Theoretical estimation of lifetimes of the lowest metastable states in Sc III and Y III

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Abstract

Lifetimes of the first two metastable states in Sc2+ and Y2+ are determined using the relativistic coupled-cluster theory. There is a considerable interest in studying the electron correlation effects in these ions as their electronic configurations are similar to the neutral alkali atoms. However, their electronic structures are very different from the latter. We have made a comparative study of the correlation trends between the above doubly ionized systems with their corresponding neutral and singly ionized iso-electronic systems. The knowledge of the lifetimes of these excited states is very important in the field of astrophysics, especially for the study of post-main-sequence evolution of the chemically peculiar stars.

1. Introduction

With the recent progress in high performance computational techniques, it has now become possible to carry out accurate calculations on heavy atomic systems using the powerful relativistic many-body theories [1–3] which otherwise are computationally expensive. However, it is quite difficult to treat all the heavy atomic systems by a single many-body theory due to the large differences in their electronic structures and because of their limitations. Among the various existing atomic many-body theories, the relativistic coupled-cluster (RCC) theory has been successfully applied earlier to a wide range of atomic properties [4] including the lifetime calculations of Pb+ [5] and alkaline-earth ions [6]. The role of electron correlation effects is dramatic in some of those cases. In the present work, we have carried out the lifetime calculations of the lowest 2D5/2 and 2S1/2 states in Sc III and Y III ions.

Generally, the forbidden transition lines find numerous interesting applications in astrophysics which includes the determination of the elemental abundances in different celestial objects and also in laboratory astrophysics and plasma physics studies. The spectral lines of yttrium and its doubly charged ions have been observed in the spectra of many hot stars like Ap stars [7] and these ions seem to be over abundant in Hg–Mn stars compared to their normal stellar abundances. These anomalous observations of abundances, which are significantly larger than those expected from theoretical estimations based on the s-process of neutron capture have been studied in the literature [8, 9]. Thus, the study of adjacent elements of the same row of the periodic table like, the Sr–Y–Zr triad of elements, can be used to understand the nucleo-synthetic origin of these elements and it can reveal the post-main-sequence evolution of the chemically peculiar stars, such as Hg–Mn stars [7]. The Sc III and Y III ions can also be used for the diagnostics and modelling of the stellar plasma [10]. Recently, Brage et al [11] have used the multi-configuration Hartree–Fock (MCHF) method to calculate the lifetimes of the 5P, 5D and 6D states of Y III which were measured earlier by Maniak et al [12]. However, the lifetimes of the 4d2D5/2 and 5s2S1/2 states in Y III seem to be unreported so far. Though, there are a large number of results available for the transition wavelengths of Sc III, it seems that there are no measurements of either the lifetimes or the transition probabilities of the 3d2D5/2 and 4s2S1/2 states. For this reason, we have carried out the calculations of the
lifetimes of the lowest $^2D_5/2$ and $^2S_1/2$ metastable states in Sc III and Y III employing a powerful many-body theory known as the RCC theory. The low-lying excited states and their electromagnetic decay channels are shown in figure 1. Although, the Sc III and Y III belong to K- and Rh-isoelectronic sequences, respectively, the ground states of the former two are $nd^3D_{3/2}$ states ($n = 3$ for Sc III and $n = 4$ for Y III) unlike the latter two for which the ground states are $(n + 1)s^2$. Thus, the ions considered in this work are interesting as the electron correlation effects they exhibit are different from the neutral species. We analyse the role of electron correlation effects in these cases and compare their trends with the previously studied lifetimes of the $^2D_5/2$ states in alkali atoms [13] and alkaline-earth metal ions [6].

2. Theory and method of calculation

The spontaneous emission transition probabilities for the E2 and M1 electromagnetic transitions from the state ‘i’ to the state ‘f’ are given by

$$A_{i-f}^{E2} = \frac{1.11995 \times 10^{18}}{[J_i]^3} S_{E2},$$

$$A_{i-f}^{M1} = \frac{2.69735 \times 10^{13}}{[J_i]^3} S_{M1},$$

where $[J_i] = 2J_i + 1$ is the degeneracy of the state i, $S = |\langle f|O|i\rangle|^2$ is the transition line strength (in atomic units) for the corresponding transition operator $O$ and $\lambda$ is the wavelength (in Å).

