Radiative properties of few F- and Cl- like alkali and alkaline-earth metal ions

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ABSTRACT

We present high-accuracy calculations of radiative properties such as oscillator strengths and transition probabilities, of the allowed ns ^{2}S$_{1/2}$ → np ^{2}P$_{1/2, 3/2}$ transitions and of the forbidden np ^{2}P$_{1/2}$ → np ^{2}P$_{3/2}$ transitions in the F- and Cl-like alkali and alkaline-earth ions with the ground state principal quantum number n of the respective ion. For this purpose, we have employed the Dirac–Fock, relativistic second-order many-body perturbation theory and an all-order perturbative relativistic method in the coupled-cluster (CC) theory framework. To test the validity of these methods for giving accurate results, we first evaluated the ionization potentials in the creation processes of these ions and compare them with their experimental values listed in the National Institute of Science and Technology data base. Moreover, both the allowed and forbidden transition amplitudes are estimated using the above three methods and a comparative analysis is made to follow-up the electron correlation trends in order to demonstrate the need of using a sophisticated method like the CC theory for their precise determination. For astrophysical use, we provide the most precise values of the transition properties by combining the experimental energies, which suppresses uncertainties from the calculated energies, using the transition amplitudes from the CC method. These data will be useful in the abundance analysis of the considered ions in the astronomical objects and for the diagnostic processes of astrophysical plasmas.

Key words: atomic data – line profiles.

1 INTRODUCTION

Several space missions like Hubble, *Chandra*, *Spitzer*, Lyman and the ground-based 10 metre class telescopes have enabled astrophysicists to explore a large horizon of the Universe. These facilities have the capabilities to observe the spectral lines of many atomic transitions coming out of different astronomical objects with very high resolution. These observations provide lines covering the wavelengths to a wide range starting from X-ray to infrared of the electromagnetic spectra. It is revealed that many of the radiating elements are the highly charged ions. These highly charged ions are present in the form of hot plasma in different stellar and interstellar bodies of the Universe. For example, presence of the highly charged ions at different stages of ionization of atoms having medium range nuclear charges like H to Ni have been observed in the active solar regions (Beyer & Shevelko 2003). Knowledge of transition properties of these highly charged ions, particularly for the considered highly

charged F-like and Cl-like alkali and alkaline-earth ions, present in the hot astrophysical plasmas is very useful in the diagnostic processes of plasmas. They provide information on the structural and evolutionary stages of the astronomical objects (Nahar 2005; Tayal 2012). These spectroscopic properties are also needed in determining the electron collisional rate coefficients, electron–ion recombination rate coefficients and photoionization cross-sections, etc. to explain adequately the scattering phenomena (Griem 1974; Lesage 1995; Zeippen 1995; Kimura et al. 1998; Orban et al. 2006). Accurate values of the line strengths are also required in determining the Stark broadenings of the spectral lines, which are very crucial for the astrophysical analysis (Alonso-Medina & Colon 2014).

We also give here few more examples to demonstrate explicitly about the relevance of studying spectroscopy of the considered ions for the astrophysics purposes. Liao, Zhang & Yao (2013) had examined at least 36 set of data from the *Chandra* High Energy Transmission Grating observations to detect the interstellar medium absorption lines along the sight lines of 11 low-mass X-ray binaries. In their analysis, they had observed several transitions of Mg ɪᴠ ion along with the O ɪ, Ne ɪ and Mg ɪ ions. Similarly, Pottasch & Surendiranath (2005) had analysed the spectrum of the

round-shaped planetary nebula NGC 6886 using the *Infrared Space Observatory* (*ISO*) and determined spectral line of Mg IV at 4.48 μm to confirm about the presence of this ion along with 12 other ions in this nebula. Erickson & Davidson (1995) have also advocated about the presence of Mg IV in the space plasma by analysing the interstellar spectra obtained from the Kuiper Airborne Observatory. Since the Ca abundance is an indicator of the stellar object history, therefore studying the spectral properties of the Ca ions are of lot of interest to many for a quite long time. For example, Gabriel, Fawcett & Jordan (1966) and Fawcett & Gabriel (1966) have confirmed about the existence of strong emission lines of Ca IV in the solar plasma. They identified about nine ultraviolet spectral lines in their analysis of the solar radiations. Subsequently, Feuchtgruber et al. (1997) reported about the infrared lines of Na III at 7.31 μm, of K III at 4.61 μm, of Ca IV at 3.20 μm and of Mg IV at 4.48 μm corresponding to the $2s^2 2p^5\ ^2P_{1/2} \rightarrow 2s^2 2p^5\ ^2P_{3/2}$ transition. They were observed primarily from the NGC 7027, NGC 6543 and NGC 6302 nebulae, from the Circinus galaxy, and from the Sgr A West and W51 IRS 2 by employing Short Wavelength Spectrometer on board *ISO*. Svensson & Ekberg (1968) and Smitt, Svensson & Outred (1976) also ascertained about presence of some of the spectral lines of Ca IV. In another work, Ness & Jordan (2008) reported spectral lines of Ca XII by analysing observational data from the ϵ Eridani (K2 V) star using the Low Energy Transmission Grating Spectrometer on board of *Chandra* and the *Extreme Ultraviolet Explorer*. In addition, Lanz et al. (2005) also informed about the presence of the absorption lines of Ca XII in the hot white dwarf photosphere. They argued that the observed spectra from these dwarfs are actually an amalgam of transition lines from a wide range of ions, largely comprising lines of the Si XII, S XI, S XII, Ar X, Ar XI, Ar XII, Ca XII and Fe XVI ions.

