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Radiative transition rates of 1s2s(^{3}S)3p levels for Li-like ions with $5 \leqslant Z \leqslant 10$

J.P. Santos [a,*], F. Parente [a], M.C. Martins [a], P. Indelicato [b], E.P. Benis [c], T.J.M. Zouros [d], J.P. Marques [a]

[a] Laboratório de Instrumentação, Engenharia Biomédica e Física da Radiação (LIBPhys-UNL), Departamento de Física, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Monte da Caparica, 2892-516 Caparica, Portugal
[b] Laboratoire Kastler Brossel, UPMC-Sorbonne Universités, CNRS, ENS-PSL Research University, Collège de France, Case 74; 4, place Jussieu, F-75005 Paris, France
[c] Department of Physics, University of Ioannina, GR 45110 Ioannina, Greece
[d] Department of Physics, University of Crete, P.O. Box 2208, GR 71003 Heraklion, Greece

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Energy and radiative transition rates of the 1s2s (^{1,3}S) 3p levels of Li-like ions with $5 \leqslant Z \leqslant 10$ are calculated using a multiconfiguration Dirac-Fock approach including quantum-electrodynamic and electronic correlation corrections. The importance of the electronic correlation on the radiative transition probabilities is assessed in detail.

1. Introduction

The study of highly excited few-electron ions is important for a number of reasons. Although many effects have to be taken into account such as relativity, quantum electrodynamic contributions, and electronic correlation, among others, the system is simple enough to allow for a reasonable treatment of these contributions and a comparison with experiment. Furthermore, the analysis of radiative and radiationless transitions in these systems is essential for the diagnostics of laboratory and astrophysical plasmas, and, from the theoretical point of view, in probing the wavefunctions quality.

Li-like ions, in particular, have been studied extensively in the laboratory, and in astrophysical spectra, as dielectronic and collisional often originate innershell satellite lines whose presence is important in the analysis of He-like K-shell X-ray spectra [1].

The $1s2\ell2\ell'$ configuration levels and their de-excitation have been object of particular attention, both theoretically and experimentally since, at least, 1978 [2], and numerous recent publications exist for different Z values, mainly concerning the metasTable 1s2s2p ^{4}P state [3–6].

In what concerns the 1s2s3p states, X-ray energies, Auger and radiative decay rates, as well as fluorescence yields have been computed in intermediate coupling by Chen [7]. Kato et al. [8] compared Li-like Ca and S ion line wavelengths and intensities, calculated by three different methods. Natarajan and Natarajan [9] presented X-ray rates from Li-like excited levels for ions in the range $Z = 10 - 54$.

From the experimental point of view, Rødbro et al. [10] studied the ejected-electron spectra of highly excited auto-ionizing levels of Li, Mosnier *et al.* [11] recorded Li-like silicon-ion spectra, using the beam-foil method, and Smith *et al.* [12] observed Fe XXV Kβ lines and their satellite transitions of the type $1s2\ell'3\ell'' \rightarrow 1s^2\,2\ell$ from tokamak-fusion-test-reactor plasmas with a high-resolution crystal spectrometer. Watanabe *et al.* [13] measured the X-ray emission due to the dielectronic recombination process in He-like Fe ions with an EBIT and determined the resonant strengths. The selective enhancement of 1s2s2p ^{4}P metastable states populated by cascades in single-electron transfer collisions of ions with He and H_2 targets has been studied [3–6].

In 1997, Kramida and Ivanov [14], and Kramida and M.-C. Buchet-Poulizac [15] published compilations of inner-shell excited energy levels and spectra of Li-like neon, including 1s2s3p states.

In this work, we used the multiconfiguration Dirac-Fock (MCDF) model to calculate the radiative decay probabilities for 1s2s3p configuration levels with $J = 1/2, 3/2$ of Li-like ions with $5 \leqslant Z \leqslant 10$.

* Corresponding author.
E-mail address: jps@fct.unl.pt (J.P. Santos).

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Table 1
1s2s3p Energy values (in eV). Superscripts #i are added to distinguish identical terms in the same configuration, where #1 stands for the term with the lowest energy. The values identified with * are from the NIST tables [21].

Line	Z							
	5		6	7	8	9	10	
$1s^22s\ ^2S_{1/2}$	0	0*	0	0	0	0	0	0*
$1s2s^2\ ^2S_{1/2}$	192.795	192.731*	291.662	410.729	550.576	710.885	891.670	891.52*
$1s2s3p\ ^4P_{1/2}$	220.642	220.67460*	336.145	475.879	639.862	828.120	1040.674	1040.85*
$1s2s3p\ ^4P_{3/2}$	220.646	220.67445*	336.150	475.884	639.869	828.131	1040.690	1040.85*
$1s2s3p\ ^2P^{\#1}_{3/2}$	220.801	220.77*	341.073	476.155	640.208	828.540	1041.178	1041.59*
$1s2s3p\ ^2P^{\#1}_{1/2}$	220.906	220.77*	336.357	476.282	640.227	828.578	1041.232	1041.59*
$1s2s3p\ ^2P^{\#2}_{1/2}$	224.617	224.37*	341.073	481.908	646.998	836.373	1050.057	1050.10*
$1s2s3p\ ^2P^{\#2}_{3/2}$	224.708	224.37*	336.358	481.934	647.036	836.427	1050.132	1050.10*