As shown in figure 1, the $ndD_{3/2}$ states in the considered systems can decay to the $ndD_{5/2}$ states via E2 and M1 channels; hence the total transition probabilities for the $ndD_{5/2}$ states can be expressed as

$$A_{ndD_{5/2}} = A_{ndD_{5/2}-ndD_{3/2}}^{E2} + A_{ndD_{5/2}-ndD_{3/2}}^{M1}.$$  

Similarly, the $ms^2$ states can decay to the $ndD_{5/2}$ states via E2 and M1 channels and decay to the $ndD_{5/2}$ states via E2 channel; therefore, the resulting total transition probabilities are given by

$$A_{msD_{5/2}} = A_{msD_{5/2}-ndD_{3/2}}^{E2} + A_{msD_{5/2}-ndD_{3/2}}^{M1} + A_{msD_{5/2}-ndD_{3/2}}^{E2} + A_{msD_{5/2}-ndD_{3/2}}^{M1}.$$  

In the above expressions, $n$ and $m$ represent the principal quantum numbers of the D and S states respectively; where $n = 3$ and $m = 4$ for Sc III and $n = 4$ and $m = 5$ for Y III. The expressions for the single particle reduced matrix elements of E2 and M1 operators used in our calculations can be found in [14]. The lifetimes of these states are determined by taking the inverse of their total transition probabilities.

We use the following RCC ansatz to construct the wavefunctions for the single valence electron states ($|\Psi_v\rangle$) in the considered systems:

$$|\Psi_v\rangle = e^{-\lambda} (1 + S_{v})|\Phi_0\rangle,$$

where the reference state $|\Phi_0\rangle = a_{v}^+|\Phi_0\rangle$ for the valence electron $v$ and $|\Phi_0\rangle$ is the Dirac–Fock (DF) state of the closed-shell system constructed by the Dirac–Coulomb (DC) Hamiltonian. This is the relativistic method of the universal valence coupled-cluster theory proposed by Mukherjee et al [15] and later it was expressed in compact formulation by Lindgren [16]. In the above RCC wavefunction expression, we define $T$ and $S_v$ as the closed-shell and open-shell excitation operators which excite core electrons and valence and valence–core electrons, respectively. We have considered all single, double and a subset of important triple excitations in our calculations, which is known by the name, CCSD(T) approximation in the literature [6, 17]. It has been found in many previous studies on the similar systems like those considered here that, the CCSD(T) method by its construction accounts for the correlation effects like the core-correlation, core-polarization and pair-correlation effects to all-orders [18], needed to evaluate various atomic properties to high accuracy [5, 6, 17, 18].

We solve the following equations to obtain $T$ operator amplitudes for the closed-shell configurations

$$\langle \Phi_v^e |\overline{T}_N| \Phi_0\rangle = 0,$$

where $H_N$ is the normal-order Hamiltonian, $\overline{T}_N = e^{-c^{\dagger}} H_N e^{c^{\dagger}}$ with the subscript $c$ denoting connected terms and $|\Phi_0\rangle$ represents excited states with respect to $|\Phi_0\rangle$. After obtaining the $T$ amplitudes, we solve the $S_v$ amplitudes for the single valence open-shell configurations and ionization potential (IP) of the valence electron $v$ using the following equations:

$$\langle \Phi_v^e |\overline{T}_N S_v | \Phi_v^e\rangle = -\langle \Phi_v^e |\overline{T}_N | \Phi_v^e\rangle + \langle \Phi_v^e | S_v | \Phi_v^e\rangle,$$

$$\langle \Phi_v^e |\overline{T}_N[1 + S_v] | \Phi_v^e\rangle.$$

The above equations are solved iteratively until self-consistent high accuracy amplitudes are obtained.