The objective of the present study is to provide accurate radiative properties of both the allowed and forbidden transitions of the above mentioned F-like and Cl-like ions which are of immense interest in astrophysics. Accurate calculations of these atomic data demand for using powerful many-body methods that are capable of incorporating the relativistic along with the electron correlation effects appropriately. In fact, a very few results for these ions have been reported earlier with whom we also compare our calculations. Our results can be appended with the atomic data bases like CHIANTI (Young et al. 2003) for various astrophysical application purposes.

2 METHOD OF CALCULATIONS

The expressions for the dominant emission transition probabilities due to the E1, E2 and M1 channels in an atomic transition ($|\Psi_i\rangle \rightarrow |\Psi_f\rangle$) from the higher level state $|\Psi_i\rangle$ to the lower level state $|\Psi_f\rangle$ are given by

$$A_{if}^{E1} = \frac{2.0261 \times 10^{-6}}{\lambda_{if}^3 g_i} S_{if}^{E1} \tag{1}$$

$$A_{if}^{E2} = \frac{1.1195 \times 10^{-22}}{\lambda_{if}^5 g_i} S_{if}^{E2} \tag{2}$$

and

$$A_{if}^{M1} = \frac{2.6971 \times 10^{-11}}{\lambda_{if}^3 g_i} S_{if}^{M1}, \tag{3}$$

where the quantity $S_{if}^O = |\langle\Psi_i||O||\Psi_f\rangle|^2$ is known as the line strength for the corresponding reduced matrix element $|\langle\Psi_i||O||\Psi_f\rangle|$ of a transition operator O. Later, we give these values in atomic unit

(au) which can be converted to international system (SI) units by multiplying the factors 0.7188×10^{-54} C^2 cm^2 and 0.2013×10^{-72} C^2 cm^4 to both the E1 and M1 channels and to the E2 channel, respectively. In the above expressions, $g_i = 2J_i + 1$ is the degeneracy factor of the state $|\Psi_i\rangle$ with the angular momentum J_i and the transition wavelength (λ_{if}) in cm which when substituted, the transition probabilities (A_{if}^Os) are obtained in s^{-1}.

The emission oscillator strengths (f_{if}s) due to the above transition probabilities are given by (Sobelman 2006)

$$f_{if} = 1.4992 \times 10^{-24} A_{if} \frac{g_i}{g_f} \lambda_{if}^2 \tag{4}$$

from which the absorption oscillator strengths (f_{fi}s) can be determined using the relation

$$f_{fi} = -\frac{g_f}{g_i} f_{if}, \tag{5}$$

with the degeneracy factor g_f of the state $|\Psi_f\rangle$.

The expressions for evaluating the reduced matrix elements in terms of the single particle orbitals corresponding to the E1, M1 and E2 transitions can be found elsewhere (Nandy & Sahoo 2013). The lifetime (τ) of the atomic state $|\Psi_i\rangle$ can be determined by taking the inverse of the total emission transition probabilities involving all possible spontaneous transition channels (given in s), i.e.

$$\tau_i = \frac{1}{\sum_{O,f} A_{if}^O}, \tag{6}$$

where sum over O represents for all probable decay channels and over f corresponds to transitions to all the lower states.

The considered states of the undertaken systems can be assumed to have just one electron less than a closed-shell configuration [$ns^2\ np^6$] with n being the principal quantum number of the last occupied orbital. Atomic states with closed-shell configurations are easy to determine for which we adopt a procedure to evaluate the states of our interest from these closed-shell configurations. For the same purpose, we define the [$ns^2\ np^6$] configuration as $|\Psi_0\rangle$ which is evaluated using the ansatz of the coupled-cluster (CC) theory by expressing as

$$|\Psi_0\rangle = e^T |\Phi_0\rangle, \tag{7}$$

where $|\Phi_0\rangle$ is the Dirac–Fock (DF) wavefunction for the [$ns^2\ np^6$] configuration, obtained using the Dirac–Coulomb Hamiltonian (in au for which $\hbar = 1$, $|e| = 1$ and $m_e = 1$)

