronic KX-rays will be emitted at this stage. Of course the $\Delta n > 2$ transitions feeding the $8k$ and lower muonic levels will have enough energy to knock-out K-electrons, however, their contribution is expected to be small. This is supported by the time the muons reach the $n=8$ region, were they preferably populate the circular orbits [5].

We have therefore calculated the electronic $K_{\alpha 1}$ and $K_{\alpha 2}$ transition energies for the muon in $5g$, $6h$, and $7i$ states for varying numbers of electrons present. These energies lie between the characteristic KX-rays belonging to charges Z and $(Z-1)$ (see Fig. 1). The energy shift ΔE of electron KX-ray energy due to the presence of a muon is defined as the difference between the electronic X-rays in the presence of a muon and the $(Z-1)$ characteristic X-rays (see Table 3). These shifts amount for the neutral Sn atom to 19, 37, and 59 eV for the muon in $5g$, $6h$, and $7i$ states respectively. These values are in reasonable agreement with the values for $Z=53$ obtained by Vogel [3]. However, in the calculations done here the exchange terms are treated exactly and the Breit operator is included accurately.

In addition to the shifts due to the presence of a muon the KX-ray energy increases with decreasing numbers of electrons. This is very realistic because a large number of outer electrons is probably lost due to the Auger transitions in the early stages of the muon cascade. The energy shift δE is in this case defined as the difference between the KX-ray energies of highly ionized Sn and singly ionized Sn for the same muonic state. For example in muonic Sn atom with a $7i$ muon the decrease in number of electrons to nine will increase the $K_{\alpha 1}$ energy by 157 eV. The change in energy is particularly sensitive

Table 3. Energy shifts ΔE of electronic K_α – X-rays in the presence of a $5g$, $6h$ and $7i$ muon and all possible electrons in Sn relative to the K_α-line for In

Muon state	$5g$	$6h$	$7i$
ΔE (eV)	19	37	60

Table 4. Energy shift δE of electronic $K_{\alpha 1}$ X-rays for different electron configurations with muon in $7i$ state. δE is defined as

$\delta E = E_K^{+x} - E_K^{+1}$

where x is the ionization state of muonic Sn atom

No. of electrons	$2p$-shell vacancies	Transitions	E (eV)
48	0	$1s^1 2s^2 2p^6 \ldots 5p - 1s^2 2s^2 2p^5 \ldots 5p$	0
47	1	$1s^1 2s^2 2p^5 \ldots 5p - 1s^2 2s^2 2p^4 \ldots 5p$	61
46	2	$1s^1 2s^2 2p^4 \ldots 5p - 1s^2 2s^2 2p^3 \ldots 5p$	124
45	3	$1s^1 2s^2 2p^3 \ldots 5p - 1s^2 2s^2 2p^2 \ldots 5p$	188
17	0	$1s^1 2s^2 2p^6 \ldots 3p^6 - 1s^2 2s^2 2p^5 \ldots 3p^6$	37
16	1	$1s^1 2s^2 2p^5 \ldots 3p^6 - 1s^2 2s^2 2p^4 \ldots 3p^6$	103
15	2	$1s^1 2s^2 2p^4 \ldots 3p^6 - 1s^2 2s^2 2p^3 \ldots 3p^6$	170
14	3	$1s^1 2s^2 2p^3 \ldots 3p^6 - 1s^2 2s^2 2p^2 \ldots 3p^6$	239
9	0	$1s^1 2s^2 2p^6 - 1s^2 2s^2 2p^5$	157
8	1	$1s^1 2s^2 2p^5 - 1s^2 2s^2 2p^4$	228
7	2	$1s^1 2s^2 2p^4 - 1s^2 2s^2 2p^3$	298

to the number of electrons in the L-shell. In general, for every missing electron in the $2p$-shell the KX-ray energy increases about 60 eV. Table 4 gives the shifts due to different electron configurations with the muon in $7i$ state.

The $K_{\alpha 1}$ line positions of Sn for muon in $5g$, $6h$, and $7i$ states with respect to characteristic $K_{\alpha 1}$ line of Indium ($Z=49$) are shown in Fig. 1 for 48, 17, and 9 electron Sn atoms and for one, two, and three $2p$-shell vacancies (represented as $(p)^{-1}$, $(p)^{-2}$, and $(p)^{-3}$ respectively). The length of the lines is a relative measure of the intensity based on the relative strength of Auger component of $7i-8k$, $6h-7i$, and $5g-6h$ muonic transitions (see Table 2). The intensities of lines with respect to L-shell occupation and total number of electrons present is not known. Their length has been kept uniform only for figurative reason.

From Fig. 1 one can easily see that the electronic KX-ray shifts in muonic atoms depend on the state of the muon as well as on the electron configuration. Accurate experiments could perhaps unfold the components of the shift due to the different factors discussed here. The information which electron configuration in the presence of a muon is the most dominant one is just the information which is needed to understand the details of the cascade process.

The structure of the $K_{\alpha 2}$ lines is very similar and is therefore not shown here.

Conclusion

In a measurement of X-rays with enough resolving power one expects to see a rich structure between the characteristic KX-rays belonging to the nuclear charge Z and $(Z-1)$. The KX-rays of charge Z will be emitted while the muons are being stopped in the target material. The KX-rays of charge $(Z-1)$ will be delayed by about 10^{-7} s, the time it takes for the nucleus to absorbe the muon after it has reached the $1s$ ground state. Due to the results of these calculations the structure between the normal KX-ray lines reveals valuable information on the electronic structure during the muonic cascade.

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