The transition matrix elements for the operator $O$ are calculated in the RCC approach, using the following expression:

$$\langle O \rangle = \frac{\langle \Psi_v | O | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle}} = \frac{\langle \Phi_v | O \Phi_0 \rangle}{\sqrt{\langle \Phi_v | \Phi_v \rangle}},$$

where $H_N$ is the normal-order Hamiltonian, $\overline{T}_N = e^{-c^{\dagger}} H_N e^{c^{\dagger}}$ with the subscript $c$ denoting connected terms and $|\Phi_0\rangle$ represents excited states with respect to $|\Phi_0\rangle$. After obtaining the $T$ amplitudes, we solve the $S_v$ amplitudes for the single valence open-shell configurations and ionization potential (IP) of the valence electron $v$ using the following equations:

$$\langle \Phi_v^e |\overline{T}_N S_v | \Phi_v^e\rangle = -\langle \Phi_v^e |\overline{T}_N | \Phi_v^e\rangle + \langle \Phi_v^e | S_v | \Phi_v^e\rangle,$$

$$\langle \Phi_v^e |\overline{T}_N[1 + S_v] | \Phi_v^e\rangle.$$
where $\mathcal{O} = e^T O e^T$. The above expression contains many nonlinear terms which will be computationally expensive if they are calculated directly. Hence, we follow the extended Wick’s theorem [19] to break these terms into the simple form as discussed below. First, we divide the operator $\mathcal{O}$ as the effective one-body and two-body operators and then the resulting terms will be sandwiched between the necessary $S_\nu$ operators and the resulting terms will be computed directly in the property calculations. The details of the method can be found from our earlier papers [5, 18]. The contributions from the normalization of the RCC wavefunctions (Norm.) are taken into account by

$$\text{Norm.} = \langle \Psi_f | O | \Psi_i \rangle \left\{ \frac{1}{\sqrt{N_f N_i}} - 1 \right\}, \quad (2.10)$$

where $N_v = \langle \Phi_0 | e^{T_\nu} e^{T_f} | \Phi_0 \rangle + \langle \Phi_i | \left[ S_\nu e^{T_\nu} e^{T_f} S_\nu \right] | \Phi_i \rangle$ for the corresponding valence electrons $v(= i, f)$.

3. Results and discussions

In table 1, we present the computed values of excitation energies and the transition wavelengths for the lowest D and S states of Sc$^{2+}$ and Y$^{2+}$ and compare them with the available experimental results. The calculated excitation energies are determined from the IP results of different states which are evaluated using the RCC method. We have taken experimental excitation energies of Sc III from the atomic data base of National Institute for the Standard and Technology (NIST) [20], whereas the Y III results are taken from [21]. The corresponding wavelengths ($\lambda$) are determined from these excitation energies. In order to determine more reliable results for the transition probabilities and lifetimes, it is necessary to obtain the wavelengths to high accuracy as the higher powers of $\lambda$ are involved in the calculation. Since the lifetimes of the lowest D and S states of the considered systems are not known in the literature and whose reliable values are wanted in many astrophysical applications, we use the available experimental wavelengths to determine the lifetimes accurately.

We present considered wavelengths, determined transition strengths and the individual probabilities for the E2 and M1 channels of various low-lying transitions in table 2. We also give the total probabilities for each excited state and determine their lifetimes by taking the reciprocal of these quantities in the same table. As seen from table 2, the M1 transition probabilities between the fine structure levels, i.e. the D$^{3/2} \rightarrow$ D$^{3/2}$ transitions are 5–6 orders of magnitude larger than the E2 transitions, whereas the M1 transition probabilities for the D$^{3/2} \rightarrow$ S$^{1/2}$ transitions are 4–5 orders smaller than the corresponding E2 transitions. Thus, the M1 transitions play a crucial role in determining the lifetimes of the D$^{3/2}$ states as do E2 transitions for the S$^{1/2}$ states.