$$H = \sum_i \left[c\boldsymbol{\alpha}_i \cdot \boldsymbol{p}_i + \beta_i c^2 + V_n(r_i) + \sum_{j \geq i} \frac{1}{r_{ij}} \right], \tag{8}$$

for the Dirac matrices $\boldsymbol{\alpha}_i$ and β_i, nuclear potential $V_n(r)$ and inter electronic Coulomb interaction $\frac{1}{r_{ij}}$ (in au) and T accounts for the excitations from $|\Phi_0\rangle$ to compose of excited configurations due to the electron correlations. The states of our interest can be, then, determined by annihilating the extra electron from $|\Phi_0\rangle$ and removing the additional correlation effects undertaken in the construction of $|\Psi_0\rangle$. Following the CC framework in the Fock-space formalism, we achieve this by writing (Nandy & Sahoo 2013)

$$|\Psi_a\rangle = e^T (1 + R_a) |\Phi_a\rangle, \tag{9}$$

where we define a new DF wavefunction $|\Phi_a\rangle = a_a|\Phi_0\rangle$ by removing an electron from an occupied orbital a and the operator R_a is a CC operator similar to T but takes care of the (d)excitations due to the surplus correlation effects accounted in the determination of $|\Psi_0\rangle$. Point to be noted here is that this approach still facilitates to

Table 1. Comparison between the ionization potentials (IPs) in cm^{-1} from the MBPT(2), and CCSD methods against the NIST data base (Kramida et al. 2014) of the Na III, Mg IV, K III, K XI, Ca IV and Ca XII ions.

State	DF	MBPT(2)	CCSD	CCSD(T)	NIST
F-like systems					
Na III					
$2s^2 2p^5 \, {}^2P_{3/2}$	393 739.52	371 303.68	380 357.74	381 005.08	381 390.21
$2s^2 2p^5 \, {}^2P_{1/2}$	395 365.52	372 699.46	381 820.75	382 466.98	382 756.55
$2s 2p^6 \, {}^2S_{1/2}$	676 508.80	635 005.88	645 314.20	645 871.12	645 845
Mg IV					
$2s^2 2p^5 \, {}^2P_{3/2}$	658 807.12	638 114.29	645 131.30	641 701.49	646 402
$2s^2 2p^5 \, {}^2P_{1/2}$	661 354.91	640 425.45	647 498.96	643 987.61	648 630
$2s 2p^6 \, {}^2S_{1/2}$	986 860.30	949 850.42	956 912.65	954 048.82	957 934
K XI					
$2s^2 2p^5 \, {}^2P_{3/2}$	4074 770.26	4057 179.85	4060 060.07	4058 398.44	4062 400
$2s^2 2p^5 \, {}^2P_{1/2}$	4099 478.31	4081 423.32	4084 351.55	4082 647.11	4085 895
$2s 2p^6 \, {}^2S_{1/2}$	4743 775.79	4714 656.28	4716 744.82	4715 417.22	4718 301
Ca XII					
$2s^2 2p^5 \, {}^2P_{3/2}$	4783 760.35	4766 227.90	4768 743.96	4767 383.79	4771 550
$2s^2 2p^5 \, {}^2P_{1/2}$	4815 240.49	4797 195.12	4799 761.04	4798 359.11	4801 591
$2s 2p^6 \, {}^2S_{1/2}$	5505 836.74	5476 940.49	5478 765.57	5477 621.92	5480 580
Cl-like systems					
K III					
$3s^2 3p^5 \, {}^2P_{3/2}$	256 004.54	253 921.32	255 565.14	253 635.12	255 072.8
$3s^2 3p^5 \, {}^2P_{1/2}$	258 418.28	256 153.36	257 808.32	255 833.85	257 238.2
$3s 3p^6 \, {}^2S_{1/2}$	433 922.65	387 770.75	391 031.49	388 915.67	385 682.8
Ca IV					
$3s^2 3p^5 \, {}^2P_{3/2}$	410 822.64	409 740.16	411 050.15	409 480.01	410 642.3
$3s^2 3p^5 \, {}^2P_{1/2}$	414 226.19	412 963.32	414 278.82	412 664.46	413 760.5
$3s 3p^6 \, {}^2S_{1/2}$	613 815.40	567 759.86	567 696.79	565 659.99	563 081.9

consider $|\Phi_0\rangle$ as the working reference state and both the T and R_a operators are in normal order form with respect to $|\Phi_0\rangle$. As a result, we represent these CC operators in the second quantization formulation as

$$T = T_1 + T_2 = \sum_{b,p} a_p^\dagger a_b t_b^p + \frac{1}{4} \sum_{bd,pq} a_p^\dagger a_q^\dagger a_d a_b t_{bd}^{pq} \qquad (10)$$

and

$$R_a = R_{1a} + R_{2a} = \sum_{b \neq a} a_b^\dagger a_a r_a^b + \frac{1}{2} \sum_{bd,p} a_b^\dagger a_p^\dagger a_d a_a r_{ad}^{bp}, \qquad (11)$$

where b, d and p, q represent the electrons from the core and virtual orbitals, respectively, with the excitation amplitudes denoted by t and r with the sub- and superscript indices defining the corresponding (d)excitation operations. As can be noticed from the above expressions, we consider only important singles and doubles excitations (known as CCSD method) in our calculations. Contributions from the dominant triples excitations are estimated perturbatively considering the singles, doubles and partial triples excitations (CCSD(T) method) in the procedure as demonstrated in Nandy & Sahoo (2013).