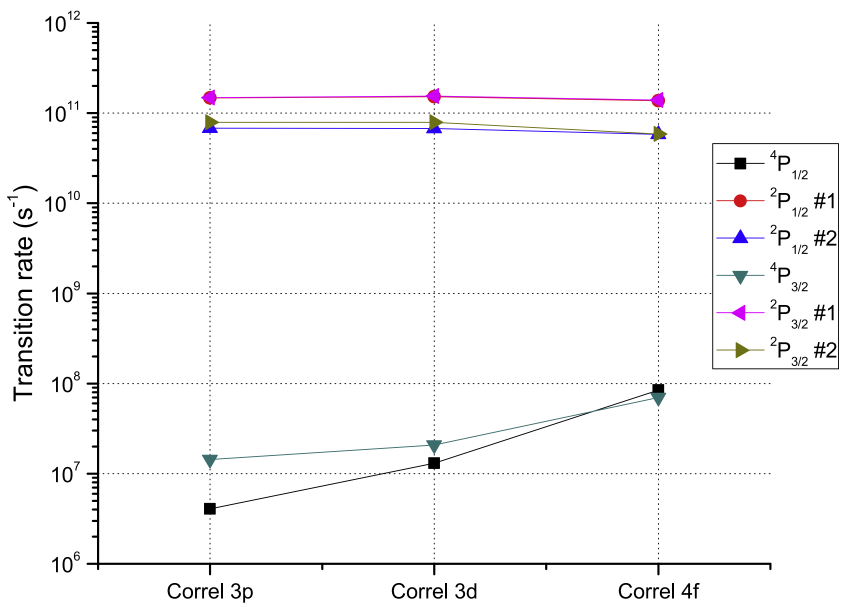

Fig. 1. Variation of the total radiative transition probabilities with correlation (Correl) for $Z = 6$.

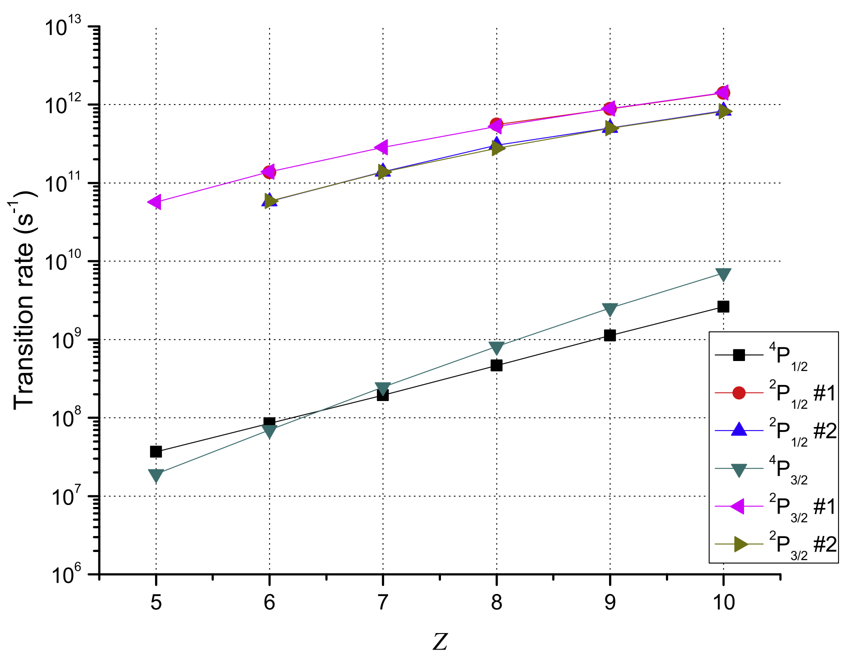

Fig. 2. Total radiative transition probabilities for 1s2s3p levels with correlation until 4f for $5 \leqslant Z \leqslant 10$.

2. Theory

The energy values of the levels were calculated within the MCDF approach using the general relativistic MultiConfiguration Dirac Fock and General Matrix Element (MDFGME) code developed by Desclaux and Indelicato [16,17]. The electrons are treated in the independent-particle model. The electronic wave functions and energies are evaluated in the Coulomb field of the nucleus and the spherically-averaged electronic field. Breit interaction, accounting for magnetic interaction and retardation effects, is included in the calculation. Quantum Electrodynamics (QED) radiative corrections to the electron-nucleus interaction, namely the self-energy and vacuum polarization, were also included. The code description and the formulas implemented can be obtained from Ref. [18].

In the calculation of the transition rate and energy values, the initial and final state wavefunctions were obtained independently in the optimized level scheme, and the formalism proposed by Löwdin [19] to treat the non-orthogonality effects was employed. Further details can be found in Ref. [20]. The length gauge was used for all radiative transition probabilities.

3. Results and conclusions

E1 radiative transitions from the 1s2s3p configuration levels may occur to levels in $1s^22s$, $1s2s^2$, and 1s2s3s configurations. However, in what concerns the latter configuration, the only energetically possible E1 transition allowed is the 1s2s3p $^4P_{5/2} \rightarrow$ 1s2s3s $^4S_{3/2}$ in an energy window far from the other transitions and, therefore, was not considered in this work.

The 1s2s3p $\rightarrow$ $1s^22s$, $1s2s^2$ initial and final level energy values, calculated with electronic correlation up to the 4f subshell for $5 \leqslant Z \leqslant 10$ are listed in Table 1. There, these values are also compared with NIST Atomic Spectra Database [21] for $Z = 5$ and $Z = 10$.

The transition probability values obtained with correlation up to 3p, 3d, and 4f subshells are plotted in Fig. 1. The variation trend with the correlation amount was found to be similar for all considered Z values. We notice that the correlation affects significantly the weakest lines, that is, the transitions from the 1s2s3p$^4P_{1/2}$ and $^4P_{3/2}$ levels, but is unimportant for the other lines. However, as Z increases, and likewise the transition probability values, the correlation effect on the weakest lines becomes less important.

In Fig. 2, the total radiative transition probability values from the 1s2s3p levels, calculated with correlation up to the 4f subshell, are plotted for all considered Z values.

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