The lifetime of the 3d$^3$D$^{3/2}$ state in Sc III is very large implying that it is a highly forbidden state. However, the

Table 1. The excitation energies and the transition wavelengths of the different low-lying transitions in Sc$^{2+}$ and Y$^{2+}$.

| Transition | Excitation energy (au) | Wavelength (Å) |
|------------|------------------------|---------------|
| This work | Experiment [20, 21] | This work | Experiment [20, 21] |
| Sc$^{2+}$ | | | |
| $3d^3D^{3/2} \rightarrow 3d^3D^{3/2}$ | 0.000 942 | 483 687 | 505 970 |
| $4s^2S^{1/2} \rightarrow 3d^3D^{3/2}$ | 0.113 984 | 3997 | 3916 |
| $3s^2S^{1/2} \rightarrow 3d^3D^{3/2}$ | 0.113 188 | 4025 | 3946 |
| Y$^{2+}$ | | | |
| $4d^2D^{5/2} \rightarrow 4d^2D^{3/2}$ | 0.003 349 | 136 051 | 138 093 |
| $5s^2S^{1/2} \rightarrow 4d^2D^{5/2}$ | 0.030 094 | 15 140 | 13 392 |
| $5s^2S^{1/2} \rightarrow 4d^2D^{3/2}$ | 0.026 706 | 17 061 | 14 830 |

Table 2. The transition probabilities ($A_s$) and the lifetimes ($\tau$) of the low-lying D and S states in Sc$^{2+}$ and Y$^{2+}$.

| Initial state | Final state | $\lambda$ (Å) | Transition channel | Strength | Individual | Total | Lifetime $\tau$ (in s) |
|--------------|-------------|---------------|-------------------|----------|------------|--------|----------------------|
| Sc$^{2+}$ | | | | | | | |
| $3d^3D^{3/2}$ | $3d^3D^{3/2}$ | 505 970 | M1 | 2.3753 | 8.2434 $\times 10^{-5}$ | 8.2434 $\times 10^{-5}$ | 12130.86 |
| | | | E2 | 2.7166 | 1.5291 $\times 10^{-4}$ | 1.5291 $\times 10^{-4}$ | 12130.86 |
| $4s^2S^{1/2}$ | $3d^3D^{3/2}$ | 3916 | M1 | 7.9497 $\times 10^{-7}$ | 1.7500 $\times 10^{-4}$ | 19.2715 | 0.0519 |
| | | | E2 | 12.9154 | 7.3854 | 7.3854 | 11.413 |
| $3d^3D^{3/2}$ | $3d^3D^{3/2}$ | 3946 | E2 | 19.5002 | 114.13 |
| Y$^{2+}$ | | | | | | | |
| $4d^2D^{5/2}$ | $4d^2D^{3/2}$ | 138 093 | M1 | 2.3821 | 4.0606 $\times 10^{-3}$ | 4.0606 $\times 10^{-3}$ | 245.89 |
| | | | E2 | 9.5972 | 3.7011 $\times 10^{-8}$ | 3.7011 $\times 10^{-8}$ | 245.89 |
| $5s^2S^{1/2}$ | $4d^2D^{3/2}$ | 13 392 | M1 | 1.1138 $\times 10^{-7}$ | 6.2544 $\times 10^{-7}$ | 9.4041 $\times 10^{-2}$ | 10.63 |
| | | | E2 | 37.6554 | 4.8952 $\times 10^{-2}$ | 4.8952 $\times 10^{-2}$ | 10.63 |
| $4d^3D^{3/2}$ | $4d^3D^{3/2}$ | 14 830 | E2 | 57.7646 | 4.5900 $\times 10^{-2}$ | 4.5900 $\times 10^{-2}$ | 10.63 |
The importance of the correlation effects and the nature of their trends in the RCC calculations of various transition amplitudes in the considered doubly ionized systems are studied and compared with the transition amplitudes of similar amplitudes in the considered doubly ionized systems. The trends in the RCC calculations etc. possibly include the truncation of the coupled-cluster series at various transition amplitude calculations and others in [6].