After obtaining wave functions of the required states in the considered systems using the above procedure, we evaluate the matrix elements between the $|\Psi_f\rangle$ and $|\Psi_i\rangle$ states as

$$\frac{\langle \Psi_f | O | \Psi_i \rangle}{\sqrt{\langle \Psi_f | \Psi_f \rangle \langle \Psi_i | \Psi_i \rangle}} = \frac{\langle \Phi_f | \{1 + R_f^\dagger\} \overline{O} \{1 + R_i\} | \Phi_i \rangle}{\sqrt{\mathcal{N}_f \mathcal{N}_i}}, \qquad (12)$$

where $\overline{O} = e^{T^\dagger} O e^T$ and $\mathcal{N}_i = \{(1 + R_i^\dagger) \overline{\mathcal{N}} (1 + R_i)\}$ with $\overline{\mathcal{N}} = e^{T^\dagger} e^T$. The evaluation procedure of these terms are described elaborately elsewhere (Nandy & Sahoo 2013).

3 RESULTS AND DISCUSSION

In Table 1, we present the ionization potentials (IPs) of the electrons from the $2p_{3/2}$, $2p_{1/2}$ and 2s orbitals of the $[2s^2 \, 2p^6]$ configuration that are obtained while calculating the $2s^2 2p^5 \, {}^2P_{3/2}$, $2s^2 2p^5 \, {}^2P_{1/2}$ and $2s 2p^6 \, {}^2S_{1/2}$ states of the F-like Na III, Mg IV, K XI and Ca XII ions, and from the $3p_{3/2}$, $3p_{1/2}$ and 3s orbitals of $[3s^2 \, 3p^6]$ in the calculations of the $3s^2 3p^5 \, {}^2P_{3/2}$, $3s^2 3p^5 \, {}^2P_{1/2}$ and $3s 3p^6 \, {}^2S_{1/2}$ atomic states of the Cl-like K III and Ca IV ions. These values are estimated using the DF, CCSD and CCSD(T) methods and considering an approximation in the CCSD method that is equivalent to the second-order many-body theory (MBPT(2) method). All these calculated results are compared against the experimental values quoted in the National Institute of Science and Technology (NIST) data base (Kramida et al. 2014) in order to assert some credence on the accuracies of the theoretical results. This table demonstrates that the CCSD method is giving more accurate IP values in many cases than the other methods.

From the theoretical perspective, the CC method is an all-order perturbative theory and it, even with the truncated CCSD and CCSD(T) approximations, satisfies the size consistent and size extensivity criterion (Shavitt & Bartlett 2009). Moreover, excellent agreement between the calculated IPs using the CCSD method, within 1 per cent accuracy, with their experimental values countenance about its potential for achieving precise theoretical results employing this method. Therefore, we employ the CCSD method to estimate the line strengths for the $nsnp^6 \, {}^2S_{1/2} \rightarrow ns^2np^5 \, {}^2P_{3/2}$ and $nsnp^6 \, {}^2S_{1/2} \rightarrow ns^2np^5 \, {}^2P_{1/2}$ transitions due to the E1 channel and for the $ns^2np^5 \, {}^2P_{1/2} \rightarrow ns^2np^5 \, {}^2P_{3/2}$ transitions through the E2 and M1 channels in the above-mentioned highly-charged alkali and alkaline-earth ions. For the comparative analysis, we also estimate

these values using the DF and MBPT(2) methods. In Table 2, we give the calculated line strengths along with the estimated values of the oscillator strengths and transition probabilities that are obtained by combining the DF, MBPT(2) and CCSD amplitudes with the wavelengths of the above transitions derived from the differences of their IPs (excitation energies) from the respective methods as given in Table 1. Differences in the line strengths are also quoted alongside the CCSD values in Table 2. Comparison among the results from the above three methods indicate the role of the correlation effects in their accurate determination. It is seen from Table 2 that the DF results for the M1 transitions are smaller than their respective MBPT and CCSD results, while it is other way around for the E1 and E2 transitions. The MBPT results for the calculated properties corresponding to the M1 and E2 transitions are higher than their CCSD results, but the E1 transition results do not follow any such definite trend.

Clearly, the ab initio results for the oscillator strengths and the transition probabilities quoted in Table 2 seem to be precarious in nature as in some cases the values are altering drastically from one method to another; especially for the transitions involving the fine structure splittings of the ground state configuration. This can be well understood as follows. Uncertainties associated with the ab initio results are, generally, twofolds; first due to the calculate wavelengths from the IPs and then from the calculated line strengths. Though the calculated energies given in Table 1 indicate that they are about 1 per cent accurate compared with the experimental values, however one can notice that the net uncertainties in the excitation energies aggregated from the IPs of both the states associated with a transition. In particular, they become extremely critical in the calculations of the states involving fine structure partners. To improve accuracies further in the fine structure splittings, it is imperative to account for the higher order relativistic corrections; i.e. the corrections due to the Breit interaction and quantum electrodynamics effects that are especially significant for the fine structure splittings. However, it should be noticed that these higher order corrections are usually insignificant in the determination of the line strengths. It can also be seen from Table 2 that, except for the E1 transitions of alkaline-earth-like ions, the differences among the line strengths obtained using all the three methods are not so large. So the uncertainties in the estimated wavelengths used in the ab initio determination of oscillator strengths and transition probabilities are culpable for making those large variations in the oscillator strengths and transition probabilities among different methods. However, the reason for getting large differences between the oscillator strengths and transition probabilities due to the E1 channel for the $nsnp^6\,^2S_{1/2} \rightarrow ns^2np^5\,^2P_{3/2, 1/2}$ transitions from the DF, MBPT(2) and CCSD methods is somewhat different. However, the reason for getting large differences between the oscillator strengths and transition probabilities due to the E1 channel for the $nsnp^6\,^2S_{1/2} \rightarrow ns^2np^5\,^2P_{3/2, 1/2}$ transitions from the DF, MBPT(2) and CCSD methods are somewhat different. It can be understood by analysing the roles of different electronic configurations that are important for determining the $ns^2np^5\,^2P_{3/2, 1/2}$ and $nsnp^6\,^2S_{1/2}$ states of the considered ions. It is not possible to investigate explicitly the same through the CC theory. However, one can follow from the calculations of similar states in the Ne II and Mg IV ions by Johnson & Kingston (1987) and in the singly ionized Ar, Kr and Xe ions by Lauer et al. (1999) using the configuration interaction method that accurate calculations of the $ns^2np^5\,^2P_{3/2, 1/2}$ states require significant contributions from the $nsnp^5\,(^{1,\,3}P^o)(n+1)$s and $nsnp^5\,(^{1,\,3}P^o)nd$ configurations, while configurations like $nsnp^4(n+1)$s and $nsnp^4nd$ are very much essential to determine the $nsnp^6\,^2S_{1/2}$ states. In our adopted Fock-space

formalism of many-body methods, the $nsnp^4(n+1)$s and $nsnp^4nd$ configurations cannot be constructed at the MBPT(2) approximation. However through the non-linear terms like T_1R_{2a} and T_2R_{2a} of our CCSD method, these configurations can be generated. This is the reason why our CCSD results are differing by large amount from their respective MBPT(2) results. That is also the reason why partial triples effects are found to contribute by quite large amount in the transitions involving the $nsnp^6\,^2S_{1/2}$ states. It indicates that our CCSD results can be improved further if full triples excitations are taken into account in the CC method. We also observe the above effects are more prominent in the ions with $n = 3$ owing to the fact that in such cases more occupied electrons are present. Since the goal of this work is to provide more accurate and reliable results for the astrophysical use, we consider the experimental wavelengths (estimated from the experimental energies given in the NIST data base; Kramida et al. 2014) and the calculated line strengths from the CCSD(T) method those are quoted in Table 2 for the determination of precise (recommended) values of the oscillator strengths and transition probabilities in the above-discussed transitions of the considered alkali and alkaline-earth ions.