We compare the correlation trends observed in the E2 transitions below: it is evident from tables 3 and 4 that the DF contributions are quite dominant in all these cases. Almost all the correlation contributions are observed to be negative of their DF and the total RCC contributions in all the three systems, in both the iso-electronic sequences considered in this work. Also, we observe that the pair-correlation contributions.

The lifetime of the $4s^2S_{1/2}$ state is a few fraction of a second. On the other hand, the lifetime of the $4d^2D_{5/2}$ state in Y III is 246 s which is also a long-lived metastable state, whereas the $5s^2S_{1/2}$ state has a lifetime of only 10 s. The transition probabilities of the states given in table 2 will be very useful in astrophysics for the accurate determination of the abundances of these elements. We estimate that the calculated lifetime results can have an error bar of less than 2%. The source of errors includes the truncation of the coupled-cluster series at the partial inclusion of triple excitations to CCSD, the omission of higher order relativistic effects like QED corrections in the amplitude calculations etc.

| Transition | 3d $^2D_{3/2}$ | 3d $^2D_{5/2}$ | 4s $^2S_{1/2}$ | 3d $^2D_{5/2}$ |
|------------|----------------|----------------|----------------|----------------|
| DF (O)     | $-63.0538$    | $-1.5492$      | $-5.0192$      | $-1.5491$      |
| $\Omega - O$ | $0.0010$  | $4.7387 \times 10^{-4}$ | $0.0001$  | $1.2875 \times 10^{-2}$ |
| $\Omega S_{1s} + S_{1s} \Omega$ | $10.2998$ | $-3.0444 \times 10^{-2}$ | $0.9186$ | $-2.9343 \times 10^{-2}$ |
| $\Omega S_{2s} + S_{2s} \Omega$ | $0.0230$  | $-3.1263 \times 10^{-6}$ | $0.0921$  | $-2.5193 \times 10^{-5}$ |
| Others     | $0.0033$      | $-1.0656 \times 10^{-6}$ | $0.0031$  | $-6.2382 \times 10^{-7}$ |
| Total      | $-51.7215$    | $1.5489$        | $-3.9146$     | $-1.5287$      |

Table 3. Different correlation contributions of M1 and E2 transitions arising between the low-lying D and S states in the K- iso-electronic sequence. All the results are given in atomic units.

The importance of the correlation effects and the nature of their trends in the RCC calculations of various transition amplitudes in the considered doubly ionized systems are studied and compared with the transition amplitudes of similar states in the iso-electronic neutral and singly ionized systems and these comparative results are explicitly given in tables 3 and 4 for K- and Rb- iso-electronic systems, respectively. Interestingly, the members of these iso-electronic sequences have different energy level distributions; the neutral and singly ionized systems have $2S_{1/2}$ states as their ground states, whereas the doubly ionized systems have $2D_{3/2}$ states as their ground states. Also, in the singly ionized systems, D states are the first excited states, whereas the first excited states in the doubly ionized systems are the S states. However, in the neutral systems D states are the higher excited states. Obviously, these energy level structures will participate differently in giving different correlation contributions and we discuss the major correlation terms in the RCC calculations in detail below. There are no relativistic results available for the corresponding transition amplitudes in the neutral systems, however a few non-relativistic results have been reported to our knowledge (see [13] and references therein). The E2 transition amplitudes derived from the transition probabilities presented in [13] matches approximately with the DF results of the S–D$_{3/2}$ transition amplitudes reported in this work. We had also reported the M1 and E2 transition amplitudes of the singly ionized systems in our previous work [6]. However, we have determined these quantities again using the same exponents of the Gaussian type orbitals (GTOs) as those used for the doubly ionized systems in order to make a comparative study of the electron correlation effects at the same level of approximation. We have also discussed the difference between our method of calculations and others in [6].