In Table 3, we present the experimental wavelengths and the recommended values of the oscillator strengths and transition probabilities in the considered ions due to the E1, M1 and E2 channels through the above mentioned procedure. From the wavelength values, it can be realized that the lines corresponding to all the allowed (E1) transitions fall in the extreme ultraviolet region, while the M1 and E2 transition lines of the Na III, Mg IV, K III and Ca IV ions lie mostly in the infrared region. However, the M1 and E2 transition lines of the K XI and Ca XII ions are in the near ultraviolet region. As has been stated in Introduction, these lines are of immense interest for the astrophysical studies. It is seen from Table 3 that the transition probabilities due to the M1 channel are dominating over the E2 channel, as anticipated, in the forbidden transitions in all the considered ions. Again, the magnitudes of the forbidden transition probabilities are becoming larger with increase in size of the ion owing to wider fine structure splittings. Naturally, the transition probabilities due to the E1 channels are found to be much higher in these ions and are much larger compared to the forbidden transitions. Using these transition probabilities, the lifetimes of the studied atomic states of the above alkali and alkaline-earth ions are estimated and given in Table 3. A few more results for the lifetimes of the fine structure levels in the K XI ion are also available in the literature (Trabert et al. 2001). Trabert et al. (2001) had measured the corresponding lifetime in K XI using the Livermore electron beam ion trap of EBIT-2. They had also estimated the M1 transition probability between the corresponding fine structure splitting from this lifetime measurement by neglecting the contribution from the E2 channel, which is insignificantly small. Their value for the lifetime of the $2S^2 2p^5\,^2P_{3/2}$ state is 4.44 ± 0.10 s and the M1 transition probability of the $2S^2 2p^5\,^2P_{3/2} \rightarrow 2S^2 2p^5\,^2P_{1/2}$ transition is 224 ± 6 s^{-1}. In another work, Kaufman & Sugar (1986) had also calculated the lifetime of the $2S^2 2p^5\,^2P_{3/2}$ state as 4.27 s. Similarly, Krueger & Czyzak (1965) had estimated the M1 transition probability for the above transition in the Ca XII ion by analysing a fitting procedure to reproduce the experimental energies from their computed energies in the LS intermediate coupling scheme. Mason (1975) had also evaluated transition probability for this transition by employing the SUPER-STRUCTURE atomic many-body program of Eissner & Nussabaumer (1969). This program essentially deals with the non-relativistic mechanics, but Mason (1975) had evaluated this quantity considering the Breit–Pauli approximation. None the less our results are in reasonably good agreement with these

Table 2. The line strengths (S_{ik}) in atomic unit (au) from the DF, MBPT(2) and CCSD methods and the corresponding ab initio values for the oscillator strengths (f_{ik}) and the transition rates (A_{ik}) in s^{-1} of the $ns^2 2p^5\,^2P_{1/2} \rightarrow ns^2 np^5\,^2P_{3/2}$ and the $nsnp^6\,^2S_{1/2} \rightarrow ns^2 np^5\,^2P_{1/2,\,3/2}$ transitions from all the three methods in the considered alkali and alkaline-earth ions. Differences in the estimated S_{ik} values from the CCSD and CCSD(T) methods (CCSD(T)−CCSD values) are given in the parentheses alongside the CCSD results. The notation [x] to be read as $\times 10^x$.

Transition ($|\Psi_i\rangle \rightarrow |\Psi_f\rangle$)	S_{ik}(au)			f_{ik}			A_{ik} (s^{-1})		
	DF	MBPT	CCSD	DF	MBPT	CCSD	DF	MBPT	CCSD
Na III									
F-like systems									
$2s^2 2p^5\,^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\,^2P_{3/2}$	1.331	1.468	1.414(0.001)	2.189[−8]	2.073[−8]	2.090[−8]	0.077	0.054	0.060
$\xrightarrow{E2} 2s^2 2p^5\,^2P_{3/2}$	0.531	0.488	0.465(−0.002)	9.591[−14]	5.578[−14]	6.115[−14]	3.381[−7]	1.449[−7]	1.745[−7]
$2s^2 2p^6\,^2S_{1/2} \xrightarrow{E1} 2s^2 2p^5\,^2P_{1/2}$	0.396	0.245	0.269(−0.001)	0.168	0.097	0.107	8.906[9]	4.480[9]	4.992[9]
$\xrightarrow{E1} 2s^2 2p^5\,^2P_{3/2}$	0.795	0.503	0.543(−0.002)	0.170	0.100	0.108	1.822[10]	9.338[9]	1.024[10]
Mg IV									
$2s^2 2p^5\,^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\,^2P_{3/2}$	1.332	1.432	1.395(0.001)	3.430[−8]	3.347[−8]	3.338[−8]	0.297	0.239	0.250
$\xrightarrow{E2} 2s^2 2p^5\,^2P_{3/2}$	0.275	0.243	0.239(~0)	1.906[−13]	1.259[−13]	1.332[−13]	1.650[−6]	8.971[−7]	9.959[−7]
$2s^2 2p^6\,^2S_{1/2} \xrightarrow{E1} 2s^2 2p^5\,^2P_{1/2}$	0.301	0.192	0.209(~0)	0.148	0.090	0.098	1.053[10]	5.758[9]	6.267[9]
$\xrightarrow{E1} 2s^2 2p^5\,^2P_{3/2}$	0.605	0.389	0.420(~0)	0.150	0.092	0.099	2.165[10]	1.195[10]	1.289[10]
K XI									
$2s^2 2p^5\,^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\,^2P_{3/2}$	1.332	1.359	1.348(~0)	3.326[−7]	3.332[−7]	3.312[−7]	270.89	261.25	260.59
$\xrightarrow{E2} 2s^2 2p^5\,^2P_{3/2}$	0.017	0.015	0.015(~0)	1.070[−11]	8.903[−12]	8.958[−12]	8.711[−3]	6.972[−3]	7.048[−3]
$2s^2 2p^6\,^2S_{1/2} \xrightarrow{E1} 2s^2 2p^5\,^2P_{1/2}$	0.082	0.063	0.065(~0)	0.080	0.060	0.062	2.216[10]	1.624[10]	1.667[10]
$\xrightarrow{E1} 2s^2 2p^5\,^2P_{3/2}$	0.166	0.128	0.131(~0)	0.084	0.064	0.065	5.025[10]	3.690[10]	3.761[10]
Ca XII									
$2s^2 2p^5\,^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\,^2P_{3/2}$	1.329	1.355	1.345(~0)	4.230[−7]	4.241[−7]	4.219[−7]	559.29	542.59	541.48
$\xrightarrow{E2} 2s^2 2p^5\,^2P_{3/2}$	0.013	0.011	0.011(~0)	1.702[−11]	1.374[−11]	1.381[−11]	0.022	0.018	0.018
$2s^2 2p^6\,^2S_{1/2} \xrightarrow{E1} 2s^2 2p^5\,^2P_{1/2}$	0.072	0.056	0.057(~0)	0.075	0.058	0.059	2.397[10]	1.787[10]	1.812[10]
$\xrightarrow{E1} 2s^2 2p^5\,^2P_{3/2}$	0.146	0.114	0.116(~0)	0.080	0.061	0.062	5.566[10]	4.154[10]	4.217[10]
K III									
Cl-like systems									
$3s^2 3p^5\,^2P_{1/2} \xrightarrow{M1} 3s^2 3p^5\,^2P_{3/2}$	1.332	1.737	1.428(0.001)	3.249[−8]	3.919[−8]	3.238[−8]	0.253	0.260	0.217
$\xrightarrow{E2} 3s^2 3p^5\,^2P_{3/2}$	4.640	3.602	3.764(−0.001)	2.739[−12]	1.682[−12]	1.783[−12]	2.128[−5]	1.117[−5]	1.197[−5]
$3s^2 3p^6\,^2S_{1/2} \xrightarrow{E1} 3s^2 3p^5\,^2P_{1/2}$	1.164	0.125	0.322(−0.008)	0.308	0.025	0.064	6.376[9]	2.895[8]	7.701[8]
$\xrightarrow{E1} 3s^2 3p^5\,^2P_{3/2}$	2.338	0.247	0.653(−0.015)	0.314	0.025	0.068	1.334[10]	6.001[8]	1.644[9]
Ca IV									
$3s^2 3p^5\,^2P_{1/2} \xrightarrow{M1} 3s^2 3p^5\,^2P_{3/2}$	1.332	1.703	1.411(0.001)	4.582[−8]	5.549[−8]	4.606[−8]	0.708	0.769	0.641
$\xrightarrow{E2} 3s^2 3p^5\,^2P_{3/2}$	2.775	2.129	2.259(−0.001)	4.594[−12]	2.992[−12]	3.192[−12]	7.096[−5]	4.145[−5]	4.436[−5]
$3s^2 3p^6\,^2S_{1/2} \xrightarrow{E1} 3s^2 3p^5\,^2P_{1/2}$	0.943	0.127	0.270(−0.005)	0.284	0.030	0.063	7.594[9]	4.762[8]	9.892[8]
$\xrightarrow{E1} 3s^2 3p^5\,^2P_{3/2}$	1.896	0.242	0.543(−0.010)	0.290	0.029	0.064	1.607[10]	9.676[8]	2.115[9]

Table 3. Experimental values for the wavelengths (λ) in Å, the recommended values of the oscillator strengths (f_{ik}) and the transition rates (A_{ik}) in s^{-1} of the $ns^2 2p^5\ ^2P_{1/2} \rightarrow ns^2 np^5\ ^2P_{3/2}$ and the $nsnp^6\ ^2S_{1/2} \rightarrow ns^2 np^5\ ^2P_{1/2,\ 3/2}$ transitions along with the lifetimes of the excited states in the considered alkali and alkaline-earth ions. The notation $[x]$ to be read as $\times 10^x$.