Various important correlation contributions like core-correlation, pair-correlation and core-polarization effects are highlighted through the $\Omega - O$, $\Omega S_{1s}$ + h.c. and $\Omega S_{2s}$ + h.c. RCC terms, respectively, where $O$ is the corresponding transition operator and h.c. stands for Hermitian conjugate. Contributions from higher order correlation effects are given by ‘Others’. We also present the contribution of the normalization term, Norm. given in equation (2.10) and the total RCC result which is the sum of all the RCC terms. The difference between the DF and the RCC results give the total contribution of the correlation effects.

We compare the correlation trends observed in the E2 transitions below: it is evident from the tables 3 and 4 that the DF contributions are quite dominant in all these cases. Almost all the correlation contributions are observed to be negative of their DF and the total RCC contributions in all the three systems, in both the iso-electronic sequences considered in this work. Also, we observe that the pair-correlation contributions.
are the dominant correlation contributions in all the ions, in both the iso-electronic sequences. They are about (10–16)% for the transitions in K+, more than 15% for the transitions in Ca+ and around (8–10)% for the transitions in Sc2+ in the K- iso-electronic sequence (cf table 3). However, it varies from 12 to 22% in Rb-, (10–11)% in Sr+ and about (5–6)% in Y2+ in the Rb- iso-electronic sequence (cf table 4). Thus, when compared to the neutral and singly ionized systems, the doubly ionized systems have the smallest pair-correlation effects. The core-polarization contributions are the second largest correlation contributions in all the transitions considered. More or less, these contributions are larger in the doubly ionized systems when compared to the neutral and singly ionized counterparts in their corresponding iso-electronic sequences. It varies from 0.04 to 4.4% among the various transitions belonging to the K- iso-electronic sequence, whereas it varies from 0.1 to 4% for the various transitions in Rb- iso-electronic sequence. The core-correlation contributions in the neutral atoms are smaller than the doubly ionized systems by almost 2 orders of magnitude in both the sequences. They are about 10^{-3}% for the neutral atoms and ~10^{-16}% for the doubly ionized systems. However, the core-correlation contributions of many of the singly ionized systems are negligibly small.

The correlation trends observed in the M1 transitions are compared below: the DF contribution for the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} M1 transitions are almost same for all the ions in both the K- (n = 3) and Rb- (n = 4) iso-electronic sequences. We can decompose the relativistic M1 operator into the non-relativistic part, i.e., L + 2S plus a relativistic corrections part. As the orbital angular momentum, L and the spin angular momentum, S are the same for all the ions for this transition, it can be implied that, the relativistic corrections are quite small for the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} M1 transitions. Also, it is observed in both the iso-electronic sequences that the DF results for the M1 transitions in the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions are about 6–7 orders of magnitude larger than the (n + 1)s\textsuperscript{2}S\textsubscript{1/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions. In contrast, it can be seen that the electron correlation effects in the (n + 1)s\textsuperscript{2}S\textsubscript{1/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions are quite large compared to that in the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions. We observe a particular trend in the correlation terms in the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions in both the sequences that the pair-correlation contribution is the largest among the other correlation terms and it varies from 1.9 to 2.3% in K- iso-electronic sequence and from 1.7 to 3.6% in Rb- iso-electronic sequence. However, despite observing the larger correlation contributions in different RCC terms of (n + 1)s\textsuperscript{2}S\textsubscript{1/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions compared to those of the nd\textsuperscript{2}D\textsubscript{3/2} \rightarrow nd\textsuperscript{2}D\textsubscript{3/2} transitions, we do not see any particular trend among the various correlation contributions in the former.

4. Conclusion

We have determined the lifetimes of the lowest 2\textsuperscript{D}3/2 and 2\textsuperscript{S}1/2 metastable states in Sc2+ and Y2+ employing the relativistic coupled-cluster theory which seem to be unreported so far in the literature. We have discussed various correlation contributions for the E2 and M1 transition amplitudes arising in the transitions between the above states and compared the correlation trends of these doubly ionized systems with their corresponding singly ionized and neutral counterparts in K- and Rb- iso-electronic sequences, respectively. The transition
probabilities and the lifetime estimations of these states find interesting applications in astrophysics in understanding the post-main-sequence evolution of the chemically peculiar stars.

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