System	Transition ($|\Psi_i\rangle \rightarrow |\Psi_f\rangle$)	λ_{if} (Å)	f_{ik}	A_{ik} (s^{-1}) Present	Others	τ_i (s) Present	Others
			F-like systems				
Na III	$2s^2 2p^5\ ^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\ ^2P_{3/2}$	73188.23	1.954[−8]	4.867[−2]		20.546	
	$\xrightarrow{E2} 2s^2 2p^5\ ^2P_{3/2}$		4.957[−14]	1.234[−7]			
	$2s2p^6\ ^2S_{1/2} \xrightarrow{E1} 2s^2 2p^6\ ^2P_{1/2}$	380.10	0.106	4.930[9]		6.64[−11]	
	$\xrightarrow{E1} 2s^2 2p^5\ ^2P_{3/2}$	378.14	0.107	1.012[10]			
Mg IV	$2s^2 2p^5\ ^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\ ^2P_{3/2}$	44883.30	3.136[−8]	0.207		4.81	
	$\xrightarrow{E2} 2s^2 2p^5\ ^2P_{3/2}$		1.110[−13]	7.348[−7]			
	$2s2p^6\ ^2S_{1/2} \xrightarrow{E1} 2s^2 2p^6\ ^2P_{1/2}$	323.31	9.750[−2]	6.261[9]		5.23[−11]	
	$\xrightarrow{E1} 2s^2 2p^5\ ^2P_{3/2}$	320.99	9.872[−2]	1.286[10]			
K XI	$2s^2 2p^5\ ^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\ ^2P_{3/2}$	4256.22	3.201[−7]	235.75	224 ± 6[a]	4.24[−3]	4.44 ± 0.10[−3][a] 4.27[−3][b]
	$\xrightarrow{E2} 2s^2 2p^5\ ^2P_{3/2}$		8.240[−12]	6.063[−3]			
	$2s2p^6\ ^2S_{1/2} \xrightarrow{E1} 2s^2 2p^6\ ^2P_{1/2}$	158.13	6.211[−2]	1.666[10]		1.85[−11]	
	$\xrightarrow{E1} 2s^2 2p^5\ ^2P_{3/2}$	152.46	6.491[−2]	3.746[10]			
Ca XII	$2s^2 2p^5\ ^2P_{1/2} \xrightarrow{M1} 2s^2 2p^5\ ^2P_{3/2}$	3328.78	4.080[−7]	491.95	487.9[c] 560.5[d]	2.03[−3]	
	$\xrightarrow{E2} 2s^2 2p^5\ ^2P_{3/2}$		1.301[−11]	1.568[−2]			
	$2s2p^6\ ^2S_{1/2} \xrightarrow{E1} 2s^2 2p^6\ ^2P_{1/2}$	147.28	5.901[−2]	1.826[10]		1.66[−11]	
	$\xrightarrow{E1} 2s^2 2p^5\ ^2P_{3/2}$	141.04	6.221[−2]	4.200[10]			
			Cl-like systems				
K III	$3s^2 3p^5\ ^2P_{1/2} \xrightarrow{M1} 3s^2 3p^5\ ^2P_{3/2}$	46180.84	3.126[−8]	0.195		5.114	
	$\xrightarrow{E2} 3s^2 3p^5\ ^2P_{3/2}$		1.604[−12]	1.003[−5]			
	$3s3p^6\ ^2S_{1/2} \xrightarrow{E1} 3s^2 3p^6\ ^2P_{1/2}$	778.85	6.080[−2]	6.732[8]		4.73[−10]	
	$\xrightarrow{E1} 3s^2 3p^5\ ^2P_{3/2}$	765.64	6.293[−2]	1.441[9]			
Ca IV	$3s^2 3p^5\ ^2P_{1/2} \xrightarrow{M1} 3s^2 3p^5\ ^2P_{3/2}$	32071.84	4.449[−8]	0.577		1.733	
	$\xrightarrow{E2} 3s^2 3p^5\ ^2P_{3/2}$		2.871[−12]	3.722[−5]			
	$3s3p^6\ ^2S_{1/2} \xrightarrow{E1} 3s^2 3p^6\ ^2P_{1/2}$	669.70	5.978[−2]	8.946[8]		3.50[−10]	
	$\xrightarrow{E1} 3s^2 3p^5\ ^2P_{3/2}$	656	6.131[−2]	1.912[9]			

Notes. [a](Trabert et al. 2001), [b](Kaufman & Sugar 1986), [c](Krueger & Czyzak 1965), [d](Mason 1975).

literature values; however, we believe that our results are more accurate compared to the other available calculations due to consideration of a four component relativistic theory and the CCSD(T) method for their determination. In addition we provide data for the other ions, which were not investigated earlier using a suitable relativistic method.

4 CONCLUSION

By employing relativistic many-body methods in the CC framework, we have determined the line strengths of the low-lying transitions of many highly charged alkali and alkaline-earth ions. Very accurate values of the oscillator strengths and transition probabilities in these ions are estimated by combining the calculated line strengths with the experimental wavelengths. Importance of using a more powerful many-body method in the relativistic theory is demonstrated by presenting ab initio results from three different methods at various levels of approximation. Our results are also compared with the available few literature data and found to be quite good agreement with them. The reported transition properties

are going to be very useful in the abundance analysis of these ions in various astrophysical objects and for analysing the diagnostic processes of the astrophysical plasmas.

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